

# Atoms, molecules, solids, and surfaces: Applications of the approximation for exchange and correlation

Physical Review B

46, 6671-6687

DOI: [10.1103/physrevb.46.6671](https://doi.org/10.1103/physrevb.46.6671)

Citation Report

#	ARTICLE	IF	CITATIONS
1	Magnetism with generalized-gradient-approximation density functionals. Physical Review B, 1992, 46, 11570-11577.	1.1	107
2	General-potential study of the electronic and magnetic structure of FeCo. Physical Review B, 1992, 46, 11145-11148.	1.1	36
3	Polarizabilities, charge states, and vibrational modes of isolated fullerene molecules. Physical Review B, 1992, 46, 13584-13591.	1.1	166
4	Densityâ€functional thermochemistry. II. The effect of the Perdewâ€™Wang generalizedâ€gradient correlation correction. Journal of Chemical Physics, 1992, 97, 9173-9177.	1.2	1,565
5	Chemical applications of density functional theory: Fâˆ³ anion dissociation (Fâˆ³ â†’ F2 + Fâˆ). Chemical Physics Letters, 1993, 211, 265-271.	1.2	22
6	Self-compression of metallic clusters under surface tension. Solid State Communications, 1993, 88, 795-801.	0.9	33
7	Properties of ordered intermetallic alloys: first-principles and approximate methods. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1993, 170, 49-57.	2.6	27
8	Local density and gradient-corrected functionals for short-range correlation: Antiparallel-spin and non-RPA contributions. International Journal of Quantum Chemistry, 1993, 48, 93-100.	1.0	32
9	Density-Functional and ab initio computational studies of palladium clusters. International Journal of Quantum Chemistry, 1993, 48, 263-268.	1.0	8
10	Densityâ€functional thermochemistry. III. The role of exact exchange. Journal of Chemical Physics, 1993, 98, 5648-5652.	1.2	91,707
11	Polarization and charge transfer during the dissociation of H2 on Al(110). Surface Science, 1993, 297, L68-L72.	0.8	20
12	Madelung field and electron correlation in physisorption. Surface Science, 1993, 298, 251-258.	0.8	4
13	Accurate optimized-potential-model solutions for spherical spin-polarized atoms: Evidence for limitations of the exchange-only local spin-density and generalized-gradient approximations. Physical Review A, 1993, 47, 2800-2811.	1.0	241
14	Exact exchange-only potentials and the virial relation as microscopic criteria for generalized gradient approximations. Physical Review B, 1993, 47, 13164-13174.	1.1	723
15	Electronic origins of the magnetic phase transitions in zinc-blende Mn chalcogenides. Physical Review B, 1993, 48, 6111-6115.	1.1	71
16	The physics of simple metal clusters: self-consistent jellium model and semiclassical approaches. Reviews of Modern Physics, 1993, 65, 677-732.	16.4	1,557
17	First-principles study of the structural and electronic properties of Cu clusters. Physical Review B, 1993, 47, 9715-9722.	1.1	81
18	Analytic Second Derivatives of the Potential Energy Surface. Israel Journal of Chemistry, 1993, 33, 331-344.	1.0	93

#	ARTICLE	IF	CITATIONS
19	Tight bound and convexity constraint on the exchange-correlation-energy functional in the low-density limit, and other formal tests of generalized-gradient approximations. <i>Physical Review B</i> , 1993, 48, 11638-11645.	1.1	159
20	A study of the energetics of the Cl <sub>2</sub> /MgO(001) interface using correlation corrected periodic Hartree-Fock theory. <i>Journal of Chemical Physics</i> , 1993, 98, 6387-6391.	1.2	25
21	Nonlocal density functional calculations: Comparison of two implementation schemes. <i>Journal of Chemical Physics</i> , 1993, 98, 2971-2974.	1.2	20
22	Effect of semicore banding on heavy-alkali-metal lattice constants: Corrections to the frozen-core approximation. <i>Physical Review B</i> , 1993, 47, 16101-16106.	1.1	6
23	Electronic states of group-IV endohedral atoms in C <sub>28</sub> . <i>Physical Review B</i> , 1993, 48, 17556-17561.	1.1	36
24	Pressure dependence of the elastic moduli in aluminum-rich Al-Li compounds. <i>Physical Review B</i> , 1993, 47, 2493-2500.	1.1	397
25	Fixed-spin-moment calculations on bcc and fcc iron using the generalized gradient approximation. <i>Physical Review B</i> , 1993, 47, 566-569.	1.1	44
26	Calculations of pressure-induced phase transitions in silica. <i>Journal of Geophysical Research</i> , 1993, 98, 22147-22155.	3.3	24
27	Ab initio liquid water. <i>Journal of Chemical Physics</i> , 1993, 99, 9080-9089.	1.2	579
28	Crystal-structure calculations with distorted ions. <i>Physical Review B</i> , 1993, 48, 2889-2908.	1.1	55
29	Weighted-density-approximation ground-state studies of solids. <i>Physical Review B</i> , 1993, 48, 14099-14103.	1.1	27
30	Full-potential calculations using the generalized gradient approximation: Structural properties of transition metals. <i>Physical Review B</i> , 1993, 48, 18304-18307.	1.1	132
31	Pair interactions of rare-gas atoms as a test of exchange-energy-density functionals in regions of large density gradients. <i>Physical Review A</i> , 1993, 47, 4681-4690.	1.0	188
32	Electronic structure of the CoO molecule. <i>Physical Review A</i> , 1993, 48, 2679-2685.	1.0	22
33	Ab initio correlation calculation for metallic lithium. <i>Journal of Chemical Physics</i> , 1993, 99, 6799-6809.	1.2	19
34	Periodic Hartree-Fock study of a weakly bonded layer structure: Brucite Mg(OH) <sub>2</sub> . <i>Physical Review B</i> , 1993, 47, 3522-3529.	1.1	51
35	Expectation values in density-functional theory, and kinetic contribution to the exchange-correlation energy. <i>Physical Review B</i> , 1993, 47, 1167-1173.	1.1	45
36	Application of gradient corrections to density-functional theory for atoms and solids. <i>Physical Review B</i> , 1993, 48, 14944-14952.	1.1	89

#	ARTICLE	IF	CITATIONS
37	First-principles evaluation of dynamical response and plasmon dispersion in metals. Physical Review Letters, 1993, 70, 3955-3958.	2.9	100
38	Properties of monovacancies and self-interstitials in bcc Li: An ab initio pseudopotential study. Physical Review B, 1993, 48, 7676-7678.	1.1	43
39	Theoretical study of linear and bent CrCO, NiCO, and CuCO. Journal of Chemical Physics, 1993, 98, 8041-8050.	1.2	82
40	Self-consistent spline augmented-plane-wave calculation: Ground-state properties of Cu. Physical Review B, 1993, 48, 17703-17714.	1.1	20
41	Electronic-structure calculations of cobalt clusters. Physical Review B, 1993, 47, 13611-13614.	1.1	94
42	Shape of small silicon clusters. Physical Review Letters, 1993, 71, 727-730.	2.9	174
43	Role of nonlocal exchange correlation in activated adsorption. Physical Review Letters, 1993, 70, 3971-3974.	2.9	170
44	Formation energies of metallic voids, edges, and steps: Generalized liquid-drop model. Physical Review B, 1993, 47, 16460-16463.	1.1	26
45	Weighted-density exchange and local-density Coulomb correlation energy functionals for finite systems: Application to atoms. Physical Review A, 1993, 48, 4197-4212.	1.0	42
46	Electronic-structure investigations of siloxenic clusters and films. Physical Review B, 1993, 48, 17400-17405.	1.1	6
47	On the structural properties of NaCl: an ab initio study of the B1-B2 phase transition. Journal of Physics Condensed Matter, 1993, 5, 2969-2976.	0.7	90
48	A super-cell approach for the study of localized defects in solids: carbon substitution in bulk silicon. Journal of Physics Condensed Matter, 1994, 6, 8573-8583.	0.7	9
49	Positron annihilation in II-VI compound semiconductors: theory. Journal of Physics Condensed Matter, 1994, 6, 8809-8827.	0.7	46
50	Modeling CVD diamond with density functional theory. Nanotechnology, 1994, 5, 172-178.	1.3	3
51	Implementation of an approximate self-energy correction scheme in the orthogonalized linear combination of atomic orbitals method of band-structure calculations. Physical Review B, 1994, 49, 10958-10967.	1.1	8
52	Boron hydride analogues of the fullerenes. Physical Review B, 1994, 50, 4787-4794.	1.1	24
53	Core-cancellation functions for evaluating exchange-correlation functionals in first-principles pseudopotential calculations. Physical Review B, 1994, 49, 2351-2361.	1.1	13
54	Is the Local Density Approximation Exact for Short Wavelength Fluctuations?. Physical Review Letters, 1994, 73, 1283-1286.	2.9	56



#	ARTICLE	IF	CITATIONS
55	Improvement on the correlated-Hartree-Fock method and application to atoms. Physical Review A, 1994, 49, 2354-2362.	1.0	8
56	Quantum-mechanical calculation of the solid-state equilibrium $\text{MgO}+\hat{1}\pm\text{-Al}_2\text{O}_3\hat{2}\pm,\text{MgAl}_2\text{O}_4(\text{spinel})$ versus pressure. Physical Review B, 1994, 49, 14179-14187.	1.1	169
57	Gradient-free exchange-correlation functional beyond the local-spin-density approximation. Physical Review A, 1994, 50, 3766-3774.	1.0	14
58	Calculation of atomic forces using the linearized-augmented-plane-wave method. Physical Review B, 1994, 50, 8846-8848.	1.1	13
59	Local and nonlocal density functional studies of FeCr. Journal of Applied Physics, 1994, 76, 6688-6690.	1.1	16
60	Tests of nonlocal kinetic energy functionals. Journal of Chemical Physics, 1994, 100, 4446-4452.	1.2	71
61	Calculations of the total energy, electron-phonon interaction, and Stoner parameter for metals. Physical Review B, 1994, 50, 7255-7261.	1.1	67
62	Relationship between Slater and Kohn-Sham exchange potentials. Physical Review B, 1994, 49, 14197-14201.	1.1	29
63	Fermi surface of noble metals: Full-potential generalized-gradient-approximation calculations. Physical Review B, 1994, 50, 11183-11186.	1.1	7
64	Electronic properties off-electron metals using the generalized gradient approximation. Physical Review B, 1994, 50, 7291-7294.	1.1	134
65	Attachment of Two Electrons to $\text{C}_6\text{O}_4^{4-}$ : Coulomb Barriers in Doubly Charged Anions. Physical Review Letters, 1994, 73, 2821-2824.	2.9	109
66	Simple but efficient correlation functional from a model pair-correlation function. Physical Review B, 1994, 49, 7874-7886.	1.1	43
67	Magnetic structures of hcp bulk gadolinium. Physical Review B, 1994, 49, 4348-4351.	1.1	43
68	Ab initiodetermination of the bulk properties of MgO. Physical Review B, 1994, 49, 8574-8582.	1.1	96
69	High-Dimensional Quantum Dynamics of Adsorption and Desorption of $\text{H}_2$ at Cu(111). Physical Review Letters, 1994, 73, 3121-3124.	2.9	145
70	Bonding in the molybdenum silicides. Physical Review B, 1994, 50, 10742-10760.	1.1	42
71	Surface Corrugation in the Dissociative Adsorption of $\text{H}_2$ on Cu(100). Physical Review Letters, 1994, 73, 1404-1407.	2.9	213
72	Ab initio study of ZnO (101 $\hat{\text{A}}^0$ ) surface relaxation. Physical Review B, 1994, 49, 11153-11158.	1.1	92

#	ARTICLE	IF	CITATIONS
73	Why the local-spin-density approximation fails to predict the energy bands of Gd correctly. <i>Physical Review B</i> , 1994, 49, 1608-1611.	1.1	38
74	Density functionals for exchange and correlation energies: Exact conditions and comparison of approximations. <i>International Journal of Quantum Chemistry</i> , 1994, 49, 539-548.	1.0	60
75	A correlation-energy functional from a correlation-factor model. <i>International Journal of Quantum Chemistry</i> , 1994, 49, 549-557.	1.0	6
76	An analysis of nonlocal density functionals in chemical bonding. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 711-730.	1.0	29
77	Ionization potentials of atoms calculated with a nonlocal exchange and a local correlation functional. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 993-1010.	1.0	9
78	Applicability to atoms of a large set of correlation energy functionals. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 1027-1038.	1.0	5
79	Density-Functional LCAO calculations for solids: Comparison between Hartree-Fock and Kohn-Sham structural properties. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 633-644.	1.0	27
80	A study of small systems containing H and O atoms using nonlocal functionals: comparisons with ab initio and experiment. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 655-666.	1.0	19
81	A test for the Wilson-Levy correlation energy functional. <i>Chemical Physics Letters</i> , 1994, 217, 566-570.	1.2	16
82	Statistical model for delocalized $\pi$ bonding in the C <sub>60</sub> molecule. <i>Chemical Physics Letters</i> , 1994, 218, 229-233.	1.2	1
83	Density functional LCAO calculation of periodic systems. A posteriori correction of the Hartree-Fock energy of covalent and ionic crystals. <i>Chemical Physics Letters</i> , 1994, 220, 145-153.	1.2	104
84	The coupling between adsorption dynamics and the surface structure: H <sub>2</sub> on Si(100). <i>Chemical Physics Letters</i> , 1994, 229, 645-649.	1.2	65
85	Density-functional based determination of the CH <sub>3</sub> -CH <sub>4</sub> hydrogen exchange reaction barrier. <i>Chemical Physics Letters</i> , 1994, 230, 54-60.	1.2	20
86	Nonlocal correlation functional involving the Laplacian of the density. <i>Chemical Physics Letters</i> , 1994, 230, 419-428.	1.2	65
87	Proton transfer in model hydrogen-bonded systems by a density functional approach. <i>Chemical Physics Letters</i> , 1994, 231, 295-300.	1.2	99
88	Calculation of spin-spin coupling constants using density functional theory. <i>Chemical Physics Letters</i> , 1994, 221, 91-99.	1.2	192
89	A density functional study of the simplest hydrogen abstraction reaction. Effect of self-interaction correction. <i>Chemical Physics Letters</i> , 1994, 221, 100-108.	1.2	334
90	Theoretical study of passivated small fullerenes C <sub>24</sub> X <sub>4</sub> (X = N, P, As) and their isoelectronic equivalents (BN) <sub>12</sub> X <sub>4</sub> . <i>Chemical Physics Letters</i> , 1994, 225, 448-453.	1.2	22

#	ARTICLE	IF	CITATIONS
92	A reassessment of electron-gas density-functional calculations of short range repulsive potentials for rare gas atoms. <i>Chemical Physics</i> , 1994, 188, 205-220.	0.9	14
93	Structural phase transformation and ground state properties of cadmium telluride. <i>Solid State Communications</i> , 1994, 91, 607-610.	0.9	11
95	Exchange-correlation potential with correct asymptotic behavior. <i>Physical Review A</i> , 1994, 49, 2421-2431.	1.0	1,343
96	Fullerene molecules and tubules polarizabilities, vibrational modes and nanocapillarity. <i>Computational Materials Science</i> , 1994, 2, 536-542.	1.4	14
97	Generalized-gradient-approximation description of band splittings in transition-metal oxides and fluorides. <i>Physical Review B</i> , 1994, 49, 10170-10175.	1.1	130
98	Calculated electronic structure of metastable phases of Cu. <i>Physical Review B</i> , 1994, 49, 4463-4466.	1.1	14
99	The electronic structure of magnetic transition metallic materials. <i>Reports on Progress in Physics</i> , 1994, 57, 1289-1344.	8.1	61
100	Applications of Engel and Vosko's generalized gradient approximation in solids. <i>Physical Review B</i> , 1994, 50, 7279-7283.	1.1	359
101	A theoretical study of oxygen adsorption on Ge(001). <i>Surface Science</i> , 1994, 311, 126-138.	0.8	17
102	The energetics and dynamics of H <sub>2</sub> dissociation on Al(110). <i>Surface Science</i> , 1994, 304, 131-144.	0.8	48
103	Fermi surface of alkali metals using the full-potential linear muffin-tin orbital method and the generalized gradient approximation. <i>Physical Review B</i> , 1994, 50, 18003-18006.	1.1	4
104	Implementation of gradient-corrected exchange-correlation potentials in Car-Parrinello total-energy calculations. <i>Physical Review B</i> , 1994, 50, 4954-4957.	1.1	1,021
105	Calculated enthalpies of mixing of MnO/MgO and NiO/MgO. <i>Journal of Materials Chemistry</i> , 1994, 4, 825-829.	6.7	13
106	An implementation of analytic second derivatives of the gradient-corrected density functional energy. <i>Journal of Chemical Physics</i> , 1994, 100, 7429-7442.	1.2	214
107	Density-functional calculation of the electronic structure and equilibrium geometry of iron pyrite (FeS <sub>2</sub> ). <i>Physical Review B</i> , 1994, 50, 8214-8220.	1.1	40
108	All-electron local-density and generalized-gradient calculations of the structural properties of semiconductors. <i>Physical Review B</i> , 1994, 50, 14947-14951.	1.1	172
109	Density-functional calculations for small iron clusters: Fe <sub>n</sub> , Fe <sub>n</sub> <sup>+</sup> , and Fe <sub>n</sub> <sup>2+</sup> . <i>Physical Review B</i> , 1994, 49, 11842-11852.	1.1	134
110	Iron at high pressure: Linearized-augmented-plane-wave computations in the generalized-gradient approximation. <i>Physical Review B</i> , 1994, 50, 6442-6445.	1.1	225

#	ARTICLE	IF	CITATIONS
111	Multidimensional Potential Energy Surface for H <sub>2</sub> Dissociation over Cu(111). Physical Review Letters, 1994, 73, 1400-1403.	2.9	334
112	ACRES: Adaptive Coordinate Real-Space Electronic Structure. Materials Research Society Symposia Proceedings, 1995, 408, 139.	0.1	0
113	First-Principles Calculation of the Structure of Mercury. Materials Research Society Symposia Proceedings, 1995, 408, 383.	0.1	1
114	Dissociative Adsorption and Desorption Processes of Cl <sub>2</sub> /GaAs(001) Surfaces. Materials Research Society Symposia Proceedings, 1995, 408, 451.	0.1	0
115	A density-functional study of van der Waals forces: rare gas diatomics. Chemical Physics Letters, 1995, 233, 134-137.	1.2	493
116	The backbone <sup>15</sup> N chemical shift tensor of the gramicidin channel. A molecular dynamics and density functional study. Chemical Physics Letters, 1995, 239, 186-194.	1.2	31
117	Cr <sub>2</sub> in density-functional theory: approximate spin projection. Chemical Physics Letters, 1995, 244, 427-432.	1.2	79
118	Density functional LCAO calculations of periodic systems. Effect of an $\hat{\epsilon}^{-1}$ a posteriori correction of the Hartree-Fock energy on the physical properties of ionic sulfur compounds. Chemical Physics Letters, 1995, 246, 263-268.	1.2	12
119	Investigations using the Becke-Roussel exchange functional. Chemical Physics Letters, 1995, 246, 381-386.	1.2	32
120	On the accuracy of density functionals and their basis set dependence: An extensive study on the main group homonuclear diatomic molecules Li <sub>2</sub> to Br <sub>2</sub> . Journal of Computational Chemistry, 1995, 16, 576-585.	1.5	98
121	Step structure in the atomic Kohn-Sham potential. Zeitschrift für Physik D-Atoms Molecules and Clusters, 1995, 33, 229-238.	1.0	59
122	Density functional theory including Van Der Waals forces. International Journal of Quantum Chemistry, 1995, 56, 247-255.	1.0	100
123	Density functional LCAO calculations for solids: Comparison among Hartree-Fock, DFT local density approximation, and DFT generalized gradient approximation structural properties. International Journal of Quantum Chemistry, 1995, 56, 337-344.	1.0	33
124	On the gradient expansion of the exchange energy within linear response theory and beyond. International Journal of Quantum Chemistry, 1995, 56, 351-361.	1.0	22
125	Nonlocal functionals for exchange and correlation in density functional theory: Application to atoms and to small atomic clusters. International Journal of Quantum Chemistry, 1995, 56, 499-508.	1.0	2
126	Proton transfer in small model systems: A density functional study. International Journal of Quantum Chemistry, 1995, 56, 697-705.	1.0	27
127	Comparison of the performance of various gradient-corrected exchange and correlation functionals in density functional theory: Case studies of CO and N <sub>2</sub> O molecules. International Journal of Quantum Chemistry, 1995, 56, 753-762.	1.0	12
128	Nonlocal density functional calculations of the jellium metal surface. International Journal of Quantum Chemistry, 1995, 56, 847-860.	1.0	0

#	ARTICLE	IF	CITATIONS
129	Exchange and correlation in density functional theory. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 49-59.	1.0	11
130	Determining and extending the domain of exchange and correlation functionals. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 61-78.	1.0	80
131	Why gold is the noblest of all the metals. <i>Nature</i> , 1995, 376, 238-240.	13.7	2,902
132	An adiabatic model of chemisorbed molecules: electron spectroscopy and excited-state potential-energy surfaces. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 1995, 72, 9-18.	0.8	6
133	Electric field gradients, isomer shifts and hyperfine fields from band structure calculations in NiI2. <i>Hyperfine Interactions</i> , 1995, 95, 257-263.	0.2	13
134	Chemisorbed-molecule potential energy surfaces and DIET processes. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 1995, 101, 22-30.	0.6	21
135	On the ab initio evaluation of dynamical electronic response in metals and its comparison with experiment. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 1995, 96, 550-564.	0.6	22
136	Band splittings in AF transition metal compounds using the generalized gradient approximation. <i>Journal of Magnetism and Magnetic Materials</i> , 1995, 140-144, 173-174.	1.0	1
137	Theoretical study of the vibrational spectra of the transition metal carbonyls M(CO) <sub>6</sub> [M=Cr, Mo, W], M(CO) <sub>5</sub> [M=Fe, Ru, Os], and M(CO) <sub>4</sub> [M=Ni, Pd, Pt]. <i>Journal of Chemical Physics</i> , 1995, 102, 8474-8484.	1.2	395
138	Construction of tight-binding-like potentials on the basis of density-functional theory: Application to carbon. <i>Physical Review B</i> , 1995, 51, 12947-12957.	1.1	1,950
139	First principles calculation of preparing mechanism for H <sub>2</sub> desorption from Si(100) $\hat{a}^{\sim}2\hat{A}-1$ . <i>Journal of Chemical Physics</i> , 1995, 103, 1232-1234.	1.2	43
140	Density functional based studies of transition states and barriers for hydrogen exchange and abstraction reactions. <i>Journal of Chemical Physics</i> , 1995, 102, 9345-9349.	1.2	65
141	Interaction of hydrogen with the Be(0001) surface. <i>Physical Review B</i> , 1995, 51, 13748-13759.	1.1	37
142	Electronic structure and enhancement of magnetic moments in the ferromagnetic nitride Fe <sub>16</sub> N <sub>2</sub> . <i>Physical Review B</i> , 1995, 52, 6193-6196.	1.1	8
143	Generalized local approximation to the exchange potential. <i>Physical Review B</i> , 1995, 52, 16476-16485.	1.1	16
144	Use of the generalized gradient approximation in pseudopotential calculations of solids. <i>Physical Review B</i> , 1995, 51, 9521-9525.	1.1	73
145	All-electron study of gradient corrections to the local-density functional in metallic systems. <i>Physical Review B</i> , 1995, 51, 4105-4109.	1.1	202
146	Remanence coercivity of recording media in the high speed regime. <i>IEEE Transactions on Magnetics</i> , 1995, 31, 2892-2894.	1.2	27

#	ARTICLE	IF	CITATIONS
147	Theory of lithium islands and monolayers: Electronic structure and stability. <i>Physical Review B</i> , 1995, 51, 2457-2466.	1.1	10
148	Effect of nonlocal corrections to the local-density approximation on total-energy calculations of K, Rb, and Cs. <i>Physical Review B</i> , 1995, 52, 1441-1443.	1.1	7
149	Six-Dimensional Quantum Dynamics of Adsorption and Desorption of H <sub>2</sub> at Pd(100): Steering and Steric Effects. <i>Physical Review Letters</i> , 1995, 75, 2718-2721.	2.9	358
150	Energy expressions in density-functional theory using line integrals. <i>Physical Review A</i> , 1995, 51, 170-178.	1.0	64
151	Density-functional calculations for cerium metal. <i>Physical Review B</i> , 1995, 51, 4618-4621.	1.1	24
152	Theoretical investigation of the high-pressure crystal structures of Ce and Th. <i>Physical Review B</i> , 1995, 52, 13169-13176.	1.1	32
153	Escaping the symmetry dilemma through a pair-density interpretation of spin-density functional theory. <i>Physical Review A</i> , 1995, 51, 4531-4541.	1.0	335
154	Theoretical zero-temperature phase diagram for neptunium metal. <i>Physical Review B</i> , 1995, 52, 1631-1639.	1.1	29
155	Barriers for hydrogen atom diffusion on the Si(100)-1 surface. <i>Journal of Chemical Physics</i> , 1995, 102, 8249-8254.	1.2	45
156	Dissociation of H <sub>2</sub> on Cu(100): Dynamics on a new two-dimensional potential energy surface. <i>Journal of Chemical Physics</i> , 1995, 102, 3873-3883.	1.2	73
157	Theory of Adsorption and Desorption of H <sub>2</sub> /Si(001). <i>Physical Review Letters</i> , 1995, 74, 952-955.	2.9	94
158	Density-functional calculation of the bulk and surface geometry of beryllium. <i>Physical Review B</i> , 1995, 51, 13653-13659.	1.1	33
159	Electronic and magnetic structure of KNiF <sub>3</sub> perovskite. <i>Physical Review B</i> , 1995, 52, 2381-2389.	1.1	79
160	Exact Exchange Potential Band-Structure Calculations by the Linear Muffin-Tin Orbital Atomic-Sphere Approximation Method for Si, Ge, C, and MnO. <i>Physical Review Letters</i> , 1995, 74, 2989-2992.	2.9	122
161	Structure, stability, and vibrational properties of polymerized C <sub>60</sub> . <i>Physical Review B</i> , 1995, 52, 14963-14970.	1.1	139
162	Si adatom binding and diffusion on the Si(100) surface: Comparison of ab initio, semiempirical and empirical potential results. <i>Journal of Chemical Physics</i> , 1995, 102, 1044-1056.	1.2	71
163	Direct pathway for sticking/desorption of H <sub>2</sub> on Si(100). <i>Physical Review B</i> , 1995, 51, 13432-13440.	1.1	84
164	Density-functional-based construction of transferable nonorthogonal tight-binding potentials for Si and SiH. <i>Physical Review B</i> , 1995, 52, 11492-11501.	1.1	133

#	ARTICLE	IF	CITATIONS
165	Local Chemical Reactivity of a Metal Alloy Surface. <i>Physical Review Letters</i> , 1995, 74, 3487-3490.	2.9	210
166	Theoretical study of the stability of beryllium oxide (110) and (001) surfaces in dense wurtzite and layered graphitic phases. <i>Physical Review B</i> , 1995, 52, 17480-17490.	1.1	13
167	Theoretical investigation of the pressure-induced metallization and the collapse of the antiferromagnetic state of NiI <sub>2</sub> . <i>Physical Review B</i> , 1995, 51, 4122-4127.	1.1	13
168	Magnetic interactions and the cooperative Jahn-Teller effect in KCuF <sub>3</sub> . <i>Physical Review B</i> , 1995, 52, 10150-10159.	1.1	83
169	Bulk and surface magnetism and interplanar spacings in Gd from first-principles calculations. <i>Physical Review B</i> , 1995, 52, 4420-4426.	1.1	48
170	Semilocal density functionals for exchange and correlation: Theory and applications. <i>Theoretical and Computational Chemistry</i> , 1995, 2, 29-74.	0.2	13
171	Development, implementation and applications of efficient methodologies for density functional calculations. <i>Theoretical and Computational Chemistry</i> , 1995, 2, 169-219.	0.2	5
172	Symmetry and density-functional exchange and correlation. <i>Theoretical and Computational Chemistry</i> , 1995, , 151-167.	0.2	2
173	Ground state properties of titaniumdiboride. <i>High Pressure Research</i> , 1995, 13, 335-341.	0.4	12
174	Local density and generalized gradient approximation studies of KNbO <sub>3</sub> and BaTiO <sub>3</sub> . <i>Ferroelectrics</i> , 1995, 164, 143-152.	0.3	58
175	Structural phase transitions and specific-heat coefficients of alkaline-earth metals. <i>Journal of Physics Condensed Matter</i> , 1995, 7, 1283-1286.	0.7	8
176	Superexchange interaction in K <sub>2</sub> NiF <sub>4</sub> : an ab initio Hartree-Fock study. <i>Journal of Physics Condensed Matter</i> , 1995, 7, 7997-8007.	0.7	26
177	Electronic and magnetic properties of embedded Rh clusters in Ni matrix. <i>Journal of Physics Condensed Matter</i> , 1995, 7, 7367-7372.	0.7	5
178	Electronic Band Structures of LaMO <sub>3</sub> (M = Ti, V, Cr,..., Ni, Cu) in the Local Spin-Density Approximation. <i>Springer Series in Solid-state Sciences</i> , 1995, , 95-105.	0.3	10
179	DMol, a standard tool for density functional calculations: Review and advances. <i>Theoretical and Computational Chemistry</i> , 1995, , 221-254.	0.2	107
180	Gradient correction for positron states in solids. <i>Physical Review B</i> , 1995, 51, 7341-7344.	1.1	196
181	Poisoning of Pd(100) for the dissociation of H <sub>2</sub> : a theoretical study of co-adsorption of hydrogen and sulphur. <i>Surface Science</i> , 1995, 329, L605-L610.	0.8	85
182	The interaction of hydrogen with the (110) surface of NiAl. <i>Surface Science</i> , 1995, 331-333, 811-817.	0.8	53



#	ARTICLE	IF	CITATIONS
183	First-principles molecular dynamics study of acetylene adsorption on the Si(001) surface. <i>Surface Science</i> , 1995, 341, L1091-L1095.	0.8	81
184	Electronic factors determining the reactivity of metal surfaces. <i>Surface Science</i> , 1995, 343, 211-220.	0.8	2,087
185	Correlation energy density from ab initio first- and second-order density matrices: A benchmark for approximate functionals. <i>Journal of Chemical Physics</i> , 1995, 103, 10085-10094.	1.2	35
186	Constraints on the crystalline structure of the inner core: Mechanical instability of BCC iron at high pressure. <i>Geophysical Research Letters</i> , 1995, 22, 125-128.	1.5	66
187	First-principles prediction of the high-pressure phase transition and electronic structure of FeO: Implications for the chemistry of the lower mantle and core. <i>Geophysical Research Letters</i> , 1995, 22, 1001-1004.	1.5	42
188	An introduction to density functional theory in chemistry. <i>Theoretical and Computational Chemistry</i> , 1995, , 1-27.	0.2	46
189	High-Pressure Elasticity of Iron and Anisotropy of Earth's Inner Core. <i>Science</i> , 1995, 267, 1972-1975.	6.0	254
190	Theoretical study of electronic, magnetic, and structural properties of $\alpha$ -Fe <sub>2</sub> O <sub>3</sub> (hematite). <i>Physical Review B</i> , 1995, 51, 7441-7450.	1.1	273
191	Theoretical stability limit of diamond at ultrahigh pressure. <i>Physical Review B</i> , 1995, 52, 15035-15038.	1.1	37
192	The calculation of NMR and ESR spectroscopy parameters using density functional theory. <i>Theoretical and Computational Chemistry</i> , 1995, 2, 273-347.	0.2	139
193	Association and insertion complexes of nickel with water and methanol studied using Kohn-Sham theory. <i>Theoretica Chimica Acta</i> , 1995, 91, 129-146.	0.9	8
194	Extension of the local-spin-density exchange-correlation approximation to multiplet states. <i>Theoretica Chimica Acta</i> , 1995, 91, 147-156.	0.9	96
195	Density functional calculations of the structures and bond energies of Cr(CO) <sub>6</sub> and (η <sup>6</sup> -C <sub>6</sub> H <sub>6</sub> )Cr(CO) <sub>2</sub> (CX) (X=O, S) complexes. <i>Theoretica Chimica Acta</i> , 1995, 91, 157-167.	0.9	1
196	Ab initio Force-Constant Method for Phonon Dispersions in Alkali Metals. <i>Physical Review Letters</i> , 1995, 74, 1791-1794.	2.9	185
197	Application of generalized gradient approximations: The diamond- $\beta$ -tin phase transition in Si and Ge. <i>Physical Review B</i> , 1995, 52, 2550-2556.	1.1	153
198	Electronic structure, total energies, and STM images of clean and oxygen-covered Al(111). <i>Physical Review B</i> , 1995, 52, 14954-14962.	1.1	118
199	Ab initio calculations of structural and electronic properties of gallium solid-state phases. <i>Physical Review B</i> , 1995, 52, 9988-9998.	1.1	145
200	Generalized-gradient approximations to density-functional theory: A comparative study for atoms and solids. <i>Physical Review B</i> , 1996, 53, 1180-1185.	1.1	228



#	ARTICLE	IF	CITATIONS
201	Influence of gradient corrections to the local-density-approximation on the calculation of hyperfine fields in ferromagnetic Fe, Co, and Ni. <i>Physical Review B</i> , 1996, 53, 9776-9783.	1.1	53
202	Ab initio molecular dynamics simulation of liquid water: Comparison of three gradient-corrected density functionals. <i>Journal of Chemical Physics</i> , 1996, 105, 1142-1152.	1.2	597
203	Interactions Between Adsorbate Particles. <i>Handbook of Surface Science</i> , 1996, , 577-650.	0.3	21
204	Assignment of Relative Configuration to Acyclic Compounds Based on <sup>13</sup> C NMR Shifts. A Density Functional and Molecular Mechanics Study. <i>Journal of Organic Chemistry</i> , 1996, 61, 8083-8088.	1.7	45
205	Electron Densities of Homonuclear Diatomic Molecules As Calculated from Density Functional Theory. <i>The Journal of Physical Chemistry</i> , 1996, 100, 5274-5280.	2.9	20
206	First-principles theory of iron up to earth-core pressures: Structural, vibrational, and elastic properties. <i>Physical Review B</i> , 1996, 53, 14063-14072.	1.1	240
207	Dynamics, Spin Fluctuations, and Bonding in Liquid Silicon. <i>Physical Review Letters</i> , 1996, 76, 2077-2080.	2.9	59
208	An ab Initio Hartree-Fock Study of the Cubic and Tetragonal Phases of Bulk Tungsten Trioxide. <i>Journal of the American Chemical Society</i> , 1996, 118, 12174-12182.	6.6	120
209	Intrinsic Aptitude of Cationic Methyl- and Ethylpalladium To Associate Ethylene and To Further Undergo Subsequent Migratory Insertion. A Theoretical Study. <i>Organometallics</i> , 1996, 15, 5542-5550.	1.1	38
210	Density functional theory of time-dependent phenomena. , 1996, , 81-172.		476
211	Elementary Concepts in Density Functional Theory. <i>Theoretical and Computational Chemistry</i> , 1996, , 3-24.	0.2	12
212	Andersen's force theorem and the local stress field. <i>Physical Review B</i> , 1996, 53, 7143-7146.	1.1	75
213	Density-functional thermochemistry. IV. A new dynamical correlation functional and implications for exact-exchange mixing. <i>Journal of Chemical Physics</i> , 1996, 104, 1040-1046.	1.2	2,426
214	Ab initio quantum dynamics of adsorption/desorption on a 3-D potential. <i>Surface Science</i> , 1996, 345, 125-137.	0.8	31
215	Theory of adsorption of Cl <sub>2</sub> molecules on GaAs(001) surfaces. <i>Surface Science</i> , 1996, 357-358, 322-326.	0.8	18
216	Six-dimensional quantum dynamics of adsorption and desorption of H <sub>2</sub> at Pd(100): no need for a molecular precursor adsorption state. <i>Surface Science</i> , 1996, 357-358, 614-618.	0.8	43
217	Geometric and electronic factors determining the differences in reactivity of H <sub>2</sub> on Cu(100) and Cu(111). <i>Surface Science</i> , 1996, 359, 45-53.	0.8	100
218	Disagreement between experimental and theoretical metal surface relaxations. <i>Surface Science</i> , 1996, 360, 297-301.	0.8	46

#	ARTICLE	IF	CITATIONS
219	A comparison of quantum and classical dynamics of H <sub>2</sub> dissociation on Cu(111). Surface Science, 1996, 364, 219-234.	0.8	42
220	Hydrogen-induced structural changes on NiAl(110). Surface Science, 1996, 365, L639-L646.	0.8	18
221	Infrared intensities and Raman-scattering activities within density-functional theory. Physical Review B, 1996, 54, 7830-7836.	1.1	579
222	Microscopic mechanisms in heterogeneous catalysis: H <sub>2</sub> dissociation on clean and S covered Pd (1 0 0). Applied Physics A: Materials Science and Processing, 1996, 63, 583-593.	1.1	11
223	Density Functional for van der Waals Forces at Surfaces. Physical Review Letters, 1996, 77, 2029-2032.	2.9	108
224	First-principles finite-temperature simulation of surface dynamics: Si(111)-(7 Å <sup>-1</sup> × 7). Surface Science, 1996, 368, 152-162.	0.8	7
225	Ab initio calculations of adsorbate hydrogen-bond strength: ammonia on Pt(111). Surface Science, 1996, 368, 253-257.	0.8	35
226	Electronic Structure and Properties of Solids. The Journal of Physical Chemistry, 1996, 100, 13263-13274.	2.9	111
227	CO Chemisorption at Metal Surfaces and Overlayers. Physical Review Letters, 1996, 76, 2141-2144.	2.9	1,293
228	Abinitio pseudopotential study of Fe, Co, and Ni employing the spin-polarized LAPW approach. Physical Review B, 1996, 53, 10685-10689.	1.1	53
229	Calculation of positron states and annihilation in solids: A density-gradient-correction scheme. Physical Review B, 1996, 53, 16201-16213.	1.1	199
230	van der Waals Interactions in Density-Functional Theory. Physical Review Letters, 1996, 76, 102-105.	2.9	474
231	Structure and Stability of a High-Coverage(1 Å <sup>-1</sup> ) Oxygen Phase on Ru(0001). Physical Review Letters, 1996, 77, 3371-3374.	2.9	220
232	Nuclear magnetic resonance spin-spin coupling constants from density functional theory: Problems and results. Journal of Chemical Physics, 1996, 105, 8793-8800.	1.2	146
233	NMR Spin-Spin Coupling Constants from Density Functional Theory with Slater-Type Basis Functions. The Journal of Physical Chemistry, 1996, 100, 5286-5290.	2.9	90
234	Cohesive energy of 3d transition metals: Density functional theory atomic and bulk calculations. Physical Review B, 1996, 54, 5326-5333.	1.1	204
235	Generalized gradient approximation for the exchange-correlation hole of a many-electron system. Physical Review B, 1996, 54, 16533-16539.	1.1	5,433
236	Prediction of Nitrogen and Oxygen NMR Chemical Shifts in Organic Compounds by Density Functional Theory. The Journal of Physical Chemistry, 1996, 100, 16881-16891.	2.9	51

#	ARTICLE	IF	CITATIONS
237	Quantum Chemistry and Molecular Processes. The Journal of Physical Chemistry, 1996, 100, 13213-13225.	2.9	232
238	The theory of CVD diamond growth. Diamond and Related Materials, 1996, 5, 236-241.	1.8	17
239	Spin dynamics in magnets: Equation of motion and finite temperature effects. Physical Review B, 1996, 54, 1019-1035.	1.1	287
240	Quantum Steering Effects in the Dissociative Adsorption of H <sub>2</sub> on Rh(100). Physical Review Letters, 1996, 77, 1119-1122.	2.9	63
241	Density-functional study of the ground- and excited-spin states of [M <sub>2</sub> Cl <sub>9</sub> ] <sup>3-</sup> (M = Mo or W) face-shared dimers: consequences for structural variation in A <sub>3</sub> M <sub>2</sub> Cl <sub>9</sub> complexes. Journal of the Chemical Society Dalton Transactions, 1996, , 4485-4491.	1.1	12
242	The structure and binding energy of K <sup>+</sup> ether complexes: A comparison of MP2, RI-MP2, and density functional methods. Journal of Chemical Physics, 1996, 105, 1940-1950.	1.2	58
243	Binding energy of the ring form of (H <sub>2</sub> O) <sub>6</sub> : Comparison of the predictions of conventional and localized orbital MP2 calculations. Journal of Chemical Physics, 1996, 105, 11091-11099.	1.2	104
244	Ab Initio Pseudopotential Calculations of Carbon Impurities in Si. Materials Research Society Symposia Proceedings, 1996, 438, 33.	0.1	0
245	Ab Initio Pseudopotential Calculations of Carbon Impurities In Si. Materials Research Society Symposia Proceedings, 1996, 439, 59.	0.1	7
246	First-Principles Calculations Of Diffusion Of Chlorine Atoms In GaAs. Materials Research Society Symposia Proceedings, 1996, 442, 529.	0.1	0
247	Lattice distortion and magnetism of Fe impurity in Cu and Ag. Materials Transactions, JIM, 1996, 37, 279-282.	0.9	3
248	Generalized gradient approximations to density functional theory: comparison with exact results. Theoretical and Computational Chemistry, 1996, , 295-326.	0.2	34
249	Nonlocal Weighted Density Approximation to exchange, correlation and kinetic energy in Density Functional Theory. Theoretical and Computational Chemistry, 1996, , 239-294.	0.2	0
250	Adsorption complexes on oxides: Density functional model cluster studies. Theoretical and Computational Chemistry, 1996, , 569-619.	0.2	24
251	DFT Study of Nickel: Towards the MD Simulation of the Nickel-Water Interface. Theoretical and Computational Chemistry, 1996, 4, 649-677.	0.2	1
252	Anisotropy of Growth of the Close-Packed Surfaces of Silver. Physical Review Letters, 1996, 77, 1095-1098.	2.9	133
253	Recent Developments in Configuration Interaction and Density Functional Theory Calculations of Radical Hyperfine Structure.. Advances in Quantum Chemistry, 1996, 27, 297-369.	0.4	83
254	Generalized Gradient Approximation Made Simple. Physical Review Letters, 1996, 77, 3865-3868.	2.9	157,044

#	ARTICLE	IF	CITATIONS
255	Harmonic Vibrational Frequencies: An Evaluation of Hartree-Fock, Møller-Plesset, Quadratic Configuration Interaction, Density Functional Theory, and Semiempirical Scale Factors. <i>The Journal of Physical Chemistry</i> , 1996, 100, 16502-16513.	2.9	6,586
256	Structural, elastic, and high-pressure properties of cubic TiC, TiN, and TiO. <i>Physical Review B</i> , 1996, 53, 3072-3079.	1.1	259
257	A Density Functional Approach to Hardness, Polarizability, and Valency of Molecules in Chemical Reactions. <i>The Journal of Physical Chemistry</i> , 1996, 100, 12295-12298.	2.9	180
258	Density functionals: Where do they come from, why do they work?. <i>Topics in Current Chemistry</i> , 1996, , 1-30.	4.0	40
259	Designing surface alloys with specific active sites. <i>Catalysis Letters</i> , 1996, 40, 131-135.	1.4	77
260	Theoretical and experimental studies of F <sub>3</sub> SiCO <sup>+</sup> and F <sub>3</sub> SiOC <sup>+</sup> . <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1996, 153, 161-172.	1.9	7
261	An ab initio Hartree-Fock investigation of galena (PbS). <i>Chemical Physics Letters</i> , 1996, 257, 627-632.	1.2	38
262	Theoretical study of the structural evolution of small hydrogenated silicon clusters: Si <sub>6</sub> H <sub>x</sub> . <i>Chemical Physics Letters</i> , 1996, 261, 346-352.	1.2	54
263	Applications of density functional theory approaching chemical accuracy to the study of typical carbon-carbon and carbon-hydrogen bonds. <i>Computational and Theoretical Chemistry</i> , 1996, 369, 29-37.	1.5	12
264	Structure of the optimized effective Kohn-Sham exchange potential and its gradient approximations. <i>International Journal of Quantum Chemistry</i> , 1996, 57, 17-33.	1.0	17
265	Comparison shopping for a gradient-corrected density functional. <i>International Journal of Quantum Chemistry</i> , 1996, 57, 309-319.	1.0	276
266	Accurate density functional calculations on large systems. <i>International Journal of Quantum Chemistry</i> , 1996, 58, 123-132.	1.0	10
267	Calculations of molecules, clusters, and solids with a simplified LCAO-DFT-LDA scheme. <i>International Journal of Quantum Chemistry</i> , 1996, 58, 185-192.	1.0	684
268	Electronic and geometrical structure of bulk rutile studied with Hartree-Fock and density functional methods. <i>International Journal of Quantum Chemistry</i> , 1996, 58, 297-306.	1.0	31
269	A comparison of Hartree-Fock, MP2, and DFT results for the HCN dimer and crystal. , 1996, 60, 767-778.		23
270	On the optimal mixing of the exchange energy and the electron-electron interaction part of the exchange-correlation energy. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 1375-1384.	1.0	22
271	Linear response and quasiparticle calculations as probes of the Kohn-Sham eigenvalues in metals. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 1457-1468.	1.0	2
272	Zr@Si <sub>20</sub> : a strongly bound Si endohedral system. <i>Chemical Physics Letters</i> , 1996, 254, 249-256.	1.2	99

#	ARTICLE	IF	CITATIONS
273	35/37Cl NMR chemical shifts and nuclear quadrupole couplings for some small chlorine compounds: experimental and theoretical study. <i>Chemical Physics Letters</i> , 1996, 258, 330-335.	1.2	24
274	First-principles molecular dynamics simulation of water dissociation on TiO <sub>2</sub> (110). <i>Chemical Physics Letters</i> , 1996, 261, 246-252.	1.2	160
275	Force calculation and atomic-structure optimization for the full-potential linearized augmented plane-wave code WIEN. <i>Computer Physics Communications</i> , 1996, 94, 31-48.	3.0	177
276	Ab Initio ECP/DFT Calculation and Interpretation of Carbon and Oxygen NMR Chemical Shift Tensors in Transition-Metal Carbonyl Complexes. <i>Chemistry - A European Journal</i> , 1996, 2, 24-30.	1.7	52
277	NMR Chemical Shift Anomaly and Bonding in Piano-Stool Carbonyl and Related Complexes—an Ab Initio ECP/DFT Study. <i>Chemistry - A European Journal</i> , 1996, 2, 348-358.	1.7	25
278	Solvent Effect on the NMR Chemical Shieldings in Water Calculated by a Combination of Molecular Dynamics and Density Functional Theory. <i>Chemistry - A European Journal</i> , 1996, 2, 452-457.	1.7	90
279	Analysis of <sup>13</sup> C and <sup>17</sup> O Chemical Shift Tensors and an ELF View of Bonding in Fe <sub>2</sub> (CO) <sub>9</sub> and Rh <sub>6</sub> (CO) <sub>16</sub> . <i>Chemische Berichte</i> , 1996, 129, 527-533.	0.2	31
280	Interpretation of <sup>31</sup> P NMR Coordination Shifts for Phosphane Ligands. Ab Initio ECP/DFT Study of Chemical Shift Tensors in M(CO) <sub>5</sub> L [M = Cr, Mo, W; L = PH <sub>3</sub> , P(CH <sub>3</sub> ) <sub>3</sub> , PF <sub>3</sub> , PCl <sub>3</sub> ]. <i>Chemische Berichte</i> , 1996, 129, 535-544.	0.2	40
281	The magnetic properties of 4d impurities in Ag <sub>n</sub> clusters. <i>Solid State Communications</i> , 1996, 97, 429-433.	0.9	1
282	Electronic ground state of MnO, FeO, CoO and NiO within the LSDA + U approximation. <i>Solid State Communications</i> , 1996, 100, 457-461.	0.9	42
283	The shape of the Fermi surface. <i>Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics</i> , 1996, 383, 127-132.	1.5	7
284	Density functional based structure optimization for molecules containing heavy elements: analytical energy gradients for the Douglas-Kroll-Hess scalar relativistic approach to the LCGTO-DF method. <i>Chemical Physics</i> , 1996, 210, 413-425.	0.9	127
285	Electronic, magnetic and crystal structure of Cr <sub>2</sub> O <sub>3</sub> by theoretical methods. <i>Journal of Physics and Chemistry of Solids</i> , 1996, 57, 1735-1741.	1.9	106
286	Direct orbital-free calculations using DFT and one-electron Green's functions: applications to atoms. <i>Chemical Physics Letters</i> , 1996, 263, 507-512.	1.2	1
287	Construction of the adiabatic connection. <i>Chemical Physics Letters</i> , 1996, 263, 499-506.	1.2	164
288	Adaptive coordinate, real-space electronic structure calculations on parallel computers. <i>Solid State Communications</i> , 1996, 99, 57-61.	0.9	46
289	Steering and re-vibrational effects on dissociative adsorption and associative desorption of H <sub>2</sub> Pd(100). <i>Progress in Surface Science</i> , 1996, 53, 187-196.	3.8	44
290	Magnetism of the Rh <sub>13</sub> cluster. <i>Physica Status Solidi (B): Basic Research</i> , 1996, 195, 549-552.	0.7	1

#	ARTICLE	IF	CITATIONS
291	Structure, Stability, and Bonding of Transition-Metal $\pi$ -Boryl Complexes. A Molecular Orbital Study. The Journal of Physical Chemistry, 1996, 100, 6509-6517.	2.9	68
292	The Douglas-Kroll-Hess Approach to Relativistic Density Functional Theory: Methodological Aspects and Applications to Metal Complexes and Clusters. Theoretical and Computational Chemistry, 1996, , 497-566.	0.2	82
293	Density Functional Theory. , 1996, , 1-35.		11
294	The fcc - bcc structural transition: I. A band theoretical study for Li, K, Rb, Ca, Sr, and the transition metals Ti and V. Journal of Physics Condensed Matter, 1996, 8, 799-815.	0.7	69
295	Generalized gradient correction for exchange: Deduction from the oscillator model. Physical Review A, 1996, 53, 3143-3150.	1.0	11
296	Pseudopotential variational quantum Monte Carlo approach to bcc lithium. Physical Review B, 1996, 54, 8393-8397.	1.1	15
297	Electronic structure of cerium in the self-interaction-corrected local-spin-density approximation. Physical Review B, 1996, 53, 4275-4286.	1.1	127
298	Magnetic properties of M <sub>13</sub> clusters (M=Y, Zr, Nb, Mo, and Tc). Physical Review B, 1996, 54, 11907-11910.	1.1	31
299	Dynamics of H <sub>2</sub> dissociation on Cu(100): Effects of surface defects. Journal of Chemical Physics, 1996, 104, 9994-10000.	1.2	12
300	Sum-over- $\epsilon$ states density functional perturbation theory: Prediction of reliable <sup>13</sup> C, <sup>15</sup> N, and <sup>17</sup> O nuclear magnetic resonance chemical shifts. Journal of Chemical Physics, 1996, 105, 8995-9006.	1.2	64
301	A Kohn-Sham study of CH <sub>4</sub> , C <sub>6</sub> H <sub>6</sub> , and O <sub>3</sub> using functionals incorporating exact exchange. Journal of Chemical Physics, 1996, 104, 4166-4172.	1.2	17
302	Generalized-gradient functionals in adaptive curvilinear coordinates. Physical Review B, 1996, 54, 1568-1574.	1.1	29
303	Adhesion in NiAl-Cr from first principles. Physical Review B, 1996, 53, 13883-13890.	1.1	65
304	Generalized Gradient Theory for Silica Phase Transitions. Physical Review Letters, 1996, 76, 660-663.	2.9	313
305	Investigation of density functionals to predict both ground-state properties and band structures. Physical Review B, 1996, 54, 8420-8429.	1.1	23
306	Theoretical study of O adlayers on Ru(0001). Physical Review B, 1996, 54, 2868-2872.	1.1	160
307	D <sub>2</sub> dissociative adsorption on and associative desorption from Si(100): Dynamic consequences of an ab initio potential energy surface. Journal of Chemical Physics, 1996, 104, 3075-3091.	1.2	30
308	Potential-energy surface for H <sub>2</sub> dissociation over Pd(100). Physical Review B, 1996, 53, 4926-4932.	1.1	129

#	ARTICLE	IF	CITATIONS
309	Constraint Satisfaction in Local and Gradient Susceptibility Approximations: Application to a van der Waals Density Functional. <i>Physical Review Letters</i> , 1996, 76, 1780-1783.	2.9	177
310	Laser-induced desorption of NO from NiO(100): Ab initio calculations of potential surfaces for intermediate excited states. <i>Journal of Chemical Physics</i> , 1996, 104, 10030-10040.	1.2	73
311	Electronic structure of Pu compounds with group-IIIb metals: Two regimes of behavior. <i>Physical Review B</i> , 1996, 54, R17265-R17268.	1.1	26
312	An analytical six-dimensional potential energy surface for dissociation of molecular hydrogen on Cu(100). <i>Journal of Chemical Physics</i> , 1996, 104, 7344-7358.	1.2	118
313	Density dependence of the electronic supershells in the homogeneous jellium model. <i>Physical Review B</i> , 1996, 54, 5168-5177.	1.1	22
314	Puckering models for the Si(113) surface reconstruction. <i>Physical Review B</i> , 1996, 54, 13744-13747.	1.1	19
315	Ab initio study of a CO monolayer adsorbed on the (101̄,0) surface of ZnO. <i>Journal of Chemical Physics</i> , 1996, 104, 3348-3351.	1.2	32
316	A theoretical study of CH <sub>4</sub> dissociation on pure and gold-alloyed Ni(111) surfaces. <i>Journal of Chemical Physics</i> , 1996, 105, 5595-5604.	1.2	262
317	Investigation of the reliability of density functional methods: Reaction and activation energies for Si-Si bond cleavage and H <sub>2</sub> elimination from silanes. <i>Journal of Chemical Physics</i> , 1996, 104, 148-158.	1.2	112
318	Straightforward gradient approximation for the exchange energy of s <sup>2</sup> p-bonded solids. <i>Physical Review B</i> , 1996, 54, 17392-17401.	1.1	13
319	Mechanism of Poisoning the Catalytic Activity of Pd(100) by a Sulfur Adlayer. <i>Physical Review Letters</i> , 1996, 76, 3380-3383.	2.9	71
320	Relevance of relativistic exchange-correlation functionals and of finite nuclei in molecular density-functional calculations. <i>Physical Review A</i> , 1996, 54, 4775-4782.	1.0	89
321	Competition between vibrational excitation and dissociation in collisions of H <sub>2</sub> with Cu(100). <i>Physical Review B</i> , 1996, 53, 10397-10401.	1.1	54
322	Local Isoelectronic Reactivity of Solid Surfaces. <i>Physical Review Letters</i> , 1996, 77, 1560-1563.	2.9	48
323	Diffusion Monte Carlo study of jellium surfaces: Electronic densities and pair correlation functions. <i>Physical Review B</i> , 1996, 54, 17199-17207.	1.1	43
324	Improving energies by using exact electron densities. <i>Physical Review A</i> , 1996, 53, R2915-R2917.	1.0	22
325	Adsorption of CO on TiO <sub>2</sub> (110) studied by means of a cluster model surrounded by multipoles obtained from slab calculations. <i>Physical Review B</i> , 1996, 54, 14812-14821.	1.1	36
326	Gradient expansion of the exchange energy from second-order density response theory. <i>Physical Review B</i> , 1996, 54, 17402-17413.	1.1	159



#	ARTICLE	IF	CITATIONS
327	Optimized effective-potential calculations of Ge and GaAs. Physical Review B, 1996, 54, 7891-7896.	1.1	43
328	Hydrogen adsorption on the (100) surfaces of rhodium and palladium: the influence of non-local exchange - correlation interactions. Journal of Physics Condensed Matter, 1996, 8, 7659-7675.	0.7	52
329	On the Accuracy of the Total Energy Pseudopotential Scheme Applied to Small Molecules. The Journal of Physical Chemistry, 1996, 100, 6093-6096.	2.9	19
330	Reference-State Density Functional Theory. The Journal of Physical Chemistry, 1996, 100, 6104-6106.	2.9	11
331	LCAO-LDA calculation of Compton profiles in hexagonal BN; comparison with experiments. Journal of Physics Condensed Matter, 1996, 8, 10425-10434.	0.7	2
332	Alternative density functional theory for atoms and molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 1996, 29, L173-L179.	0.6	17
333	Density functional theory, the exchange hole, and the molecular bond. Theoretical and Computational Chemistry, 1996, , 207-238.	0.2	11
334	Charge-Transfer Complexes: Stringent Tests for Widely Used Density Functionals. The Journal of Physical Chemistry, 1996, 100, 12265-12276.	2.9	188
335	Structural and electronic properties of pyrope garnet : anab initiostudy. Journal of Physics Condensed Matter, 1996, 8, 8815-8828.	0.7	20
336	Magnetic properties of icosahedral clusters. Journal of Physics Condensed Matter, 1997, 9, 4925-4930.	0.7	0
337	Calculation of the phonon frequencies of in an anharmonic model. Journal of Physics Condensed Matter, 1997, 9, 7063-7070.	0.7	1
338	Comparison of the spherically averaged pseudopotential model with the stabilized jellium model. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, 3583-3596.	0.6	6
339	First-principles studies of the thermodynamic properties of bulk Li. Journal of Physics Condensed Matter, 1997, 9, 2135-2148.	0.7	19
340	Density-functional exchange-correlation potential and orbital eigenvalues for the Ne-Atom. Physica Scripta, 1997, 55, 459-463.	1.2	1
341	Anab initiostudy of muons in ethanal. Journal of Physics Condensed Matter, 1997, 9, 3241-3257.	0.7	6
342	Gradient-corrected correlation with nearly exact Kohn-Sham exchange: Calculations for Si and Ge. Physical Review B, 1997, 55, 9432-9438.	1.1	41
343	Anomalous atomic volume of $\hat{1}\pm$ -Pu. Physical Review B, 1997, 55, 15353-15355.	1.1	38
344	Ab initiostudy of the anomalies in the He-atom-scattering spectra of H/Mo(110) and H/W(110). Physical Review B, 1997, 56, 13503-13518.	1.1	34



#	ARTICLE	IF	CITATIONS
345	Fractional occupation numbers in density-functional theory. <i>Physical Review A</i> , 1997, 56, 2665-2669.	1.0	27
346	Proton-Induced Plasticity in Hydrogen Clusters. <i>Physical Review Letters</i> , 1997, 78, 3669-3672.	2.9	39
347	Tight-binding computations of elastic anisotropy of Fe, Xe, and Si under compression. <i>Physical Review B</i> , 1997, 56, 8575-8589.	1.1	99
348	Relativistic calculations on the adsorption of CO on the (111) surfaces of Ni, Pd, and Pt within the zeroth-order regular approximation. <i>Physical Review B</i> , 1997, 56, 13556-13562.	1.1	161
349	Six-dimensional quantum dynamics of dissociative chemisorption of H <sub>2</sub> on Cu(100). <i>Journal of Chemical Physics</i> , 1997, 107, 3309-3323.	1.2	74
350	Dynamics of hydrogen dissociation on Pt{100}: Steering, screening and thermal roughening effects. <i>Journal of Chemical Physics</i> , 1997, 106, 8896-8904.	1.2	43
351	First-Principles Determination of the Dispersion Interaction between Fullerenes and Their Intermolecular Potential. <i>Physical Review Letters</i> , 1997, 79, 3873-3876.	2.9	106
352	Xe <sup>129</sup> adsorbed in AlPO <sub>4</sub> -11 molecular sieve: Molecular dynamics simulation of adsorbate dynamics and NMR chemical shift. <i>Journal of Chemical Physics</i> , 1997, 107, 6470-6478.	1.2	23
353	Application of the generalized-gradient approximation to rare-gas dimers. <i>Physical Review A</i> , 1997, 56, R2495-R2498.	1.0	110
354	Novel Diffusion Mechanism on the GaAs(001) Surface: The Role of Adatom-Dimer Interaction. <i>Physical Review Letters</i> , 1997, 79, 5278-5281.	2.9	175
355	Surface Relaxation and Ferromagnetism of Rh(001). <i>Physical Review Letters</i> , 1997, 78, 1299-1302.	2.9	70
356	Hydrogen-Induced Polymorphism of the Pd(110) Surface. <i>Physical Review Letters</i> , 1997, 79, 1329-1332.	2.9	25
357	Anomalous Behavior of Ru for Catalytic Oxidation: A Theoretical Study of the Catalytic Reaction CO + 1/2 O <sub>2</sub> → CO <sub>2</sub> . <i>Physical Review Letters</i> , 1997, 78, 1500-1503.	2.9	121
358	Six-Dimensional Quantum Dynamics of Dissociative Chemisorption of (v=0, j=0) H <sub>2</sub> on Cu(100). <i>Physical Review Letters</i> , 1997, 78, 3583-3586.	2.9	121
359	Charge Density of MgO: Implications of Precise New Measurements for Theory. <i>Physical Review Letters</i> , 1997, 78, 4777-4780.	2.9	95
360	Total Energy Spectra of Complete Sets of Magnetic States for fcc-Fe Films on Cu(100). <i>Physical Review Letters</i> , 1997, 79, 507-510.	2.9	126
361	Generalized gradient approximation: An improved density-functional theory for accurate orbital eigenvalues. <i>Physical Review B</i> , 1997, 55, 16103-16109.	1.1	69
362	Calculated specific-heat coefficients of nonmagnetic closed-packed metals. <i>Physical Review B</i> , 1997, 55, 9200-9202.	1.1	1

#	ARTICLE	IF	CITATIONS
363	LDA simulations of pressure-induced anomalies and electric-field gradients for Zn and Cd. <i>Physical Review B</i> , 1997, 56, 7206-7214.	1.1	65
364	Adaptive-coordinate real-space electronic-structure calculations for atoms, molecules, and solids. <i>Physical Review B</i> , 1997, 55, 10289-10301.	1.1	187
365	Adaptive-coordinate electronic structure of $\text{TiO}_2$ . <i>Physical Review B</i> , 1997, 56, 14979-14984.	1.1	15
366	Jahn-Teller distortion and magnetic structures in $\text{LaMnO}_3$ . <i>Physical Review B</i> , 1997, 56, 12154-12160.	1.1	164
367	Molecular Precursors in the Dissociative Adsorption of $\text{O}_2$ on $\text{Pt}(111)$ . <i>Physical Review Letters</i> , 1997, 79, 4481-4484.	2.9	309
368	Density Functional Theory: A Useful Tool for the Study of Free Radicals. <i>Advances in Quantum Chemistry</i> , 1997, , 293-309.	0.4	17
369	The calculation of $^{17}\text{O}$ chemical shielding in transition metal oxo complexes. I. Comparison of DFT and ab initio approaches, and mechanisms of relativity-induced shielding. <i>Journal of Chemical Physics</i> , 1997, 106, 9201-9212.	1.2	81
370	First-principles study of the structural and electronic properties of ethylene adsorption on $\text{Si}(100)-(2\times 1)$ surface. <i>Journal of Chemical Physics</i> , 1997, 107, 3981-3985.	1.2	77
371	Density Functional Theory of Crystal Field Quasiparticle Excitations and the Ab Initio Calculation of Spin Hamiltonian Parameters. <i>Physical Review Letters</i> , 1997, 79, 2546-2549.	2.9	34
372	Linear Response and the Exchange-Correlation Hole within a Screened-Exchange Density Functional Theory. <i>Physical Review Letters</i> , 1997, 78, 3515-3518.	2.9	20
373	Adsorbate Reorganization at Steps: $\text{NO}$ on $\text{Pd}(211)$ . <i>Physical Review Letters</i> , 1997, 79, 4441-4444.	2.9	68
374	Energies of strained silica rings. <i>Physical Review B</i> , 1997, 55, 14784-14793.	1.1	82
375	Investigation of $\text{Al}$ phonons in $\text{YBa}_2\text{Cu}_3\text{O}_7$ by means of linearized-augmented-plane-wave atomic-force calculations. <i>Physical Review B</i> , 1997, 56, 14766-14770.	1.1	20
376	Quantum-mechanical calculation of $\text{H}$ on $\text{Ni}(001)$ using a model potential based on first-principles calculations. <i>Physical Review B</i> , 1997, 56, 2258-2266.	1.1	56
377	Pressure-induced phase transitions in $\text{Pa}$ metal from first-principles theory. <i>Physical Review B</i> , 1997, 56, 10719-10721.	1.1	24
378	Ab initio study of point defects in $\text{CdF}_2$ . <i>Physical Review B</i> , 1997, 56, 15665-15671.	1.1	23
379	The oxygen vacancy at the surface and in bulk $\text{MgO}$ : An embedded-cluster study. <i>Journal of Chemical Physics</i> , 1997, 107, 9645-9658.	1.2	138
380	Strain dependence of surface diffusion: $\text{Ag}$ on $\text{Ag}(111)$ and $\text{Pt}(111)$ . <i>Physical Review B</i> , 1997, 55, 6750-6753.	1.1	171

#	ARTICLE	IF	CITATIONS
381	Ionic and electronic processes at ionic surfaces induced by atomic-force-microscope tips. <i>Physical Review B</i> , 1997, 56, 15332-15344.	1.1	62
382	Simplified generalized-gradient approximation and anharmonicity: Benchmark calculations on molecules. <i>Physical Review B</i> , 1997, 55, 7454-7459.	1.1	140
383	Ab initio study of step formation and self-diffusion on Ag(100). <i>Physical Review B</i> , 1997, 55, 13916-13924.	1.1	66
384	Site symmetry dependence of repulsive interactions between chemisorbed oxygen atoms on Pt{100}-(1Å-1). <i>Journal of Chemical Physics</i> , 1997, 106, 1210-1215.	1.2	63
385	Giant lifetimes of optically excited states and the elusive structure of sodiumnitroprusside. <i>Journal of Chemical Physics</i> , 1997, 107, 10067-10074.	1.2	102
386	Protonated hydrogen clusters. <i>Journal of Chemical Physics</i> , 1997, 107, 9482-9492.	1.2	66
387	Density Functional Study of the First-Row Transition-Metal Monoxides*. <i>Zeitschrift Fur Physikalische Chemie</i> , 1997, 200, 39-49.	1.4	12
388	Theoretical study of epitaxial growths on As-covered Si(100) surfaces. , 0, , .		0
389	Chapter 13 Density-functional theory of epitaxial growth of metals. <i>Chemical Physics of Solid Surfaces</i> , 1997, 8, 490-544.	0.3	17
390	The energy diagram of NiO within an LCAO-LSDA+U approach. <i>Journal of Physics Condensed Matter</i> , 1997, 9, 647-661.	0.7	23
391	A Comparison of N <sub>2</sub> and CO Adsorption on Ru(001). <i>Zeitschrift Fur Physikalische Chemie</i> , 1997, 198, 113-122.	1.4	27
392	Atoms embedded in an electron gas: the generalized gradient approximation. <i>Physica Scripta</i> , 1997, 55, 499-506.	1.2	9
393	Vibrational Properties of Liquid Crystal Molecules from Ab Initio Computer Simulation. <i>Molecular Crystals and Liquid Crystals</i> , 1997, 302, 433-438.	0.3	2
394	Theoretical Study of Native Point Defects in AlN and InN. <i>Materials Research Society Symposia Proceedings</i> , 1997, 482, 910.	0.1	4
395	Ab Initio Pseudopotential Calculations of Dopant Diffusion in Si. <i>Materials Research Society Symposia Proceedings</i> , 1997, 469, 151.	0.1	13
396	Elasticity, Thermal Properties, and Molecular Dynamics Using Non-Empirical Tight-Binding. <i>Materials Research Society Symposia Proceedings</i> , 1997, 491, 501.	0.1	0
398	Evaluation of the performance of non-local and hybrid density functional theory methods for pi-radical hyperfine structures. <i>Molecular Physics</i> , 1997, 91, 827-834.	0.8	12
399	Correlation potentials and functionals in Hartree-Fock-Kohn-Sham theory. <i>Journal of Chemical Physics</i> , 1997, 107, 1536-1543.	1.2	22

#	ARTICLE	IF	CITATIONS
400	Ab initio calculations of Ru, Pd, and Ag cluster structure with 55, 135, and 140 atoms. Journal of Chemical Physics, 1997, 106, 1856-1862.	1.2	71
401	Correlated Capped Subsystem Method for the Calculation of Substituent Effects on Bond Energies. Journal of Physical Chemistry A, 1997, 101, 1193-1197.	1.1	24
402	Density-functional-based predictions of Raman and IR spectra for small Si clusters. Physical Review B, 1997, 55, 2549-2555.	1.1	71
403	Ab initio density functional studies of transition-metal sulphides: II. Electronic structure. Journal of Physics Condensed Matter, 1997, 9, 11107-11140.	0.7	109
404	An ab initio Hartree - Fock study of the magnetic states of the polymorphs of MnS. Journal of Physics Condensed Matter, 1997, 9, 7105-7118.	0.7	21
405	Proton Affinity and Acidity of Hypohalous Acids: A Density Functional Study. Journal of Physical Chemistry A, 1997, 101, 5022-5025.	1.1	15
406	Monodeprotonated Free Base Porphyrin. Journal of Physical Chemistry B, 1997, 101, 1496-1497.	1.2	18
407	Probing the Balance between Localization and Delocalization of the Metal-Based Electrons in Face-Shared Octahedral Complexes. Inorganic Chemistry, 1997, 36, 3242-3247.	1.9	61
408	Numerical Determination of the Topological Properties of the Electronic Charge Density in Molecules and Solids Using Density Functional Theory. Journal of Physical Chemistry A, 1997, 101, 6976-6982.	1.1	16
409	Transition Metal Oxide Chemistry: Electronic Structure Study of WO <sub>3</sub> , ReO <sub>3</sub> , and NaWO <sub>3</sub> . Journal of Physical Chemistry B, 1997, 101, 3945-3952.	1.2	107
410	Ab Initio Molecular Dynamics Study of the Desorption of D <sub>2</sub> from Si(100). Physical Review Letters, 1997, 79, 701-704.	2.9	67
411	Cation Siting and Dynamical Properties of Zeolite Offretite from First-Principles Molecular Dynamics. Journal of Physical Chemistry B, 1997, 101, 9932-9939.	1.2	39
412	First-principles spin-polarized calculations on the reduced and reconstructed TiO <sub>2</sub> (110) surface. Physical Review B, 1997, 55, 15919-15927.	1.1	191
413	The GaAs(001)-(2 × 4) Surface: Structure, Chemistry, and Adsorbates. Journal of Physical Chemistry B, 1997, 101, 1498-1509.	1.2	24
414	A Numerical Method for the Topological Analysis of the Laplacian of the Electronic Charge Density in Molecules and Solids. Journal of Physical Chemistry A, 1997, 101, 2178-2184.	1.1	19
415	Structure and Bonding of the Noble Gas-Metal Carbonyl Complexes M(CO) <sub>5</sub> Ng (M = Cr, Mo, W and Ng) Tj ETQ <sub>11</sub> 1 0.784314 rgB	1.1	51
416	A Quantum Chemical View of Density Functional Theory. Journal of Physical Chemistry A, 1997, 101, 5383-5403.	1.1	576
417	An orbital-based density difference index for the comparison of electron density distributions. Journal of Chemical Physics, 1997, 107, 6693-6698.	1.2	3

#	ARTICLE	IF	CITATIONS
418	Broken-Symmetry and Approximate Spin-Projected Potential Energy Curves for Bimetallic Systems: A Density Functional Study of $M_2Cl_9$ , $M = Cr^{III}$ , $Mo^{III}$ , $W^{III}$ , and $Re^{IV}$ . <i>Journal of Physical Chemistry A</i> , 1997, 101, 6265-6272.	1.1	66
419	Experimental and Theoretical Studies of $SiFn(CO)_2^+$ Cations with $n = 2$ and $3$ : A Search for Pentacoordinate Cationic Silicon. <i>Journal of Physical Chemistry A</i> , 1997, 101, 7258-7264.	1.1	7
420	Structural stability in uranium. <i>Journal of Physics Condensed Matter</i> , 1997, 9, L549-L555.	0.7	32
421	Recent Developments in Multiple Scattering Theory and Density Functional Theory for Molecules and Solids. , 1997, , 1-58.		0
422	Van Der Waals Interactions from Density Functional Theories: , 1997, , 337-382.		4
423	Ab initiodensity functional studies of transition-metal sulphides: I. Crystal structure and cohesive properties. <i>Journal of Physics Condensed Matter</i> , 1997, 9, 11085-11106.	0.7	118
424	Describing van der Waals Interaction in diatomic molecules with generalized gradient approximations: The role of the exchange functional. <i>Journal of Chemical Physics</i> , 1997, 107, 7921-7925.	1.2	282
425	$H_2$ dissociative adsorption on Pd(111). <i>Physical Review B</i> , 1997, 56, 15396-15403.	1.1	151
426	Assessment of Basis Set and Functional Dependencies in Density Functional Theory: A Studies of Atomization and Reaction Energies. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1927-1934.	1.1	61
427	Periodic unrestricted Hartree-Fock study of corundumlike $Ti_2O_3$ and $V_2O_3$ . <i>Physical Review B</i> , 1997, 55, 16122-16131.	1.1	44
428	Relativistic band structure calculation of cubic and hexagonal SiC polytypes. <i>Journal of Applied Physics</i> , 1997, 82, 5496-5508.	1.1	284
429	Calculation of the momentum distributions of positron annihilation radiation in Ge. <i>Journal of Physics Condensed Matter</i> , 1997, 9, 8147-8154.	0.7	4
430	On the structural, electronic and magnetic properties of spinel. <i>Journal of Physics Condensed Matter</i> , 1997, 9, 10715-10724.	0.7	27
431	Ab initio simulation of the metal/nonmetal transition in expanded fluid mercury. <i>Physical Review B</i> , 1997, 55, 7539-7548.	1.1	131
432	Comparison of the projector augmented-wave, pseudopotential, and linearized augmented-plane-wave formalisms for density-functional calculations of solids. <i>Physical Review B</i> , 1997, 55, 2005-2017.	1.1	230
433	Ab-Initio Total Energy Studies of the Static and Dynamical Properties of Ice Ih. <i>Journal of Physical Chemistry B</i> , 1997, 101, 6146-6150.	1.2	62
434	Self-diffusion of adatoms, dimers, and vacancies on Cu(100). <i>Physical Review B</i> , 1997, 56, 7643-7655.	1.1	145
435	A new gradient-corrected exchange-correlation density functional. <i>Molecular Physics</i> , 1997, 91, 847-860.	0.8	18

#	ARTICLE	IF	CITATIONS
436	Structural properties of plutonium from first-principles theory. <i>Physical Review B</i> , 1997, 55, 1997-2004.	1.1	97
437	Magnetic properties of cobalt clusters embedded in a copper matrix. <i>Physical Review B</i> , 1997, 55, 3677-3682.	1.1	36
438	The theoretical charge density of silicon: experimental testing of exchange and correlation potentials. <i>Journal of Physics Condensed Matter</i> , 1997, 9, 7541-7561.	0.7	124
439	The future of the total energy pseudopotential technique and its application to minerals. <i>Phase Transitions</i> , 1997, 61, 41-49.	0.6	2
440	Theoretical investigations of the elastic constants in Laves phases. <i>Intermetallics</i> , 1997, 5, 449-465.	1.8	71
441	The influence of generalized gradient corrections on the structural and electronic properties of tellurium. <i>Computational Materials Science</i> , 1997, 8, 335-340.	1.4	14
442	Large structural and magnetic phase stability of VS and VSe. <i>Journal of Alloys and Compounds</i> , 1997, 246, 166-176.	2.8	12
443	Fluorination of diamond $\text{C}^{13}$ C4F9I and CF3I photochemistry on diamond (100). <i>Surface Science</i> , 1997, 370, 209-231.	0.8	21
444	The surface chemistry of metal-oxygen interactions: a first-principles study of O:Rh(110). <i>Surface Science</i> , 1997, 370, 166-178.	0.8	35
445	Adsorption of atomic and molecular oxygen on the MgO (001) surface. <i>Surface Science</i> , 1997, 374, 373-386.	0.8	79
446	The energetics of N2O dissociation on CaO(001). <i>Surface Science</i> , 1997, 376, 169-176.	0.8	24
447	Study of CO oxidation over Ru(0001) at high gas pressures. <i>Surface Science</i> , 1997, 377-379, 808-812.	0.8	14
448	Structures and energetics of Si6Hx and Si6H+x clusters. <i>Surface Science</i> , 1997, 377-379, 1046-1050.	0.8	4
449	Influence of potassium adatoms on the dissociative adsorption of hydrogen on Pd(100). <i>Surface Science</i> , 1997, 380, L446-L454.	0.8	24
450	Surface-induced antiparallel coupling at the surface of a B2-ordered FeCr alloy. <i>Surface Science</i> , 1997, 381, 117-122.	0.8	2
451	Trends in atom/molecule-surface van der Waals interactions. <i>Surface Science</i> , 1997, 383, 88-94.	0.8	16
452	A systematic study of the surface energetics and structure of TiO2(110) by first-principles calculations. <i>Surface Science</i> , 1997, 385, 386-394.	0.8	224
453	CO adsorption and dissociation on Pt(111) and Ni(111) surfaces. <i>Surface Science</i> , 1997, 386, 67-72.	0.8	91

#	ARTICLE	IF	CITATIONS
454	Effect of kinks and concerted diffusion mechanisms on mass transport and growth on stepped metal surfaces. <i>Surface Science</i> , 1997, 387, 167-182.	0.8	80
455	Energetics of void enlargement in thermally grown ultrathin Si-oxide on Si(001). <i>Surface Science</i> , 1997, 387, L1057-L1061.	0.8	4
456	DIET in the bulk: evidence for hot electron cleavage of Si-H bonds in SiO <sub>2</sub> films. <i>Surface Science</i> , 1997, 390, 112-118.	0.8	10
457	Exchange and correlation energy in density functional theory: Comparison of accurate density functional theory quantities with traditional Hartree-Fock based ones and generalized gradient approximations for the molecules Li <sub>2</sub> , N <sub>2</sub> , F <sub>2</sub> . <i>Journal of Chemical Physics</i> , 1997, 107, 5007-5015.	1.2	194
458	Theoretical investigations of structural and vibronic properties of YBa <sub>2</sub> Cu <sub>3</sub> O <sub>7</sub> by first-principles atomic-force calculations. <i>Physica C: Superconductivity and Its Applications</i> , 1997, 282-287, 1635-1636.	0.6	2
459	Fermi surface-analysis of YBa <sub>2</sub> Cu <sub>3</sub> O <sub>7</sub> by full-potential LAPW calculations. <i>Physica C: Superconductivity and Its Applications</i> , 1997, 282-287, 1637-1638.	0.6	0
460	First-principles calculation of the phonon frequencies in <sup>57</sup> Fe. <i>Physics of the Solid State</i> , 1997, 39, 148-152.	0.2	3
461	Modified local exchange and kinetic energy functionals for atomic systems. <i>Computational and Theoretical Chemistry</i> , 1997, 390, 1-9.	1.5	4
462	Review of quantum Monte Carlo methods and their applications. <i>Computational and Theoretical Chemistry</i> , 1997, 394, 75-85.	1.5	23
463	Study on europium chalcogenides by means of density functional theory. <i>Computational and Theoretical Chemistry</i> , 1997, 417, 9-17.	1.5	1
464	Physical origin of exchange diffusion on fcc(100) metal surfaces. <i>Physical Review B</i> , 1997, 56, R15569-R15572.	1.1	104
465	Structure sensitivity in adsorption: CO interaction with stepped and reconstructed Pt surfaces. <i>Catalysis Letters</i> , 1997, 46, 31-35.	1.4	453
466	Pseudopotentials for clusters. <i>Il Nuovo Cimento A</i> , 1997, 110, 1183-1189.	0.2	1
467	First-principles calculation of Cu(1 0 0)c(2 Å <sup>-2</sup> )Cu <sub>3</sub> d surface alloy formation energy: Improvement by generalized gradient approximation. <i>Physica B: Condensed Matter</i> , 1997, 237-238, 359-360.	1.3	14
468	Surface electronic structure and reactivity of transition and noble metals1Communication presented at the First Francqui Colloquium, Brussels, 19 <sup>th</sup> -20 February 1996.1. <i>Journal of Molecular Catalysis A</i> , 1997, 115, 421-429.	4.8	1,166
469	Dissociative adsorption of H <sub>2</sub> on the Pd(111) surface. <i>Journal of Molecular Catalysis A</i> , 1997, 119, 69-76.	4.8	43
470	Catalytic properties of F-centres at the magnesium oxide surface: hydrogen abstraction from methane. <i>Journal of Molecular Catalysis A</i> , 1997, 119, 253-262.	4.8	48
471	From silicon to RNA: The coming of age of ab initio molecular dynamics. <i>Solid State Communications</i> , 1997, 102, 107-120.	0.9	171



#	ARTICLE	IF	CITATIONS
472	Electronic structure of La <sub>0.5</sub> Ca <sub>0.5</sub> MnO <sub>3</sub> . Solid State Communications, 1997, 102, 621-626.	0.9	25
473	Methodological study of Becke3-LYP density functional adapted to the determination of accurate infrared signature for hydrogen-bonded complexes. Journal of Molecular Structure, 1997, 416, 1-9.	1.8	20
474	Conformational and vibrational analyses of 2-methoxyethanol and 2-(methylthio)ethanol by density functional theory. Journal of Molecular Structure, 1997, 413-414, 217-226.	1.8	11
475	Thermodynamics of hydrogen bonding from molecular orbital theory: 1. Water. AIChE Journal, 1997, 43, 1589-1596.	1.8	28
476	Simple tests for density functional methods. Journal of Computational Chemistry, 1997, 18, 1534-1545.	1.5	25
477	On-top pair-density interpretation of spin density functional theory, with applications to magnetism. International Journal of Quantum Chemistry, 1997, 61, 197-205.	1.0	97
478	Direct approximation of the long- and short-range components of the exchange-correlation Kohn-Sham potential. International Journal of Quantum Chemistry, 1997, 61, 231-243.	1.0	31
479	Differences between ab initio and density functional electron densities. International Journal of Quantum Chemistry, 1997, 61, 245-252.	1.0	8
480	Density functional study of atomic electron affinities using a nonlocal exchange and a local correlation functional. International Journal of Quantum Chemistry, 1997, 61, 253-261.	1.0	3
481	Additive density functional correlation corrections to single particle theories. International Journal of Quantum Chemistry, 1997, 61, 281-285.	1.0	3
482	Why the generalized gradient approximation works and how to go beyond it. International Journal of Quantum Chemistry, 1997, 61, 287-293.	1.0	126
483	Systematic study of the lowest energy states of Pd, Pd <sub>2</sub> , and Pd <sub>3</sub> . International Journal of Quantum Chemistry, 1997, 61, 515-523.	1.0	48
484	Benchmark comparison of gradient-dependent and local density calculations for bulk silicon and aluminum. International Journal of Quantum Chemistry, 1997, 61, 641-646.	1.0	6
485	Density-gradient analysis for density functional theory: Application to atoms. International Journal of Quantum Chemistry, 1997, 61, 835-845.	1.0	81
486	A nonlocal correlation energy density functional from a Coulomb hole model. International Journal of Quantum Chemistry, 1997, 62, 603-616.	1.0	24
487	Density functional study of the relationship between energy, hardness, and polarizability of molecules in nonequilibrium situations. International Journal of Quantum Chemistry, 1997, 63, 917-926.	1.0	6
488	Accurate density-functional calculations on large systems. International Journal of Quantum Chemistry, 1997, 64, 193-203.	1.0	17
489	Coupling-constant dependence of atomization energies. International Journal of Quantum Chemistry, 1997, 64, 285-295.	1.0	174



#	ARTICLE	IF	CITATIONS
490	Extension of the LAP functional to include parallel spin correlation. International Journal of Quantum Chemistry, 1997, 64, 427-446.	1.0	77
491	Electronic structure and properties of the carbonyls TiCO and Ti7CO and carbenes TiCH2 and Ti7CH2 by density functional methods. International Journal of Quantum Chemistry, 1997, 65, 65-73.	1.0	3
492	Real-space multigrid methods for large-scale electronic structure problems. International Journal of Quantum Chemistry, 1997, 65, 531-543.	1.0	22
493	Systematic study of the lowest energy states of Aun (n=1-4) using DFT. International Journal of Quantum Chemistry, 1997, 65, 749-758.	1.0	49
494	White and Bird's Formulation of Gradient-Corrected Exchange-Correlation Potentials Applied to Atoms. Journal of Computational Physics, 1997, 136, 599-602.	1.9	2
495	The adiabatic connection method: a non-empirical hybrid. Chemical Physics Letters, 1997, 265, 115-120.	1.2	212
496	The adsorption of atomic nitrogen on Ru(0001): geometry and energetics. Chemical Physics Letters, 1997, 264, 680-686.	1.2	77
497	Atomic reference energies for density functional calculations. Chemical Physics Letters, 1997, 265, 481-489.	1.2	154
498	Higher-order gradient corrections for exchange-correlation functionals. Chemical Physics Letters, 1997, 266, 16-22.	1.2	31
499	Ab initio molecular dynamics simulation of methanol adsorbed in chabazite. Chemical Physics Letters, 1997, 266, 397-402.	1.2	100
500	Anharmonic force fields from density functional theory. Chemical Physics Letters, 1997, 273, 71-78.	1.2	99
501	Electronic structure of $\hat{1}\pm$ -MnS (alabandite): an ab initio study. Chemical Physics Letters, 1997, 273, 83-90.	1.2	37
502	Toward reliable adiabatic connection models free from adjustable parameters. Chemical Physics Letters, 1997, 274, 242-250.	1.2	706
503	Structure of chemisorbed acetylene on the Si(001)-(2 $\text{\AA}$ -1) surface and the effect of coadsorbed atomic hydrogen. Chemical Physics Letters, 1997, 278, 97-101.	1.2	28
504	Ab initio gradient corrected density functional molecular dynamics: investigation of structural and dynamical properties of the Li8 cluster. Chemical Physics Letters, 1997, 279, 129-139.	1.2	34
505	DFT calculations of the binding energy of metallocenes. Chemical Physics Letters, 1997, 281, 226-232.	1.2	71
506	Linear-scaling DFT-pseudopotential calculations on parallel computers. Computer Physics Communications, 1997, 102, 1-16.	3.0	61
507	Density-functional theory calculations for poly-atomic systems: electronic structure, static and elastic properties and ab initio molecular dynamics. Computer Physics Communications, 1997, 107, 187-222.	3.0	660

#	ARTICLE	IF	CITATIONS
508	Protonation of [Ru(C5Me5) (3-C6H9)] (C6H9 = methylpentadienyl): fluxionality and structure of an agostic complex. <i>Inorganica Chimica Acta</i> , 1997, 259, 197-202.	1.2	8
509	Density functional theory. <i>Coordination Chemistry Reviews</i> , 1998, 178-180, 699-721.	9.5	213
510	Hydrogenation-induced structural evolution of small silicon clusters: The case of Si6Hx+. <i>Chemical Physics Letters</i> , 1998, 284, 12-18.	1.2	17
511	Dynamical observation of the catalytic activation of methanol in zeolites. <i>Chemical Physics Letters</i> , 1998, 283, 402-408.	1.2	56
512	First-principles molecular dynamics study of CO adsorption on the Si(001) surface. <i>Chemical Physics Letters</i> , 1998, 287, 131-136.	1.2	21
513	A study of the reaction $H + O_2 \rightarrow HO_2 \rightarrow O + OH$ at four levels of density-functional theory. <i>Chemical Physics Letters</i> , 1998, 287, 195-201.	1.2	5
514	The dynamics of the H + D/Si(001) reaction: a trajectory study based on ab initio potentials. <i>Chemical Physics Letters</i> , 1998, 288, 396-402.	1.2	26
515	A dynamical density functional study of CO migration in the Reppe carbonylation. <i>Chemical Physics Letters</i> , 1998, 291, 57-63.	1.2	11
516	Vibrational frequency and chemisorption site: a DFT-periodic study of NO on Pd (111) and Rh (111) surfaces. <i>Chemical Physics Letters</i> , 1998, 291, 15-23.	1.2	139
517	Exchange and correlation Kohn-Sham functionals for the helium atom: locality and homogeneity. <i>Chemical Physics Letters</i> , 1998, 294, 314-318.	1.2	2
518	Tests of a density functional with Laplacian terms: activation barriers and bond-stretching energies. <i>Chemical Physics Letters</i> , 1998, 295, 467-474.	1.2	15
519	Gradient correction to the exchange pair-correlation function of the weighted spin-density approximation in the density functional formalism. <i>Chemical Physics Letters</i> , 1998, 296, 307-312.	1.2	1
520	Excitation energies in density functional theory: comparison of several methods for the H2O, N2, CO and C2H4 molecules. <i>Chemical Physics Letters</i> , 1998, 296, 489-493.	1.2	28
521	Effect of Strain on the Reactivity of Metal Surfaces. <i>Physical Review Letters</i> , 1998, 81, 2819-2822.	2.9	2,001
522	The viscosity of liquid iron at the physical conditions of the Earth's core. <i>Nature</i> , 1998, 392, 805-807.	13.7	259
523	Room-temperature magnetoresistance in an oxide material with an ordered double-perovskite structure. <i>Nature</i> , 1998, 395, 677-680.	13.7	1,883
524	Exchange and correlation interactions and band structure of non-close-packed solids. <i>Physics of the Solid State</i> , 1998, 40, 1802-1805.	0.2	7
525	Ab initio Methods for the Study of Molecular Systems for Nanometer Technology: Toward the First-Principles Design of Molecular Computers. <i>Annals of the New York Academy of Sciences</i> , 1998, 852, 68-94.	1.8	15

#	ARTICLE	IF	CITATIONS
526	Energy bands and chemical bonding in the novel hydride nitrides Sr <sub>2</sub> (H)N and Ba <sub>2</sub> (H)N. <i>Journal of Physics and Chemistry of Solids</i> , 1998, 59, 915-922.	1.9	4
527	Accurate ab initio energetics of extended systems via explicit correlation embedded in a density functional environment. <i>Chemical Physics Letters</i> , 1998, 295, 129-134.	1.2	189
528	Accurate finite-element multi-grid (FEM-MG) description for angular momentum and spin dependences of Kohn-Sham density functionals for axially restricted calculations on first-row atoms and dimers. <i>Chemical Physics Letters</i> , 1998, 295, 439-446.	1.2	9
529	Vibrations and dissociation of molecules in strong electric fields: N <sub>2</sub> , NaCl, H <sub>2</sub> O and SF <sub>6</sub> . <i>Computational and Theoretical Chemistry</i> , 1998, 434, 229-237.	1.5	22
530	Binding schemes of adsorbates at metal surfaces: theoretical cluster studies. <i>Computational and Theoretical Chemistry</i> , 1998, 458, 81-92.	1.5	12
531	First-principles determinations of magneto-crystalline anisotropy and magnetostriction in bulk and thin-film transition metals. <i>Journal of Magnetism and Magnetic Materials</i> , 1998, 177-181, 1216-1219.	1.0	58
532	Electronic structure and magnetic properties of 2Fe/Pd and 2Pd/Fe multilayers. <i>Journal of Magnetism and Magnetic Materials</i> , 1998, 184, 293-301.	1.0	10
533	The electronic and magnetic properties of Y <sub>n+1</sub> Co <sub>3n+5</sub> B <sub>2n</sub> (n=0, 1, 2, 3, and ∞) systems. <i>Journal of Magnetism and Magnetic Materials</i> , 1998, 185, 322-330.	1.0	33
534	Ab Initio Hartree-Fock Study of the Energies of Mixing of MnO-NiO, MgO-MnO, and CaO-MnO Solid Solutions. <i>Journal of Solid State Chemistry</i> , 1998, 137, 261-275.	1.4	21
535	Ab Initio Quantum Mechanical Study of the Structure and Stability of the Alkaline Earth Metal Oxides and Peroxides. <i>Journal of Solid State Chemistry</i> , 1998, 140, 103-115.	1.4	57
536	Self-consistent field calculations using two-body density functionals for correlation energy component: I. Atomic systems. <i>Journal of Computational Chemistry</i> , 1998, 19, 1887-1898.	1.5	6
537	Atmospheric chemistry of acetone: Kinetic study of the CH <sub>3</sub> C(O)CH <sub>2</sub> O <sub>2</sub> +NO/NO <sub>2</sub> reactions and decomposition of CH <sub>3</sub> C(O)CH <sub>2</sub> O <sub>2</sub> NO <sub>2</sub> . <i>International Journal of Chemical Kinetics</i> , 1998, 30, 475-489.	1.0	32
538	A scattering theoretic approach to scalar relativistic corrections on bonding. <i>International Journal of Quantum Chemistry</i> , 1998, 69, 423-433.	1.0	264
539	Atomic kinetic- and exchange-energy functionals by means of local-scaling transformations. <i>International Journal of Quantum Chemistry</i> , 1998, 69, 503-512.	1.0	8
540	Virial exchange-correlation energy density in Hooke's atom. <i>International Journal of Quantum Chemistry</i> , 1998, 69, 533-540.	1.0	16
541	A theoretical study of rare-gas diatomic molecules with the generalized-gradient approximation to density functional theory. <i>International Journal of Quantum Chemistry</i> , 1998, 69, 619-627.	1.0	37
542	Density functional investigations of carboxyl free radicals: Formyloxyl, acetyloxyl, and benzoyloxyl radicals. <i>International Journal of Quantum Chemistry</i> , 1998, 70, 253-267.	1.0	34
543	Oxygen binding to iron-porphyrin: A density functional study using both LSD and LSD+GC schemes. , 1998, 70, 387-394.		22

#	ARTICLE	IF	CITATIONS
544	High pressure studies on YNi <sub>2</sub> B <sub>2</sub> C and LuNi <sub>2</sub> B <sub>2</sub> C: ADXRD, thermoelectric power, resistivity, and electronic structure. <i>Journal of Physics and Chemistry of Solids</i> , 1998, 59, 2201-2204.	1.9	2
545	Density functionals and van der Waals interactions at surfaces. <i>Progress in Surface Science</i> , 1998, 59, 149-165.	3.8	5
546	Can 5d transition-metal monolayers BE magnetic on ferromagnetic substrate?. <i>Solid State Communications</i> , 1998, 106, 665-667.	0.9	6
547	Electronic structure of stishovite. <i>Solid State Communications</i> , 1998, 108, 37-42.	0.9	11
548	Different adsorbate binding mechanisms of hydrocarbons: Theoretical studies for Cu(111)â€“C <sub>2</sub> H <sub>2</sub> and Cu(111)â€“C <sub>2</sub> H <sub>4</sub> . <i>Applied Catalysis A: General</i> , 1998, 172, 85-95.	2.2	35
549	Full-potential linear-muffin-tin orbital atomic-sphere approximation calculations of the electric field gradient in HCP metals. <i>Physica B: Condensed Matter</i> , 1998, 245, 376-382.	1.3	5
550	Electronic structure of TiO <sub>2</sub> (110) surface as a function of surface ligand configuration. <i>Applied Surface Science</i> , 1998, 130-132, 587-592.	3.1	8
551	Reactions at surfaces studied by ab initio dynamics calculations. <i>Surface Science Reports</i> , 1998, 32, 291-340.	3.8	346
552	Density functional. Theory and application to atoms and molecules. <i>Physics Reports</i> , 1998, 298, 1-79.	10.3	151
553	Design of a Surface Alloy Catalyst for Steam Reforming. <i>Science</i> , 1998, 279, 1913-1915.	6.0	951
554	Ab initiomolecular-dynamics studies of the graphitization of flat and stepped diamond (111) surfaces. <i>Physical Review B</i> , 1998, 58, 13167-13175.	1.1	52
555	Development and assessment of new exchange-correlation functionals. <i>Journal of Chemical Physics</i> , 1998, 109, 6264-6271.	1.2	1,374
556	Electronic structure of tin monochalcogenides from SnO to SnTe. <i>Physical Review B</i> , 1998, 58, 1896-1906.	1.1	286
557	Complex magnetic behavior at the surface of B <sub>2</sub> ordered FeCr alloy. <i>Computational Materials Science</i> , 1998, 10, 273-277.	1.4	3
558	The electronic structure of colossal magnetoresistive manganites. <i>Computational Materials Science</i> , 1998, 10, 240-244.	1.4	6
559	Density functionals from LDA to GGA. <i>Computational Materials Science</i> , 1998, 11, 122-127.	1.4	137
560	Ab initio pseudopotential calculations of dopant diffusion in Si. <i>Computational Materials Science</i> , 1998, 12, 309-318.	1.4	45
561	Effect of generalized gradient corrections on lanthanide cohesive properties. <i>Journal of Alloys and Compounds</i> , 1998, 275-277, 472-475.	2.8	14

#	ARTICLE	IF	CITATIONS
562	Ab-initio calculations of the 6D potential energy surfaces for the dissociative adsorption of H <sub>2</sub> on the (100) surfaces of Rh, Pd and Ag. Surface Science, 1998, 397, 116-136.	0.8	88
563	The dynamics of H absorption in and adsorption on Cu(111). Surface Science, 1998, 397, 382-394.	0.8	111
564	Atomic and electronic structure of Cu clusters on MgO. Surface Science, 1998, 402-404, 413-417.	0.8	36
565	The adsorption of small molecules on the TiO <sub>2</sub> anatase (101) surface by first-principles molecular dynamics. Surface Science, 1998, 402-404, 219-222.	0.8	88
566	Structural and electronic properties of the MoS <sub>2</sub> (101̄,0) edge-surface. Surface Science, 1998, 407, 237-250.	0.8	108
567	The adsorption and dissociation of ROH molecules on TiO <sub>2</sub> (110). Surface Science, 1998, 409, 336-349.	0.8	192
568	A theoretical study of adsorbate-adsorbate interactions on Ru(0001). Surface Science, 1998, 414, 315-329.	0.8	123
569	Hydrogen adsorption on palladium: a comparative theoretical study of different surfaces. Surface Science, 1998, 411, 123-136.	0.8	198
570	The surface energy of metals. Surface Science, 1998, 411, 186-202.	0.8	2,342
571	Ab initio study of the dissociative adsorption of H <sub>2</sub> on the Pd(110) surface. Surface Science, 1998, 412-413, 518-526.	0.8	44
572	Mechanism of single atom switch on silicon. Surface Science, 1998, 415, L1037-L1045.	0.8	47
573	First principles calculation of oxygen adsorption and reconstruction of Cu(110) surface. Surface Science, 1998, 415, 194-211.	0.8	80
574	Poisoning of hydrogen dissociation at Pd (100) by adsorbed sulfur studied by ab-initio quantum dynamics and ab-initio molecular dynamics. Surface Science, 1998, 416, L1095-L1100.	0.8	49
575	N <sub>2</sub> and HF vibrations on LiF(001): the effect of surface coverage. Surface Science, 1998, 411, 23-34.	0.8	4
576	Nature of the Three-Electron Bond in H <sub>2</sub> S~SH <sub>2</sub> +H <sub>2</sub> . Journal of Physical Chemistry A, 1998, 102, 9549-9553.	1.1	102
577	Induced phase shift in interlayer magnetic exchange coupling: Magnetic layer doping. Physical Review B, 1998, 58, 6367-6377.	1.1	10
578	A Theoretical Study of Bonding in Lanthanide Trihalides by Density Functional Methods. Journal of Physical Chemistry A, 1998, 102, 6812-6820.	1.1	94
579	Density functionals for non-relativistic coulomb systems. , 1998, , 8-59.		22

#	ARTICLE	IF	CITATIONS
580	Adsorption of thiophene on RuS <sub>2</sub> : An ab initio density-functional study. <i>Physical Review B</i> , 1998, 58, R1782-R1785.	1.1	14
581	Diffusion of Atomic Oxygen in SiO <sub>2</sub> . <i>Physical Review Letters</i> , 1998, 81, 3447-3450.	2.9	141
582	Theoretical Study of the Geometric and Electronic Structures and Spectra of trans-ME <sub>2</sub> (PH <sub>3</sub> ) <sub>4</sub> Complexes (M = Mo, W; E = S, Se, Te). <i>Inorganic Chemistry</i> , 1998, 37, 674-678.	1.9	0
583	Ab initio molecular polarisabilities of liquid crystals: Application to DOBAMBC and 5CB. <i>Europhysics Letters</i> , 1998, 44, 578-584.	0.7	24
584	Chemisorption of Organics on Platinum. 1. The Interstitial Electron Model. <i>Journal of Physical Chemistry B</i> , 1998, 102, 9481-9491.	1.2	70
585	Density Functional Study of the Conformations and Vibrations of 1,2-Dimethoxyethane. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2691-2699.	1.1	56
586	Phonon dispersion relation in rhodium: Ab initio calculations and neutron-scattering investigations. <i>Physical Review B</i> , 1998, 57, 324-333.	1.1	39
587	Ab initio study of the martensitic bcc-hcp transformation in iron. <i>Physical Review B</i> , 1998, 58, 5296-5304.	1.1	115
588	Molecular Structures, Tautomerism, and Carbon Nucleophilicity of Free-Base Inverted Porphyrins and Carbaporphyrins: A Density Functional Theoretical Study. <i>Journal of Physical Chemistry B</i> , 1998, 102, 10459-10467.	1.2	76
589	Theoretical Study of the Mechanism of the Addition of Diazomethane to Ethylene and Formaldehyde. Comparison of Conventional ab Initio and Density Functional Methods. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10106-10112.	1.1	27
590	Compression mechanisms in quasimolecular X <sub>3</sub> (X=As,Sb,Bi) solids. <i>Physical Review B</i> , 1998, 58, 14812-14822.	1.1	36
591	Chemisorption and Transformation of CH <sub>x</sub> Fragments (x = 0-3) on a Pd(111) Surface: A Periodic Density Functional Study. <i>Journal of Physical Chemistry B</i> , 1998, 102, 1578-1585.	1.2	92
592	Sequential Ligation of Mg <sup>+</sup> , Fe <sup>+</sup> , (c-C <sub>5</sub> H <sub>5</sub> )Mg <sup>+</sup> , and (c-C <sub>5</sub> H <sub>5</sub> )Fe <sup>+</sup> with Ammonia in the Gas Phase: Transition from Coordination to Solvation in the Sequential Ligation of Mg <sup>+</sup> . <i>Journal of Physical Chemistry A</i> , 1998, 102, 9803-9810.	1.1	48
593	Systematic Experimental and Quantum Chemical Investigation into the Structures, the Stability, and the Spectroscopic Properties of Alkylindium(I) Compounds: Tetrameric In <sub>4</sub> [C(SiMeRR) <sub>3</sub> ] <sub>4</sub> versus Monomeric InC(SiMeRR) <sub>3</sub> Derivatives. <i>Organometallics</i> , 1998, 17, 5009-5017.	1.1	64
594	Orbital and magnetic orderings in localized d <sub>2g</sub> systems, YTiO <sub>3</sub> and YVO <sub>3</sub> : Comparison with a more itinerant system LaMnO <sub>3</sub> . <i>Physical Review B</i> , 1998, 58, 6831-6836.	1.1	114
595	Atmospheric Chemistry of the Phenoxy Radical, C <sub>6</sub> H <sub>5</sub> O (̂): UV Spectrum and Kinetics of Its Reaction with NO, NO <sub>2</sub> , and O <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 1998, 102, 7964-7974.	1.1	110
596	Direct Porphyrin-Aryl Orbital Overlaps in Some meso-Tetraarylporphyrins. <i>Journal of the American Chemical Society</i> , 1998, 120, 6227-6230.	6.6	38
597	The Surface Structure of Sulfated Zirconia: Periodic ab Initio Study of Sulfuric Acid Adsorbed on ZrO <sub>2</sub> (101) and ZrO <sub>2</sub> (001). <i>Journal of the American Chemical Society</i> , 1998, 120, 13503-13512.	6.6	168

#	ARTICLE	IF	CITATIONS
598	Reassessment of the Electronic and Molecular Structure, Bonding, and Stability of Zerovalent Nickel Acetylene Complexes by the Density Functional Method. <i>Organometallics</i> , 1998, 17, 4724-4733.	1.1	26
599	Energetics and electronic structure of stacking faults in AlN, GaN, and InN. <i>Physical Review B</i> , 1998, 57, R15052-R15055.	1.1	298
600	Density functional theory for calculation of elastic properties of orthorhombic crystals: Application to TiSi <sub>2</sub> . <i>Journal of Applied Physics</i> , 1998, 84, 4891-4904.	1.1	1,565
601	A new inhomogeneity parameter in density-functional theory. <i>Journal of Chemical Physics</i> , 1998, 109, 2092-2098.	1.2	276
602	Chapter 2 Electronic Structure Calculations for Semiconductors under Pressure. <i>Semiconductors and Semimetals</i> , 1998, 54, 49-144.	0.4	8
603	Chemical Bonding in XeF <sub>2</sub> , XeF <sub>4</sub> , KrF <sub>2</sub> , KrF <sub>4</sub> , RnF <sub>2</sub> , XeCl <sub>2</sub> , and XeBr <sub>2</sub> : From the Gas Phase to the Solid State. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10647-10654.	1.1	47
604	Electronic Structure of Host Lattices for Intercalation Compounds: SnS <sub>2</sub> , SnSe <sub>2</sub> , ZrS <sub>2</sub> , and TaS <sub>2</sub> . <i>Chemistry of Materials</i> , 1998, 10, 3422-3428.	3.2	19
605	Exchange-Correlation Energy Density from Virial Theorem. <i>Journal of Physical Chemistry A</i> , 1998, 102, 4911-4917.	1.1	86
606	Adsorption of Thiophene on the Catalytically Active Surface of MoS <sub>2</sub> : An Ab Initio Local-Density-Functional Study. <i>Physical Review Letters</i> , 1998, 80, 1481-1484.	2.9	128
607	Ab initio study of iron and iron hydride: I. Cohesion, magnetism and electronic structure of cubic Fe and FeH. <i>Journal of Physics Condensed Matter</i> , 1998, 10, 5081-5111.	0.7	40
608	Improving virtual Kohn-Sham orbitals and eigenvalues: Application to excitation energies and static polarizabilities. <i>Journal of Chemical Physics</i> , 1998, 109, 10180-10189.	1.2	886
609	Ab initio calculation of the lithium-tin voltage profile. <i>Physical Review B</i> , 1998, 58, 15583-15588.	1.1	254
610	Calculations of near-edge x-ray-absorption spectra of gas-phase and chemisorbed molecules by means of density-functional and transition-potential theory. <i>Physical Review B</i> , 1998, 58, 8097-8110.	1.1	467
611	Pseudopotential study of binding properties of solids within generalized gradient approximations: The role of core-valence exchange correlation. <i>Physical Review B</i> , 1998, 57, 2134-2145.	1.1	197
612	Structure and Energetics of Water Adsorbed at TiO <sub>2</sub> Anatase (101) and (001) Surfaces. <i>Physical Review Letters</i> , 1998, 81, 2954-2957.	2.9	883
613	The Hematite (α-Fe <sub>2</sub> O <sub>3</sub> ) (0001) Surface: Evidence for Domains of Distinct Chemistry. <i>Physical Review Letters</i> , 1998, 81, 1038-1041.	2.9	490
614	Island morphology and adatom self-diffusion on Pt(111). <i>Physical Review B</i> , 1998, 57, 1881-1889.	1.1	90
615	Interpretation of Activation Volumes for Water Exchange Reactions Revisited: Ab Initio Calculations for Al <sup>3+</sup> , Ga <sup>3+</sup> , and In <sup>3+</sup> , and New Experimental Data. <i>Journal of the American Chemical Society</i> , 1998, 120, 6569-6577.	6.6	95



#	ARTICLE	IF	CITATIONS
616	Ab initio self-consistent calculations of the Compton profiles and polarizabilities of diamond and cubic boron nitride. <i>Journal of Physics Condensed Matter</i> , 1998, 10, 557-575.	0.7	10
617	Chemisorption of Organics on Platinum. 2. Chemisorption of C <sub>2</sub> H <sub>x</sub> and CH <sub>x</sub> on Pt(111). <i>Journal of Physical Chemistry B</i> , 1998, 102, 9492-9500.	1.2	98
618	Adsorption of Methanol on TiO <sub>2</sub> (110): A First-Principles Investigation. <i>Journal of Physical Chemistry B</i> , 1998, 102, 2017-2026.	1.2	127
619	Exchange functionals with improved long-range behavior and adiabatic connection methods without adjustable parameters: The mPW and mPW1PW models. <i>Journal of Chemical Physics</i> , 1998, 108, 664-675.	1.2	3,068
620	Using the Exact Kohn-Sham Exchange Energy Density Functional and Potential to Study Errors Introduced by Approximate Correlation Functionals. <i>Advances in Quantum Chemistry</i> , 1998, , 151-165.	0.4	0
621	Structural stability of compounds (M = Al, Ni, Cu) studied by ab initio total-energy calculations and high-pressure x-ray diffraction. <i>Journal of Physics Condensed Matter</i> , 1998, 10, 2933-2945.	0.7	24
622	Derivation of a Generalized Gradient Approximation: The PW91 Density Functional. , 1998, , 81-111.		163
623	d-to-s bonding in GaN. <i>Journal of Physics Condensed Matter</i> , 1998, 10, 7155-7162.	0.7	4
624	Some ground-state properties of 3d and 4d metals studied using the generalized gradient approximation. <i>Journal of Physics Condensed Matter</i> , 1998, 10, 1285-1291.	0.7	11
625	First-principles calculation of hyperfine fields in ternary compounds and their carbides. <i>Journal of Physics Condensed Matter</i> , 1998, 10, 10999-11014.	0.7	3
626	Study of the structures of solid hydrogen at megabar pressures by means of first-principles calculations. <i>Journal of Physics Condensed Matter</i> , 1998, 10, 11191-11201.	0.7	2
627	Kohn-Sham density functionals accurately solved by a finite-element multi-grid (FEM-MG) method for lighter atoms and diatomic molecules. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 1998, 31, 4743-4754.	0.6	9
628	First-principles study of the equilibrium structures of clusters. <i>Journal of Physics Condensed Matter</i> , 1998, 10, 5851-5860.	0.7	5
629	Anomalous hydrogen adsorption sites found for the c(2 $\sqrt{3}$ ×2)-3H phases formed on the Re(10 $\bar{1}$ ,0) and Ru(10 $\bar{1}$ ,0) surfaces. <i>Journal of Chemical Physics</i> , 1998, 108, 8671-8679.	1.2	34
630	Structural and electronic properties of small Cu <sub>n</sub> clusters using generalized-gradient approximations within density functional theory. <i>Journal of Chemical Physics</i> , 1998, 109, 6626-6630.	1.2	78
631	Density functional analysis of <sup>13</sup> C and <sup>1</sup> H chemical shifts and bonding in mercurimethanes and organomercury hydrides: The role of scalar relativistic, spin-orbit, and substituent effects. <i>Journal of Chemical Physics</i> , 1998, 108, 3648-3659.	1.2	72
632	Transferability of first principles derived torsional potentials for mesogenic molecules and fragments. <i>Molecular Physics</i> , 1998, 93, 947-954.	0.8	3
633	Theoretical investigation of the high-pressure phases of Ce. <i>Physical Review B</i> , 1998, 57, 2091-2101.	1.1	22



#	ARTICLE	IF	CITATIONS
634	First-principles diffusion-barrier calculation for atomic oxygen on Pt(111). Physical Review B, 1998, 57, R4289-R4292.	1.1	80
635	First-principles theory of inelastic currents in a scanning tunneling microscope. Physical Review B, 1998, 58, 8038-8041.	1.1	52
636	Activation energy for the decay of two-dimensional islands on Cu(100). Physical Review B, 1998, 58, R7556-R7559.	1.1	34
637	Pressure-induced phase transitions in solid Si, SiO <sub>2</sub> , and Fe: Performance of local-spin-density and generalized-gradient-approximation density functionals. Physical Review B, 1998, 58, 11266-11272.	1.1	77
638	Surface-tip interactions in noncontact atomic-force microscopy on reactive surfaces: Si(111). Physical Review B, 1998, 58, 10835-10849.	1.1	194
639	Energetics of hydrogen in amorphous silicon: An ab initio study. Physical Review B, 1998, 57, 12859-12868.	1.1	53
640	Gaussian-basis LDA and GGA calculations for alkali-metal equations of state. Physical Review B, 1998, 57, 11834-11837.	1.1	37
641	Structure and dynamics of Rh surfaces. Physical Review B, 1998, 57, 4768-4775.	1.1	25
642	Many-body effects on bandwidths in ionic, noble gas, and molecular solids. Physical Review B, 1998, 58, 9579-9583.	1.1	76
643	Nonlinear magneto-optics of Fe monolayers from first principles: Structural dependence and spin-orbit coupling strength. Physical Review B, 1998, 58, 5093-5105.	1.1	15
644	Molecular orientation with visible light: Reflectance-anisotropy spectroscopy of 3-thiophene carboxylate on Cu(110) surfaces. Physical Review B, 1998, 58, 10883-10889.	1.1	44
645	Electronic topological and structural transition in AuIn <sub>2</sub> under pressure. Physical Review B, 1998, 57, 773-776.	1.1	59
646	Kohn-Sham potentials and exchange and correlation energy densities from one- and two-electron density matrices for Li <sub>2</sub> , N <sub>2</sub> , and F <sub>2</sub> . Physical Review A, 1998, 57, 1729-1742.	1.0	58
647	Magnetic transition in Mn <sub>n</sub> (n=2-8) clusters. Physical Review B, 1998, 58, 5632-5636.	1.1	131
648	A spin-density polarization index. Journal of Chemical Physics, 1998, 108, 2824-2830.	1.2	4
649	Effective homogeneity of the exchange-correlation energy functional. Physical Review A, 1998, 58, 3524-3527.	1.0	22
650	Exchange energy in density-functional theory: A nonlocal approximation based on a self-consistent determination of the $I_{\pm}$ parameter of the Slater $X_{\pm}$ theory. Physical Review A, 1998, 57, 4306-4310.	1.0	6
651	Simple model for complex structures. Physical Review B, 1998, 57, 1320-1323.	1.1	22

#	ARTICLE	IF	CITATIONS
652	Ab initio calculation of the potential energy surface for the dissociation of H <sub>2</sub> on the sulfur-covered Pd(100) surface. <i>Physical Review B</i> , 1998, 57, 15572-15584.	1.1	42
653	High-pressure studies on YNi <sub>2</sub> B <sub>2</sub> C at room temperature. <i>Physical Review B</i> , 1998, 58, 3377-3380.	1.1	23
654	Reversed spin polarization at the Co(001)-HfO <sub>2</sub> (001) interface. <i>Physical Review B</i> , 1998, 58, 15422-15425.	1.1	15
655	Electronic structure, chemical bonding, phase stability, and ground-state properties of YNi <sub>2-x</sub> (Co/Cu) <sub>x</sub> B <sub>2</sub> C. <i>Physical Review B</i> , 1998, 58, 3381-3393.	1.1	39
656	Ab initio quantum and molecular dynamics of the dissociative adsorption of hydrogen on Pd(100). <i>Physical Review B</i> , 1998, 57, 2493-2506.	1.1	158
657	Low-Symmetry Diffusion Barriers in Homoepitaxial Growth of Al(111). <i>Physical Review Letters</i> , 1998, 81, 637-640.	2.9	98
658	Cohesive properties of the lanthanides: Effect of generalized gradient corrections and crystal structure. <i>Physical Review B</i> , 1998, 58, 4345-4351.	1.1	56
659	Spin-density-functional-based search for half-metallic antiferromagnets. <i>Physical Review B</i> , 1998, 57, 10613-10619.	1.1	213
660	First principles calculation of the activity of cytochrome P450. <i>Physical Review E</i> , 1998, 57, 4618-4621.	0.8	22
661	Highly Site-Specific H <sub>2</sub> Adsorption on Vicinal Si(001) Surfaces. <i>Physical Review Letters</i> , 1998, 81, 5596-5599.	2.9	100
662	Alkali Promotion of N <sub>2</sub> Dissociation over Ru(0001). <i>Physical Review Letters</i> , 1998, 80, 4333-4336.	2.9	185
663	Adsorption of CO on Rh(100) studied by ab initio local-density functional calculations. <i>Journal of Chemical Physics</i> , 1998, 109, 5585-5595.	1.2	46
664	Nature of bonding forces between two hydrogen-passivated silicon wafers. <i>Physical Review B</i> , 1998, 58, 16118-16122.	1.1	7
665	Interaction between atoms and surfaces: A bond-pair description based on an extended Anderson model. <i>Physical Review B</i> , 1998, 58, 5007-5021.	1.1	36
666	C <sub>24</sub> : Ring or fullerene?. <i>Journal of Chemical Physics</i> , 1998, 108, 3213-3217.	1.2	31
667	Exchange-correlation density functional beyond the gradient approximation. <i>Physical Review A</i> , 1998, 57, 189-199.	1.0	69
668	H-induced reconstructions on Pd(110). <i>Physical Review B</i> , 1998, 57, 12482-12491.	1.1	45
669	Oxygen adsorption on the Ru(101 $\bar{1}$ 0) surface: Anomalous coverage dependence. <i>Physical Review B</i> , 1998, 57, 15487-15495.	1.1	68

#	ARTICLE	IF	CITATIONS
670	Density-functional study of the magnetic and metal-insulator transition of bcc hydrogen. <i>Physical Review B</i> , 1998, 58, 12680-12683.	1.1	11
671	Adsorption of CO on Pd(100): Steering into less favored adsorption sites. <i>Physical Review B</i> , 1998, 57, 10110-10114.	1.1	43
672	Magnetic and electronic properties of rhodium clusters. <i>Physical Review A</i> , 1998, 58, 2196-2202.	1.0	72
673	A combined molecular dynamicsâ€“ab initio study of H <sub>2</sub> adsorption on ideal, relaxed, and temperature-reconstructed MgO(111) surfaces. <i>Journal of Chemical Physics</i> , 1998, 109, 7515-7521.	1.2	31
674	Applications of the generalized gradient approximation to ferroelectric perovskites. <i>Physical Review B</i> , 1998, 58, 11959-11963.	1.1	76
675	Thermal isomerization in Cs <sub>4</sub> Cl <sub>3</sub> . <i>Physical Review A</i> , 1998, 58, 744-747.	1.0	6
676	First-principles theory of Ta up to 10 Mbar pressure: Structural and mechanical properties. <i>Physical Review B</i> , 1998, 57, 10340-10350.	1.1	96
677	Nature of the surface chemical bond in N <sub>2</sub> on Ni(100) studied by x-ray-emission spectroscopy and ab initio calculations. <i>Physical Review B</i> , 1998, 57, 9274-9284.	1.1	61
678	First principles study of adsorbed Cu <sub>n</sub> (n=1â€“4) microclusters on MgO(100): Structural and electronic properties. <i>Journal of Chemical Physics</i> , 1998, 108, 5044-5054.	1.2	137
679	High Pressure Polymorphism in Silica. <i>Physical Review Letters</i> , 1998, 80, 2145-2148.	2.9	205
680	Excitonic correlations in the intermetallic Fe <sub>2</sub> VAl. <i>Physical Review B</i> , 1998, 58, 6855-6861.	1.1	155
681	STM-Induced Hydrogen Desorption via a Hole Resonance. <i>Physical Review Letters</i> , 1998, 80, 2618-2621.	2.9	131
682	Embrittlement and the Bistable Crystal Structure of Zirconium Hydride. <i>Physical Review Letters</i> , 1998, 80, 2233-2236.	2.9	64
683	Al Dimer Dynamics on Al(111). <i>Physical Review Letters</i> , 1998, 81, 172-175.	2.9	52
684	Effect of exchange-correlation functionals and symmetry constraints of electronic structure on the trajectories of reactive molecular collisions. <i>Physical Review A</i> , 1998, 57, 899-905.	1.0	10
685	First-Principles Study of the As-Mediated Growths of Si and Ge on Si(100). <i>Surface Review and Letters</i> , 1998, 05, 77-80.	0.5	1
686	Recent Developments in the Local-Scaling Transformation Version of Density Functional Theory. <i>Advances in Quantum Chemistry</i> , 1998, , 49-70.	0.4	12
687	Digging into the Exchange-Correlation Energy: The Exchange-Correlation Hole. , 1998, , 19-29.		2

#	ARTICLE	IF	CITATIONS
688	Why Density-Gradient Corrections Improve Atomization Energies and Barrier Heights. <i>Advances in Quantum Chemistry</i> , 1998, 33, 1-9.	0.4	2
689	In Search of the Correlation Potential. <i>Advances in Quantum Chemistry</i> , 1998, , 71-83.	0.4	0
690	Quantum Chemical Molecular Dynamics. <i>Advances in Quantum Chemistry</i> , 1998, 33, 167-187.	0.4	5
691	A first-principles Hartree-Fock description of MnO at high pressures. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1998, 77, 1063-1075.	0.6	3
692	N <sub>2</sub> Interaction with Fe Surfaces. <i>Israel Journal of Chemistry</i> , 1998, 38, 279-284.	1.0	8
693	First-principles Hartree-Fock description of the electronic structure of monoclinic <i>C<sub>2/m</sub></i> Li <sub>x</sub> MnO <sub>2</sub> (1 ≤ x ≤ 0). <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1998, 77, 1077-1092.	0.6	19
694	Coadsorption of CO and O on Ru(0001): A Structural Analysis by Density Functional Theory. <i>Israel Journal of Chemistry</i> , 1998, 38, 409-414.	1.0	10
695	Molecular processes on oxide surfaces studied by first-principles calculations. <i>Mineralogical Magazine</i> , 1998, 62, 669-685.	0.6	16
696	Twenty to thirty years of DV-X $\alpha$ calculations: A survey of accuracy and applications. <i>Advances in Quantum Chemistry</i> , 1998, , 1-47.	0.4	9
697	Ab Initio Study of Changes in the Magnetism of Iron During the BCC-HCP Phase Transformation. <i>Materials Research Society Symposia Proceedings</i> , 1998, 538, 523.	0.1	1
698	First Principles Calculations for Lithiated Manganese Oxides. <i>Materials Research Society Symposia Proceedings</i> , 1998, 548, 137.	0.1	4
699	Theoretical study of benzothiophene hydrodesulfurization on MoS <sub>2</sub> . <i>Studies in Surface Science and Catalysis</i> , 1999, 127, 327-334.	1.5	24
700	Absolute total energy of small copper clusters in an all-electron mixed-basis approach with the generalized-gradient approximation. <i>Journal of Materials Research</i> , 1999, 14, 980-983.	1.2	2
701	Dispersion Coefficients for van der Waals Complexes, Including C <sub>60</sub> ⋯C <sub>60</sub> . <i>Physica Scripta</i> , 1999, 60, 211-216.	1.2	26
702	Electronic and magnetic structure of Mn-Ni alloys in two and three dimensions. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 6359-6372.	0.7	22
703	Unusual multilayer relaxation of the Mo(111) surface induced by hydrogen. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 1873-1888.	0.7	11
704	Theoretical Study of Na Clusters by First Principle Molecular Dynamics Calculations. <i>Chinese Physics Letters</i> , 1999, 16, 262-263.	1.3	4
705	Ab initio and molecular dynamics studies of cation⋯water interactions. <i>Theoretical and Computational Chemistry</i> , 1999, 7, 431-469.	0.2	6

#	ARTICLE	IF	CITATIONS
706	Comparison of Hartree-Fock and density functional theory structure factors and charge density in diamond, silicon and germanium. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 5827-5843.	0.7	6
707	Structural properties of magnetic Heusler alloys. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 2017-2026.	0.7	230
708	Ab Initio Study of Hydrogen Desorption from Diamond C(100) Surfaces. <i>Japanese Journal of Applied Physics</i> , 1999, 38, L783-L785.	0.8	8
709	SYNTHESIS, CRYSTAL STRUCTURE AND QUANTUM CHEMICAL CALCULATIONS OF $[\text{Ge}(\text{OH})(\text{Hcdta})] \cdot \text{H}_2\text{O}$ ( $\text{H4cdta} = \text{trans-CYCLOHEXANE-1,2-DIAMINETETRAACETIC ACID}$ ). <i>Main Group Metal Chemistry</i> , 1999, 22, .	0.6	1
710	Atomic structure and charge transfer in liquid Rb-Te mixtures: An ab initio molecular-dynamics simulation. <i>Physical Review B</i> , 1999, 59, 3514-3520.	1.1	13
711	Diffusion of Pt dimers on Pt(111). <i>Physical Review B</i> , 1999, 59, 9846-9849.	1.1	28
712	Bond Activation at Monatomic Steps: NO Dissociation at Corrugated Ru(0001). <i>Physical Review Letters</i> , 1999, 83, 3681-3684.	2.9	183
713	Reaction channels for the catalytic oxidation of CO on Pt(111). <i>Physical Review B</i> , 1999, 59, 5960-5967.	1.1	100
714	Variations in the Nature of Metal Adsorption on Ultrathin $\text{Al}_2\text{O}_3$ Films. <i>Physical Review Letters</i> , 1999, 82, 4050-4053.	2.9	175
715	Anisotropic intermolecular interactions in van der Waals and hydrogen-bonded complexes: What can we get from density functional calculations?. <i>Journal of Chemical Physics</i> , 1999, 111, 7727-7735.	1.2	91
716	Atomic and electronic structure and interatomic potentials at a polar ceramic/metal interface: $\{222\}\text{MgO}/\text{Cu}$ . <i>Physical Review B</i> , 1999, 60, 16094-16102.	1.1	48
717	Anomalous behavior of the semiconducting gap in $\text{WO}_3$ from first-principles calculations. <i>Physical Review B</i> , 1999, 59, 2684-2693.	1.1	121
718	Rotational effects in six-dimensional quantum dynamics for reaction of $\text{H}_2$ on Cu(100). <i>Journal of Chemical Physics</i> , 1999, 110, 7008-7020.	1.2	52
719	Electronic structure of magnetic $\text{Sr}_2\text{RuO}_4$ . <i>Physical Review B</i> , 1999, 59, 9894-9897.	1.1	30
720	Effect of the cluster size in modeling the $\text{H}_2$ desorption and dissociative adsorption on Si(001). <i>Journal of Chemical Physics</i> , 1999, 110, 3986-3994.	1.2	162
721	Structural and electronic properties of chemisorbed oxygen on Rh(111). <i>Physical Review B</i> , 1999, 59, 15533-15543.	1.1	127
722	Model of noncontact scanning force microscopy on ionic surfaces. <i>Physical Review B</i> , 1999, 59, 2436-2448.	1.1	134
723	Electron affinities of the first- and second-row atoms: Benchmark ab initio and density-functional calculations. <i>Physical Review A</i> , 1999, 60, 1034-1045.	1.0	95

#	ARTICLE	IF	CITATIONS
724	Mechanisms of self-diffusion on Pt(110). <i>Physical Review B</i> , 1999, 60, R5149-R5152.	1.1	45
725	Role of generalized-gradient approximation in structural and electronic properties of bulk and surface of $\text{In}^{2-}\text{GaN}$ and GaAs. <i>Physical Review B</i> , 1999, 59, 3008-3014.	1.1	24
726	Theoretical analysis of hydrogen chemisorption on Pd(111), Re(0001) and PdML/Re(0001), ReML/Pd(111) pseudomorphic overlayers. <i>Physical Review B</i> , 1999, 60, 6146-6154.	1.1	207
727	Electron transfer reactions on Cs/MoS <sub>2</sub> (0002) with chlorine, oxygen, and water: High resolution x-ray photoelectron spectroscopy and theoretical study. <i>Journal of Chemical Physics</i> , 1999, 111, 1636-1649.	1.2	11
728	Combined photoelectron spectroscopy and ab initio study of the hypermetallic Al <sub>3</sub> C molecule. <i>Journal of Chemical Physics</i> , 1999, 110, 8980-8985.	1.2	44
729	Atomic and molecular hydrogen interacting with Pt(111). <i>Journal of Chemical Physics</i> , 1999, 111, 11155-11163.	1.2	197
730	Molecular N <sub>2</sub> chemisorption-specific adsorption on step defect sites on Pt surfaces. <i>Journal of Chemical Physics</i> , 1999, 111, 8651-8658.	1.2	56
731	Brønsted acid sites in gmelinite. <i>Journal of Chemical Physics</i> , 1999, 111, 7537-7545.	1.2	28
732	Effect of rotation and vibration on nuclear magnetic resonance chemical shifts: Density functional theory calculations. <i>Journal of Chemical Physics</i> , 1999, 110, 7153-7159.	1.2	26
733	Benchmark calculations of chemical reactions in density functional theory: Comparison of the accurate Kohn-Sham solution with generalized gradient approximations for the H <sub>2</sub> +H and H <sub>2</sub> +H <sub>2</sub> reactions. <i>Journal of Chemical Physics</i> , 1999, 111, 4056-4067.	1.2	74
734	The Pt <sup>4+</sup> cation has an extremely large negative <sup>31</sup> P nuclear magnetic resonance chemical shift, due to spin-orbit coupling: A quantum-chemical prediction and its confirmation by solid-state nuclear magnetic resonance spectroscopy. <i>Journal of Chemical Physics</i> , 1999, 110, 3897-3902.	1.2	46
735	Electronic structure of the layered manganite LaSr <sub>2</sub> Mn <sub>2</sub> O <sub>7</sub> . <i>Physical Review B</i> , 1999, 60, 10758-10762.	1.1	28
736	First-principles investigation of tip-surface interaction on a GaAs(110) surface: Implications for atomic force and scanning tunneling microscopies. <i>Physical Review B</i> , 1999, 60, 11631-11638.	1.1	66
737	X-ray measurement of the electron static structure factor in LiF. <i>Physical Review B</i> , 1999, 59, 12853-12859.	1.1	2
738	Correcting overbinding in local-density-approximation calculations. <i>Physical Review B</i> , 1999, 59, 14992-15001.	1.1	103
739	Polyanionic and octet phases in the K-Sb system. I. Crystalline intermetallic compounds. <i>Physical Review B</i> , 1999, 59, 829-842.	1.1	17
740	Interpretation of x-ray emission spectra: NO adsorbed on Ru(001). <i>Journal of Chemical Physics</i> , 1999, 111, 4704-4713.	1.2	21
741	Theoretical study of the structural phase transformation of BeO under pressure. <i>Physical Review B</i> , 1999, 59, 13501-13504.	1.1	52

#	ARTICLE	IF	CITATIONS
742	A reexamination of exchange energy functionals. <i>Journal of Chemical Physics</i> , 1999, 111, 5656-5667.	1.2	21
743	Time-dependent density functional calculations on the electronic absorption spectrum of free base porphyrin. <i>Journal of Chemical Physics</i> , 1999, 111, 2499-2506.	1.2	168
744	Hydrogen Electrochemistry and Stress-Induced Leakage Current in Silica. <i>Physical Review Letters</i> , 1999, 83, 372-375.	2.9	312
745	Atomic geometry and energetics of vacancies and antisites in cubic boron nitride. <i>Applied Physics Letters</i> , 1999, 74, 2984-2986.	1.5	39
746	The adiabatic molecule-metal surface interaction: Theoretical approaches. <i>Reviews of Modern Physics</i> , 1999, 71, 231-265.	16.4	133
747	Ammonia adsorbed on Cu(110): An angle resolved x-ray spectroscopic and ab initio study. <i>Journal of Chemical Physics</i> , 1999, 110, 4880-4890.	1.2	38
748	Two-Dimensional Quantum Rotation of Adsorbed H <sub>2</sub> . <i>Physical Review Letters</i> , 1999, 83, 124-127.	2.9	44
749	Initial Stages of Growth of Copper on MgO(100): A First Principles Study. <i>Physical Review Letters</i> , 1999, 83, 2761-2764.	2.9	49
750	Successful Test of a Seamless van der Waals Density Functional. <i>Physical Review Letters</i> , 1999, 82, 2123-2126.	2.9	188
751	Structure and Dynamics of Small Metallic Clusters on an Insulating Metal-Oxide Surface: Copper on MgO(100). <i>Physical Review Letters</i> , 1999, 83, 3242-3245.	2.9	70
752	Ab Initio Based Tight-Binding Hamiltonian for the Dissociation of Molecules at Surfaces. <i>Physical Review Letters</i> , 1999, 82, 1209-1212.	2.9	36
753	Nitrogen Adsorption and Hydrogenation on a MoFe <sub>6</sub> S <sub>9</sub> Complex. <i>Physical Review Letters</i> , 1999, 82, 4054-4057.	2.9	70
754	Metal-on-Metal Bonding and Rebonding Revisited. <i>Physical Review Letters</i> , 1999, 82, 5301-5304.	2.9	24
755	Surface diffusion potential energy surfaces from first principles: CO chemisorbed on Pt{110}. <i>Journal of Chemical Physics</i> , 1999, 111, 9461-9464.	1.2	46
756	Anharmonic adlayer vibrations on the Si(111):H surface. <i>Physical Review B</i> , 1999, 59, 10996-11013.	1.1	35
757	Geometric and electronic structure of vanadium pentoxide: a density functional bulk and surface study. <i>Physical Review B</i> , 1999, 59, 10583-10590.	1.1	184
758	Trends in the chemical reactivity of surfaces studied by ab initio quantum-dynamics calculations. <i>Physical Review B</i> , 1999, 59, 13297-13300.	1.1	67
759	First-principles calculation of structural and magnetic properties for Fe monolayers and bilayers on W(110). <i>Physical Review B</i> , 1999, 60, 16192-16197.	1.1	89



#	ARTICLE	IF	CITATIONS
760	Simulation of tip-surface interactions in atomic force microscopy of an InP(110) surface with a Si tip. <i>Physical Review B</i> , 1999, 60, 11639-11644.	1.1	46
761	Analysis of the MgO structure factors. <i>Physical Review B</i> , 1999, 60, 8569-8574.	1.1	13
762	Calculated polarizabilities of intermediate-size Si clusters. <i>Physical Review A</i> , 1999, 59, 3685-3689.	1.0	73
763	Dependence of energy gaps and effective masses on atomic positions in hexagonal SiC. <i>Journal of Applied Physics</i> , 1999, 86, 5036-5039.	1.1	32
764	Ab initio calculation of optical-mode frequencies in compressed solid hydrogen. <i>Physical Review B</i> , 1999, 59, 13741-13753.	1.1	25
765	Density-functional study of hydrogen chemisorption on vicinal Si(001) surfaces. <i>Physical Review B</i> , 1999, 59, 2790-2800.	1.1	34
766	Inverted vibrational distributions from N <sub>2</sub> recombination at Ru(001): Evidence for a metastable molecular chemisorption well. <i>Journal of Chemical Physics</i> , 1999, 110, 6954-6962.	1.2	73
767	Transformation of molecular oxygen on a platinum surface: A theoretical calculation of STM images. <i>Physical Review B</i> , 1999, 59, 15437-15445.	1.1	64
768	Unified treatment of asymptotic van der Waals forces. <i>Physical Review B</i> , 1999, 59, 4708-4713.	1.1	89
769	Theoretical study of the pressure-concentration diagram for the Ce-Th alloy system. <i>Physical Review B</i> , 1999, 60, 9372-9376.	1.1	7
770	Structural and electronic properties of Si <sub>1-x</sub> C <sub>x</sub> alloys and the band alignment in Si <sub>1-x</sub> C <sub>x</sub> /Si(001) heterostructure. <i>Physical Review B</i> , 1999, 59, 15013-15018.	1.1	4
771	ELECTRON DENSITY FUNCTIONAL THEORY. <i>International Journal of Modern Physics B</i> , 1999, 13, 511-523.	1.0	4
772	An ab initio study of the structural and physical properties of a novel rigid-rod polymer: PIPD. <i>Polymer</i> , 1999, 40, 1313-1323.	1.8	45
773	Electronic structure of NaNO <sub>2</sub> in the ferroelectric phase. <i>Solid State Communications</i> , 1999, 112, 495-498.	0.9	5
774	Modeling STM tips by single adsorbed atoms on W(100) films: 5d transition metal atoms. <i>Solid State Communications</i> , 1999, 113, 245-250.	0.9	49
775	Model structures and properties of the electron density distribution for low quartz at pressure: a study of the SiO bond. <i>Journal of Molecular Structure</i> , 1999, 485-486, 13-25.	1.8	36
776	Calculation of cohesion and changes in electronic structure due to impurity segregation at boundaries in iron. <i>Acta Materialia</i> , 1999, 47, 4069-4075.	3.8	14
777	Prediction of <sup>29</sup> Si MAS NMR chemical shifts in zeolites using density functional theory. <i>Microporous and Mesoporous Materials</i> , 1999, 30, 111-117.	2.2	12

#	ARTICLE	IF	CITATIONS
778	Experimental and theoretical studies of gas-phase reactions of SiF <sub>x</sub> <sup>+</sup> (x = 1-3) with ammonia: intramolecular H-atom transfer reactions with SiF <sub>3</sub> <sup>+</sup> and F <sub>2</sub> Si(NH <sub>2</sub> ). International Journal of Mass Spectrometry, 1999, 185-187, 381-392.	0.7	8
779	Experimental and theoretical studies of the basicity and proton affinity of SiF <sub>4</sub> and the structure of SiF <sub>4</sub> H <sup>+</sup> . Journal of the American Society for Mass Spectrometry, 1999, 10, 848-855.	1.2	5
780	Influence of generalized gradient approximations on theoretical hyperfine fields of paramagnetic defects. Physica B: Condensed Matter, 1999, 273-274, 88-91.	1.3	3
781	Fracture and dislocation properties: an ab-initio electronic structure approach. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1999, 260, 80-93.	2.6	13
782	The C-type defect on Si(001) as a hydrogen-vacancy complex. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1999, 58, 48-51.	1.7	4
783	Ab initio study on the topological Li insertion in titanium oxide. Journal of Power Sources, 1999, 81-82, 393-396.	4.0	10
784	Network transformation processes during oxidation of silicon. Microelectronic Engineering, 1999, 48, 89-94.	1.1	4
785	Investigating the effects of silicon tip contamination in noncontact scanning force microscopy (SFM). Applied Surface Science, 1999, 144-145, 608-612.	3.1	24
786	Approximation of the exchange-correlation Kohn-Sham potential with a statistical average of different orbital model potentials. Chemical Physics Letters, 1999, 302, 199-207.	1.2	409
787	On the performance of density functional theory for symmetry-breaking problems. Chemical Physics Letters, 1999, 302, 425-430.	1.2	128
788	Metal-coated fullerenes: electronic, geometrical and vibrational properties of C <sub>60</sub> M <sub>62</sub> (M=Ti and V). Chemical Physics Letters, 1999, 303, 373-378.	1.2	11
789	Relativistic density functional investigation of Pu(H <sub>2</sub> O) <sub>n</sub> <sup>3+</sup> clusters. Chemical Physics Letters, 1999, 310, 347-354.	1.2	29
790	Rotational effects in the dissociation of H <sub>2</sub> on metal surfaces studied by ab initio quantum-dynamics calculations. Chemical Physics Letters, 1999, 311, 1-7.	1.2	32
791	Hydrogen abstraction rates via density functional theory. Chemical Physics Letters, 1999, 312, 262-268.	1.2	26
792	Ab initio pseudopotentials for electronic structure calculations of poly-atomic systems using density-functional theory. Computer Physics Communications, 1999, 119, 67-98.	3.0	1,313
793	Enhancement of surface self-diffusion of platinum atoms by adsorbed hydrogen. Nature, 1999, 398, 134-136.	13.7	221
794	Pairing in dense lithium. Nature, 1999, 400, 141-144.	13.7	375
795	The melting curve of iron at the pressures of the Earth's core from ab initio calculations. Nature, 1999, 401, 462-464.	13.7	270

#	ARTICLE	IF	CITATIONS
796	Cu underpotential deposition on Au(111) and Au(100). Can this be explained in terms of the energetics of the Cu/Au system?. <i>Electrochimica Acta</i> , 1999, 45, 691-697.	2.6	31
797	The chemisorption of spin polarised NO on Ag{111}. <i>Chemical Physics Letters</i> , 1999, 300, 639-644.	1.2	53
798	DFT investigation of the adsorption of atomic hydrogen on a cluster-model graphite surface. <i>Chemical Physics Letters</i> , 1999, 300, 157-162.	1.2	352
799	Ab initio study of surface structural changes during methanol synthesis over Zn/Cu(111). <i>Chemical Physics Letters</i> , 1999, 304, 91-97.	1.2	48
800	First-principles theoretical studies of the structural, electronic and magnetic properties of Co{1010}-A. <i>Chemical Physics Letters</i> , 1999, 309, 434-440.	1.2	12
801	Prediction of a nanoporous sp <sup>2</sup> -carbon framework structure by combining graph theory with quantum mechanics. <i>Chemical Physics Letters</i> , 1999, 312, 536-541.	1.2	25
802	Nitrogen Adsorption and Dissociation on Fe(111). <i>Journal of Catalysis</i> , 1999, 182, 479-488.	3.1	150
803	DFT Calculations of Unpromoted and Promoted MoS <sub>2</sub> -Based Hydrodesulfurization Catalysts. <i>Journal of Catalysis</i> , 1999, 187, 109-122.	3.1	393
804	Chemisorption of Methane on Ni(100) and Ni(111) Surfaces with Preadsorbed Potassium. <i>Journal of Catalysis</i> , 1999, 187, 238-244.	3.1	94
805	Electric field gradient and atomic position for Se in MoSe <sub>2</sub> . , 1999, 120/121, 423-426.		2
806	Electric field gradients at V, Nb and Ta in A15 alloys. , 1999, 120/121, 157-161.		2
807	Towards standard methods for benchmark quality ab initio thermochemistryâ€”W1 and W2 theory. <i>Journal of Chemical Physics</i> , 1999, 111, 1843-1856.	1.2	947
808	Density functional calculations on small platinum clusters: Pt n q ( n =1â€“4, q =0,Â±1). <i>Computational and Theoretical Chemistry</i> , 1999, 493, 233-240.	1.5	44
809	Interaction of H <sub>2</sub> O clusters with hydrogen-terminated and clean Si(001) surfaces. <i>Thin Solid Films</i> , 1999, 343-344, 397-400.	0.8	12
810	Dynamic crystal field in heavy fermion systems. <i>Journal of Magnetism and Magnetic Materials</i> , 1999, 192, 553-563.	1.0	2
811	Magnetism, magneto-crystalline anisotropy, magnetostriction and MOKE at surfaces and interfaces. <i>Journal of Magnetism and Magnetic Materials</i> , 1999, 203, 1-5.	1.0	15
812	Spinâ€“orbit induced magnetic phenomena in bulk metals and their surfaces and interfaces. <i>Journal of Magnetism and Magnetic Materials</i> , 1999, 200, 498-514.	1.0	227
813	Crystal Structures and Electrical and Optical Properties of MgIn <sub>2</sub> â€“xGa <sub>x</sub> O <sub>4</sub> Solid Solutions. <i>Journal of Solid State Chemistry</i> , 1999, 142, 206-213.	1.4	34

#	ARTICLE	IF	CITATIONS
814	NMR vs. molecular modelling. Part IIâ€”steroid chemical shift calculations. <i>Magnetic Resonance in Chemistry</i> , 1999, 37, 103-106.	1.1	35
815	NMR vs. molecular modelling. Part IIIâ€”a DFT-GIAO study of a series of 2-X-fluorobenzenes. <i>Magnetic Resonance in Chemistry</i> , 1999, 37, 107-109.	1.1	20
816	Magnetic and redox properties in hydroxo- and alkoxo-bridged Fe(III) binuclear complexes: A density functional study. <i>International Journal of Quantum Chemistry</i> , 1999, 72, 61-71.	1.0	14
817	The antiparallel electron correlation coefficient and Coulomb hole structure. <i>International Journal of Quantum Chemistry</i> , 1999, 74, 1-6.	1.0	0
818	Relativistic effects on geometry and electronic structure of small Pd <sub>n</sub> species (n=1, 2, 4). <i>International Journal of Quantum Chemistry</i> , 1999, 74, 405-416.	1.0	26
819	Density functional study of small molecules and transition-metal carbonyls using revised PBE functionals. <i>International Journal of Quantum Chemistry</i> , 1999, 75, 863-873.	1.0	164
820	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs. , 1999, 75, 889-909.		598
821	Understanding reactivity with Kohn-Sham molecular orbital theory: E2-SN2 mechanistic spectrum and other concepts. <i>Journal of Computational Chemistry</i> , 1999, 20, 114-128.	1.5	515
822	From explicit to implicit density functionals. <i>Journal of Computational Chemistry</i> , 1999, 20, 31-50.	1.5	156
823	The role of $\pi$ -type nonbonding orbitals for spin-orbit induced NMR chemical shifts: DFT study of <sup>13</sup> C and <sup>19</sup> F shifts in the series CF <sub>3</sub> IF <sub>n</sub> (n=0, 2, 4, 6). <i>Journal of Computational Chemistry</i> , 1999, 20, 1304-1313.	1.5	37
824	Analysis of XPS valence band spectra of polymers using a density-functional theory based calculation of model oligomers. <i>Journal of Polymer Science Part A</i> , 1999, 37, 95-103.	2.5	14
825	Ab Initio Density Functional Theory Studies of Hydrogen Adsorption at the V <sub>2</sub> O <sub>5</sub> (010) Surface. <i>Physica Status Solidi A</i> , 1999, 173, 195-208.	1.7	26
826	Ab initio calculation of the lattice dynamics and phase diagram of boron nitride. <i>Physical Review B</i> , 1999, 59, 8551-8559.	1.1	359
827	Structure and electronic properties of amorphous WO <sub>3</sub> . <i>Physical Review B</i> , 1999, 60, 16463-16474.	1.1	88
828	First-principles calculations for phonons in AgGaX <sub>2</sub> (X = Se, Te) chalcopyrite crystals. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 9673-9678.	0.7	16
829	Optimization of Gaussian basis sets for density-functional calculations. <i>Physical Review A</i> , 1999, 60, 2840-2847.	1.0	250
830	From ultrasoft pseudopotentials to the projector augmented-wave method. <i>Physical Review B</i> , 1999, 59, 1758-1775.	1.1	61,625
831	Density functional study of the Feâ€”CO bond dissociation energies of Fe(CO) <sub>5</sub> . <i>Journal of Chemical Physics</i> , 1999, 110, 778-783.	1.2	61

#	ARTICLE	IF	CITATIONS
832	Effects of spin polarization on the structural and electronic properties of supercritical fluid selenium:ab initiomolecular-dynamics simulations. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 8829-8838.	0.7	17
833	Retardation of O diffusion through polycrystalline Pt by Be doping. <i>Physical Review B</i> , 1999, 59, 16047-16052.	1.1	12
834	Structure, Chemical Bonding, and Nuclear Quadrupole Interactions of $^{125}\text{Cd}(\text{OH})_2$ : Experiment and First Principles Calculations. <i>Inorganic Chemistry</i> , 1999, 38, 2860-2867.	1.9	28
835	Elastic and optical properties of $\alpha$ - and $\beta$ - $\text{Al}_2\text{O}_3$ . <i>Physical Review B</i> , 1999, 59, 12777-12787.	1.1	152
836	Structural stability of higher-energy phases and its relation to the atomic configurations of extended defects: The example of Cu. <i>Physical Review B</i> , 1999, 60, 844-850.	1.1	44
837	Exact exchange Kohn-Sham formalism applied to semiconductors. <i>Physical Review B</i> , 1999, 59, 10031-10043.	1.1	358
838	Ab initio studies of the formation of a $\text{Y}_{1-x}\text{Ni}_x$ superstructure with ordered Y vacancies. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 1177-1187.	0.7	19
839	Intergrain tunneling magnetoresistance in polycrystals of the ordered double perovskite $\text{Sr}_2\text{FeReO}_6$ . <i>Physical Review B</i> , 1999, 59, 11159-11162.	1.1	438
840	Structural and vibrational properties of carbon monoxide adlayers on the copper (001) surface. <i>Journal of Chemical Physics</i> , 1999, 110, 4619-4633.	1.2	24
841	Ab initio studies on the structural and magnetic properties of FeCu superlattices. <i>Physical Review B</i> , 1999, 60, 3025-3028.	1.1	25
842	Spectroscopy of low-coordinated surface sites: Theoretical study of MgO. <i>Physical Review B</i> , 1999, 59, 2417-2430.	1.1	164
843	Conformations and Barriers of Haloethyl Radicals ( $\text{CH}_2\text{XCH}_2$ , X = F, Cl, Br, I): Ab Initio Studies. <i>Journal of Physical Chemistry A</i> , 1999, 103, 6638-6649.	1.1	49
844	Impeded Dimer Formation in the High-Pressure Crystal Structure of Formic Acid. <i>Physical Review Letters</i> , 1999, 82, 3464-3467.	2.9	67
845	Density functional calculations of nuclear magnetic shieldings using the zeroth-order regular approximation (ZORA) for relativistic effects: ZORA nuclear magnetic resonance. <i>Journal of Chemical Physics</i> , 1999, 110, 7689-7698.	1.2	464
846	Electronic structure of 3d-transition-metal oxides: on-site Coulomb repulsion versus covalency. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 1657-1682.	0.7	151
847	First-Principles Theory of Surface Thermodynamics and Kinetics. <i>Physical Review Letters</i> , 1999, 83, 2993-2996.	2.9	181
848	Electronic properties of ppp-oligomers investigated from first-principles. <i>Synthetic Metals</i> , 1999, 101, 673-674.	2.1	9
849	First-principles elastic constants for the hcp transition metals Fe, Co, and Re at high pressure. <i>Physical Review B</i> , 1999, 60, 791-799.	1.1	355

#	ARTICLE	IF	CITATIONS
850	Density-functional calculations for III-V nitrides using the local-density approximation and the generalized gradient approximation. <i>Physical Review B</i> , 1999, 59, 5521-5535.	1.1	641
851	Improved adsorption energetics within density-functional theory using revised Perdew-Burke-Ernzerhof functionals. <i>Physical Review B</i> , 1999, 59, 7413-7421.	1.1	6,206
852	Frenkel-Kontorova Model of Vacancy-Line Interactions on Ga/Si(112). <i>Physical Review Letters</i> , 1999, 83, 1818-1821.	2.9	50
853	Ab initio study of hydrogen adsorption on the ZnO (101̄,0) surface. <i>Surface Science</i> , 1999, 422, 1-7.	0.8	43
854	Nitrogen adsorption on Fe(111), (100), and (110) surfaces. <i>Surface Science</i> , 1999, 422, 8-16.	0.8	97
855	First principles study on the geometry and stability of the Ge atom in initial Ge growth on the Si(001) surface. <i>Surface Science</i> , 1999, 423, 32-42.	0.8	15
856	Structural, electronic and magnetic properties of nickel surfaces. <i>Surface Science</i> , 1999, 423, 1-11.	0.8	116
857	The structure of Si(112):Ga-(N̄-1) reconstructions. <i>Surface Science</i> , 1999, 423, L265-L270.	0.8	34
858	Reaction channels for the catalytic oxidation of CO on Pt(111). <i>Surface Science</i> , 1999, 433-435, 58-62.	0.8	47
859	Dependence of stretching frequency on surface coverage and adsorbate-adsorbate interactions: a density-functional theory approach of CO on Pd (111). <i>Surface Science</i> , 1999, 425, 68-80.	0.8	180
860	Adsorption of transition metal atoms on oxygen vacancies and regular sites of the MgO(001) surface. <i>Surface Science</i> , 1999, 426, 123-139.	0.8	165
861	Electric field dependent structural and vibrational properties of the Si(100)-H(2̄-1) surface and its implications for STM induced hydrogen desorption. <i>Surface Science</i> , 1999, 429, 327-337.	0.8	22
862	Oxygen adsorption on Pt(110)-(1̄-2): new high-coverage structures. <i>Surface Science</i> , 1999, 430, L533-L539.	0.8	37
863	Hydrogen, sulphur and chlorine coadsorption on Pd(111): a theoretical study of poisoning and promotion. <i>Surface Science</i> , 1999, 430, 176-191.	0.8	70
864	Ethylene, sulphur, and chlorine coadsorption on Pd(111): a theoretical study of poisoning and promotion. <i>Surface Science</i> , 1999, 430, 192-198.	0.8	24
865	Molecular precursors in the dissociative adsorption of O <sub>2</sub> on Ni(111). <i>Surface Science</i> , 1999, 433-435, 756-760.	0.8	40
866	Density-functional theory study of the catalytic oxidation of CO over transition metal surfaces. <i>Surface Science</i> , 1999, 433-435, 119-126.	0.8	58
867	Theoretical study of the hydrogen relay dissociation of water molecules on Si(001) surfaces. <i>Surface Science</i> , 1999, 438, 9-17.	0.8	22

#	ARTICLE	IF	CITATIONS
868	Methyl chemisorption on Ni(111) and C H M multicentre bonding: a density functional theory study. <i>Surface Science</i> , 1999, 437, 362-376.	0.8	84
869	Density functional study of the structural and electronic properties of RuS <sub>2</sub> (111). <i>Surface Science</i> , 1999, 439, 163-172.	0.8	16
870	Predicting lateral surface interactions through density functional theory: application to oxygen on Rh(100). <i>Surface Science</i> , 1999, 441, 410-424.	0.8	58
871	Primary slip system of $\hat{\mu}$ -iron and anisotropy of the Earth's inner core. <i>Physics of the Earth and Planetary Interiors</i> , 1999, 110, 147-156.	0.7	40
872	(100) Silicon oxidation: first principle investigation of basic mechanisms. <i>Journal of Non-Crystalline Solids</i> , 1999, 245, 150-153.	1.5	9
873	Calculation of the <sup>13</sup> C NMR chemical shift of ether linkages in lignin derived geopolymers. <i>Geochimica Et Cosmochimica Acta</i> , 1999, 63, 193-205.	1.6	22
874	A density functional study of lithium bulk and surfaces. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 5007-5019.	0.7	74
875	The electronic structure and chemical bonding of hypermetallic Al <sub>5</sub> C by ab initio calculations and anion photoelectron spectroscopy. <i>Journal of Chemical Physics</i> , 1999, 111, 4993-4998.	1.2	45
876	DENSITYFUNCTIONALTHEORY OFBIOLOGICALLYRELEVANTMETALCENTERS. <i>Annual Review of Physical Chemistry</i> , 1999, 50, 221-249.	4.8	250
877	AB Initio Liquids: Simulating Liquids Based on First Principles. , 1999, , 439-457.		2
878	Ab Initio Methods. <i>Springer Series in Solid-state Sciences</i> , 1999, , 7-138.	0.3	5
879	Magnetism and magneto-structural effects in transition-metal sulphides. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 8197-8222.	0.7	60
880	Polymorphism in silica studied in the local density and generalized-gradient approximations. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 3833-3874.	0.7	174
881	A first-principles potential energy surface for Eley-Rideal reaction dynamics of H atoms on Cu(111). <i>Journal of Chemical Physics</i> , 1999, 110, 2240-2249.	1.2	68
882	Eley-Rideal and hot-atom reactions of H(D) atoms with D(H)-covered Cu(111) surfaces; quasiclassical studies. <i>Journal of Chemical Physics</i> , 1999, 110, 11038-11046.	1.2	80
883	Role of the Zeolitic Environment in Catalytic Activation of Methanol. <i>Journal of the American Chemical Society</i> , 1999, 121, 3292-3302.	6.6	116
884	Competition between the ionic and covalent character in the series of boron compounds BP, BAs, and BSb. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 5781-5796.	0.7	53
885	In-Plane Aromaticity in 1,3-Dipolar Cycloadditions. Solvent Effects, Selectivity, and Nucleus-Independent Chemical Shifts. <i>Journal of the American Chemical Society</i> , 1999, 121, 6737-6746.	6.6	222



#	ARTICLE	IF	CITATIONS
886	First-principles theory of ultrathin magnetic films. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 9347-9363.	0.7	28
887	Tetracoordinated Planar Carbon in the Al <sub>4</sub> C-Anion. A Combined Photoelectron Spectroscopy and ab Initio Study. <i>Journal of the American Chemical Society</i> , 1999, 121, 6033-6038.	6.6	297
888	Theoretical Studies of Low-Spin Six-Coordinate Iron(III) Porphyrins Relevant to Cytochromes b: Variable Electronic Configurations, Ligand Noninnocence, and Macrocyclic Ruffling. <i>Journal of Physical Chemistry B</i> , 1999, 103, 1363-1367.	1.2	60
889	Adhesion energy of Cu atoms on the MgO(001) surface. <i>Journal of Chemical Physics</i> , 1999, 110, 4873-4879.	1.2	140
890	Role of surface vacancies and water products in metal nucleation: Pt/MgO(100). <i>Surface Science</i> , 1999, 437, L741-L747.	0.8	95
891	Ground and Excited State Properties and Vibronic Coupling Analysis of the Creutz-Taube Ion, [(NH <sub>3</sub> ) <sub>5</sub> Ru-pyrazine-Ru(NH <sub>3</sub> ) <sub>5</sub> ] <sup>5+</sup> , Using DFT. <i>Journal of the American Chemical Society</i> , 1999, 121, 11418-11424.	6.6	82
892	Quantum Dynamics of H <sub>2</sub> <sup>+</sup> Surface Scattering: H <sub>2</sub> <sup>+</sup> LiF(001) and H <sub>2</sub> <sup>+</sup> Cu(100). <i>Journal of Physical Chemistry B</i> , 1999, 103, 9397-9414.	1.2	3
893	Dimer Cations of Cyanoacetylene: Theoretical Isomers and Their Laboratory Production in the Absence and Presence of C <sub>6</sub> O <sub>2</sub> <sup>+</sup> . Implications for Interstellar/Circumstellar Chemistry. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7528-7534.	1.1	21
894	Mapped Interpolation Scheme for Single-Point Energy Corrections in Reaction Rate Calculations and a Critical Evaluation of Dual-Level Reaction Path Dynamics Methods. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1140-1149.	1.1	254
895	Half-metallic ferrimagnetism in Mn <sub>2</sub> VAl. <i>Physical Review B</i> , 1999, 60, 13006-13010.	1.1	215
896	A first principles and mean field investigation of the conformational properties of 5CB. <i>Molecular Physics</i> , 1999, 97, 541-550.	0.8	15
897	Fast Electron Transfer Across Semiconductor-Molecule Interfaces: GaAs/Co(Cp) <sub>2</sub> /O. <i>Journal of Physical Chemistry B</i> , 1999, 103, 2122-2141.	1.2	48
898	ĭ- and ĭf-Coordinated Al in AlC <sub>2</sub> - and AlCSi-. A Combined Photoelectron Spectroscopy and ab Initio Study. <i>Journal of the American Chemical Society</i> , 1999, 121, 10193-10197.	6.6	36
899	Catalysis from first principles. <i>Studies in Surface Science and Catalysis</i> , 1999, , 3-10.	1.5	12
900	Scaling Factors for the Prediction of the Frequencies of the Ring Modes in Benzene Derivatives. <i>Journal of Physical Chemistry A</i> , 1999, 103, 11366-11377.	1.1	36
901	Reaction of Laser-Ablated Uranium Atoms with CO: Infrared Spectra of the CUO, CUO <sup>-</sup> , OUCCO, (ĭ-2-C <sub>2</sub> )UO <sub>2</sub> , and U(CO) <sub>x</sub> (x = 1-6) Molecules in Solid Neon. <i>Journal of the American Chemical Society</i> , 1999, 121, 9712-9721.	6.6	125
902	A Major, pH-Induced Stereochemical Switch of Pairs of trans-Oriented Ligands in Complexes of trans-a <sub>2</sub> PtII (a = NH <sub>3</sub> , CH <sub>3</sub> NH <sub>2</sub> ). <i>Inorganic Chemistry</i> , 1999, 38, 3160-3166.	1.9	38
903	Density functional predictions for magnetizabilities and nuclear shielding constants. <i>Molecular Physics</i> , 1999, 97, 757-768.	0.8	58

#	ARTICLE	IF	CITATIONS
904	Bis(arene) Actinide Sandwich Complexes, $(\eta^6\text{-C}_6\text{H}_3\text{R}_3)_2\text{An}$ : Linear or Bent?. Journal of the American Chemical Society, 1999, 121, 10243-10244.	6.6	22
905	Prediction of $^{195}\text{Pt}$ NMR Chemical Shifts by Density Functional Theory Computations: The Importance of Magnetic Coupling and Relativistic Effects in Explaining Trends. Journal of Physical Chemistry A, 1999, 103, 7535-7543.	1.1	75
906	Density Functional Study on Activation and Ion-Pair Formation in Group IV Metallocene and Related Olefin Polymerization Catalysts. Organometallics, 1999, 18, 4624-4636.	1.1	119
907	Density Functional (DFT) Study of the Anti-Syn Isomerization of the Butenyl Group in Cationic and Neutral (Butenyl)(butadiene)(monoligand)nickel(II) Complexes. Organometallics, 1999, 18, 3045-3060.	1.1	48
908	Phase diagram of MgO from density-functional theory and molecular-dynamics simulations. Physical Review B, 1999, 60, 15084-15093.	1.1	77
909	Ab Initio Calculations of $^1\text{H}$ and $^{13}\text{C}$ Chemical Shifts in Anhydrodeoxythymidines. Journal of Physical Chemistry A, 1999, 103, 4089-4093.	1.1	13
910	Hydrogen Bonding in Water Clusters: Pair and Many-Body Interactions from Symmetry-Adapted Perturbation Theory. Journal of Physical Chemistry A, 1999, 103, 6811-6819.	1.1	92
911	Intermediate Range Order and Bonding Character in Disordered Network-Forming Systems. Journal of the American Chemical Society, 1999, 121, 2943-2944.	6.6	59
912	Lithium Intercalation into Vanadium Pentoxide: A Theoretical Study. Chemistry of Materials, 1999, 11, 1990-1998.	3.2	122
913	$\text{Fe}(\text{N}_2)_n$ ( $n = 1-5$ ): Structure, Bonding, and Vibrations from Density Functional Theory. Inorganic Chemistry, 1999, 38, 3895-3903.	1.9	29
914	Theoretical Density Functional Analysis of Maleic Anhydride Chemisorption on Pd(111), Re(0001), and Bimetallic PdML/Re(0001) and PdML/Mo(110) Pseudomorphic Overlayers. Journal of Physical Chemistry B, 1999, 103, 8973-8983.	1.2	28
915	Role of Steps in $\text{N}_2$ Activation on Ru(0001). Physical Review Letters, 1999, 83, 1814-1817.	2.9	706
916	Full-potential KKR calculations for metals and semiconductors. Physical Review B, 1999, 60, 5202-5210.	1.1	112
917	Computational Materials Science: The Era of Applied Quantum Mechanics. Physics Today, 1999, 52, 30-35.	0.3	45
918	Dimer Reconstruction at Metal-Silicide/Silicon Interfaces: A First-Principles Study. Materials Research Society Symposia Proceedings, 1999, 564, 103.	0.1	0
919	First-Principles Calculations of Positron Annihilation in Solids. Materials Research Society Symposia Proceedings, 1999, 579, 249.	0.1	3
920	Dynamics of Silicon Oxidation. Materials Research Society Symposia Proceedings, 1999, 592, 30.	0.1	4
921	Excitation Spectra in the Time-Dependent Density-Functional Theory with Gradient Correction. Materials Research Society Symposia Proceedings, 1999, 579, 75.	0.1	0

#	ARTICLE	IF	CITATIONS
922	First-Principles Studies on the Structural and Magnetic Properties of 3d/(Cu, Ag, Au) Multilayers. Materials Transactions, JIM, 1999, 40, 1228-1236.	0.9	5
923	Ab initio-Monte Carlo Studies on the Finite-Temperature Properties of FeAu Superlattice. Materials Transactions, JIM, 2000, 41, 601-604.	0.9	3
924	Analysis of chemical bond in metal clusters: I. Alkali metal and alkaline earth metals. Advances in Quantum Chemistry, 2000, 37, 237-254.	0.4	3
925	Ab-initio study of the vacancy formation in Keggin and Linqvist heteropolyanion. Studies in Surface Science and Catalysis, 2000, 130, 1199-1204.	1.5	4
926	A Comparative Study of the Influence of the Local Density Approximation and the Generalized Gradient Approximation on the Calculated Properties of the III-Nitride (110) Surfaces. Materials Research Society Symposia Proceedings, 2000, 639, 11461.	0.1	0
927	Calculation Of Positron Characteristics In Silicon Carbide. Materials Research Society Symposia Proceedings, 2000, 640, 1.	0.1	1
928	Grain boundary structure in B2 Fe-Al ordered alloys: an atomic-scale simulation. Materials Research Society Symposia Proceedings, 2000, 652, 1.	0.1	0
929	Atomic Scale Simulation of the Effect of Hydrogen on Dislocations in Zr. Materials Research Society Symposia Proceedings, 2000, 653, 1.	0.1	0
930	Variation of parameters in Becke-3 hybrid exchange-correlation functional. Journal of Computational Chemistry, 2000, 21, 227-238.	1.5	39
931	Density functional study of small molybdenum clusters. International Journal of Quantum Chemistry, 2000, 76, 105-112.	1.0	32
932	Ensuring proper short-range and asymptotic behavior of the exchange-correlation Kohn-Sham potential by modeling with a statistical average of different orbital model potentials. International Journal of Quantum Chemistry, 2000, 76, 407-419.	1.0	106
933	Density functional study for stacking energy of cytosine dimer: Ab initio MO calculations based on Slater-type basis set. International Journal of Quantum Chemistry, 2000, 76, 677-685.	1.0	14
934	Scaling factors for the prediction of vibrational spectra. I. Benzene molecule. International Journal of Quantum Chemistry, 2000, 77, 661-684.	1.0	405
935	Recent developments in ab initio thermodynamics. , 2000, 77, 871-879.		26
936	CRYSTAL and EMBED, two computational tools for the ab initio study of electronic properties of crystals. International Journal of Quantum Chemistry, 2000, 77, 1032-1048.	1.0	46
937	Density Functional Study of Possible Intermediates in the Mechanism of Olefin Cyclopropanation Catalyzed by Metal Carboxylates. European Journal of Inorganic Chemistry, 2000, 2000, 1073-1078.	1.0	13
938	Density functional study of dimers of dimethylnitramine. International Journal of Quantum Chemistry, 2000, 80, 184-192.	1.0	62
939	Hydrogen Bonding Effects on the 15N and 1H Shielding Tensors in Nucleic Acid Base Pairs. Journal of Magnetic Resonance, 2000, 145, 142-146.	1.2	41

#	ARTICLE	IF	CITATIONS
940	Surface chemistry in three dimensions: CO dissociation between two surfaces. <i>Chemical Physics Letters</i> , 2000, 322, 307-311.	1.2	2
941	Application of the scaling properties of the correlation energy functional to local and gradient-dependent forms. <i>Chemical Physics Letters</i> , 2000, 322, 371-376.	1.2	0
942	A density functional theory study of the anthracene anion. <i>Chemical Physics Letters</i> , 2000, 330, 180-187.	1.2	30
943	Artificial symmetry breaking in radicals is avoided by the use of the Ensemble-Referenced Kohn-Sham (REKS) method. <i>Chemical Physics Letters</i> , 2000, 332, 409-419.	1.2	24
944	Assessment of exchange correlation functionals. <i>Chemical Physics Letters</i> , 2000, 316, 160-166.	1.2	104
945	Chlorine adsorption on the Cu(111) surface. <i>Chemical Physics Letters</i> , 2000, 317, 282-289.	1.2	120
946	Pentaprismane and hypostrophene from first-principles, with plane waves. <i>Chemical Physics Letters</i> , 2000, 317, 381-387.	1.2	23
947	The adsorption of aromatics on sp-metals: benzene on Al(111). <i>Chemical Physics Letters</i> , 2000, 318, 43-48.	1.2	65
948	Remarkable low symmetry hydrogen bonding network in the structure of $\text{ReCl}_2(\text{NCMe})(\text{NO})(\text{PMe}_3)_2$ . <i>Inorganica Chimica Acta</i> , 2000, 306, 153-159.	1.2	24
949	Regional density functional theory for crystal growth in GaN. <i>Journal of Crystal Growth</i> , 2000, 221, 765-771.	0.7	10
950	Correlated ab initio molecular orbital (MP3, MP4) and density functional (PW91, MPW91) studies on the conformations of 1,2-diphenylethane. <i>Journal of Molecular Structure</i> , 2000, 554, 183-190.	1.8	9
951	FP-LAPW and pseudopotential calculations of the structural phase transformations of GaN under high-pressure. <i>Solid State Communications</i> , 2000, 116, 389-393.	0.9	27
952	Tip-surface interactions in noncontact atomic force microscopy on reactive surfaces. <i>Progress in Surface Science</i> , 2000, 64, 179-191.	3.8	15
953	Comparison of elastic constants and electronic structures in the series of the alkaline-earth selenides: a quantum chemical approach. <i>Journal of Physics and Chemistry of Solids</i> , 2000, 61, 1707-1715.	1.9	45
954	Ab initio calculations of elastic properties and electronic structure of calcium selenide. <i>Journal of Physics and Chemistry of Solids</i> , 2000, 61, 603-608.	1.9	4
955	The roles of charged and neutral oxidising species in silicon oxidation from ab initio calculations. <i>Microelectronics Reliability</i> , 2000, 40, 567-570.	0.9	17
956	Theoretical study of penetration reaction of fluorine atoms and ions into hydrogen-terminated Si(111) thin film. <i>Thin Solid Films</i> , 2000, 374, 143-149.	0.8	5
957	Ab initio molecular dynamics simulation of methanol interacting with acidic zeolites of different framework structure. <i>Microporous and Mesoporous Materials</i> , 2000, 35-36, 379-385.	2.2	77

#	ARTICLE	IF	CITATIONS
958	Atomic-scale computational materials science. <i>Acta Materialia</i> , 2000, 48, 71-92.	3.8	163
959	Electronic structure of SnO <sub>2</sub> (110) surface. <i>Materials Science in Semiconductor Processing</i> , 2000, 3, 103-107.	1.9	53
960	Molecular aspects of the H <sub>2</sub> activation on MoS <sub>2</sub> based catalysts – the role of dynamic surface arrangements. <i>Journal of Molecular Catalysis A</i> , 2000, 163, 117-122.	4.8	59
961	Stereoselective synthesis of cyclobutyl $\pm$ -aminocyclopropyl carboxylic acid derivatives. <i>Tetrahedron: Asymmetry</i> , 2000, 11, 4903-4914.	1.8	15
962	Static electronic properties on various surface orientations of Al crystal undergoing electromigration. <i>Applied Surface Science</i> , 2000, 159-160, 167-173.	3.1	22
963	Theory of hydrogen extraction from hydrogenated diamond surfaces. <i>Applied Surface Science</i> , 2000, 159-160, 599-602.	3.1	7
964	First-principle analysis of the dissociative adsorption of formic acid on rutile TiO <sub>2</sub> (110). <i>Applied Surface Science</i> , 2000, 166, 370-375.	3.1	47
965	Structure and dynamics from combined neutron scattering and first-principles studies. <i>Chemical Physics</i> , 2000, 261, 205-216.	0.9	52
966	Localisation of adsorbate-induced demagnetisation: CO chemisorbed on Ni{110}. <i>Chemical Physics Letters</i> , 2000, 327, 125-130.	1.2	102
967	Theoretical evidence of bound metastable states in the doubly ionized nickel dimer Ni <sup>2+</sup> . <i>Chemical Physics Letters</i> , 2000, 332, 481-486.	1.2	8
968	Adsorbate/substrate bonding in Co{100}/K-c(2 $\times$ 2) elucidated through first-principles theory. <i>Chemical Physics Letters</i> , 2000, 317, 372-380.	1.2	21
969	The basis set convergence of the density functional energy for H <sub>2</sub> . <i>Chemical Physics Letters</i> , 2000, 317, 400-403.	1.2	18
970	First-principles structural determination of Si(001)-C <sub>2</sub> H <sub>2</sub> chemisorbed surface. <i>Applied Surface Science</i> , 2000, 159-160, 19-24.	3.1	6
971	Formation energy of threefold coordinated oxygen in SiO <sub>2</sub> systems. <i>Applied Surface Science</i> , 2000, 166, 451-454.	3.1	11
972	The interaction of ammonia with small iron clusters: infrared spectra and density functional calculations of Fe <sub>n</sub> (NH <sub>3</sub> ) <sub>m</sub> and Fe <sub>n</sub> (ND <sub>3</sub> ) <sub>m</sub> complexes. <i>Chemical Physics</i> , 2000, 262, 41-51.	0.9	18
973	Electronic structure of NaNO <sub>2</sub> in the ferroelectric phase and paraelectric phase. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2000, 269, 252-256.	0.9	6
974	Flat band – steep band scenario and superconductivity – the case of calcium. <i>Solid State Sciences</i> , 2000, 2, 31-38.	1.5	36
975	Electronic structure of La <sub>0.65</sub> Pb <sub>0.35</sub> MnO <sub>3</sub> perovskite studied by X-ray photoemission spectroscopy. <i>Journal of Magnetism and Magnetic Materials</i> , 2000, 217, 44-48.	1.0	10

#	ARTICLE	IF	CITATIONS
976	Nonlinear magnetoelastic coupling coefficients in Fe from an ab initio calculation. Journal of Magnetism and Magnetic Materials, 2000, 220, 8-12.	1.0	24
977	Magnetoelastic effects in ultrathin epitaxial Ni films: an ab initio study. Journal of Magnetism and Magnetic Materials, 2000, 222, 245-250.	1.0	12
978	X-ray photoemission spectra of La <sub>0.7</sub> Sr <sub>0.3</sub> MnO <sub>3</sub> perovskite. Journal of Magnetism and Magnetic Materials, 2000, 212, 107-111.	1.0	18
979	Ab initio calculation of structural and magnetic properties for Fe mono- and bilayers on Mo(110). Journal of Magnetism and Magnetic Materials, 2000, 213, 12-18.	1.0	24
980	Atomistic modelling of radiation effects: Towards dynamics of exciton relaxation. Nuclear Instruments & Methods in Physics Research B, 2000, 166-167, 1-12.	0.6	18
981	Molecular modeling of inhibition of hydroxyapatite by phosphocitrate. Computational and Theoretical Chemistry, 2000, 529, 73-82.	1.5	37
982	An ab initio molecular orbital theory and density functional theory study of the conformational free energies of methyltetrahydro-2H-thiopyrans. Computational and Theoretical Chemistry, 2000, 529, 225-239.	1.5	17
983	Density functional vibrational analysis of N-methylthiourea and three deuterated analogues. Computational and Theoretical Chemistry, 2000, 499, 175-183.	1.5	3
984	The role of the kinetic energy density in approximations to the exchange energy. Computational and Theoretical Chemistry, 2000, 501-502, 59-64.	1.5	28
985	New perspectives of the weighted spin-density approximation: gradient corrections and the valence-only approach. Computational and Theoretical Chemistry, 2000, 501-502, 153-166.	1.5	1
986	Density-functional study of Pt 13 and Pt 55 cuboctahedral clusters. Computational and Theoretical Chemistry, 2000, 501-502, 251-259.	1.5	48
987	Transverse relaxation optimized triple-resonance NMR experiments for nucleic acids. Journal of Biomolecular NMR, 2000, 16, 291-302.	1.6	87
988	Nuclear quadrupole interaction in metals: Experiments, calculations, models. , 2000, 129, 493-509.		7
989	Making gold less noble. Catalysis Letters, 2000, 64, 101-106.	1.4	641
990	Edge termination of MoS <sub>2</sub> and CoMoS catalyst particles. Catalysis Letters, 2000, 64, 95-99.	1.4	130
991	Ab Initio Study of the H <sub>2</sub> â€“H <sub>2</sub> S/MoS <sub>2</sub> Gasâ€“Solid Interface: The Nature of the Catalytically Active Sites. Journal of Catalysis, 2000, 189, 129-146.	3.1	350
992	Theoretical Studies of Stability and Reactivity of CH <sub>x</sub> Species on Ni(111). Journal of Catalysis, 2000, 189, 16-30.	3.1	187
993	Electronic Factors Governing Ethylene Hydrogenation and Dehydrogenation Activity of Pseudomorphic PdML/Re(0001), PdML/Ru(0001), Pd(111), and PdML/Au(111) Surfaces. Journal of Catalysis, 2000, 191, 301-317.	3.1	364

#	ARTICLE	IF	CITATIONS
994	Structure, Energetics, and Electronic Properties of the Surface of a Promoted MoS <sub>2</sub> Catalyst: An ab Initio Local Density Functional Study. <i>Journal of Catalysis</i> , 2000, 190, 128-143.	3.1	321
995	Title is missing!. <i>Topics in Catalysis</i> , 2000, 11/12, 271-278.	1.3	21
996	Vacancies in Metals: From First-Principles Calculations to Experimental Data. <i>Physical Review Letters</i> , 2000, 85, 3862-3865.	2.9	226
997	Growth and structure of ultrathin vanadium oxide layers on Pd(111). <i>Physical Review B</i> , 2000, 61, 13945-13954.	1.1	124
998	Electronic and magnetic structure of the (001) surfaces of V, Cr, and V/Cr. <i>Physical Review B</i> , 2000, 62, R11937-R11940.	1.1	58
999	Structure and dynamics of liquid iron under Earth's core conditions. <i>Physical Review B</i> , 2000, 61, 132-142.	1.1	245
1000	Reaction of NO <sub>2</sub> with Zn and ZnO: Photoemission, XANES, and Density Functional Studies on the Formation of NO <sub>3</sub> . <i>Journal of Physical Chemistry B</i> , 2000, 104, 319-328.	1.2	371
1001	Electronic structure of the Cu <sub>2</sub> MnAl Heusler alloy. <i>Journal of Physics Condensed Matter</i> , 2000, 12, 2997-3012.	0.7	40
1002	Geometric and Electronic Structures of V and Cr Clusters.. <i>Hyomen Kagaku</i> , 2000, 21, 462-467.	0.0	6
1003	Investigation of Hydrogen Chemisorption on GaAs (111)A Ga Surface by In Situ Monitoring and Ab Initio Calculation. <i>Japanese Journal of Applied Physics</i> , 2000, 39, 6174-6179.	0.8	1
1004	Magnetic moment and atomic volume in supersaturated Fe-Cu solid solutions: Ab initio calculations compared with experiments. <i>Journal of Materials Research</i> , 2000, 15, 653-658.	1.2	11
1005	Defect structure in homoepitaxial non-stoichiometric strontium titanate thin films. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , 2000, 80, 621-637.	0.8	114
1006	Breakdown of intermediate-range order in liquid GeSe <sub>2</sub> at high temperatures. <i>Journal of Physics Condensed Matter</i> , 2000, 12, L697-L704.	0.7	29
1007	The relationship between interlayer spacing and magnetic ordering in gadolinium. <i>Journal of Physics Condensed Matter</i> , 2000, 12, 10441-10456.	0.7	5
1008	A high-pressure structural study of propionic acid and the application of CCD detectors in high-pressure single-crystal x-ray diffraction. <i>Journal of Physics Condensed Matter</i> , 2000, 12, L613-L618.	0.7	17
1009	Molecular Adsorption on Ultrafine Precious Metal Particles Studied by Density Functional Calculation. <i>Japanese Journal of Applied Physics</i> , 2000, 39, 4261-4265.	0.8	1
1010	Rubidium at high pressure and temperature. <i>Journal of Physics Condensed Matter</i> , 2000, 12, 921-931.	0.7	9
1011	Title is missing!. <i>Journal of Physics Condensed Matter</i> , 2000, 12, 1239-1252.	0.7	68



#	ARTICLE	IF	CITATIONS
1012	A generalized Frenkel-Kontorova model of the Ga/Si(112) dimerized overlayer system with vacancies. Chinese Physics B, 2000, 9, 611-614.	1.3	1
1013	Overlayers, interlayers, and surface alloys of Mn on the Cu(111) surface. Physical Review B, 2000, 62, 4726-4732.	1.1	33
1014	First-principles investigation of the quantum-well system Na on Cu(111). Physical Review B, 2000, 61, 13973-13982.	1.1	87
1015	Calculated polarizabilities of small Si clusters. Physical Review A, 2000, 61, .	1.0	47
1016	Host-guest interactions in an organic crystal: 1,2-hydroquinone clathrate with Ne and HF guests. Journal of Chemical Physics, 2000, 112, 835-840.	1.2	15
1017	Adsorbate-induced vacancy formation and substrate relaxation on Cr(100). Physical Review B, 2000, 62, 5163-5167.	1.1	25
1018	Work-function anisotropy in noble metals: Contributions from d states and effects of the surface atomic structure. Physical Review B, 2000, 61, 8489-8495.	1.1	57
1019	Pairing, $\pi$ -bonding, and the role of nonlocality in a dense lithium monolayer. Physical Review B, 2000, 62, 8494-8499.	1.1	34
1020	Structure of liquid GeSe: A first principle study. Journal of Chemical Physics, 2000, 113, 5425.	1.2	24
1021	Electronic structure and magnetic coupling in sodium electro sodalite: All-electron density functional calculations. Journal of Chemical Physics, 2000, 113, 5466.	1.2	11
1022	Pressure-induced interlinking of carbon nanotubes. Physical Review B, 2000, 62, 12648-12651.	1.1	116
1023	Local chemistry of Al and P impurities in silica. Physical Review B, 2000, 61, 12590-12593.	1.1	34
1024	A density functional theory study of CH <sub>2</sub> and H adsorption on Ni(111). Journal of Chemical Physics, 2000, 112, 6006-6014.	1.2	52
1025	First principles analysis of hydrogen chemisorption on Pd-Re alloyed overlayers and alloyed surfaces. Journal of Chemical Physics, 2000, 112, 5435-5439.	1.2	72
1026	Molecular electronic structure using auxiliary field Monte Carlo, plane-waves, and pseudopotentials. Journal of Chemical Physics, 2000, 112, 1679-1684.	1.2	19
1027	Atom-by-atom and concerted hopping of adatom pairs on an open metal surface. Physical Review B, 2000, 61, R2456-R2459.	1.1	12
1028	Interactions of atomic hydrogen with Cu(111), Pt(111), and Pd(111). Journal of Applied Physics, 2000, 88, 6897-6901.	1.1	83
1029	First-principles formation energies of monovacancies in bcc transition metals. Physical Review B, 2000, 61, 2579-2586.	1.1	91

#	ARTICLE	IF	CITATIONS
1030	Complex reconstruction of $\text{Fe}^3$ -iron multilayers on Cu(100): Ab initio local-spin-density investigations. Physical Review B, 2000, 61, 16129-16136.	1.1	33
1031	Dimensional crossover of the exchange-correlation density functional. Physical Review B, 2000, 62, 2321-2329.	1.1	21
1032	How Carbon Monoxide Adsorbs in Different Sites. Physical Review Letters, 2000, 85, 3309-3312.	2.9	157
1033	First-principles investigation of the stability of 3d monolayer/Fe(001) against bilayer formation. Journal of Applied Physics, 2000, 87, 5935-5937.	1.1	10
1034	Structure and energetics of $\text{Si}_n\text{Ni}_m$ clusters: Growth pathways in a heterogeneous cluster system. Journal of Chemical Physics, 2000, 112, 1295-1305.	1.2	33
1035	Positron energy levels in semiconductors. Physical Review B, 2000, 61, 15848-15853.	1.1	24
1036	Structure and magnetism of $\text{Fe}^3$ -Fe overlayers on face-centered-cubic Co(001) substrates. Physical Review B, 2000, 62, 9575-9585.	1.1	14
1037	Structure, elastic moduli, and thermodynamics of sodium and potassium at ultrahigh pressures. Physical Review B, 2000, 61, 14420-14424.	1.1	41
1038	Dissociation and sticking of $\text{H}_2$ on the Ni(111), (100), and (110) substrate. Physical Review B, 2000, 62, 8295-8305.	1.1	191
1039	Exchange energy in the local Airy gas approximation. Physical Review B, 2000, 62, 10046-10050.	1.1	98
1040	Theoretical and Computational Study of High-Pressure Structures in Barium. Physical Review Letters, 2000, 84, 5580-5583.	2.9	45
1041	Theory of Single Molecule Vibrational Spectroscopy and Microscopy. Physical Review Letters, 2000, 85, 2997-3000.	2.9	230
1042	Nature of Metal-Ceramic Adhesion: Computational Experiments with Co on TiC. Physical Review Letters, 2000, 85, 1898-1901.	2.9	77
1043	Image potential and the exchange-correlation weighted density approximation functional. Physical Review B, 2000, 62, 16063-16068.	1.1	19
1044	Interface energy and electron structure for Fe/VN. Physical Review B, 2000, 61, 2221-2229.	1.1	77
1045	Dielectric response of oxides in the weighted density approximation. Physical Review B, 2000, 62, 12724-12729.	1.1	79
1046	The electronic structure and chemical bonding of aluminum acetylide: $\text{Al}_2\text{C}_2$ and $\text{Al}_2\text{C}_2^{\text{H}}$ : An experimental and theoretical investigation. Journal of Chemical Physics, 2000, 113, 2671-2679.	1.2	34
1047	Phonon-induced decay of a quantum-well hole: One monolayer Na on Cu(111). Physical Review B, 2000, 61, 2343-2348.	1.1	40

#	ARTICLE	IF	CITATIONS
1048	Simplified embedding schemes for the quantum-chemical description of neutral and charged point defects in SiO <sub>2</sub> and related dielectrics. <i>Journal of Chemical Physics</i> , 2000, 113, 10744-10752.	1.2	27
1049	Quadrupole moments of the halogen nuclei. <i>Physical Review B</i> , 2000, 61, 13588-13592.	1.1	36
1050	Unusual bridged site for adsorbed oxygen adatoms: Theory and experiment for Ir{100}-(1 $\times$ 2)-O. <i>Journal of Chemical Physics</i> , 2000, 112, 10460-10466.	1.2	65
1051	Electronic Fine Structure in the Electron-Hole Plasma in SrB <sub>6</sub> . <i>Physical Review Letters</i> , 2000, 84, 3903-3906.	2.9	42
1052	Atomic and Electronic Origins of a Type-C Defect on Si(001). <i>Physical Review Letters</i> , 2000, 84, 4128-4131.	2.9	8
1053	Nature, Strength, and Consequences of Indirect Adsorbate Interactions on Metals. <i>Physical Review Letters</i> , 2000, 85, 1910-1913.	2.9	175
1054	Efficient Total Energy Calculations from Self-Energy Models. <i>Physical Review Letters</i> , 2000, 85, 5611-5614.	2.9	32
1055	An extensive study of gradient approximations to the exchange-correlation and kinetic energy functionals. <i>Journal of Chemical Physics</i> , 2000, 112, 5639-5653.	1.2	43
1056	Vibrationally resolved photoelectron spectra of CuCN $\tilde{\nu}$ and AgCN $\tilde{\nu}$ and ab initio studies of the structure and bonding in CuCN. <i>Journal of Chemical Physics</i> , 2000, 112, 3627-3632.	1.2	42
1057	Hyperfine fields and local lattice relaxation at 4d and 5sp impurities in bcc iron. <i>Physical Review B</i> , 2000, 62, 461-467.	1.1	36
1058	A first principles study of CH <sub>3</sub> dehydrogenation on Ni(111). <i>Journal of Chemical Physics</i> , 2000, 112, 8120-8125.	1.2	53
1059	First-principles characterization of a heteroceramic interface: ZrO <sub>2</sub> (001) deposited on an $\tilde{\nu}$ -Al <sub>2</sub> O <sub>3</sub> (11 $\tilde{\nu}$ 02) substrate. <i>Physical Review B</i> , 2000, 62, 16968-16983.	1.1	61
1060	Ge(001) surface reconstruction studied using a first-principles calculation and a Monte Carlo simulation. <i>Physical Review B</i> , 2000, 61, 1965-1970.	1.1	57
1061	Ground-state interpretation of x-ray emission spectroscopy on adsorbates: CO adsorbed on Cu(100). <i>Physical Review B</i> , 2000, 61, 16229-16240.	1.1	72
1062	Surface topography of the Si(111)-7 $\tilde{\nu}$ 7 reconstruction. <i>Physical Review B</i> , 2000, 62, 15319-15322.	1.1	14
1063	Electronic and magnetic structures in metallic thin films. <i>Physical Review B</i> , 2000, 62, 500-507.	1.1	15
1064	Parameter-free exchange functional. <i>Physical Review B</i> , 2000, 62, 15527-15531.	1.1	33
1065	Comparison of the electronic structure and surface geometry of the metastable Cs+O overlayers on Ru(0001). <i>Physical Review B</i> , 2000, 61, 8455-8461.	1.1	6

#	ARTICLE	IF	CITATIONS
1066	Energetics of carbon and oxygen impurities and their interaction with vacancies in cubic boron nitride. <i>Physical Review B</i> , 2000, 62, 10135-10141.	1.1	33
1067	Dynamics of hydrogen dissociation at the sulfur-covered Pd(100) surface. <i>Physical Review B</i> , 2000, 61, 8425-8432.	1.1	32
1068	Highly reactive dissociative adsorption of hydrogen molecules on partially H-covered Si(001) surfaces: A density-functional study. <i>Physical Review B</i> , 2000, 62, 12932-12939.	1.1	50
1069	Magnetism of the V(001) surface in the generalized gradient approximation. <i>Physical Review B</i> , 2000, 61, R3780-R3783.	1.1	29
1070	Exchange interaction and magnetic phase transition in layered Fe/Au(001) superlattices. <i>Physical Review B</i> , 2000, 62, 3354-3360.	1.1	21
1071	H <sub>2</sub> adsorbed in a two-dimensional quantum rotor state on a stepped copper surface. <i>Physical Review B</i> , 2000, 61, 16921-16932.	1.1	33
1072	Structural, electronic, and magnetic properties of thin Mn/Cu(100) films. <i>Physical Review B</i> , 2000, 61, 11492-11505.	1.1	64
1073	Local-density approach and quasiparticle levels for generalized Hubbard Hamiltonians. <i>Physical Review B</i> , 2000, 62, 4309-4331.	1.1	57
1074	Theoretical investigation of water formation on Rh and Pt Surfaces. <i>Journal of Chemical Physics</i> , 2000, 112, 9986-9995.	1.2	61
1075	Quantum-size colloid metal systems. <i>Russian Chemical Reviews</i> , 2000, 69, 821-843.	2.5	77
1076	Perspective on inhomogeneous electron gas, 2000, , 259-262.		4
1077	Adsorption energetics and bonding from femtomole calorimetry and from first principles theory. <i>Advances in Catalysis</i> , 2000, 45, 207-259.	0.1	43
1078	Chapter 193 RBa <sub>2</sub> Cu <sub>3</sub> O <sub>7</sub> compounds: Electronic theory and physical properties. <i>Fundamental Theories of Physics</i> , 2000, 30, 453-489.	0.1	0
1079	Chemisorption and repulsive physisorption potentials from a unified treatment. <i>Journal of Physics Condensed Matter</i> , 2000, 12, 8369-8386.	0.7	2
1080	Equilibrium properties of delta-Pu: LDA+U calculations (LDAequiv local density approximation). <i>Journal of Physics Condensed Matter</i> , 2000, 12, 1723-1733.	0.7	95
1081	Fully unconstrained noncollinear magnetism within the projector augmented-wave method. <i>Physical Review B</i> , 2000, 62, 11556-11570.	1.1	707
1082	Molecular calculations of excitation energies and (hyper)polarizabilities with a statistical average of orbital model exchange-correlation potentials. <i>Journal of Chemical Physics</i> , 2000, 112, 1344-1352.	1.2	699
1083	A density functional study of CuO <sub>2</sub> molecules: structural stability, bonding and temperature effects. <i>Chemical Physics Letters</i> , 2000, 331, 290-298.	1.2	14

#	ARTICLE	IF	CITATIONS
1084	Dangling Bond Defects at Si <sup>+</sup> /SiO <sub>2</sub> Interfaces: Atomic Structure of the Pb Center. <i>Physical Review Letters</i> , 2000, 85, 2773-2776.	2.9	104
1085	The electronic and electrochemical properties of the ZrV <sub>2</sub> and Zr(V <sub>0.75</sub> Ni <sub>0.25</sub> ) <sub>2</sub> systems. <i>Journal of Alloys and Compounds</i> , 2000, 302, 299-303.	2.8	7
1086	The electronic and electrochemical properties of the LaNi <sub>5</sub> , LaNi <sub>4</sub> Al and LaNi <sub>3</sub> AlCo systems. <i>Journal of Alloys and Compounds</i> , 2000, 307, 290-296.	2.8	34
1087	Concentration fluctuations on intermediate range distances in liquid GeSe <sub>2</sub> : the critical role of ionicity. <i>Computational Materials Science</i> , 2000, 17, 115-121.	1.4	15
1088	Dissociation pathways of oxygen on copper (110) surface: a first principles study. <i>Computational Materials Science</i> , 2000, 17, 133-140.	1.4	23
1089	Electron spin localisation and correlation effects for point defects in semi-ionic solids. <i>Computational Materials Science</i> , 2000, 17, 312-318.	1.4	7
1090	Ab initio pseudopotential calculations on the effect of Mn doped on lattice parameters of L1 <sub>0</sub> TiAl. <i>Intermetallics</i> , 2000, 8, 637-641.	1.8	19
1091	Neutral and anionic CuO <sub>2</sub> : an ab initio study. <i>Computational Materials Science</i> , 2000, 17, 539-543.	1.4	13
1092	Electronic and structural properties of BaTe. <i>Computational Materials Science</i> , 2000, 17, 81-87.	1.4	28
1093	Ab initio free energy calculations on the polymorphs of iron at core conditions. <i>Physics of the Earth and Planetary Interiors</i> , 2000, 117, 123-137.	0.7	89
1094	Adsorption and energetics of isolated CO molecules on Pd(111). <i>Surface Science</i> , 2000, 453, 25-31.	0.8	68
1095	Density functional theory calculations of adsorption of water at calcium oxide and calcium fluoride surfaces. <i>Surface Science</i> , 2000, 452, 9-19.	0.8	83
1096	Density functional study of the structural and electronic properties of RuS <sub>2</sub> (111): II. Hydrogenated surfaces. <i>Surface Science</i> , 2000, 457, 285-293.	0.8	14
1097	Spectroscopic characterisation and chemical reactivity of silicon monoxide layers deposited on Cu(100). <i>Surface Science</i> , 2000, 458, 229-238.	0.8	14
1098	Pathways to dissociation of O <sub>2</sub> on Cu (110) surface: first principles simulations. <i>Surface Science</i> , 2000, 459, 104-114.	0.8	46
1099	A density functional theory study of CO and atomic oxygen chemisorption on Pt(111). <i>Surface Science</i> , 2000, 458, 1-14.	0.8	112
1100	First-principles study of the adsorption of atomic H on Ni (111), (100) and (110). <i>Surface Science</i> , 2000, 459, 287-302.	0.8	294
1101	Adsorption, diffusion, and dissociation of NO, N and O on flat and stepped Ru(0001). <i>Surface Science</i> , 2000, 459, 323-348.	0.8	140

#	ARTICLE	IF	CITATIONS
1102	Ab initio pseudopotential study of dehydrogenation of methanol on oxygen modified Ag(110) surface. Surface Science, 2000, 459, 213-222.	0.8	16
1103	Dissociative adsorption of formic acid and diffusion of formate on the TiO <sub>2</sub> (110) surface: the role of hydrogen. Surface Science, 2000, 461, 191-198.	0.8	82
1104	Ultrathin aluminum oxide films: Al-sublattice structure and the effect of substrate on ad-metal adhesion. Surface Science, 2000, 464, 108-116.	0.8	59
1105	Energetics and structure of stoichiometric SnO <sub>2</sub> surfaces studied by first-principles calculations. Surface Science, 2000, 463, 93-101.	0.8	269
1106	A density functional theory study of the surface relaxation and reactivity of Cu <sub>2</sub> O(100). Surface Science, 2000, 464, 223-232.	0.8	33
1107	The energetics and structure of oxygen vacancies on the SnO <sub>2</sub> (110) surface. Surface Science, 2000, 467, 35-48.	0.8	87
1108	Comprehensive characterization of the (2 $\sqrt{3}$ -2)-O and the CO-induced overlayers on Pd(111). Surface Science, 2000, 468, 176-186.	0.8	57
1109	Limits of perturbation theory: first principles simulations of scanning tunneling microscopy scans on Fe(100). Surface Science, 2000, 466, L795-L801.	0.8	29
1110	Scanning tunneling microscopy of binary alloys: first principles calculation of the current for PtX(100) surfaces.. Surface Science, 2000, 447, 51-61.	0.8	79
1111	Activated non-dissociative adsorption on a compound surface: CO on NiAl(110). Surface Science, 2000, 446, 187-192.	0.8	8
1112	Electron-stimulated bond rearrangements on the H/Si(100)-3 $\sqrt{3}$ -1 surface. Surface Science, 2000, 446, 211-218.	0.8	19
1113	Formic Acid Adsorption on Dry and Hydrated TiO <sub>2</sub> Anatase (101) Surfaces by DFT Calculations. Journal of Physical Chemistry B, 2000, 104, 1300-1306.	1.2	402
1114	Electronic and structural properties of germania polymorphs. Physical Review B, 2000, 62, 14703-14711.	1.1	47
1115	The Silabenzenes: Structure, Properties, and Aromaticity. Organometallics, 2000, 19, 1477-1487.	1.1	115
1116	Studies on the Behavior of Mixed-Metal Oxides and Desulfurization: Reaction of H <sub>2</sub> S and SO <sub>2</sub> with Cr <sub>2</sub> O <sub>3</sub> (0001), MgO(100), and Cr <sub>x</sub> Mg <sub>1-x</sub> O(100). Journal of the American Chemical Society, 2000, 122, 12362-12370.	6.6	75
1117	An ab initio study of hydrogen in forsterite and a possible mechanism for hydrolytic weakening. Journal of Geophysical Research, 2000, 105, 18977-18982.	3.3	87
1118	Structure and Energetics of SiO <sub>2</sub> Polymorphs by Quantum-Mechanical and Semiclassical Approaches. Journal of Physical Chemistry B, 2000, 104, 7259-7265.	1.2	40
1119	A computer simulation study of domain walls in NH <sub>4</sub> Cl. Journal of Physics Condensed Matter, 2000, 12, 2093-2101.	0.7	1

#	ARTICLE	IF	CITATIONS
1120	Electronic Structure and Bonding at the Al-terminated Al(111) $\sqrt{3}\times\sqrt{3}$ -Al <sub>2</sub> O <sub>3</sub> (0001) Interface: A First Principles Study. Materials Research Society Symposia Proceedings, 2000, 654, 421.	0.1	5
1121	First-Principles Molecular Dynamics Simulations of H <sub>2</sub> O on $\sqrt{3}\times\sqrt{3}$ -Al <sub>2</sub> O <sub>3</sub> (0001). Journal of Physical Chemistry B, 2000, 104, 5527-5540.	1.2	213
1122	Density Functional Theory Study of Redox Pairs. 1. Dinuclear Iron Complexes That Undergo Multielectron Redox Reactions Accompanied by a Reversible Structural Change. Journal of the American Chemical Society, 2000, 122, 9143-9154.	6.6	61
1123	Second-order optical response in semiconductors. Physical Review B, 2000, 61, 5337-5352.	1.1	545
1124	Transition-Metal Systems in Biochemistry Studied by High-Accuracy Quantum Chemical Methods. Chemical Reviews, 2000, 100, 421-438.	23.0	559
1126	Studies on the Behavior of Mixed-Metal Oxides: A Structural, Electronic, and Chemical Properties of $\sqrt{2}\times\sqrt{2}$ -FeMoO <sub>4</sub> . Journal of Physical Chemistry B, 2000, 104, 8145-8152.	1.2	49
1127	Tractable nonlocal correlation density functionals for flat surfaces and slabs. Physical Review B, 2000, 62, 6997-7006.	1.1	130
1128	Ammonia synthesis at low temperatures. Journal of Chemical Physics, 2000, 112, 5343-5347.	1.2	217
1129	Structural and Acidic Properties of Mordenite. An ab Initio Density-Functional Study. Journal of Physical Chemistry B, 2000, 104, 4593-4607.	1.2	158
1130	Electron correlation in chemical bonds. Journal of Chemical Physics, 2000, 112, 4014-4019.	1.2	29
1131	Implementation of the projector augmented-wave LDA+U method: Application to the electronic structure of NiO. Physical Review B, 2000, 62, 16392-16401.	1.1	494
1132	Insight into Microscopic Reaction Pathways in Heterogeneous Catalysis. Journal of the American Chemical Society, 2000, 122, 9866-9867.	6.6	146
1133	Theoretical Study of the MoS <sub>2</sub> (100) Surface: A Chemical Potential Analysis of Sulfur and Hydrogen Coverage. Journal of Physical Chemistry B, 2000, 104, 11220-11229.	1.2	172
1134	Hydrogen Bonding in DNA Base Pairs: A Reconciliation of Theory and Experiment. Journal of the American Chemical Society, 2000, 122, 4117-4128.	6.6	418
1135	Synthesis, Characterization, and Structural and Theoretical Analysis of Gd <sub>4</sub> B <sub>3</sub> C <sub>4</sub> : A Novel Rare Earth Metal Borocarbide Containing Two Different Boron-Carbon Arrangements. Inorganic Chemistry, 2000, 39, 5895-5900.	1.9	25
1136	Ground state gas and solution phase conformational dynamics of polar processes: Furfural systems. Journal of Chemical Physics, 2000, 113, 7519-7529.	1.2	33
1137	Energetics of hydrogen chemisorbed on Cu(110): A first principles calculations study. Journal of Chemical Physics, 2000, 113, 6926-6932.	1.2	32
1138	First-principles study of NH <sub>3</sub> exposed Si(001)2 $\times$ 1: Relation between N 1s core-level shifts and atomic structure. Applied Physics Letters, 2000, 76, 553-555.	1.5	42



#	ARTICLE	IF	CITATIONS
1139	Density functional theory analysis of the local chemical bonds in the periodic tantalum dichalcogenides TaX <sub>2</sub> (X=S, Se, Te). <i>Journal of Chemical Physics</i> , 2000, 113, 5879-5890.	1.2	29
1140	Local density approximation and generalized gradient approximation calculations for oxygen and silicon vacancies in silica. <i>Journal of Chemical Physics</i> , 2000, 112, 9543-9548.	1.2	27
1141	Radial moments of the electron density: Gas phase results and the effects of solvation. <i>Journal of Chemical Physics</i> , 2000, 112, 1113-1121.	1.2	4
1142	1,3-Dipolar Cycloadditions of Diazomethane to Chiral Electron-Deficient Olefins: The Origin of the $\pi$ -Facial Diastereoselection. <i>Journal of Organic Chemistry</i> , 2000, 65, 388-396.	1.7	35
1143	Bond Scission in a Perfect Polyethylene Chain and the Consequences for the Ultimate Strength. <i>Macromolecules</i> , 2000, 33, 9098-9108.	2.2	32
1144	Heterogeneous Catalysis through Subsurface Sites. <i>Journal of the American Chemical Society</i> , 2000, 122, 1796-1801.	6.6	94
1145	A Combined Density Functional and Molecular Dynamics Study on Ethylene Insertion into the Cp <sub>2</sub> ZrEt <sup>+</sup> MeB(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> Ion-Pair. <i>Organometallics</i> , 2000, 19, 5182-5189.	1.1	81
1146	Experimental Observation of Pentaatomic Tetracoordinate Planar Carbon-Containing Molecules. <i>Journal of the American Chemical Society</i> , 2000, 122, 7681-7687.	6.6	230
1147	Precursor-mediated adsorption of oxygen on the (111) surfaces of platinum-group metals. <i>Physical Review B</i> , 2000, 62, 4744-4755.	1.1	319
1148	Structure and properties of isolated liquid crystal molecules: jet spectroscopy and ab initio calculations of 4-cyanobiphenyl. <i>Liquid Crystals</i> , 2000, 27, 845-850.	0.9	5
1149	A Simple Relativistic Correction to the Nuclear Spin-Spin Coupling Constant. <i>Journal of Physical Chemistry A</i> , 2000, 104, 113-120.	1.1	38
1150	Reactions of Laser-Ablated U and Th with CO <sub>2</sub> : Neon Matrix Infrared Spectra and Density Functional Calculations of OUCO, OThCO, and Other Products. <i>Journal of the American Chemical Society</i> , 2000, 122, 11440-11449.	6.6	63
1151	First-Principles Periodic Density Functional Study of the Hydrogenation of Maleic Anhydride to Succinic Anhydride over Palladium(111). <i>Journal of Physical Chemistry B</i> , 2000, 104, 9449-9459.	1.2	23
1152	Effect of the Environment on $\gamma$ -Al <sub>2</sub> O <sub>3</sub> (0001) Surface Structures. <i>Physical Review Letters</i> , 2000, 84, 3650-3653.	2.9	473
1153	Why Does the Tetrakis(trimethylphosphine)iridium(III) Hydrido-chloride Cation Adopt the Sterically and Electronically Unfavorable $\eta^5$ -Cis Geometry?. <i>Organometallics</i> , 2000, 19, 4608-4612.	1.1	9
1154	A Comparative Theoretical Study of the Hydrogen, Methyl, and Ethyl Chemisorption on the Pt(111) Surface. <i>Journal of the American Chemical Society</i> , 2000, 122, 4129-4144.	6.6	198
1155	O/N Ordering in Y <sub>2</sub> Si <sub>3</sub> O <sub>3</sub> N <sub>4</sub> with the Melilite-type Structure from First-Principles Calculations. <i>Chemistry of Materials</i> , 2000, 12, 1071-1075.	3.2	27
1156	Theoretical Studies of Stability and Reactivity of C <sub>2</sub> Hydrocarbon Species on Pt Clusters, Pt(111), and Pt(211). <i>Journal of Physical Chemistry B</i> , 2000, 104, 2299-2310.	1.2	121

#	ARTICLE	IF	CITATIONS
1157	Theoretical Study of the Adsorption of Acetylene on the Si(001) Surface. <i>Journal of Physical Chemistry B</i> , 2000, 104, 8259-8267.	1.2	106
1158	Magnetic Exchange in $[Mn_2(\frac{1}{4}-O)_3(tmtacn)_2]^{2+}$ : Metal-Metal Bonding or Superexchange?. <i>Inorganic Chemistry</i> , 2000, 39, 491-495.	1.9	20
1159	Density-functional study of bulk and surface properties of titanium nitride using different exchange-correlation functionals. <i>Physical Review B</i> , 2000, 62, 2899-2907.	1.1	386
1160	The Importance of Transient States at Higher Coverages in Catalytic Reactions. <i>Journal of the American Chemical Society</i> , 2000, 122, 1150-1153.	6.6	84
1161	CO Adsorption on Molybdenum Nitride's $\beta$ -Mo <sub>2</sub> N(100) Surface: Formation of NCO Species? A Density Functional Study. <i>Journal of Physical Chemistry B</i> , 2000, 104, 11972-11976.	1.2	29
1162	Phase transformations and electronic properties in mixed-metal oxides: Experimental and theoretical studies on the behavior of NiMoO <sub>4</sub> and MgMoO <sub>4</sub> . <i>Journal of Chemical Physics</i> , 2000, 112, 935-945.	1.2	111
1163	Interaction of SO <sub>2</sub> with MgO(100) and Cu/MgO(100): Decomposition Reactions and the Formation of SO <sub>3</sub> and SO <sub>4</sub> . <i>Journal of Physical Chemistry B</i> , 2000, 104, 7439-7448.	1.2	77
1164	The Coupling of Protonation and Reduction in Proteins with Multiple Redox Centers: Theory, Computational Method, and Application to Cytochrome c <sub>3</sub> . <i>Journal of Physical Chemistry B</i> , 2000, 104, 6293-6301.	1.2	54
1165	Electronic Structure Study of the N <sub>2</sub> O Isomers Using Post-Hartree-Fock and Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2000, 104, 1304-1310.	1.1	33
1166	A Density Functional Study of Ion-Pair Formation and Dissociation in the Reaction between Boron- and Aluminum-Based Lewis Acids with (1,2-Me <sub>2</sub> Cp) <sub>2</sub> ZrMe <sub>2</sub> . <i>Organometallics</i> , 2000, 19, 1841-1849.	1.1	110
1167	Adsorption and Decomposition of H <sub>2</sub> S on MgO(100), NiMgO(100), and ZnO(0001) Surfaces: A First-Principles Density Functional Study. <i>Journal of Physical Chemistry B</i> , 2000, 104, 3630-3638.	1.2	159
1168	Molecular Hardness, Polarizability and Valency Variation of Formamide and Thioformamide on Internal Rotation: A Density Functional Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2975-2979.	1.1	27
1169	Gas-Phase Reaction Pathways of Aluminum Organometallic Compounds with Dimethylaluminum Hydride and Alane as Model Systems. <i>Journal of Physical Chemistry A</i> , 2000, 104, 7881-7891.	1.1	8
1170	Proton Affinity and Protonation Sites of Aniline. Energetic Behavior and Density Functional Reactivity Indices. <i>Journal of Physical Chemistry A</i> , 2000, 104, 4017-4021.	1.1	79
1171	Density Functional Theory Calculations on the Interaction of Ethene with the {111} Surface of Platinum. <i>Journal of Physical Chemistry B</i> , 2000, 104, 6439-6446.	1.2	49
1172	Comparison of the Accurate Kohn-Sham Solution with the Generalized Gradient Approximations (GGAs) for the S <sub>N</sub> 2 Reaction F <sup>-</sup> + CH <sub>3</sub> F → FCH <sub>3</sub> + F <sup>-</sup> : A Qualitative Rule To Predict Success or Failure of GGAs. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8558-8565.	1.1	151
1173	Structures of Furanosides: A Study of the Conformational Space of Methyl $\beta$ -D-Lyxofuranoside by Density Functional Methods. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5291-5297.	1.1	13
1174	Theoretical Study of the CF <sub>2</sub> CH <sub>2</sub> + HF + CF <sub>4</sub> → CH <sub>3</sub> F + HF + CF <sub>4</sub> Reaction. <i>Journal of Physical Chemistry A</i> , 2000, 104, 9535-9541.	1.1	4

#	ARTICLE	IF	CITATIONS
1175	â€œNapoleon Hatâ€•Structure of Tetraatomic Molecules. A Combined Photoelectron Spectroscopy and Ab Initio Study of $\text{CAISi}_2$ - and Its Neutral. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5358-5365.	1.1	6
1176	Thermodynamic Stability of Fe/O Solid Solution at Inner-Core Conditions. <i>Geophysical Research Letters</i> , 2000, 27, 2417-2420.	1.5	17
1177	Density functional theory: An introduction. <i>American Journal of Physics</i> , 2000, 68, 69-79.	0.3	194
1178	Fundamental Electronic and Optical Properties. <i>Springer Series in Materials Science</i> , 2000, , 181-241.	0.4	0
1179	The Role of Orbital Interactions in Determining the Interlayer Spacing in Graphite Slabs. <i>Journal of the American Chemical Society</i> , 2000, 122, 11871-11875.	6.6	31
1180	Theoretical surface science and catalysisâ€”calculations and concepts. <i>Advances in Catalysis</i> , 2000, 45, 71-129.	0.1	1,776
1181	Ab Initio Molecular Orbital and Density Functional Studies on the Stable Structures and Vibrational Properties of <i>trans</i> - and <i>cis</i> -Azobenzenes. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8114-8120.	1.1	81
1182	Quasiparticle Calculations in Solids. <i>Solid State Physics</i> , 2000, 54, 1-218.	1.3	514
1183	An Accurate Description of the Bergman Reaction Using Restricted and Unrestricted DFT: A Stability Test, Spin Density, and On-Top Pair Densityâ€. <i>Journal of Physical Chemistry A</i> , 2000, 104, 1748-1761.	1.1	250
1184	The bonding of CO to metal surfaces. <i>Journal of Chemical Physics</i> , 2000, 112, 1946-1958.	1.2	165
1185	Density functional studies of $\text{UO}_2^{2+}$ and $\text{AnF}_6$ ( $\text{An}=\text{U}$ , $\text{Np}$ , and $\text{Pu}$ ) using scalar-relativistic effective core potentials. <i>Journal of Chemical Physics</i> , 2000, 113, 7345-7350.	1.2	58
1186	Calculated equilibrium properties, electronic structures and structural stabilities of Th, Pa, U, Np and Pu. <i>Journal of Physics Condensed Matter</i> , 2000, 12, 5819-5829.	0.7	25
1187	THEORETICAL STUDIES OF ATOMIC-SCALE PROCESSES RELEVANT TO CRYSTAL GROWTH. <i>Annual Review of Physical Chemistry</i> , 2000, 51, 623-653.	4.8	121
1188	Fundamentals of the Electronic Structure of Surfaces. <i>Handbook of Surface Science</i> , 2000, , 1-91.	0.3	6
1189	Density Functional Study of the Reppe Carbonylation of Acetylene. <i>Organometallics</i> , 2000, 19, 4104-4116.	1.1	23
1190	Oxygen Vacancies as Active Sites for Water Dissociation on Rutile $\text{TiO}_2(110)$ . <i>Physical Review Letters</i> , 2001, 87, 266104.	2.9	884
1191	Band structure and optical parameters of the $\text{SnO}_2(110)$ surface. <i>Physical Review B</i> , 2001, 64, .	1.1	115
1192	Adsorption of Cu and Pd on $\hat{1}\pm\text{-Al}_2\text{O}_3(0001)$ surfaces with different stoichiometries. <i>Journal of Chemical Physics</i> , 2001, 115, 11261-11267.	1.2	89

#	ARTICLE	IF	CITATIONS
1193	Coexistence of Atomic and Molecular Chemisorption States:H <sub>2</sub> /Pd(210). Physical Review Letters, 2001, 87, 096103.	2.9	70
1194	Band structure ofMgB <sub>2</sub> with different lattice constants. Physical Review B, 2001, 65, .	1.1	48
1195	Clean Oxide Surfaces: a theoretical review. Chemical Physics of Solid Surfaces, 2001, 9, 35-93.	0.3	9
1196	Structural stability and lattice defects in copper:Ab initio, tight-binding, and embedded-atom calculations. Physical Review B, 2001, 63, .	1.1	1,756
1197	Theoretical Study of Oxygen Adsorption on Graphite and the (8,0) Single-walled Carbon Nanotube. Journal of Physical Chemistry B, 2001, 105, 11227-11232.	1.2	258
1198	High-pressure phases of group IV and III-V semiconductors. Reports on Progress in Physics, 2001, 64, 483-516.	8.1	230
1199	Energetics of native defects in ZnO. Journal of Applied Physics, 2001, 90, 824-828.	1.1	360
1200	Density Functional Theory Calculations of Hydrogen-Containing Defects in Forsterite, Periclase, and $\pm$ -Quartz. Journal of Physical Chemistry B, 2001, 105, 9747-9754.	1.2	53
1201	Tetragonal Y-doped zirconia: Structure and ion conductivity. Physical Review B, 2001, 64, .	1.1	145
1202	Comparison of Steric and Electronic Requirements for C <sup>+</sup> C and C <sup>+</sup> H Bond Activation. Chelating vs Nonchelating Case. Journal of the American Chemical Society, 2001, 123, 9064-9077.	6.6	118
1203	Crystal Chemistry of the Olivine-Type Li(Mn <sub>[sub y]</sub> Fe <sub>[sub 1<sup>~</sup>y]</sub> )PO <sub>[sub 4]</sub> and (Mn <sub>[sub y]</sub> Fe <sub>[sub ]</sub> )Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Society, 2001, 148, A960.	1.3	375
1204	Atomic and ionic processes of silicon oxidation. Physical Review B, 2001, 63, .	1.1	70
1205	CF <sub>2</sub> XCFCF <sub>2</sub> and CF <sub>2</sub> XCFCF <sub>2</sub> Radicals (X = Cl, Br, I): Ab Initio and DFT Studies and Comparison with Experiments. Journal of Physical Chemistry A, 2001, 105, 3623-3632.	1.1	40
1206	Electronic coupling between molybdenum and tungsten quadruple bonds in molecular squares and extended chains linked by oxalate, acetylenedicarboxylate, and perfluoroterephthalate bridges. Israel Journal of Chemistry, 2001, 41, 187-195.	1.0	7
1207	Surface electronic structures of superconducting thin filmMgB <sub>2</sub> (0001). Physical Review B, 2001, 64, .	1.1	25
1208	Second nearest-neighbor modified embedded atom method potentials for bcc transition metals. Physical Review B, 2001, 64, .	1.1	519
1209	Computer simulations for shock-compressed liquid deuterium: Failure of density-functional theory and molecular dynamics. Physical Review B, 2001, 64, .	1.1	13
1210	Electronic and magnetic properties ofLa <sub>2</sub> FeCrO <sub>6</sub> :Superexchange interaction for ad <sup>5</sup> d <sup>3</sup> system. Physical Review B, 2001, 63, .	1.1	52

#	ARTICLE	IF	CITATIONS
1211	Effect of GGA on the half-metallicity of the itinerant ferromagnet CoS <sub>2</sub> . <i>Physical Review B</i> , 2001, 64, .	1.1	135
1212	Modeling STM tips by single adsorbed atoms on W(100) films: 3d and 4d transition-metal atoms. <i>Physical Review B</i> , 2001, 64, .	1.1	44
1213	Ab initio calculations on etching of graphite and diamond surfaces by atomic hydrogen. <i>Physical Review B</i> , 2001, 63, .	1.1	32
1214	Role of disorder in incorporation energies of oxygen atoms in amorphous silica. <i>Physical Review B</i> , 2001, 63, .	1.1	56
1215	An ab Initio Theory and Density Functional Theory (DFT) Study of Conformers of Tetrahydro-2H-pyran. <i>Journal of Physical Chemistry A</i> , 2001, 105, 10123-10132.	1.1	33
1216	Upper Limit of the O-H...O Hydrogen Bond. Ab Initio Study of the Kaolinite Structure. <i>Journal of Physical Chemistry B</i> , 2001, 105, 10812-10817.	1.2	109
1217	Light-Atom Location in Adsorbed Benzene by Experiment and Theory. <i>Physical Review Letters</i> , 2001, 87, 216102.	2.9	47
1218	A density functional theory study of hydroxyl and the intermediate in the water formation reaction on Pt. <i>Journal of Chemical Physics</i> , 2001, 114, 513.	1.2	173
1219	Catalytic Water Formation on Platinum: A First-Principles Study. <i>Journal of the American Chemical Society</i> , 2001, 123, 4235-4242.	6.6	314
1220	Electronic structure of doped LaMnO <sub>3</sub> perovskite studied by x-ray photoemission spectroscopy. <i>Journal of Physics Condensed Matter</i> , 2001, 13, 5519-5525.	0.7	8
1221	Computational Studies of the Interactions of Oxygen with Platinum Clusters. <i>Journal of Physical Chemistry B</i> , 2001, 105, 9943-9952.	1.2	118
1222	Charge Distribution in Bis-Dioxolene Radical Metal Complexes. Synthesis and DFT Characterization of Dinuclear Co(III) and Cr(III) Complexes with a Mixed-Valent, S=1/2 Semiquinone-Catecholate Ligand. <i>Inorganic Chemistry</i> , 2001, 40, 1582-1590.	1.9	58
1223	Giant Anharmonicity and Nonlinear Electron-Phonon Coupling in MgB <sub>2</sub> : A Combined First-Principles Calculation and Neutron Scattering Study. <i>Physical Review Letters</i> , 2001, 87, 037001.	2.9	381
1224	The origin of the electron distribution in SnO. <i>Journal of Chemical Physics</i> , 2001, 114, 758.	1.2	96
1225	Study of relativistic effects on nuclear shieldings using density-functional theory and spin-orbit pseudopotentials. <i>Journal of Chemical Physics</i> , 2001, 114, 61.	1.2	101
1226	A Study of the Mechanism of the Reaction between Ozone and the Chlorine Atom Using Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4065-4070.	1.1	18
1227	Ab initio molecular dynamics simulation of the Ag(111)-water interface. <i>Journal of Chemical Physics</i> , 2001, 115, 7196-7206.	1.2	81
1228	Tunable Adsorption on Carbon Nanotubes. <i>Physical Review Letters</i> , 2001, 87, 116802.	2.9	184

#	ARTICLE	IF	CITATIONS
1229	First-principles study of the stability of BN and C. <i>Physical Review B</i> , 2001, 64, .	1.1	105
1230	Exohydrogenated single-wall carbon nanotubes. <i>Physical Review B</i> , 2001, 64, .	1.1	103
1231	Modeling disorder in amorphous silica with embedded clusters: The peroxy bridge defect center. <i>Physical Review B</i> , 2001, 64, .	1.1	39
1232	Role of the core-valence interaction for pseudopotential calculations with exact exchange. <i>Physical Review B</i> , 2001, 64, .	1.1	113
1233	Optical properties of copper and silver in the energy range 2.5–9.0 eV. <i>Physical Review B</i> , 2001, 64, .	1.1	116
1234	Numerical atomic orbitals for linear-scaling calculations. <i>Physical Review B</i> , 2001, 64, .	1.1	992
1235	Nitrogen 1s core-level shifts at the NH <sub>3</sub> saturated Si(100)-2×1 surface: a first-principles study. <i>Surface Science</i> , 2001, 490, L614-L618.	0.8	19
1236	Kinetics of heterogeneous catalytic reactions: Analysis of reaction schemes. <i>Advances in Catalysis</i> , 2001, , 161-264.	0.1	83
1237	Electronic structure of superconducting non-oxide perovskite MgCNi <sub>3</sub> . <i>Journal of Physics Condensed Matter</i> , 2001, 13, L595-L600.	0.7	32
1238	Quantum Monte Carlo simulations of solids. <i>Reviews of Modern Physics</i> , 2001, 73, 33-83.	16.4	1,813
1239	Effect of Particle Size on the Adsorption of O and S Atoms on Pt: A Density-Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2001, 105, 7739-7747.	1.2	65
1240	Oxygen Dissociation at Pt Steps. <i>Physical Review Letters</i> , 2001, 87, 056103.	2.9	189
1241	A Comparison of the Adsorption and Diffusion of Hydrogen on the {111} Surfaces of Ni, Pd, and Pt from Density Functional Theory Calculations. <i>Journal of Physical Chemistry B</i> , 2001, 105, 4889-4894.	1.2	184
1242	A Quantum Chemical Approach to the Study of Reaction Mechanisms of Redox-Active Metalloenzymes. <i>Journal of Physical Chemistry B</i> , 2001, 105, 9375-9386.	1.2	101
1243	Density-functional study of charge disordering in Cs <sub>2</sub> Au(I)Au(III)Cl <sub>6</sub> under pressure. <i>Physical Review B</i> , 2001, 63, .	1.1	31
1244	Molecular Dynamics Simulations of Pd Deposition on the ±-Al <sub>2</sub> O <sub>3</sub> (0001) Surface. <i>Journal of Physical Chemistry B</i> , 2001, 105, 12111-12117.	1.2	30
1245	Cluster embedding in an elastic polarizable environment: Density functional study of Pd atoms adsorbed at oxygen vacancies of MgO(001). <i>Journal of Chemical Physics</i> , 2001, 115, 8157-8171.	1.2	116
1246	Electronic properties of CdSe and Cd <sub>1-x</sub> FexSe wurtzite compounds: theoretical ab-initio investigation. <i>Journal of Alloys and Compounds</i> , 2001, 328, 139-142.	2.8	4

#	ARTICLE	IF	CITATIONS
1247	A density functional study of small Ni <sub>x</sub> Sn clusters with x=1-4. Computational Materials Science, 2001, 20, 57-65.	1.4	7
1248	Electronic structure of the polar ZnO{0001}-surfaces. Computational Materials Science, 2001, 22, 24-31.	1.4	54
1249	Electronic structure of twist grain-boundaries in ZnO and the effect of Sb doping. Computational Materials Science, 2001, 22, 38-43.	1.4	18
1250	Cation polarizability from first-principles: Sn <sup>2+</sup> . Computational Materials Science, 2001, 22, 94-98.	1.4	20
1251	Screening of the possible boron-based n-type thermoelectric conversion materials on the basis of the calculated densities of states of metal borides and doped $\beta$ -boron. Intermetallics, 2001, 9, 721-734.	1.8	40
1252	Cu, Ag, and Au atoms adsorbed on TiO <sub>2</sub> (110): cluster and periodic calculations. Surface Science, 2001, 471, 21-31.	0.8	131
1253	Density-functional study of the adsorption of benzene on the (111), (100) and (110) surfaces of nickel. Surface Science, 2001, 472, 133-153.	0.8	124
1254	STM-induced void formation at the Al <sub>2</sub> O <sub>3</sub> /Ni <sub>3</sub> Al(111) interface. Surface Science, 2001, 472, L157-L163.	0.8	14
1255	Stress induced nanostructure in a Pd monolayer on Ni(110): a first principles theoretical study. Surface Science, 2001, 472, L139-L144.	0.8	23
1256	Adsorption sites and STM images of C <sub>2</sub> H <sub>2</sub> on Si(100): a first-principles study. Surface Science, 2001, 475, 83-88.	0.8	38
1257	The structure of carbon adsorbed on Ir{100}: LEED $I$ - $V$ analysis and benchmarking of DFT. Surface Science, 2001, 478, 49-56.	0.8	13
1258	Synergetic effects in CO adsorption on Cu-Pd(111) alloys. Surface Science, 2001, 477, 59-75.	0.8	110
1259	Quenching surface states with the tip: STM scans on Fe(100). Surface Science, 2001, 482-485, 1113-1118.	0.8	8
1260	Si(001)/In-4 $\times$ 3 surface: a first principles total energy calculation. Surface Science, 2001, 482-485, 1468-1473.	0.8	5
1261	Benzene on silicon: combining STM experiments with first principles studies. Surface Science, 2001, 482-485, 1181-1185.	0.8	23
1262	The structure of the oxygen induced (1 $\times$ 5) reconstruction of V(100). Surface Science, 2001, 480, 11-24.	0.8	39
1263	Formation of a new type of chromium oxide by deposition of chromium onto water precovered Cu(111). Surface Science, 2001, 480, 73-83.	0.8	11
1264	Substrate reconstruction and electronic surface states: Ag(001). Surface Science, 2001, 486, 65-72.	0.8	20



#	ARTICLE	IF	CITATIONS
1265	Disproportionation of dimethylalane on aluminum surfaces. Part II. Quantum chemistry studies. Surface Science, 2001, 488, 303-324.	0.8	3
1266	The first-principle study of the iodine-modified silver surfaces. Surface Science, 2001, 487, 77-86.	0.8	21
1267	Nonmetal-to-metal transition in Mg films on the Mo(112) surface. Surface Science, 2001, 488, 7-14.	0.8	6
1268	First-principles study on the geometries and electronic structures of clean and hydrogen-adsorbed NbC(111) surface. Surface Science, 2001, 488, 256-268.	0.8	14
1269	The effect of strain for N <sub>2</sub> dissociation on Fe surfaces. Surface Science, 2001, 489, 135-143.	0.8	48
1270	Structure and energetics of Cu(100) vicinal surfaces. Surface Science, 2001, 489, 151-160.	0.8	22
1271	Unsaturated cyclic-hydrocarbon molecules on a Si(0 0 1) surface. Surface Science, 2001, 493, 131-137.	0.8	17
1272	Density-functional bridge between surfaces and interfaces. Surface Science, 2001, 493, 253-270.	0.8	31
1273	Behavior of H atom in adsorption states on metal surfaces – localization and delocalization. Surface Science, 2001, 493, 271-277.	0.8	36
1274	Atom bridge made from magnetic materials: atomic configuration and magnetic properties. Surface Science, 2001, 493, 757-762.	0.8	16
1275	Structural and electronic properties of silver surfaces: ab initio pseudopotential density functional study. Surface Science, 2001, 490, 125-132.	0.8	48
1276	A first principles survey of stoichiometric (1 $\bar{1}$ –2) reconstructions on the rutile surface. Surface Science, 2001, 495, 211-233.	0.8	23
1277	First-principles study of the interaction of oxygen with the SnO <sub>2</sub> (110) surface. Surface Science, 2001, 490, 221-236.	0.8	98
1278	A theoretical investigation of the binding of TiCl <sub>n</sub> to MgCl <sub>2</sub> . Surface Science, 2001, 490, 237-250.	0.8	35
1279	Investigation of vinyl phosphonic acid/hydroxylated $\gamma$ -Al <sub>2</sub> O <sub>3</sub> ( $\gamma$ ) reaction enthalpies. Surface Science, 2001, 494, 1-20.	0.8	48
1280	A DFT study of the adsorption of thiophene on Ni(100). Surface Science, 2001, 492, 27-33.	0.8	35
1281	First-principles calculations for V <sub>x</sub> O <sub>y</sub> grown on Pd(111). Surface Science, 2001, 492, 329-344.	0.8	66
1282	Adsorption and dissociation of O <sub>2</sub> on Cu(): thermochemistry, reaction barrier and the effect of strain. Surface Science, 2001, 494, 131-144.	0.8	175

#	ARTICLE	IF	CITATIONS
1283	Comparative theory of missing-row reconstructions: Pt{110}, Pt{211} and Pt{311}. Surface Science, 2001, 494, 159-165.	0.8	39
1284	Minority metallic surface states of a half-metallic ferrimagnet. Surface Science, 2001, 494, L793-L798.	0.8	53
1285	Is there theoretical evidence for a metallic carbon polymorph with space group symmetry at ambient conditions?. Diamond and Related Materials, 2001, 10, 2225-2227.	1.8	24
1286	Electronic and Chemical Properties of Ce <sub>0.8</sub> Zr <sub>0.2</sub> O <sub>2</sub> (111) Surfaces: Photoemission, XANES, Density-Functional, and NO <sub>2</sub> Adsorption Studies. Journal of Physical Chemistry B, 2001, 105, 7762-7770.	1.2	118
1287	First-principles studies of the stability of Zintl ions in alkali-tin alloys: I. Crystalline intermetallic compounds. Journal of Physics Condensed Matter, 2001, 13, 959-980.	0.7	10
1288	Ligand Dependence of Metal-Metal Bonding in the d <sup>3</sup> d <sup>3</sup> Dimers M <sub>2</sub> X <sub>9</sub> n- (M <sup>III</sup> = Cr, Mo, W; M <sup>IV</sup> = Mn, Tc, Re;) $\frac{1}{1.9} \frac{1}{0.784314} \frac{1}{27}$	1.9	27
1289	A theoretical study of a sulfur impurity in diamond. Diamond and Related Materials, 2001, 10, 449-452.	1.8	58
1290	Covalent origin of adsorbate-induced demagnetization at ferromagnetic surfaces. Physical Review B, 2001, 64, .	1.1	23
1291	An Electronic Structure of Ferroelectric PbZr <sub>0.5</sub> Ti <sub>0.5</sub> O <sub>3</sub> . Chinese Physics Letters, 2001, 18, 826-828.	1.3	12
1292	A density functional theory study of the reaction of C+O, C+N, and C+H on close packed metal surfaces. Journal of Chemical Physics, 2001, 114, 5792-5795.	1.2	35
1293	Softened C-H modes of adsorbed methyl and their implications for dehydrogenation: An ab initio study. Journal of Chemical Physics, 2001, 114, 2523-2526.	1.2	61
1294	Ab initio investigation of the adsorption of benzene in mordenite. Journal of Chemical Physics, 2001, 114, 3703-3712.	1.2	36
1295	Interaction between Metallic p Orbitals and the $\pi$ Orbitals of Organic Molecules: The Binding between Ethylene and Aluminum. Journal of Physical Chemistry B, 2001, 105, 641-645.	1.2	14
1296	Combined Computational and Experimental Investigation of SO <sub>x</sub> Adsorption on MgO. Journal of Physical Chemistry B, 2001, 105, 6972-6979.	1.2	75
1297	Structure and Stability of N <sub>6</sub> Isomers and Their Spectroscopic Characteristics. Journal of Physical Chemistry A, 2001, 105, 4107-4113.	1.1	95
1298	CO Adsorption on Pt-Ru Surface Alloys and on the Surface of Pt-Ru Bulk Alloy. Journal of Physical Chemistry B, 2001, 105, 9533-9536.	1.2	90
1299	Alloying Effects on N-O Stretching Frequency: A Density Functional Theory Study of the Adsorption of NO on Pd <sub>3</sub> Mn (100) and (111) Surfaces. Journal of Physical Chemistry B, 2001, 105, 3027-3033.	1.2	14
1300	The Failure of Generalized Gradient Approximations (GGAs) and Meta-GGAs for the Two-Center Three-Electron Bonds in He <sub>2</sub> <sup>+</sup> , (H <sub>2</sub> O) <sub>2</sub> <sup>+</sup> , and (NH <sub>3</sub> ) <sub>2</sub> <sup>+</sup> . Journal of Physical Chemistry A, 2001, 105, 9211-9218.	1.1	83

#	ARTICLE	IF	CITATIONS
1301	Adsorption of benzene on Si(100)-(2 $\times$ 1): $\epsilon$ f Adsorption energies and STM image analysis byab initiomethods. Physical Review B, 2001, 63, .	1.1	91
1302	FeMo Cofactor of Nitrogenase: A Density Functional Study of States MN, MOX, MR, and MI. Journal of the American Chemical Society, 2001, 123, 12392-12410.	6.6	181
1303	Nitrogen bonding configurations at nitrided Si(001) surfaces andSi(001) $\hat{\sim}$ SiO <sub>2</sub> interfaces: A first-principles study of core-level shifts. Physical Review B, 2001, 63, .	1.1	58
1304	Full band calculation of doping-induced band-gap narrowing inp-type GaAs. Physical Review B, 2001, 64, .	1.1	25
1305	Theoretical Modeling of a Copper Site in a Cu(II) $\hat{\sim}$ Y Zeolite. Journal of Physical Chemistry B, 2001, 105, 1149-1156.	1.2	42
1306	Density Functional Studies of Oxidized and Reduced Methane Monooxygenase. Optimized Geometries and Exchange Coupling of Active Site Clusters. Inorganic Chemistry, 2001, 40, 5251-5266.	1.9	33
1307	Coverage-Dependent Adsorption of CH <sub>3</sub> S and (CH <sub>3</sub> S) <sub>2</sub> on Au(111): A Density Functional Theory Study. Journal of Physical Chemistry B, 2001, 105, 9509-9513.	1.2	230
1308	An ab Initio Study of Hydrogen Bonding Effects on the <sup>15</sup> N and <sup>1</sup> H Chemical Shielding Tensors in the Watson $\hat{\sim}$ Crick Base Pairs. Journal of Physical Chemistry A, 2001, 105, 1357-1365.	1.1	26
1309	Dynamical Density Functional Study of the Multistep CO Insertion into Zirconium $\hat{\sim}$ Carbon Bonds Anchored to a Calix[4]arene Moiety. Organometallics, 2001, 20, 4031-4039.	1.1	12
1310	Beyond Classical Stoichiometry: $\hat{\sim}$ Experiment and Theory. Journal of Physical Chemistry A, 2001, 105, 10759-10775.	1.1	119
1311	Theoretical Study of the Oxidative Addition of Ammonia to Various Unsaturated Low-Valent Transition Metal Species. Organometallics, 2001, 20, 1860-1874.	1.1	41
1312	An Insight into Alkali Promotion: $\hat{\sim}$ A Density Functional Theory Study of CO Dissociation on K/Rh(111). Journal of the American Chemical Society, 2001, 123, 12596-12604.	6.6	139
1313	A Density Functional Study of the Competing Processes Occurring in Solution during Ethylene Polymerization by the Catalyst (1,2-Me <sub>2</sub> Cp) <sub>2</sub> ZrMe <sup>+</sup> . Organometallics, 2001, 20, 905-913.	1.1	59
1314	First-principles structural stability study of nonstoichiometry-related planar defects in SrTiO <sub>3</sub> and BaTiO <sub>3</sub> . Journal of Applied Physics, 2001, 89, 5622-5629.	1.1	29
1315	First Principle Study to Correlate Location and Activity of Ruthenium Oxide Incorporated in Alkali-Metal Hexatitanates. Journal of Physical Chemistry B, 2001, 105, 3463-3469.	1.2	5
1316	Boron $\hat{\sim}$ Nitrogen (BN) Substitution Patterns in C/BN Hybrid Fullerenes: $\hat{\sim}$ C <sub>60</sub> -2x(BN) <sub>x</sub> (x = 1 $\hat{\sim}$ 7). Journal of Physical Chemistry A, 2001, 105, 8376-8384.	1.1	49
1317	DFT Study on Ferroelectricity of BaTiO <sub>3</sub> . Journal of Physical Chemistry B, 2001, 105, 5766-5771.	1.2	70
1318	Energetics of Oxidized and Reduced Methane Monooxygenase Active Site Clusters in the Protein Environment. Inorganic Chemistry, 2001, 40, 5267-5278.	1.9	28

#	ARTICLE	IF	CITATIONS
1319	Dynamical and optical properties of warm dense hydrogen. <i>Physical Review B</i> , 2001, 63, .	1.1	135
1320	A Periodic Density Functional Theory Analysis of the Effect of Water Molecules on Deprotonation of Acetic Acid over Pd(111). <i>Journal of Physical Chemistry B</i> , 2001, 105, 9171-9182.	1.2	66
1321	On the Aromaticity of Square Planar Ga <sub>4</sub> <sup>2-</sup> and In <sub>4</sub> <sup>2-</sup> in Gaseous NaGa <sub>4</sub> <sup>-</sup> and NaIn <sub>4</sub> <sup>-</sup> Clusters. <i>Journal of the American Chemical Society</i> , 2001, 123, 8825-8831.	6.6	217
1322	Theoretical Calculation of Bond Dissociation Energies and Enthalpies of Formation for Halogenated Molecules. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6729-6742.	1.1	66
1323	Three Conformational Polymorphs of Di- <sup>1</sup> / <sub>4</sub> -chlorotetrakis(1-methylboratabenzene)diyttrium:Â Synthesis, X-ray Structures, Quantum Chemical Calculations, and Lattice Energy Minimizations1. <i>Inorganic Chemistry</i> , 2001, 40, 3117-3123.	1.9	27
1324	First-Principles Pseudo-Potential Study of the Pd(110)-c(2 $\sqrt{2}$ -2)-Ethylene Adsorption System. <i>Journal of Physical Chemistry B</i> , 2001, 105, 8149-8154.	1.2	9
1325	Ambient pressure phase diagram of plutonium: A unified theory for $\delta$ -Pu and $\epsilon$ -Pu. <i>Europhysics Letters</i> , 2001, 55, 525-531.	0.7	137
1326	Mechanism of Olefin Cyclopropanation by Diazomethane Catalyzed by Palladium Dicarboxylates. A Density Functional Study. <i>Journal of the American Chemical Society</i> , 2001, 123, 6157-6163.	6.6	53
1327	Density functional theory calculations of proton-containing defects in forsterite. <i>Radiation Effects and Defects in Solids</i> , 2001, 154, 255-259.	0.4	3
1328	Electronic Structure Study of CO Adsorption on the Fe(001) Surface. <i>Journal of Physical Chemistry B</i> , 2001, 105, 164-172.	1.2	74
1329	1,2-FCI Rearrangement as an Intermediate Step in the Unimolecular 1,3-HCl Elimination from Chlorofluoropropanesâ€. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1622-1625.	1.1	27
1330	Quantum Chemical Descriptions of FOOF:Â The Unsolved Problem of Predicting Its Equilibrium Geometry. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3269-3276.	1.1	33
1331	The CO/Pt(111) Puzzle. <i>Journal of Physical Chemistry B</i> , 2001, 105, 4018-4025.	1.2	642
1332	First-principles density-functional study of metal-carbonitride interface adhesion: Co/TiC(001) and Co/TiN(001). <i>Physical Review B</i> , 2001, 64, .	1.1	112
1333	INSULATING OXIDES IN LOW DIMENSIONALITY: A THEORETICAL REVIEW. <i>Surface Review and Letters</i> , 2001, 08, 121-167.	0.5	30
1334	Superconductivity of MgB <sub>2</sub> : Covalent Bonds Driven Metallic. <i>Physical Review Letters</i> , 2001, 86, 4366-4369.	2.9	811
1335	Ab initio study of hydrogen adsorption to single-walled carbon nanotubes. <i>Physical Review B</i> , 2001, 63, .	1.1	161
1336	Theoretical Study of the Interaction of Molecular Hydrogen with PdCu(111) Bimetallic Surfaces. <i>Journal of Physical Chemistry B</i> , 2001, 105, 1817-1822.	1.2	29

#	ARTICLE	IF	CITATIONS
1337	A First Principles Density Functional Study of Au Deposition on TiN (001) Surface. International Journal of Molecular Sciences, 2001, 2, 263-270.	1.8	7
1338	Ab-initio modelling of atomic and molecular Hydrogen adsorption in graphite. Materials Research Society Symposia Proceedings, 2001, 677, 4111.	0.1	0
1339	Stoichiometry and Adhesion of Al/WC. Materials Research Society Symposia Proceedings, 2001, 677, 4251.	0.1	1
1340	Ab-initio modelling of atomic and molecular Hydrogen adsorption in graphite. Materials Research Society Symposia Proceedings, 2001, 677, 471.	0.1	1
1341	Parameter Optimization of Tersoff Interatomic Potentials Using a Genetic Algorithm.. JSME International Journal Series A-Solid Mechanics and Material Engineering, 2001, 44, 207-213.	0.4	7
1342	Full-Potential KKR Calculations for Point Defect Energies in Metals, based on the Generalized-Gradient Approximation: I. Vacancy Formation Energies in fcc and bcc Metals. Materials Transactions, 2001, 42, 2206-2215.	0.4	38
1343	Full-Potential KKR Calculations for Point Defect Energies in Metals, based on the Generalized-Gradient Approximation: II. Impurity-Impurity Interaction Energies and Phase Diagrams. Materials Transactions, 2001, 42, 2216-2224.	0.4	21
1344	Bipyridinium Molecular Switch: $\langle I \rangle$ Ab-initio $\langle I \rangle$ Electronic Structure Calculation. Materials Transactions, 2001, 42, 2276-2278.	0.4	4
1345	Mechanisms for enzymatic reactions involving formation or cleavage of O-O bonds. Theoretical and Computational Chemistry, 2001, , 95-143.	0.2	2
1346	Electronic structure and properties in perovskite CaTiO <sub>3</sub> from first principle. Ferroelectrics, 2001, 259, 127-132.	0.3	3
1347	Proton trapping and diffusion in SiO <sub>2</sub> thin films: a first-principles study. Applied Surface Science, 2001, 172, 41-46.	3.1	8
1348	Pressure-induced structural change of the tetrafluoro-p-benzoquinone (p-fluoranil) crystal from ab initio total energy calculations. Chemical Physics, 2001, 264, 9-19.	0.9	3
1349	Study of the local atomic strain field in a Zr-doped TiAl intermetallic alloy by EXAFS and ab initio FLAPW calculations. Ultramicroscopy, 2001, 86, 265-272.	0.8	5
1350	Electronic structure of KTa <sub>0.5</sub> Nb <sub>0.5</sub> O <sub>3</sub> in the ferroelectric phase and paraelectric phase. Physics Letters, Section A: General, Atomic and Solid State Physics, 2001, 285, 390-394.	0.9	12
1351	Theoretical study on the fine structure of PbFe <sub>0.5</sub> Nb <sub>0.5</sub> O <sub>3</sub> . Physics Letters, Section A: General, Atomic and Solid State Physics, 2001, 288, 45-48.	0.9	13
1352	Adiabatic potential-energy surface of O <sub>2</sub> /Al(111): rare entrance-channel barriers but molecularly chemisorbed state apt for abstraction. Solid State Communications, 2001, 117, 531-535.	0.9	47
1353	First-principles study on the tendency to ferroelectricity of CaTiO <sub>3</sub> . Solid State Communications, 2001, 117, 461-464.	0.9	23
1354	First-principles study on the optical properties of NaNO <sub>2</sub> in the ferroelectric and paraelectric phase. Solid State Communications, 2001, 119, 665-669.	0.9	0

#	ARTICLE	IF	CITATIONS
1355	First-principles study on the optical properties of SrHfO <sub>3</sub> and SrTiO <sub>3</sub> . <i>Solid State Communications</i> , 2001, 120, 133-136.	0.9	30
1356	First-principles study of the electronic structure of NaTaO <sub>3</sub> . <i>Solid State Communications</i> , 2001, 120, 137-140.	0.9	25
1357	X-ray photoemission spectra and electronic structure of GdCo <sub>4</sub> B. <i>Solid State Communications</i> , 2001, 120, 407-411.	0.9	12
1358	The different roles of charged and neutral atomic and molecular oxidising species in silicon oxidation from ab initio calculations. <i>Solid-State Electronics</i> , 2001, 45, 1233-1240.	0.8	21
1359	Lattice dynamics of Mg <sub>2</sub> SiO <sub>4</sub> . <i>Journal of Molecular Structure</i> , 2001, 596, 3-6.	1.8	13
1360	Metal-metal interaction in polynuclear complexes with cyanide bridges: synthesis, characterisation, and theoretical studies. <i>Journal of Organometallic Chemistry</i> , 2001, 632, 94-106.	0.8	10
1361	A density functional study of the structures, vibrations and bond energies of dinitrogen phosphine complexes of the first transition series. <i>Journal of Organometallic Chemistry</i> , 2001, 635, 165-172.	0.8	5
1362	Hartree-Fock and density functional calculations of the elastic constants of CaO. <i>Journal of Physics and Chemistry of Solids</i> , 2001, 62, 661-663.	1.9	4
1363	Individually selecting multi-reference CI and its application to biradicalic cyclizations. <i>Computers &amp; Chemistry</i> , 2001, 25, 15-38.	1.2	23
1364	Bornane-2,10-sultam: a highly efficient chiral controller and mechanistic probe for the intermolecular Pauson-Khand reaction. <i>Tetrahedron: Asymmetry</i> , 2001, 12, 1837-1850.	1.8	14
1365	Calculation of debye temperature for crystalline structures—a case study on Ti, Zr, and Hf. <i>Acta Materialia</i> , 2001, 49, 947-961.	3.8	138
1366	On the nature of RuS <sub>2</sub> HDS active sites: insight from ab initio theory. <i>Journal of Molecular Catalysis A</i> , 2001, 174, 239-244.	4.8	8
1367	Parallel between infrared characterisation and ab initio calculations of CO adsorption on sulphided Mo catalysts. <i>Catalysis Today</i> , 2001, 70, 255-269.	2.2	111
1368	A combined experimental and theoretical approach to the study of methane activation over oxide catalysts. <i>Catalysis Today</i> , 2001, 71, 3-10.	2.2	6
1369	Transferable tight-binding parameters for ferromagnetic and paramagnetic iron. <i>Physica B: Condensed Matter</i> , 2001, 296, 125-128.	1.3	85
1370	First-principles calculations for point-defect energies in metals and phase diagrams of binary alloys. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2001, 312, 72-76.	2.6	6
1371	First principles study of isotope effect in hydrogen-bonded K <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub> : I stable structures. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2001, 79, 31-44.	1.7	8
1372	First principles study of isotope effect in hydrogen-bonded K <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub> . <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2001, 79, 98-112.	1.7	6

#	ARTICLE	IF	CITATIONS
1373	Ab initio molecular dynamics simulation of hydration and ion-exchange processes in low Al-zeolites. <i>Microporous and Mesoporous Materials</i> , 2001, 42, 1-19.	2.2	14
1374	First principles calculation of the free energy barrier for the reaction of methanol in a zeolite catalyst. <i>Microporous and Mesoporous Materials</i> , 2001, 48, 375-381.	2.2	16
1375	Self-assembly directed by NH <sub>4</sub> <sup>+</sup> hydrogen bonding: new molecular assemblies derived from N,N-tetramethyl-1,2-diaminoethane and malonic or fumaric acid incorporating $\sigma$ -proton transferred <sup>TM</sup> hydrogen bonds. <i>Journal of Supramolecular Chemistry</i> , 2001, 1, 201-205.	0.4	1
1376	Electronic factors in catalysis: the volcano curve and the effect of promotion in catalytic ammonia synthesis. <i>Applied Catalysis A: General</i> , 2001, 222, 19-29.	2.2	225
1377	Reaction kinetics measurements and analysis of reaction pathways for conversions of acetic acid, ethanol, and ethyl acetate over silica-supported Pt. <i>Applied Catalysis A: General</i> , 2001, 222, 369-392.	2.2	113
1378	Density functional study of small Ni <sub>n</sub> clusters, with n=2-6, 8, using the generalized gradient approximation. <i>International Journal of Quantum Chemistry</i> , 2001, 85, 22-33.	1.0	39
1379	Configuration interaction calculation of electronic tensors in transition metal complexes. <i>International Journal of Quantum Chemistry</i> , 2001, 83, 104-114.	1.0	71
1380	Generalized spin density functional theory for noncollinear molecular magnetism II?Influence of gradient correction and self-interaction correction. <i>International Journal of Quantum Chemistry</i> , 2001, 85, 421-431.	1.0	20
1381	Quantum mechanics simulation of protein dynamics on long timescale. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 44, 484-489.	1.5	140
1382	Theoretical study of the mechanism of peptide ring formation in green fluorescent protein. <i>International Journal of Quantum Chemistry</i> , 2001, 81, 169-186.	1.0	30
1383	Theoretical investigation of the cyclic GaO <sub>2</sub> and GaS <sub>2</sub> molecules at DFT and correlated wave function levels. <i>International Journal of Quantum Chemistry</i> , 2001, 81, 222-231.	1.0	6
1384	Model potential density functional study of small cobalt clusters, Co <sub>n</sub> , n=3. <i>International Journal of Quantum Chemistry</i> , 2001, 81, 422-430.	1.0	36
1385	Density functional finite cluster method for polarizability of large BeN three-dimensional systems. <i>Journal of Computational Chemistry</i> , 2001, 22, 230-240.	1.5	2
1386	Ab initio quantum chemistry and molecular dynamics simulations studies of LiPF <sub>6</sub> /poly(ethylene oxide) interactions. <i>Journal of Computational Chemistry</i> , 2001, 22, 641-654.	1.5	76
1387	Chemistry with ADF. <i>Journal of Computational Chemistry</i> , 2001, 22, 931-967.	1.5	8,854
1388	A high-resolution electron momentum spectroscopy and density functional theory study into the complete valence electronic structure of allene. <i>Journal of Computational Chemistry</i> , 2001, 22, 1321-1333.	1.5	14
1389	Parametrization of the Becke3-LYP hybrid functional for a series of small molecules using quantum molecular similarity techniques. <i>Journal of Computational Chemistry</i> , 2001, 22, 1666-1678.	1.5	21
1390	Density functional studies of AnF <sub>6</sub> (An=U, Np, and Pu) and UF <sub>6</sub> ?nCl <sub>n</sub> (n=1-6) using hybrid functionals: geometries and vibrational frequencies. <i>Journal of Computational Chemistry</i> , 2001, 22, 2010-2017.	1.5	38



#	ARTICLE	IF	CITATIONS
1391	Crystal Structures and $^{29}\text{Si}$ NMR Calculations of Amino-Functionalized Silyllithium Compounds. <i>European Journal of Inorganic Chemistry</i> , 2001, 2001, 1013-1018.	1.0	31
1392	Effects of Oxidation on the Nanoscale Mechanisms of Crack Formation in Aluminum. <i>ChemPhysChem</i> , 2001, 2, 55-59.	1.0	39
1394	Magnetic Interactions as Supramolecular Function: Structure and Magnetic Properties of Hydrogen-Bridged Dinuclear Copper(II) Complexes. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 4207-4210.	7.2	71
1395	Luminescent $\text{FeSi}_2/\text{Si}(111)$ Structures Induced by Heteroepitaxial Stress. <i>Physica Status Solidi (B): Basic Research</i> , 2001, 223, 253-257.	0.7	8
1396	Theoretical Studies of Stoichiometric TiC. <i>Physica Status Solidi (B): Basic Research</i> , 2001, 225, 265-270.	0.7	10
1397	Theoretical Study of Hydrogen Adsorption and Diffusion on $\text{TiN}(100)$ Surface. <i>Physica Status Solidi (B): Basic Research</i> , 2001, 226, 29-36.	0.7	11
1398	Electronic Structure of Vanadium Dioxide: Ab initio Density Functional Theory Studies of Periodic and Local Systems. <i>Physica Status Solidi A</i> , 2001, 187, 137-149.	1.7	9
1399	Ab initio Calculations of GaN Initial Growth Processes on $\text{GaAs}(111)\text{A}$ and $\text{GaAs}(111)\text{B}$ Surfaces. <i>Physica Status Solidi A</i> , 2001, 188, 553-556.	1.7	1
1400	Electronic Structure of Uranium Digermanide. <i>Crystal Research and Technology</i> , 2001, 36, 1105-1112.	0.6	3
1401	HARES: an efficient method for first-principles electronic structure calculations of complex systems. <i>Computer Physics Communications</i> , 2001, 137, 341-360.	3.0	37
1402	Amorphous $\text{WO}_3$ : a first-principles approach. <i>Electrochimica Acta</i> , 2001, 46, 1989-1993.	2.6	52
1403	Interaction of halogen atom with $\text{Ag}(110)$ : ab initio pseudopotential density functional study. <i>Chemical Physics Letters</i> , 2001, 334, 411-418.	1.2	21
1404	Systematic prediction of crystal structures. <i>Chemical Physics Letters</i> , 2001, 337, 36-42.	1.2	52
1405	Theoretical prediction of the state-state correlation among doublet state $\text{AlSO}$ isomers. <i>Chemical Physics Letters</i> , 2001, 338, 142-150.	1.2	13
1406	Transition states and rearrangement mechanisms from hybrid eigenvector-following and density functional theory.. <i>Chemical Physics Letters</i> , 2001, 341, 185-194.	1.2	155
1407	Theoretical study of the structures and properties of $\text{SrSiAl}_2\text{O}_3\text{N}_2$ and $\text{Ce}_4[\text{Si}_4\text{O}_4\text{N}_6]\text{O}$ . <i>Chemical Physics Letters</i> , 2001, 343, 622-626.	1.2	7
1408	NO reduction over $\text{Pt}(1\ 0\ 0)$ : reaction rates from first principles. <i>Chemical Physics Letters</i> , 2001, 343, 383-389.	1.2	32
1409	Ab initio study of ammonia adsorption states on an ice surface I: structures, adsorption energies and linear dependences on coverage ratio. <i>Chemical Physics Letters</i> , 2001, 348, 107-114.	1.2	12

#	ARTICLE	IF	CITATIONS
1410	Ab initio and DFT studies for accurate description of van der Waals interaction between He atoms. Chemical Physics Letters, 2001, 348, 139-146.	1.2	48
1411	Ab initio study of ammonia adsorption states on an ice surface II: theoretical characterization of the surface bound state. Chemical Physics Letters, 2001, 350, 141-146.	1.2	6
1412	The role of adsorbates in the electrochemical oxidation of ammonia on noble and transition metal electrodes. Journal of Electroanalytical Chemistry, 2001, 506, 127-137.	1.9	323
1413	Short- and intermediate-range structure of liquid GeSe <sub>2</sub> . Physical Review B, 2001, 64, .	1.1	77
1414	Hydrogen bonding and stacking interactions of nucleic acid base pairs: A density-functional-theory based treatment. Journal of Chemical Physics, 2001, 114, 5149-5155.	1.2	978
1415	Thermodynamics of hexagonal-close-packed iron under Earth's core conditions. Physical Review B, 2001, 64, .	1.1	252
1416	Electronic structure and physical properties of early transition metal mononitrides: Density-functional theory LDA, GGA, and screened-exchange LDA FLAPW calculations. Physical Review B, 2001, 63, .	1.1	454
1417	Structure and electrical levels of point defects in monoclinic zirconia. Physical Review B, 2001, 64, .	1.1	307
1418	Mechanical Properties and Formation Mechanisms of a Wire of Single Gold Atoms. Physical Review Letters, 2001, 87, .	2.9	379
1419	Pd-Mn Silica-Supported Catalysts. Journal of Catalysis, 2001, 198, 243-255.	3.1	7
1420	The NO+CO Reaction Catalyzed by Flat, Stepped, and Edged Pd Surfaces. Journal of Catalysis, 2001, 199, 171-176.	3.1	146
1421	Morphology and Surface Properties of Boehmite ( $\gamma$ -AlOOH): A Density Functional Theory Study. Journal of Catalysis, 2001, 201, 236-246.	3.1	218
1422	NO Reduction by CO on the Pt(100) Surface. Journal of Catalysis, 2001, 204, 118-128.	3.1	71
1423	Optimized LiFePO <sub>4</sub> for Lithium Battery Cathodes. Journal of the Electrochemical Society, 2001, 148, A224.	1.3	1,703
1424	Surface waves on NiAl(110). Physical Review B, 2001, 63, .	1.1	28
1425	Adsorption properties of SO <sub>2</sub> on ultrafine precious metal particles studied using density functional calculation. Applied Surface Science, 2001, 177, 180-188.	3.1	10
1426	The structural character of AlS <sub>2</sub> species in quartet state: prediction at density functional theory and the correlated-wave function levels. Chemical Physics, 2001, 271, 229-238.	0.9	5
1427	Theoretical approaches of the isomerization mechanism of GaSO isomers in doublet states at density functional theory levels. Chemical Physics, 2001, 273, 103-115.	0.9	7

#	ARTICLE	IF	CITATIONS
1428	First principles study on the optical properties of cubic CaTiO <sub>3</sub> . Physics Letters, Section A: General, Atomic and Solid State Physics, 2001, 291, 338-342.	0.9	14
1429	A precise first-principles study on the non-existence of ferromagnetism in V monolayer on the Nb surface. Current Applied Physics, 2001, 1, 183-185.	1.1	2
1430	Ab initio density functional theory applied to the structure and proton dynamics of clays. Chemical Physics Letters, 2001, 333, 479-484.	1.2	45
1431	The harmonic vibrational frequencies and the geometry of the 12C6H6. Chemical Physics Letters, 2001, 340, 356-361.	1.2	17
1432	Geometry Optimization and Ground-State Properties of Complex Ceramic Oxides. Journal of the American Ceramic Society, 2001, 84, 801-805.	1.9	21
1433	Structure Models for $\hat{\Gamma}_3^+$ Aluminum Oxynitride from <i>Ab Initio</i> Calculations. Journal of the American Ceramic Society, 2001, 84, 2633-2637.	1.9	47
1434	Optimally localized Wannier functions within the Vanderbilt ultrasoft pseudo-potential formalism. Computational and Theoretical Chemistry, 2001, 544, 49-60.	1.5	12
1435	Computational characterization of energetic materials. Computational and Theoretical Chemistry, 2001, 573, 1-10.	1.5	93
1436	Research activities of the theoretical chemistry group at the University of Tokyo. Computational and Theoretical Chemistry, 2001, 573, 91-128.	1.5	13
1437	Influence of local environment on electronic properties of Co atoms in the Tm <sub>3</sub> Co <sub>11</sub> B <sub>4</sub> compound. Journal of Magnetism and Magnetic Materials, 2001, 223, 119-126.	1.0	4
1438	Accuracy of atomic-sphere approximation in electronic-structure calculations for transition-metal systems. Journal of Magnetism and Magnetic Materials, 2001, 226-230, 384-385.	1.0	3
1439	First-principles calculations for vacancy formation energies in Ni and Fe: non-local effect beyond the LSDA and magnetism. Journal of Magnetism and Magnetic Materials, 2001, 226-230, 386-387.	1.0	20
1440	Nonlinear magnetoelastic effects in ultrathin epitaxial FCC Co(001) films. Journal of Magnetism and Magnetic Materials, 2001, 224, 1-4.	1.0	16
1441	X-ray photoemission spectra of UCo <sub>4</sub> B compound. Journal of Magnetism and Magnetic Materials, 2001, 236, 243-248.	1.0	4
1442	Self-diffusion of adatoms on Ni(100) surfaces. Journal of Physics Condensed Matter, 2001, 13, L321-L328.	0.7	18
1443	Ab initio density functional study of phase stability and noncollinear magnetism in Mn. Journal of Physics Condensed Matter, 2001, 13, L681-L688.	0.7	44
1444	Silicon and carbon structures with icosahedral order, phason jumps, and disorder. Ferroelectrics, 2001, 250, 213-218.	0.3	2
1445	Electronic structure of sub-stoichiometric iron aluminide clusters. Journal of Physics Condensed Matter, 2001, 13, 8363-8374.	0.7	13

#	ARTICLE	IF	CITATIONS
1446	Density Functional Theory, Methods, Techniques, and Applications. , 2001, , 105-160.		1
1448	Accurate atomistic simulation of $\langle i \rangle a \langle /i \rangle / 2$ $\tilde{\alpha} \in 111 \tilde{\alpha} \in \%$ screw dislocations and other defects in bcc tantalum. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2001, 81, 1355-1385.	0.8	110
1449	The Valency Effect on Reaction Pathways in Heterogeneous Catalysis: Insight from Density Functional Theory Calculations. Progress in Theoretical Chemistry and Physics, 2001, , 199-215.	0.2	4
1450	Electronic properties of a grain boundary in Sb-doped ZnO. Journal of Physics Condensed Matter, 2001, 13, 9937-9943.	0.7	26
1451	Does density-functional theory predict a spin-density-wave ground state for Cr?. Journal of Physics Condensed Matter, 2001, 13, L239-L247.	0.7	20
1452	Realization of an effective ultrahigh magnetic field on a nanoscale. Journal of Physics Condensed Matter, 2001, 13, L49-L55.	0.7	4
1453	Structural and electronic properties of metal-silicide/silicon interfaces: A first-principles study. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2001, 19, 1180.	1.6	24
1454	Electronic structure of ferroelectric $\text{PbZr} \hat{A}^{1/2} \text{Ti} \hat{A}^{1/2} \text{O}_3$ by first principle. Ferroelectrics, 2001, 259, 121-126.	0.3	0
1455	Molecular Dynamics simulation of aqueous $\text{ZnCl}_2$ solutions. Molecular Physics, 2001, 99, 825-833.	0.8	37
1456	Chapter 2 Density functional theory applied to 4f and 5f elements and metallic compounds. Handbook of Magnetic Materials, 2001, 13, 87-228.	0.6	12
1457	Ab initio molecular dynamics of liquid carbon disulphide. Molecular Physics, 2001, 99, 855-863.	0.8	1
1458	Adsorption-Induced Step Formation. Physical Review Letters, 2001, 87, 126102.	2.9	65
1459	Tight-binding approach to time-dependent density-functional response theory. Physical Review B, 2001, 63, .	1.1	341
1460	Chapter 3 Magneto-optical kerr spectra. Handbook of Magnetic Materials, 2001, , 229-422.	0.6	39
1461	Atomic structures and energetics of $\text{LaNi}_5 \tilde{\alpha} \sim \text{H}$ solid solution and hydrides. Physical Review B, 2001, 64, .	1.1	54
1462	One-Dimensional Metallic Edge States in $\text{MoS}_2$ . Physical Review Letters, 2001, 87, 196803.	2.9	563
1463	First-principles study of $\text{Ca}^{2+}$ and $\text{Mn}^{2+}$ substituents in $\text{KTaO}_3$ . Physical Review B, 2001, 63, .	1.1	22
1464	First-principles study of surface and subsurface O structures at $\text{Al}(111)$ . Physical Review B, 2001, 63, .	1.1	93

#	ARTICLE	IF	CITATIONS
1465	Prediction of Electronic Excited States of Adsorbates on Metal Surfaces from First Principles. Physical Review Letters, 2001, 86, 5954-5957.	2.9	111
1466	Stability of native defects in hexagonal and cubic boron nitride. Physical Review B, 2001, 63, .	1.1	163
1467	Chain Formation of Metal Atoms. Physical Review Letters, 2001, 87, 266101.	2.9	242
1468	n- and p-type dopants for cubic silicon nitride. Applied Physics Letters, 2001, 78, 1577-1579.	1.5	22
1469	Structure Sensitive Reaction Channels of Molecular Hydrogen on Silicon Surfaces. Physical Review Letters, 2001, 86, 123-126.	2.9	52
1470	Initial stages of oxidation of (100) and (110) surfaces of iron caused by water. Physical Review B, 2001, 64, .	1.1	98
1471	Equation of state for tantalum from relativistic linear combinations of Gaussian-type orbitals calculations. Physical Review B, 2001, 64, .	1.1	14
1472	Density-functional calculation of van der Waals forces for free-electron-like surfaces. Physical Review B, 2001, 64, .	1.1	49
1473	Density-functional theory calculations of the interaction of protons and water with low-coordinated surface sites of calcium oxide. Physical Review B, 2001, 63, .	1.1	37
1474	Direct comparisons of rates for low temperature diffusion of hydrogen and deuterium on Cu(001) from quantum mechanical calculations and scanning tunneling microscopy experiments. Journal of Chemical Physics, 2001, 115, 5620-5624.	1.2	47
1475	Bond formation in titanium fulleride compounds studied through x-ray emission spectroscopy. Physical Review B, 2001, 63, .	1.1	23
1476	Electronic structure, bonding nature, and charge transfer in Ba@Si <sub>20</sub> and Si <sub>20</sub> clusters: An ab initio study. Physical Review B, 2001, 64, .	1.1	27
1477	Structure of aluminum atomic chains. Physical Review B, 2001, 64, .	1.1	61
1478	Structure and magnetism in thin films and multilayers of hexagonal ruthenium and iron. Physical Review B, 2001, 63, .	1.1	13
1479	A transversing connection between density functionals. Journal of Chemical Physics, 2001, 114, 6505-6513.	1.2	19
1480	Quantum treatment of H adsorbed on a Pt(111) surface. Physical Review B, 2001, 65, .	1.1	62
1481	All-electron and pseudopotential study of the spin-polarization of the V(001) surface: LDA versus GGA. Physical Review B, 2001, 63, .	1.1	34
1482	The performance of density functional theory for equilibrium molecular properties of symmetry breaking molecules. Journal of Chemical Physics, 2001, 114, 8257-8269.	1.2	39

#	ARTICLE	IF	CITATIONS
1483	Patterning of Si(001) with halogens: Surface structure as a function of the halogen chemical potential. <i>Physical Review B</i> , 2001, 64, .	1.1	23
1484	Coverage dependence of N <sub>2</sub> dissociation at an N, O, or H precovered Ru(0001) surface investigated with density functional theory. <i>Physical Review B</i> , 2001, 63, .	1.1	67
1485	Pseudopotential description of rare earths in oxides: The case of Er <sub>2</sub> Si <sub>2</sub> O <sub>7</sub> . <i>Physical Review B</i> , 2001, 63, .	1.1	9
1486	Further developments in the local-orbital density-functional-theory tight-binding method. <i>Physical Review B</i> , 2001, 64, .	1.1	232
1487	Computational study of Cs immobilization in the apatites Ca <sub>10</sub> (PO <sub>4</sub> ) <sub>6</sub> F <sub>2</sub> , Ca <sub>4</sub> La <sub>6</sub> (SiO <sub>4</sub> ) <sub>6</sub> F <sub>2</sub> and Ca <sub>2</sub> La <sub>8</sub> (SiO <sub>4</sub> ) <sub>6</sub> O <sub>2</sub> . <i>Physical Review B</i> , 2001, 64, .	1.1	37
1488	Electronic structure of calcium clusters. <i>Physical Review A</i> , 2001, 63, .	1.0	37
1489	Theoretical study of chlorine adsorption on the Ag(111) surface. <i>Physical Review B</i> , 2001, 63, .	1.1	57
1490	Adsorbate-induced demagnetization and restructuring of ultrathin magnetic films: CO chemisorbed on <sup>3</sup> Fe/Cu(100). <i>Physical Review B</i> , 2001, 64, .	1.1	18
1491	Magnetic coupling and site occupancy of impurities in Fe <sub>3</sub> Al. <i>Physical Review B</i> , 2001, 64, .	1.1	15
1492	Density functional theory studies of the adsorption of ethylene and oxygen on Pt(111) and Pt[ <sub>3</sub> Sn(111)]. <i>Journal of Chemical Physics</i> , 2001, 114, 4663.	1.2	80
1493	Ab initio study of hexagonal Fe/Ru multilayers. <i>Journal of Applied Physics</i> , 2001, 89, 7080-7082.	1.1	2
1494	Reconstruction of frozen-core all-electron orbitals from pseudo-orbitals. <i>Journal of Chemical Physics</i> , 2001, 115, 5791-5795.	1.2	32
1495	Adhesion of ultrathin ZrO <sub>2</sub> (111) films on Ni(111) from first principles. <i>Journal of Chemical Physics</i> , 2001, 114, 5816-5831.	1.2	112
1496	Strontium clusters: Many-body potential, energetics, and structural transitions. <i>Journal of Chemical Physics</i> , 2001, 115, 3640-3646.	1.2	25
1497	General trends in CO dissociation on transition metal surfaces. <i>Journal of Chemical Physics</i> , 2001, 114, 8244-8247.	1.2	211
1498	Density-functional description of spinel ZnFe <sub>2</sub> O <sub>4</sub> . <i>Physical Review B</i> , 2001, 63, .	1.1	32
1499	Te covered Si(001): A variable surface reconstruction. <i>Physical Review B</i> , 2001, 64, .	1.1	6
1500	Optical studies of gap, hopping energies, and the Anderson-Hubbard parameter in the zigzag-chain compound SrCuO <sub>2</sub> . <i>Physical Review B</i> , 2001, 63, .	1.1	20

#	ARTICLE	IF	CITATIONS
1501	Kinetics of fast island decay on Ag(111). <i>Physical Review B</i> , 2001, 63, .	1.1	42
1502	Nucleation of $\text{c}^{\sim}\text{B}$ on hexagonal boron nitride. <i>Physical Review B</i> , 2001, 64, .	1.1	13
1503	Spin-dependent electron momentum density in the $\text{Ni}_2\text{MnSn}$ Heusler alloy. <i>Physical Review B</i> , 2001, 63, .	1.1	21
1504	Chemical effects in rare gas adsorption: FLAPW calculations for $\text{Ag}(001)\text{c}(2\text{\AA}-2)\text{\AA}^{\sim}\text{Xe}$ . <i>Physical Review B</i> , 2001, 63, .	1.1	22
1505	Oxygen-induced $\text{Rh}_{3d5/2}$ surface core-level shifts on Rh(111). <i>Physical Review B</i> , 2001, 63, .	1.1	72
1506	Effect of tip morphology on image formation in noncontact atomic force microscopy: $\text{\AA}^{\sim}\text{InP}(110)$ . <i>Physical Review B</i> , 2001, 63, .	1.1	36
1507	Magneto-electronic properties of a ferrimagnetic semiconductor: The hybrid cupromanganite $\text{CaCu}_3\text{Mn}_4\text{O}_{12}$ . <i>Physical Review B</i> , 2001, 65, .	1.1	80
1508	Role of electron-electron correlation in the valence states of $\text{YBa}_2\text{Cu}_3\text{O}_7$ : Low-energy excitations and Fermi surface. <i>Physical Review B</i> , 2001, 64, .	1.1	8
1509	Ab initio analysis of energetics of $\text{f}$ -phase formation in Cr-based systems. <i>Physical Review B</i> , 2001, 63, .	1.1	41
1510	Parameter-free calculation of $\text{K}^{\pm}$ chemical shifts for Al, Si, and Ge oxides. <i>Physical Review B</i> , 2001, 63, .	1.1	2
1511	Bonding and physical properties of Hume-Rothery compounds with the $\text{PtHg}_4$ structure. <i>Physical Review B</i> , 2001, 63, .	1.1	30
1512	Towards 100% spin-polarized charge-injection: The half-metallic $\text{NiMnSb}/\text{CdS}$ interface. <i>Physical Review B</i> , 2001, 64, .	1.1	184
1513	Femtosecond electron dynamics of image-potential states on clean and oxygen-covered Pt(111). <i>Physical Review B</i> , 2001, 63, .	1.1	67
1514	First-principles simulation of atomic force microscopy image formation on a GaAs(110) surface: Effect of tip morphology. <i>Physical Review B</i> , 2001, 63, .	1.1	37
1515	Symmetry and site selectivity in molecular chemisorption: Benzene on $\text{Ni}\{111\}$ . <i>Journal of Chemical Physics</i> , 2001, 114, 5765-5773.	1.2	72
1516	The competition between chemical bonding and magnetism in the adsorption of atomic Ni on $\text{MgO}(100)$ . <i>Journal of Chemical Physics</i> , 2001, 115, 8172-8177.	1.2	50
1517	Relativistic spin-density-functional theory: Robust solution of single-particle equations for open-subshell atoms. <i>Physical Review B</i> , 2001, 64, .	1.1	15
1518	Comparison of global and local adaptive coordinates for density-functional calculations. <i>Physical Review B</i> , 2001, 63, .	1.1	86



#	ARTICLE	IF	CITATIONS
1519	Investigation of the Correlation Potential from Kohn-Sham Perturbation Theory. <i>Physical Review Letters</i> , 2001, 86, 2241-2244.	2.9	76
1520	Electronic structure and the x-ray photoemission spectrum of the Kondo-dense compound $UCu_5Al$ . <i>Physical Review B</i> , 2001, 64, .	1.1	9
1521	First-principle theoretical study on reliability $SiO_2$ thin films under external electric field. , 0, , .		2
1522	Hydrogen in jellium: First-principles pair interactions. <i>Physical Review B</i> , 2001, 64, .	1.1	22
1523	Origin of the $c/a$ variation in hexagonal close-packed divalent metals. <i>Physical Review B</i> , 2001, 64, .	1.1	50
1524	Growth of face-centered-cubic Fe films on Cu(100): Interdiffusion, surfactant effects, and island formation. <i>Physical Review B</i> , 2001, 64, .	1.1	29
1525	Two Disordered Phases of the $\sqrt{2}$ -Tin Structure in Binary Semiconductors. <i>Physical Review Letters</i> , 2001, 86, 5301-5304.	2.9	10
1526	Surface phase stability diagram for Pd deposits on Ni(110): A first-principles theoretical study. <i>Physical Review B</i> , 2001, 64, .	1.1	20
1527	First-principles equations of state for simulations of shock waves in silicon. <i>Physical Review B</i> , 2001, 64, .	1.1	38
1528	Density-functional calculations of semiconductor properties using a semiempirical exchange-correlation functional. <i>Physical Review B</i> , 2001, 63, .	1.1	38
1529	Thermodynamics of uniaxial phase transition: A first-principles study of the diamond-to- $\sqrt{2}$ -tin transition in Si and Ge. <i>Physical Review B</i> , 2001, 63, .	1.1	23
1530	Neglected adsorbate interactions behind diffusion prefactor anomalies on metals. <i>Physical Review B</i> , 2001, 64, .	1.1	68
1531	Atomic and electronic structures of a Boron impurity and its diffusion pathways in crystalline Si. <i>Physical Review B</i> , 2001, 64, .	1.1	85
1532	Vibrational modes of $c(4\sqrt{2}) \times c(4\sqrt{2}) \times c(4\sqrt{2})$ CO/Pt(111) from first-principles calculations. <i>Journal of Chemical Physics</i> , 2001, 114, 530.	1.2	6
1533	An experimental and theoretical investigation of the thiophene/aluminum interface. <i>Journal of Chemical Physics</i> , 2001, 114, 935.	1.2	30
1534	Luminescent $FeSi_2$ Crystal Structures Induced by Heteroepitaxial Stress on Si(111). <i>Physical Review Letters</i> , 2001, 86, 6006-6009.	2.9	83
1535	On the Constitution of Sodium at Higher Densities. <i>Physical Review Letters</i> , 2001, 86, 2830-2833.	2.9	145
1536	Symmetry Selection Rules for Vibrationally Inelastic Tunneling. <i>Physical Review Letters</i> , 2001, 86, 2593-2596.	2.9	182

#	ARTICLE	IF	CITATIONS
1537	Surface Relaxations, Current Enhancements, and Absolute Distances in High Resolution Scanning Tunneling Microscopy. <i>Physical Review Letters</i> , 2001, 87, 236104.	2.9	134
1538	First-principle electronic properties of ZrO <sub>2</sub> and HfO <sub>2</sub> crystals under external electric field. , 0, , .		2
1539	Hydrogenation of S to H <sub>2</sub> S on Pt(111): A first-principles study. <i>Journal of Chemical Physics</i> , 2001, 115, 8570-8574.	1.2	46
1540	Solving the structural model for the Si(001)–In(4Å–3) surface. <i>Applied Physics Letters</i> , 2001, 79, 203-205.	1.5	9
1541	An evaluation of the density functional approach in the zero order regular approximation for relativistic effects: Magnetic interactions in small metal compounds. <i>Journal of Chemical Physics</i> , 2001, 114, 4421.	1.2	78
1542	Mechanism of Interstitial Oxygen Diffusion in Hafnia. <i>Physical Review Letters</i> , 2002, 89, 225901.	2.9	146
1543	The Role of the Nanoscale in Surface Reactions:CO <sub>2</sub> on CdSe. <i>Physical Review Letters</i> , 2002, 89, 075506.	2.9	22
1544	Vibrational Recognition of Hydrogen-Bonded Water Networks on a Metal Surface. <i>Physical Review Letters</i> , 2002, 89, 176104.	2.9	229
1545	Stability of a Flexible Polar Ionic Crystal Surface: Metastable Alumina and One-Dimensional Surface Metallicity. <i>Physical Review Letters</i> , 2002, 88, 226101.	2.9	25
1546	Two-Dimensional Oxide on Pd(111). <i>Physical Review Letters</i> , 2002, 88, 246103.	2.9	267
1547	DFT modelling of hydrogen on Cu(110)- and (111)-type clusters. <i>Molecular Simulation</i> , 2002, 28, 807-825.	0.9	13
1548	Ab initio density functional investigation of the (001) surface of mordenite. <i>Journal of Chemical Physics</i> , 2002, 117, 7295-7305.	1.2	48
1549	Computational Methods for Homogeneous Catalysis. <i>Catalysis By Metal Complexes</i> , 2002, , 1-21.	0.6	5
1550	Surface model and exchange-correlation functional effects on the description of Pd/Al <sub>2</sub> O <sub>3</sub> (0001). <i>Journal of Chemical Physics</i> , 2002, 116, 1684-1691.	1.2	51
1551	Electronic structure and chemical bonding in nonstoichiometric molecules: Al <sub>3</sub> X <sub>2</sub> (X=C,Si,Ge). A photoelectron spectroscopy and ab initio study. <i>Journal of Chemical Physics</i> , 2002, 116, 1330-1338.	1.2	36
1552	Design of a heterostructure peapod using magic silicon clusters. <i>Physical Review B</i> , 2002, 66, .	1.1	13
1553	Adsorption and dissociation of O <sub>2</sub> on Ir(111). <i>Journal of Chemical Physics</i> , 2002, 116, 10846-10853.	1.2	67
1554	First-principles study of the adsorption of sulfur on Pt(111): S core-level shifts and the nature of the Pt-S bond. <i>Physical Review B</i> , 2002, 65, .	1.1	48

#	ARTICLE	IF	CITATIONS
1555	Assessment of time-dependent density-functional theory for the calculation of critical features in the absorption spectra of a series of aromatic donor-acceptor systems. Journal of Chemical Physics, 2002, 116, 8761-8771.	1.2	98
1556	Chemisorption of pyrrole and polypyrrole on Si(001). Physical Review B, 2002, 66, .	1.1	31
1557	Density-functional study of $S_2$ defects in alkali halides. Physical Review B, 2002, 66, .	1.1	11
1558	Energetics of transition-metal ions in low-coordination environments. Physical Review B, 2002, 66, .	1.1	2
1559	First-principles investigations for $YH_3$ (YD3): Energetics, electric-field gradients, and optical properties. Physical Review B, 2002, 66, .	1.1	19
1560	Total energy of solids: An exchange and random-phase approximation correlation study. Physical Review B, 2002, 66, .	1.1	102
1561	Delocalization and phase transitions in Pr: Theory. Physical Review B, 2002, 65, .	1.1	32
1562	Hydrogen bonding and protonation in acid-base complexes: Methanesulfonic acid-pyridine. Journal of Chemical Physics, 2002, 116, 2417-2424.	1.2	33
1563	Structural characterization of the hydrogen-covered C(100) surface by density functional theory calculations. Physical Review B, 2002, 66, .	1.1	38
1564	Adiabatic potential-energy surfaces for oxygen on Al(111). Physical Review B, 2002, 65, .	1.1	93
1565	First-principles modeling of paramagnetic Si dangling-bond defects in amorphous $SiO_2$ . Physical Review B, 2002, 66, .	1.1	47
1566	Subsystem functionals in density-functional theory: Investigating the exchange energy per particle. Physical Review B, 2002, 66, .	1.1	53
1567	Ab initio study of field evaporation from single-walled carbon nanotubes. Physical Review B, 2002, 65, .	1.1	9
1568	Thermodynamic properties of the Si- $SiO_2$ system. Journal of Chemical Physics, 2002, 117, 1843-1850.	1.2	11
1569	Density-functional study of structural and electronic properties of $N_nLi_nNa_n$ ( $1 \leq n \leq 12$ ) clusters. Physical Review A, 2002, 65, .	1.0	29
1570	Electronic structure and chemical bonding of $B_5^{+}$ and $B_5$ by photoelectron spectroscopy and ab initio calculations. Journal of Chemical Physics, 2002, 117, 7917-7924.	1.2	222
1571	Ab initio calculations for bromine adlayers on the Ag(100) and Au(100) surfaces: The $c(2\sqrt{2})$ structure. Physical Review B, 2002, 65, .	1.1	26
1572	Hydrogen adsorption on an open metal surface: $H_2/Pd(210)$ . Physical Review B, 2002, 65, .	1.1	86

#	ARTICLE	IF	CITATIONS
1573	Novel Pathway to the Growth of Diamond on Cubic $\beta$ -SiC(001). Physical Review Letters, 2002, 88, 125504.	2.9	7
1574	First-principles study of MgB <sub>2</sub> (0001) surfaces. Physical Review B, 2002, 65, .	1.1	31
1575	Atomistic and electronic structure calculation of defects at the surfaces of oxides. Radiation Effects and Defects in Solids, 2002, 157, 773-781.	0.4	12
1576	Density-functional investigation of magnetism in $\delta$ -Pu. Physical Review B, 2002, 66, .	1.1	127
1577	Interaction of Pd with $\gamma$ -Al <sub>2</sub> O <sub>3</sub> (0001): a case study of modeling the metal-oxide interface on complex substrates. Physical Review B, 2002, 65, .	1.1	55
1578	Structural Identification of Metcars. Physical Review Letters, 2002, 88, 115504.	2.9	44
1579	Magnetization-Direction-Dependent Local Electronic Structure Probed by Scanning Tunneling Spectroscopy. Physical Review Letters, 2002, 89, 237205.	2.9	116
1580	First-principles calculations of the adsorption, diffusion, and dissociation of a CO molecule on the Fe(100) surface. Physical Review B, 2002, 66, .	1.1	121
1581	Hydrogen defects in Forsterite: A test case for the embedded cluster method. Journal of Chemical Physics, 2002, 116, 2628-2635.	1.2	38
1582	Quantum mechanical behavior of an H atom on Cu(111) and Pt(111). Journal of Applied Physics, 2002, 91, 1855-1859.	1.1	20
1583	Ab initio pseudopotential study of a model tetracene/ZnSe organic-inorganic superlattice: Its electronic structure and optical responses. Journal of Applied Physics, 2002, 92, 5779-5784.	1.1	0
1584	Self-Diffusion Rates in Al from Combined First-Principles and Model-Potential Calculations. Physical Review Letters, 2002, 89, 065901.	2.9	67
1585	Kohn-Sham density-functional study of low-lying states of the iron clusters Fe <sup>n+</sup> /Fe <sup>n</sup> /Fe <sup>n-</sup> (n=1-4). Physical Review B, 2002, 66, .	1.1	58
1586	Low-Energy Linear Structures in Dense Oxygen: Implications for the $\mu$ Phase. Physical Review Letters, 2002, 88, 205503.	2.9	59
1587	Electronic properties of ferroelectric SrBi <sub>2</sub> Ta <sub>2</sub> O <sub>9</sub> , SrBi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub> , and PbBi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub> with optimized structures. Applied Physics Letters, 2002, 80, 2967-2969.	1.5	48
1588	Formation energy of Cr/Al vacancies in spinel MgCr <sub>2</sub> O <sub>4</sub> and MgAl <sub>2</sub> O <sub>4</sub> by first-principles calculations. Physical Review B, 2002, 65, .	1.1	21
1589	Energy barriers and chemical properties in the coadsorption of carbon monoxide and oxygen on Ru(0001). Physical Review B, 2002, 65, .	1.1	38
1590	First-principles electronic structure study of Ti-PTCDA contacts. Physical Review B, 2002, 65, .	1.1	25

#	ARTICLE	IF	CITATIONS
1591	Comment on "Theoretical prediction of phase transition in gold". Physical Review B, 2002, 66, .	1.1	17
1592	(3Å-3)R30°(K+CO)coadsorption structure on Pt(111): Experiment and theory. Physical Review B, 2002, 66, .	1.1	5
1593	Long-range ordering of methylidyne on Pt{110}(1Å-2). Journal of Chemical Physics, 2002, 117, 3951-3955.	1.2	3
1594	Structure and growth modes of (BaO) <sub>n</sub> (n ≈ 1/2) clusters. Journal of Chemical Physics, 2002, 116, 1339-1342.	1.2	7
1595	Importance of open-shell effects in adhesion at metal-ceramic interfaces. Physical Review B, 2002, 66, .	1.1	29
1596	Spontaneous dissociation of a conjugated molecule on the Si(100) surface. Journal of Chemical Physics, 2002, 117, 321-330.	1.2	32
1597	Electronic structure and isomer shifts of neptunium compounds. Physical Review B, 2002, 66, .	1.1	5
1598	Ab initio study on surface segregation of hydrogen from diamond C(100) surfaces. Physical Review B, 2002, 65, .	1.1	12
1599	Origin and consequences of aromatic back-bonding at a transition metal surface: Benzene on Ir{100}. Journal of Chemical Physics, 2002, 117, 819-824.	1.2	20
1600	Theoretical investigation of the pure and Zn-doped phases of Bi <sub>2</sub> O <sub>3</sub> . Physical Review B, 2002, 65, .	1.1	75
1601	Combining multideterminantal wave functions with density functionals to handle near-degeneracy in atoms and molecules. Journal of Chemical Physics, 2002, 116, 1250-1258.	1.2	146
1602	Atomic structures and bondings of $\beta$ - and spinel-Si <sub>6</sub> Al <sub>2</sub> O <sub>8</sub> by first-principles calculations. Physical Review B, 2002, 66, .	1.1	30
1603	Exchange potential from the common energy denominator approximation for the Kohn-Sham Green's function: Application to (hyper)polarizabilities of molecular chains. Journal of Chemical Physics, 2002, 116, 6435-6442.	1.2	91
1604	Electronic structure and hyperfine parameters of substitutional Al and P impurities in silica. Physical Review B, 2002, 65, .	1.1	22
1605	Structure and bonding of propyne on Cu(111) from density functional periodic and cluster models. Journal of Chemical Physics, 2002, 116, 1165-1170.	1.2	20
1606	Stability of subsurface oxygen at Rh(111). Physical Review B, 2002, 65, .	1.1	52
1607	Determination of the complete set of second-order magnetoelastic coupling constants on epitaxial films. Physical Review B, 2002, 65, .	1.1	14
1608	First-principles calculation of Li adatom structures on the Mo(112) surface. Physical Review B, 2002, 66, .	1.1	30

#	ARTICLE	IF	CITATIONS
1609	Tight-binding calculations of the band structure and total energies of the various phases of magnesium. <i>Physical Review B</i> , 2002, 65, .	1.1	40
1610	Determination of the Debye temperature of the $\gamma$ -phase Fe-Cr alloys. <i>Physical Review B</i> , 2002, 65, .	1.1	18
1611	First-principles study of nucleation, growth, and interface structure of Fe/GaAs. <i>Physical Review B</i> , 2002, 65, .	1.1	68
1612	Effect of Fock exchange on the electronic structure and magnetic coupling in NiO. <i>Physical Review B</i> , 2002, 65, .	1.1	360
1613	Comment on "Magnetism of the V(001) surface: Contradictory results from pseudopotential and linearized augmented plane-wave calculations". <i>Physical Review B</i> , 2002, 66, .	1.1	23
1614	Ground-state geometries and optical properties of $\text{Na}_8\text{Li}_x$ ( $x=0-8$ ) clusters. <i>Physical Review A</i> , 2002, 65, .	1.0	13
1615	Coverage dependence of hydrogen absorption into Pd(111). <i>Journal of Applied Physics</i> , 2002, 92, 5704-5706.	1.1	24
1616	Density-functional study of water adsorption on the $\text{PuO}_2(110)$ surface. <i>Physical Review B</i> , 2002, 65, .	1.1	136
1617	Nonlocal density-functional description of exchange and correlation in silicon. <i>Physical Review B</i> , 2002, 65, .	1.1	44
1618	First-principles investigation of $\text{MnFe}_2\text{O}_4$ . <i>Physical Review B</i> , 2002, 65, .	1.1	41
1619	Shear-strain-related nonlinear magnetoelastic properties of epitaxial films. <i>Physical Review B</i> , 2002, 65, .	1.1	14
1620	Metal nanoparticles as models of single crystal surfaces and supported catalysts: Density functional study of size effects for CO/Pd(111). <i>Journal of Chemical Physics</i> , 2002, 117, 9887-9896.	1.2	144
1621	Formation of an ordered Si dimer structure on $\text{HfB}_2(0001)$ . <i>Physical Review B</i> , 2002, 66, .	1.1	9
1622	Assigning the $(1\bar{1}-2)$ surface reconstruction on reduced rutile by first-principles energetics. <i>Physical Review B</i> , 2002, 65, .	1.1	18
1623	Chemisorption-induced disruption of surface electronic structure: Hydrogen adsorption on the $\text{Si}(100)2\times 1$ surface. <i>Physical Review B</i> , 2002, 65, .	1.1	32
1624	Surface-induced stacking transition at $\text{SiC}(0001)$ . <i>Physical Review B</i> , 2002, 66, .	1.1	47
1625	Structure and dynamics of atomic hydrogen on $\text{NiAl}(110)$ . <i>Physical Review B</i> , 2002, 65, .	1.1	7
1626	Structural and superconducting transitions in $\text{Mg}_{1-x}\text{Al}_x\text{B}_2$ . <i>Physical Review B</i> , 2002, 66, .	1.1	19

#	ARTICLE	IF	CITATIONS
1627	First-principles studies of the structural and electronic properties of pyrite FeS <sub>2</sub> . Physical Review B, 2002, 65, .	1.1	64
1628	Spontaneous magnetization of aluminum nanowires deposited on the NaCl(100) surface. Physical Review B, 2002, 66, .	1.1	31
1629	PERIODIC DFT STUDY OF ISOMORPHOUS INCORPORATION OF A V ION INTO (100) AND (001) ANATASE SURFACE LAYERS. Surface Review and Letters, 2002, 09, 1425-1430.	0.5	7
1630	Laminar Growth of Ultrathin Metal Films on Metal Oxides: Co on Hydroxylated alpha -Al <sub>2</sub> O <sub>3</sub> (0001). Science, 2002, 297, 827-831.	6.0	132
1631	Atomistic study of rare-earth compounds R <sub>2</sub> Fe <sub>17</sub> (R=Y, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Lu) and Nd <sub>2</sub> Fe <sub>17</sub> N <sub>x</sub> . Modelling and Simulation in Materials Science and Engineering, 2002, 10, 425-435.	0.8	5
1632	Vibrational properties of an H atom adsorbed on Pt(111). Surface Science, 2002, 507-510, 82-86.	0.8	19
1633	Second-order magnetoelastic effects: From the Dirac equation to the magnetic properties of ultrathin epitaxial films for magnetic thin-film applications. International Journal of Materials Research, 2002, 93, 970-973.	0.8	2
1634	Covalent bonding and bandgap formation in transition-metal aluminides: di-aluminides of group VIII transition metals. Journal of Physics Condensed Matter, 2002, 14, 5755-5783.	0.7	48
1635	Magnetic Properties of Fe Thin Films on Cu(111). Journal of the Physical Society of Japan, 2002, 71, 2983-2985.	0.7	11
1636	Tight-binding study of high-pressure phase transitions in titanium: Alpha to omega and beyond. Europhysics Letters, 2002, 60, 248-254.	0.7	28
1637	Band Structure of the Non-Oxide Perovskite MgCNi <sub>3</sub> . Chinese Physics Letters, 2002, 19, 1522-1524.	1.3	4
1638	First-principles study on molecular dissociation under metallization pressure in aromatic monomolecular crystals with iodine atoms. Journal of Physics Condensed Matter, 2002, 14, 10429-10432.	0.7	6
1639	Charge accumulation and barrier formation at grain boundaries in ZnO decorated with bismuth. Journal of Physics Condensed Matter, 2002, 14, 12717-12724.	0.7	8
1640	Chapter 10 Relativistic density functional theory: Foundations and basic formalism. Theoretical and Computational Chemistry, 2002, 11, 523-621.	0.2	39
1641	Electronic band structure and the X-ray photoemission spectrum of UCu <sub>5</sub> In. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 2002, 82, 1893-1906.	0.6	8
1642	Electron-phonon coupling at metal surfaces. Journal of Physics Condensed Matter, 2002, 14, 5959-5977.	0.7	84
1643	Dense Kondo compound UCu <sub>5</sub> Sn - electronic structure and x-ray photoemission. Journal of Physics Condensed Matter, 2002, 14, 3199-3209.	0.7	8
1644	Orbital-Free Kinetic-Energy Density Functional Theory. , 2002, , 117-184.		61



#	ARTICLE	IF	CITATIONS
1645	Quenching Studies of Lattice Vacancies in High-Purity Aluminium. <i>Materials Transactions</i> , 2002, 43, 186-198.	0.4	28
1646	First-Principles Investigation of L1 <sub>0</sub> -Disorder Phase Equilibrium in Fe-Pt System. <i>Materials Transactions</i> , 2002, 43, 2104-2109.	0.4	59
1647	Theoretical Formation Energy of Oxygen-Vacancies in Oxides. <i>Materials Transactions</i> , 2002, 43, 1426-1429.	0.4	101
1648	First-Principles Calculations of Co Impurities and Native Defects in ZnO. <i>Materials Transactions</i> , 2002, 43, 1439-1443.	0.4	20
1649	Theoretical Solution Energy of Alkaline Earth Ions in Lanthanum Chromites. <i>Materials Transactions</i> , 2002, 43, 1456-1459.	0.4	3
1650	Ab Initio Studies On Phase Behavior of Barium Titanate. <i>Materials Research Society Symposia Proceedings</i> , 2002, 718, 1.	0.1	14
1651	Nanoscale Structure/Property Correlation Through Aberration-Corrected Stem And Theory. <i>Materials Research Society Symposia Proceedings</i> , 2002, 738, 111.	0.1	1
1652	The Properties of a Na-Doped Twist Boundary in SrTiO <sub>3</sub> from First Principles. <i>Materials Research Society Symposia Proceedings</i> , 2002, 751, 1.	0.1	2
1653	Density Functional Studies of Magnetic Ordering, Lattice Distortion, and Transport in Manganites. , 2002, , 87-101.		0
1654	Oxides, Silicides, and Silicates of Zirconium and Hafnium; Density Functional Theory Study. <i>Materials Research Society Symposia Proceedings</i> , 2002, 716, 651.	0.1	0
1655	Estimation of C-H Bond Dissociation Enthalpies of Large Aromatic Hydrocarbon Compounds Using DFT Methods. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7184-7189.	1.1	76
1656	Theoretical Study of Structural and Electronic Properties of Methyl Silsesquioxanes. <i>Journal of Physical Chemistry B</i> , 2002, 106, 1709-1713.	1.2	35
1657	Novel Organotellurium(IV) Diazides and Triazides#. <i>Inorganic Chemistry</i> , 2002, 41, 1184-1193.	1.9	44
1658	Four- and Five-Coordinate CO Insertion in the Copolymerization of Carbon Monoxide and Olefins Catalyzed by Diphosphine Nickel(II) Complexes: A Dynamical Density Functional Study. <i>Organometallics</i> , 2002, 21, 2036-2040.	1.1	15
1659	Study of Thermally Treated Lithium Montmorillonite by Ab Initio Methods. <i>Journal of Physical Chemistry B</i> , 2002, 106, 12470-12477.	1.2	35
1660	Ab initioquasiharmonic equations of state for dynamically stabilized soft-mode materials. <i>Physical Review B</i> , 2002, 65, .	1.1	54
1661	Dimensional changes as a function of charge injection for trans-polyacetylene: A density functional theory study. <i>Journal of Chemical Physics</i> , 2002, 117, 7691-7697.	1.2	19
1662	Fe nanowires on vicinal Cu surfaces: Ab initio study. <i>Physical Review B</i> , 2002, 65, .	1.1	78

#	ARTICLE	IF	CITATIONS
1663	Density Functional Study of Benzene Adsorption on Pt(111). <i>Journal of Physical Chemistry B</i> , 2002, 106, 7489-7498.	1.2	166
1664	Dynamical Density Functional Study of Acetylene to Vinylidene Isomerization in (Cp)(CO) <sub>2</sub> Mn(HC≡CH). <i>Organometallics</i> , 2002, 21, 2715-2723.	1.1	48
1665	A First Principles Study of Carbon-Carbon Coupling over the {0001} Surfaces of Co and Ru. <i>Journal of Physical Chemistry B</i> , 2002, 106, 2826-2829.	1.2	67
1666	Ab Initio Structure of the (Na <sub>2</sub> [CAI <sub>4</sub> ]) <sub>2</sub> Dimer. Next Step Toward Solid Materials Containing Tetracoordinate Planar Carbon. <i>Inorganic Chemistry</i> , 2002, 41, 2795-2798.	1.9	42
1667	Density functional study on metastable bcc copper: Electronic structure and momentum density of positron-electron pairs. <i>Physical Review B</i> , 2002, 65, .	1.1	52
1668	Density Functional Theory Calculations of Solid Solutions of Fluor- and Chlorapatites. <i>Chemistry of Materials</i> , 2002, 14, 435-441.	3.2	23
1669	STM Images and Chemisorption Bond Parameters of Acetylene, Ethynyl, and Dicarbon Chemisorbed on Copper. <i>Journal of Physical Chemistry B</i> , 2002, 106, 8161-8171.	1.2	32
1670	Search for Ionic Orthocarbonates: An Ab Initio Study of Na <sub>4</sub> CO <sub>4</sub> . <i>Journal of Physical Chemistry A</i> , 2002, 106, 8951-8954.	1.1	12
1671	Peculiar Antiaromatic Inorganic Molecules of Tetrapnictogen in Na <sub>2</sub> Pn <sub>4</sub> (Pn = P, As, Sb) and Important Consequences for Hydrocarbons. <i>Inorganic Chemistry</i> , 2002, 41, 6062-6070.	1.9	66
1672	Trigonal Prismatic Structure of Tris(butadiene)molybdenum and Related Complexes Revisited: Diolefin or Metallacyclopentene Coordination?. <i>Organometallics</i> , 2002, 21, 5021-5028.	1.1	17
1673	A Comparative Theoretical Investigation of Three Sodalite Systems: Cd <sub>4</sub> S(AlO <sub>2</sub> ) <sub>6</sub> , Zn <sub>4</sub> O(BO <sub>2</sub> ) <sub>6</sub> , and Zn <sub>4</sub> S(BO <sub>2</sub> ) <sub>6</sub> . <i>Journal of Physical Chemistry B</i> , 2002, 106, 2569-2573.	1.2	8
1674	Theoretical Studies on the Insertions of Unsymmetrical Alkynes into the Metal-Carbon Bond of Phosphanickelacycles: Electronic Factors. <i>Organometallics</i> , 2002, 21, 1278-1289.	1.1	25
1675	First Principles Calculations of the Adsorption Properties of CO and NO on the Defective TiO <sub>2</sub> (110) Surface. <i>Journal of Physical Chemistry B</i> , 2002, 106, 6184-6199.	1.2	66
1676	Theoretical Analysis of the CH Stretching Overtone Vibration of 1,2-Dichloroethylene. <i>Journal of Physical Chemistry A</i> , 2002, 106, 2676-2684.	1.1	36
1677	Dramatic Cooperative Effects in Adsorption of NO <sub>x</sub> on MgO(001). <i>Journal of Physical Chemistry B</i> , 2002, 106, 7405-7413.	1.2	86
1678	A Density Functional Theory Study on the Active Center of Fe-Only Hydrogenase: Characterization and Electronic Structure of the Redox States. <i>Journal of the American Chemical Society</i> , 2002, 124, 5175-5182.	6.6	168
1679	A Dynamic Density Functional Study of the Stepwise Migratory Insertion of Isocyanides into Zirconium-Carbon Bonds Anchored to a Calix[4]arene Moiety. <i>Organometallics</i> , 2002, 21, 4090-4098.	1.1	7
1680	In Search of Covalently Bound Tetra- and Penta-Oxygen Species: A Photoelectron Spectroscopic and Ab Initio Investigation of MO <sub>4</sub> - and MO <sub>5</sub> - (M = Li, Na, K, Cs). <i>Journal of the American Chemical Society</i> , 2002, 124, 6742-6750.	6.6	15

#	ARTICLE	IF	CITATIONS
1681	Adhesion, atomic structure, and bonding at the Al(111)/Al <sub>2</sub> O <sub>3</sub> (0001) interface: A first principles study. <i>Physical Review B</i> , 2002, 65, .	1.1	212
1682	Density Functional Study of the Mechanism of a Tyrosine Phosphatase: I. Intermediate Formation. <i>Journal of the American Chemical Society</i> , 2002, 124, 10225-10235.	6.6	44
1683	Diels-Alder Reaction of Phosphaethene with 1,3-Dienes: An ab Initio Study. <i>Journal of Organic Chemistry</i> , 2002, 67, 9162-9174.	1.7	22
1684	De Novo Ligand Design: Understanding Stereoselective Olefin Binding to [( $\eta$ -5-C <sub>5</sub> H <sub>5</sub> )Re(NO)(PPh <sub>3</sub> )] <sup>+</sup> with Molecular Mechanics, Semiempirical Quantum Mechanics, and Density Functional Theory. <i>Organometallics</i> , 2002, 21, 3913-3921.	1.1	13
1685	From Local Adsorption Stresses to Chiral Surfaces: (R,R)-Tartaric Acid on Ni(110). <i>Journal of the American Chemical Society</i> , 2002, 124, 503-510.	6.6	193
1686	Al <sub>6</sub> 2- $\sigma$ Fusion of Two Aromatic Al <sub>3</sub> - Units. A Combined Photoelectron Spectroscopy and ab Initio Study of M+[Al <sub>6</sub> 2-] (M = Li, Na, K, Cu, and Au). <i>Journal of the American Chemical Society</i> , 2002, 124, 11791-11801.	6.6	124
1687	Theoretical study of oxygen-deficient SnO <sub>2</sub> (110) surfaces. <i>Physical Review B</i> , 2002, 65, .	1.1	84
1688	Shear Instability of $\alpha$ -Fe in Bulk and in Ultrathin Films. <i>Physical Review Letters</i> , 2002, 88, 056101.	2.9	47
1689	Theoretical Study of the Interactions between Cations and Anions in Group IV Transition-Metal Catalysts for Single-Site Homogeneous Olefin Polymerization. <i>Organometallics</i> , 2002, 21, 2444-2453.	1.1	79
1690	Ab Initio Studies of ClO <sub>x</sub> Reactions. 2. Unimolecular Decomposition of s-ClO <sub>3</sub> and the Bimolecular O + OClO Reaction. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8386-8390.	1.1	15
1691	Light-induced absorption changes by excitation of metastable states in Na <sub>2</sub> [Fe(CN) <sub>5</sub> NO]·2H <sub>2</sub> O single crystals. <i>Physical Review B</i> , 2002, 66, .	1.1	46
1692	Synthetic, Structural, Electrochemical, and Theoretical Studies of Heterometallic Aggregates with a [Pt <sub>2</sub> ( $\eta$ -5-S) <sub>2</sub> M] Core (M = Hg, Au). <i>Inorganic Chemistry</i> , 2002, 41, 6838-6845.	1.9	15
1693	O/Ag(100) Surface: A Density Functional Study with Slab Model. <i>Journal of Physical Chemistry B</i> , 2002, 106, 3662-3667.	1.2	30
1694	Hydrogenation of Benzene on Ni(111): A DFT Study. <i>Journal of Physical Chemistry B</i> , 2002, 106, 13299-13305.	1.2	57
1695	A Theoretical Study of Cu(II) Sites in a Faujasite-Type Zeolite: Structures and Electron Paramagnetic Resonance Hyperfine Coupling Constants. <i>Journal of Physical Chemistry B</i> , 2002, 106, 7483-7488.	1.2	30
1696	Comparisons between Density Functional Theory and Conventional ab Initio Methods for 1,2-Elimination of HF from 1,1,1-Trifluoroethane: Test Case Study for HF Elimination from Fluoroalkanes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8471-8478.	1.1	25
1697	Experimental and Theoretical Studies of the Products of Laser-Ablated Thorium Atom Reactions with H <sub>2</sub> O in Excess Argon. <i>Journal of the American Chemical Society</i> , 2002, 124, 6723-6733.	6.6	42
1698	Dissociation of CH <sub>3</sub> I on the Al(111) Surface: An STM and Density Functional Theory Study. <i>Journal of the American Chemical Society</i> , 2002, 124, 14202-14209.	6.6	13

#	ARTICLE	IF	CITATIONS
1700	Dissolution of rare-earth clusters in SiO <sub>2</sub> by Al codoping: A microscopic model. <i>Physical Review B</i> , 2002, 65, .	1.1	64
1701	Relative Stabilities of Three Low-Energy Tautomers of Cytosine: A Coupled Cluster Electron Correlation Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1381-1390.	1.1	115
1702	Semi-empirical and ab initio studies of low-temperature adsorption of oxygen and CO at [110] face of SnO <sub>2</sub> . <i>IEEE Sensors Journal</i> , 2002, 2, 416-421.	2.4	12
1703	Theoretical Study of Al <sub>n</sub> N <sub>n</sub> , Ga <sub>n</sub> N <sub>n</sub> , and In <sub>n</sub> N <sub>n</sub> (n= 4, 5, 6) Clusters. <i>Journal of Physical Chemistry B</i> , 2002, 106, 1945-1953.	1.2	89
1704	Ideal Pure Shear Strength of Aluminum and Copper. <i>Science</i> , 2002, 298, 807-811.	6.0	686
1705	Pressure-Induced Structural Changes in Liquid SiO <sub>2</sub> from Ab Initio Simulations. <i>Physical Review Letters</i> , 2002, 89, 245504.	2.9	91
1706	Parametrization and validation of a force field for liquid-crystal forming molecules. <i>Physical Review E</i> , 2002, 65, 051709.	0.8	55
1707	Broken symmetries in the crystalline and magnetic structures of f <sup>3</sup> -iron. <i>Physical Review B</i> , 2002, 66, .	1.1	136
1708	Physisorption of Molecular Hydrogen on Polycyclic Aromatic Hydrocarbons: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2002, 106, 8689-8696.	1.2	54
1709	Surface Structures and Crystal Morphology of ZnS: Computational Study. <i>Journal of Physical Chemistry B</i> , 2002, 106, 11002-11008.	1.2	116
1710	Periodic Density Functional Study of CO and OH Adsorption on Pt <sup>100</sup> /Ru Alloy Surfaces: Implications for CO Tolerant Fuel Cell Catalysts. <i>Journal of Physical Chemistry B</i> , 2002, 106, 686-692.	1.2	275
1711	New Density Functional and Atoms in Molecules Method of Computing Relative pKa Values in Solution. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11963-11972.	1.1	133
1712	Small gold clusters on stoichiometric and defected TiO <sub>2</sub> anatase (101) and their interaction with CO: A density functional study. <i>Journal of Chemical Physics</i> , 2002, 117, 353-361.	1.2	133
1713	A new correlation functional based on analysis of the Colle-Salvetti functional. <i>Journal of Chemical Physics</i> , 2002, 116, 6458-6467.	1.2	21
1714	A Periodic Density Functional Theory Study of the Dehydrogenation of Methanol over Pt(111). <i>Journal of Physical Chemistry B</i> , 2002, 106, 2559-2568.	1.2	241
1715	Atomic and molecular adsorption on Rh(111). <i>Journal of Chemical Physics</i> , 2002, 117, 6737-6744.	1.2	204
1716	Structural, electronic, and magnetic properties of a Mn monolayer on W(110). <i>Physical Review B</i> , 2002, 66, .	1.1	45
1717	First-principles simulations of metal-ceramic interface adhesion: Co/WC versus Co/TiC. <i>Physical Review B</i> , 2002, 65, .	1.1	160

#	ARTICLE	IF	CITATIONS
1718	Magnetism and electronic structure in ZnFe[sub 2]O[sub 4] and MnFe[sub 2]O[sub 4]. Journal of Applied Physics, 2002, 91, 7370.	1.1	13
1719	Time-dependent density functional calculations of fully $\pi$ -conjugated zinc oligoporphyrins. Journal of Chemical Physics, 2002, 117, 9688-9694.	1.2	44
1720	Amorphous structures of Cu, Ag, and Au nanoclusters from first principles calculations. Journal of Chemical Physics, 2002, 117, 9548-9551.	1.2	122
1721	Study of $\gamma$ -Alumina Surface Reactivity: Adsorption of Water and Hydrogen Sulfide on Octahedral Aluminum Sites. Journal of Physical Chemistry B, 2002, 106, 9359-9366.	1.2	84
1722	A Density Functional Study of Ethylene Insertion into the M-methyl (M = Ti, Zr) Bond for Different Catalysts, with a QM/MM Model for the Counterion, B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> CH <sub>3</sub> <sup>-</sup> . Israel Journal of Chemistry, 2002, 42, 403-415.	1.0	13
1723	Complementary approaches to the ab initio calculation of melting properties. Journal of Chemical Physics, 2002, 116, 6170-6177.	1.2	88
1724	Density functional theory modelling EPR spectra of Cu(II) in Y zeolite. Studies in Surface Science and Catalysis, 2002, , 1899-1906.	1.5	4
1725	Temperature-Independent Rate of Electron-Transfer between a Cobalt(II) and a Ruthenium(III) of Doublet Electronic Configuration. Journal of Physical Chemistry A, 2002, 106, 11034-11044.	1.1	29
1726	Theoretical investigation of native defects, impurities, and complexes in aluminum nitride. Physical Review B, 2002, 65, .	1.1	225
1727	Magnetoelasticity of Fe: Possible failure of ab initio electron theory with the local-spin-density approximation and with the generalized-gradient approximation. Physical Review B, 2002, 65, .	1.1	29
1728	Calculation of exchange integrals and electronic structure for manganese ferrite. Physical Review B, 2002, 66, .	1.1	25
1729	Calculation of free energies from ab initio calculation. Journal of Physics Condensed Matter, 2002, 14, 2975-3000.	0.7	54
1730	Theoretical Study of the MoS <sub>2</sub> (100) Surface: A Chemical Potential Analysis of Sulfur and Hydrogen Coverage. 2. Effect of the Total Pressure on Surface Stability. Journal of Physical Chemistry B, 2002, 106, 5659-5667.	1.2	123
1731	Band structure, Born effective charges, and lattice dynamics of CuInS <sub>2</sub> from ab initio calculations. Journal of Chemical Physics, 2002, 117, 2726-2731.	1.2	47
1732	Sodium under pressure: bcc to fcc structural transition and pressure-volume relation to 100 GPa. Physical Review B, 2002, 65, .	1.1	114
1733	Metal Substitution in the Active Site of Nitrogenase MFe <sub>7</sub> S <sub>9</sub> (M = Mo <sup>4+</sup> , V <sup>3+</sup> , Fe <sup>3+</sup> ). Inorganic Chemistry, 2002, 41, 5744-5753.	1.9	53
1734	New exchange-correlation density functionals: The role of the kinetic-energy density. Journal of Chemical Physics, 2002, 116, 9559-9569.	1.2	454
1735	Adsorption of hydrogen and deuterium atoms on the (0001) graphite surface. Journal of Chemical Physics, 2002, 117, 8486-8492.	1.2	249

#	ARTICLE	IF	CITATIONS
1736	The Effects of Lattice Motion on Eley-Rideal and Hot Atom Reactions: A Quasiclassical Studies of Hydrogen Recombination on Ni(100). Journal of Physical Chemistry B, 2002, 106, 8342-8348.	1.2	30
1737	Arene-perfluoroarene interactions in crystal engineering 8: structures of 1:1 complexes of hexafluorobenzene with fused-ring polyaromatic hydrocarbons. New Journal of Chemistry, 2002, 26, 1740-1746.	1.4	181
1738	Reversible band-gap engineering in carbon nanotubes by radial deformation. Physical Review B, 2002, 65, .	1.1	121
1739	A Density Functional Theory Analysis of the Reaction Pathways and Intermediates for Ethylene Dehydrogenation over Pd(111). Journal of Physical Chemistry B, 2002, 106, 1656-1669.	1.2	75
1740	Geometric structures, electronic properties, and vibrational frequencies of small tellurium clusters. Physical Review B, 2002, 65, .	1.1	31
1741	Theoretical Calculations of Voltage-Dependent STM Images of Acetylene on the Si(001) Surface. Journal of Physical Chemistry B, 2002, 106, 1316-1321.	1.2	24
1742	First-principles elastic and structural properties of uranium metal. Physical Review B, 2002, 66, .	1.1	119
1743	Ultrafast Electron Diffraction and Structural Dynamics: A Transient Intermediates in the Elimination Reaction of C2F4I2. Journal of Physical Chemistry A, 2002, 106, 4087-4103.	1.1	58
1744	Thermodynamical functions for crystals with large unit cells such as zircon, coffinite, fluorapatite, and iodoapatite from ab initio calculations. Physical Review B, 2002, 65, .	1.1	37
1745	N2O and NO2 formation on Pt(111): A density functional theory study. Journal of Chemical Physics, 2002, 117, 2902-2908.	1.2	54
1746	Calculating the vacancy formation energy in metals: Pt, Pd, and Mo. Physical Review B, 2002, 66, .	1.1	178
1747	Screened Coulomb interactions in metallic alloys. II. Screening beyond the single-site and atomic-sphere approximations. Physical Review B, 2002, 66, .	1.1	121
1748	Symmetry-Breaking Phenomena in Metalloporphyrin $\pi$ -Cation Radicals. Journal of the American Chemical Society, 2002, 124, 8122-8130.	6.6	65
1749	Theoretical study of disorder in Ti-substituted La <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> . Physical Review B, 2002, 65, .	1.1	84
1750	Effect of surface phosphorus on the oxidative dehydrogenation of ethane: A first-principles investigation. Journal of Chemical Physics, 2002, 117, 8080-8088.	1.2	14
1751	High-pressure and thermal properties of $\beta$ -Mg <sub>2</sub> SiO <sub>4</sub> from first-principles calculations. Journal of Chemical Physics, 2002, 117, 3340-3344.	1.2	37
1752	First Principles Study of Cu Atoms Deposited on the $\alpha$ -Al <sub>2</sub> O <sub>3</sub> (0001) Surface. Journal of Physical Chemistry B, 2002, 106, 11495-11500.	1.2	34
1753	Optical properties of point defects in SiO <sub>2</sub> from time-dependent density functional theory. Journal of Chemical Physics, 2002, 116, 825-831.	1.2	73

#	ARTICLE	IF	CITATIONS
1754	Density-functional theory studies of acetone and propanal hydrogenation on Pt(111). <i>Journal of Chemical Physics</i> , 2002, 116, 8973-8980.	1.2	54
1755	Computer Modeling of $\alpha$ -Si and $\alpha$ -Ge Polymorphs. <i>Journal of Physical Chemistry B</i> , 2002, 106, 3402-3409.	1.2	26
1756	First high-nuclearity thallium-palladium carbonyl phosphine cluster, $[Tl_2Pd_{12}(CO)_9(PEt_3)_9]^{2+}$ , and its initial mistaken identity as the unknown $Au_2Pd_{12}$ analogue: structure-to-synthesis approach concerning its formation. <i>Dalton Transactions RSC</i> , 2002, , 4116-4127.	2.3	18
1757	First-principles study for ordering and phase separation in the Fe-Pd system. <i>Journal of Physics Condensed Matter</i> , 2002, 14, 1903-1913.	0.7	45
1758	Comparative Study of $ABO_3$ Perovskite Compounds. 1. $ATiO_3$ (A = Ca, Sr, Ba, and Pb) Perovskites. <i>Journal of Physical Chemistry B</i> , 2002, 106, 9986-9992.	1.2	59
1759	Oxalate-Bridged Complexes of Dimolybdenum and Ditungsten Supported by Pivalate Ligands: $(tBuCO_2)_3M_2(\mu_4-O_2CCO_2)M_2(O_2CtBu)_3$ . Correlation of the Solid-State, Molecular, and Electronic Structures with Raman, Resonance Raman, and Electronic Spectral Data. <i>Journal of the American Chemical Society</i> , 2002, 124, 3050-3063.	6.6	74
1760	A density functional theory study of the adsorption of sulfur, mercapto, and methylthiolate on Au(111). <i>Journal of Chemical Physics</i> , 2002, 116, 784-790.	1.2	253
1761	Structural and electronic properties of $PbTiO_3$ , $PbZrO_3$ , and $PbZr_{0.5}Ti_{0.5}O_3$ : First-principles density-functional studies. <i>Journal of Chemical Physics</i> , 2002, 117, 2699-2709.	1.2	63
1762	Structure and Short Timescale Ion Dynamics of Potassium-Ammonia Graphite Intercalation Compounds. <i>Journal of Physical Chemistry B</i> , 2002, 106, 1161-1172.	1.2	4
1763	On the Resonance Energy in New All-Metal Aromatic Molecules. <i>Inorganic Chemistry</i> , 2002, 41, 532-537.	1.9	139
1764	A theoretical study of the $^{77}Se$ NMR and vibrational spectroscopic properties of $S_8$ -ring molecules. <i>Canadian Journal of Chemistry</i> , 2002, 80, 1435-1443.	0.6	19
1765	Thermodynamic stability of high-K dielectric metal oxides $ZrO_2$ and $HfO_2$ in contact with Si and $SiO_2$ . <i>Applied Physics Letters</i> , 2002, 80, 1897-1899.	1.5	346
1766	Electrochemical behaviour, IR spectroelectrochemistry and theoretical studies of tetracobalt carbonyl cluster complexes with a facial cyclooctatetraene ligand. <i>Dalton Transactions RSC</i> , 2002, , 3705.	2.3	6
1767	A hybrid quantum mechanical and empirical model for the prediction of isotropic $^{13}C$ shielding constants of organic molecules. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5498-5507.	1.3	56
1768	Ab initio study of tetragonal variants in $Ni_2MnGa$ alloy. <i>Journal of Physics Condensed Matter</i> , 2002, 14, 5325-5336.	0.7	138
1769	Search for minimum molecular programmable units. , 0, , .		12
1770	Understanding the unusual g-values and the spin density distribution of hydrogen atoms trapped in silasesquioxanes. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5458-5466.	1.3	14
1771	Binary nitrides $\hat{M}M_3N_2$ (M = Be, Mg, Ca): a theoretical study. <i>Journal of Materials Chemistry</i> , 2002, 12, 2475-2479.	6.7	48



#	ARTICLE	IF	CITATIONS
1772	Cyclooctatetraene ditungsten alkoxides: $W_2(\frac{1}{4}\text{-}\hat{1}\cdot\hat{5},\hat{1}\cdot\hat{5}\text{-COT})(OR)_4$ , where R = CH <sub>2</sub> tBu,iPr, andtBu. Dalton Transactions RSC, 2002, , 4077-4083.	2.3	8
1773	Periodic density functional embedding theory for complete active space self-consistent field and configuration interaction calculations: Ground and excited states. Journal of Chemical Physics, 2002, 116, 42.	1.2	142
1774	First-principles study of the effects of halogen dopants on the properties of intergranular films in silicon nitride ceramics. Physical Review B, 2002, 65, .	1.1	30
1775	Structure, bonding, and anharmonic librational motion of CO on Ir{100}. Journal of Chemical Physics, 2002, 116, 8097-8105.	1.2	16
1776	Composition and temperature of the Earth's core constrained by combining ab initio calculations and seismic data. Earth and Planetary Science Letters, 2002, 195, 91-98.	1.8	257
1777	Atomic hydrogen adsorption on a Stone-Wales defect in graphite. Surface Science, 2002, 496, 33-38.	0.8	55
1778	Periodic ab initio study of the hydrogenated rutile TiO <sub>2</sub> (110) surface. Surface Science, 2002, 497, 194-204.	0.8	99
1779	The virtual chemistry lab for reactions at surfaces: Is it possible? Will it be useful?. Surface Science, 2002, 500, 347-367.	0.8	78
1780	Real time chemical dynamics at surfaces. Surface Science, 2002, 500, 475-499.	0.8	51
1781	Adhesion of metal on metal. The Pt on Co case. Surface Science, 2002, 496, L51-L54.	0.8	9
1782	An STM and DFT study of the ordered structures of NO on Pd(). Surface Science, 2002, 496, 1-9.	0.8	39
1783	Effects of Co magnetism on Co/TiC() interface adhesion: a first-principles study. Surface Science, 2002, 497, 171-182.	0.8	27
1784	Superstructures of carbon on V(). Surface Science, 2002, 497, 294-304.	0.8	10
1785	Tip effects in scanning tunneling microscopy of atomic-scale magnetic structures. Surface Science, 2002, 498, L65-L70.	0.8	11
1786	Adhesion, stability, and bonding at metal/metal-carbide interfaces: Al/WC. Surface Science, 2002, 498, 321-336.	0.8	224
1787	Formation of interface states on a half-metal surface. Surface Science, 2002, 501, L185-L190.	0.8	35
1788	Theory of CO adsorption on Co{}. Surface Science, 2002, 504, 138-144.	0.8	18
1789	Stability of oxygen adsorption sites and ultrathin aluminum oxide films on Al(). Surface Science, 2002, 504, 1-10.	0.8	36

#	ARTICLE	IF	CITATIONS
1790	Adsorption of O <sub>2</sub> and NO on Pd nanocrystals supported on Al <sub>2</sub> O <sub>3</sub> /NiAl(): overlayer and edge structures. <i>Surface Science</i> , 2002, 505, 25-38.	0.8	44
1791	Ab initio molecular dynamics: recent progresses and limitations. <i>Journal of Non-Crystalline Solids</i> , 2002, 312-314, 52-59.	1.5	26
1792	Iron under Earth's core conditions: Liquid-state thermodynamics and high-pressure melting curve from ab initio calculations. <i>Physical Review B</i> , 2002, 65, .	1.1	277
1793	Electronic structure and exchange interaction in the layered perovskite Sr <sub>3</sub> Mn <sub>2</sub> O <sub>7</sub> . <i>Physical Review B</i> , 2002, 65, .	1.1	16
1794	Ab Initio Study of Field Emission from Graphitic Ribbons. <i>Physical Review Letters</i> , 2002, 88, 127601.	2.9	114
1795	Fermi surfaces of diborides: MgB <sub>2</sub> and ZrB <sub>2</sub> . <i>Physical Review B</i> , 2002, 66, .	1.1	62
1796	Quantum-based atomistic simulation of materials properties in transition metals. <i>Journal of Physics Condensed Matter</i> , 2002, 14, 2825-2857.	0.7	147
1797	Quantum Origin of the Oxygen Storage Capability of Ceria. <i>Physical Review Letters</i> , 2002, 89, 166601.	2.9	661
1798	Chemistry of Sulfur Oxides on Transition Metals I: $d$ Configurations, Energetics, Orbital Analyses, and Surface Coverage Effects of SO <sub>2</sub> on Pt(111). <i>Journal of Physical Chemistry B</i> , 2002, 106, 12575-12583.	1.2	60
1799	Density functional calculations on hydrogen in palladium-silver alloys. <i>Journal of Alloys and Compounds</i> , 2002, 330-332, 332-337.	2.8	56
1800	First-principles electronic structure calculations of BaSi <sub>7</sub> N <sub>10</sub> with both corner- and edge-sharing SiN <sub>4</sub> tetrahedra. <i>Journal of Alloys and Compounds</i> , 2002, 336, 1-4.	2.8	15
1801	Energetics of alkaline-earth metal silicides calculated using a first-principle pseudopotential method. <i>Intermetallics</i> , 2002, 10, 333-341.	1.8	70
1802	On the electronic structures of the gold tetramer clusters. <i>Computational Materials Science</i> , 2002, 25, 279-284.	1.4	9
1803	Beyond short-range order length scales in disordered materials: first principles modeling of SiSe <sub>2</sub> . <i>Computational Materials Science</i> , 2002, 24, 28-32.	1.4	2
1804	Modelling of ZrO <sub>2</sub> deposition from ZrCl <sub>4</sub> and H <sub>2</sub> O on the Si(100) surface: initial reactions and surface structures. <i>Computational Materials Science</i> , 2002, 24, 278-283.	1.4	33
1805	A density functional study of the ionisation potentials and electron affinities of small Ni <sub>x</sub> Sn clusters with $x=1-4$ . <i>Computational Materials Science</i> , 2002, 25, 363-370.	1.4	5
1806	Ab initio calculations of lattice stability of sigma-phase and phase diagram in the Cr-Fe system. <i>Computational Materials Science</i> , 2002, 25, 562-569.	1.4	27
1807	Phase diagram calculation in Co-Cr system using Ab initio determined lattice instability of sigma phase. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2002, 26, 513-522.	0.7	27

#	ARTICLE	IF	CITATIONS
1808	First-principles calculation of L10-disorder phase diagram in Fe-Pt system within the first and second nearest neighbor pair interaction energies. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2002, 26, 583-589.	0.7	26
1809	First Principles Study of the Structure and Chemistry of Mg-Based Hydrotalcite-Like Anionic Clays. Journal of Physical Chemistry B, 2002, 106, 12291-12296.	1.2	70
1810	Ab initio calculations of elastic constants and thermodynamic properties of bcc, fcc, and hcp Al crystals under pressure. Journal of Physics Condensed Matter, 2002, 14, 6989-7005.	0.7	627
1811	Probing the Electronic Structure and Aromaticity of Pentapnictogen Cluster Anions Pn <sup>5-</sup> (Pn = P, As,) Tj ETQq1 1 0.784314 rgBT /Over Chemistry A, 2002, 106, 5600-5606.	1.1	94
1812	The inherent tensile strength of iron. Philosophical Magazine Letters, 2002, 82, 141-147.	0.5	49
1813	Ab initio chemical potentials of solid and liquid solutions and the chemistry of the Earth's core. Journal of Chemical Physics, 2002, 116, 7127-7136.	1.2	107
1814	Partial Dissociation of Water on Ru(0001). Science, 2002, 295, 99-102.	6.0	464
1815	Theory of Al <sub>2</sub> O <sub>3</sub> incorporation in SiO <sub>2</sub> . Physical Review B, 2002, 65, .	1.1	11
1816	A New Insight into Fischer-Tropsch Synthesis. Journal of the American Chemical Society, 2002, 124, 11568-11569.	6.6	167
1817	Adsorption-induced restructuring of gold nanochains. Physical Review B, 2002, 66, .	1.1	102
1818	Reaction between N-Alkylhydroxylamines and Chiral Enoate Esters: A More Experimental Evidence for a Cycloaddition-like Process, a Rationale Based on DFT Theoretical Calculations, and Stereoselective Synthesis of New Enantiopure $\beta^2$ -Amino Acids. Journal of Organic Chemistry, 2002, 67, 2402-2410.	1.7	43
1819	A computational study of conformers of 1,3-dioxane (1,3-dioxacyclohexane). Computational and Theoretical Chemistry, 2002, 577, 43-54.	1.5	37
1820	Magnetism and electronic structures of Ni/Cu <sub>3</sub> Au(001). Journal of Magnetism and Magnetic Materials, 2002, 239, 33-35.	1.0	1
1821	On the magnetoelastic contribution to the magnetic anisotropy of thin epitaxial Permalloy films: an ab initio study. Journal of Magnetism and Magnetic Materials, 2002, 238, 125-128.	1.0	5
1822	Investigation of Some Ground State Properties of Lithium with the All Electron MAPW Method. Physica Status Solidi (B): Basic Research, 2002, 229, 1359-1370.	0.7	6
1823	Electronic Structure of GdNi <sub>4</sub> B Compound. Physica Status Solidi (B): Basic Research, 2002, 231, 446-450.	0.7	15
1824	The Space Group of Nd <sub>3</sub> Fe <sub>29-x</sub> Ti <sub>x</sub> : A2/m or P21/c. Physica Status Solidi (B): Basic Research, 2002, 234, 487-495.	0.7	11
1825	A First-Principles Study on Surface Magnetism of Ni <sub>x</sub> Pd <sub>1-x</sub> (x = 0, 0.5, and 1.0) Overlayers on Cu(001) and Cu <sub>3</sub> Au(001). Physica Status Solidi A, 2002, 189, 697-699.	1.7	1

#	ARTICLE	IF	CITATIONS
1827	Experimental Observation and Confirmation of Icosahedral W@Au <sub>12</sub> and Mo@Au <sub>12</sub> Molecules. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 4786-4789.	7.2	325
1828	Variations of the FeGa <sub>3</sub> Structure Type in the Systems CoIn <sub>3</sub> xZnx and CoGa <sub>3</sub> xZnx. <i>Journal of Solid State Chemistry</i> , 2002, 165, 100-110.	1.4	30
1829	A new form of the Sutton-Chen potential for the Cu-Ag alloys. <i>Superlattices and Microstructures</i> , 2002, 31, 297-313.	1.4	6
1830	Calculation of electronic g-tensors for transition metal complexes using hybrid density functionals and atomic meanfield spin-orbit operators. <i>Journal of Computational Chemistry</i> , 2002, 23, 794-803.	1.5	182
1831	Ab initio conformational studies on diols and binary diol-water systems using DFT methods. Intramolecular hydrogen bonding and 1:1 complex formation with water. <i>Journal of Computational Chemistry</i> , 2002, 23, 585-599.	1.5	104
1832	Magnetization study of UCo <sub>1-x</sub> T <sub>x</sub> Al (T=Fe, Ni) single crystals. <i>Physica B: Condensed Matter</i> , 2002, 319, 199-207.	1.3	4
1833	Electronic and structural properties of Î <sup>2</sup> -Be <sub>3</sub> N <sub>2</sub> . <i>Physica B: Condensed Matter</i> , 2002, 324, 305-311.	1.3	57
1834	A comparative study on the 1,3-dipolar cycloadditions of diazomethane and bis(diisopropylamino)phosphinodiazomethane to chiral electron-deficient olefins: reactivity and diastereoselectivity. <i>Tetrahedron: Asymmetry</i> , 2002, 13, 2593-2603.	1.8	10
1835	Modeling of alloy steels. <i>Materials Today</i> , 2002, 5, 14-23.	8.3	10
1836	Quantum chemical predictions of the vibrational spectra of polyatomic molecules.. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2002, 58, 411-440.	2.0	168
1837	Ab initio study of Mg adatom and MgO molecule adsorption and diffusion on the MgO (0 0 1) surface. <i>Applied Surface Science</i> , 2002, 188, 122-127.	3.1	20
1838	Theoretical investigation on the electronic states localized at grain boundaries in semiconductors. <i>Applied Surface Science</i> , 2002, 190, 129-133.	3.1	6
1839	Quantitative modelling in scanning force microscopy on insulators. <i>Applied Surface Science</i> , 2002, 188, 306-318.	3.1	20
1840	Combinatorial computational chemistry approach to the design of cathode materials for a lithium secondary battery. <i>Applied Surface Science</i> , 2002, 189, 313-318.	3.1	14
1841	Heats of formation for AlH, AlOH, OAlH and OAlOH and their monocations. <i>Computational and Theoretical Chemistry</i> , 2002, 581, 17-29.	1.5	39
1842	The hydration effect on the uracil frequencies: an experimental and quantum chemical study. <i>Computational and Theoretical Chemistry</i> , 2002, 585, 69-92.	1.5	66
1843	Linear and nonlinear optical properties of pyridine N-oxide molecule. <i>Computational and Theoretical Chemistry</i> , 2002, 592, 19-28.	1.5	31
1844	Comparative application of different approaches for band structure calculations on polyparaphenylene in the Parr-Pople model: III. Density functional theories. <i>Computational and Theoretical Chemistry</i> , 2002, 618, 1-34.	1.5	1

#	ARTICLE	IF	CITATIONS
1845	C3H4: density functional (DFT) study of structures and stabilities of isomers. Computational and Theoretical Chemistry, 2002, 617, 141-147.	1.5	13
1846	The use of ab initio and DFT calculations in the interpretation of ultraviolet photoelectron spectra: the rotational isomerism of anisole and thioanisole as a case study. Computational and Theoretical Chemistry, 2002, 618, 155-164.	1.5	23
1847	Materials by design and the exciting role of quantum computation/simulation. Journal of Computational and Applied Mathematics, 2002, 149, 27-56.	1.1	26
1848	Binuclear Ni(II) complexes based on bridging oxalate and tetracyanometallates.. Polyhedron, 2002, 21, 2631-2638.	1.0	25
1849	Spin-reorientation transition and electronic structure of TmCo3 compound. Journal of Magnetism and Magnetic Materials, 2002, 246, 425-433.	1.0	1
1850	Electronic structure and prediction of magnetism in metallic nanowires. Journal of Magnetism and Magnetic Materials, 2002, 249, 193-199.	1.0	16
1851	Atomic and molecular energies in terms of electrostatic potentials at nuclei. International Journal of Quantum Chemistry, 2002, 90, 459-463.	1.0	23
1852	Solution of periodic Poisson's equation and the Hartree-Fock approach for solids with extended electron states: Application to linear augmented plane wave method. International Journal of Quantum Chemistry, 2002, 89, 57-85.	1.0	14
1853	Theoretical investigation of the Ziegler-Natta catalysis in heterogeneous conditions. International Journal of Quantum Chemistry, 2002, 89, 389-396.	1.0	7
1854	Link between the kinetic- and exchange-energy functionals in the generalized gradient approximation. International Journal of Quantum Chemistry, 2002, 89, 441-446.	1.0	97
1855	Ab initio and density functional theory study of the enthalpies of formation of F2SOx and FCISOx (x=1, 2). Journal of Fluorine Chemistry, 2002, 116, 135-141.	0.9	15
1856	Density functional study of the polymorphism of Cs2C2 and Rb2C2. Solid State Communications, 2002, 121, 155-158.	0.9	4
1857	Energetics of oxygen species in crystalline and amorphous SiO2: a first-principles investigation. Solid-State Electronics, 2002, 46, 1873-1878.	0.8	5
1858	Full-coverage adsorption of water on SnO2(): the stabilisation of the molecular species. Surface Science, 2002, 512, 29-36.	0.8	27
1859	Surface relaxation and surface stress of Au(111). Surface Science, 2002, 513, 263-271.	0.8	60
1860	Magnetic properties of Fe-Ni alloy atom bridges. Surface Science, 2002, 514, 156-160.	0.8	19
1861	STM-tip induced magnetic state change of Fe atom bridge. Surface Science, 2002, 514, 161-166.	0.8	14
1862	First principles calculations for electronic band structure of single-walled carbon nanotube under uniaxial strain. Surface Science, 2002, 514, 222-226.	0.8	41

#	ARTICLE	IF	CITATIONS
1863	The structure of the oxygen-induced $c(6\sqrt{2})$ reconstruction of V(110). Surface Science, 2002, 512, 16-28.	0.8	14
1864	Reconstructions of strongly reduced SnO <sub>2</sub> (110) studied by first-principles methods. Surface Science, 2002, 513, 26-36.	0.8	52
1865	Theoretical study of the Au/TiO <sub>2</sub> ( $\bar{1}$ ) interface. Surface Science, 2002, 515, 175-186.	0.8	126
1866	Oxygen dissociation at close-packed Pt terraces, Pt steps, and Ag-covered Pt steps studied with density functional theory. Surface Science, 2002, 515, 235-244.	0.8	114
1867	A first principles study of sub-monolayer Ge on Si( $\bar{1}$ ). Surface Science, 2002, 515, 483-490.	0.8	23
1868	The characterization of SrTiO <sub>3</sub> ( $\bar{1}$ ) with MIES, UPS(HeI) and first-principles calculations. Surface Science, 2002, 515, 499-506.	0.8	53
1869	Interaction of Pd with steps on $\sqrt{3}\times\sqrt{3}$ -Al <sub>2</sub> O <sub>3</sub> ( $\bar{1}$ ). Surface Science, 2002, 518, L577-L582.	0.8	19
1870	Effect of oxide vacancies on metal island nucleation. Surface Science, 2002, 515, L481-L486.	0.8	90
1871	Structure determination of Cu( $\bar{1}$ ) $\sqrt{2}\times\sqrt{2}$ using X-ray diffraction and DFT calculations. Surface Science, 2002, 516, 16-32.	0.8	25
1872	Finite temperature studies of Te adsorption on. Surface Science, 2002, 519, 79-89.	0.8	18
1873	Computing accurate surface energies and the importance of electron self-energy in metal/metal-oxide adhesion. Surface Science, 2002, 520, L611-L618.	0.8	90
1874	Theoretical study of the structure of propene adsorbed on Pt( $\bar{1}$ ). Surface Science, 2002, 519, 250-258.	0.8	31
1875	Metal/oxide adhesion energies from first-principles. Surface Science, 2002, 520, 3-5.	0.8	33
1876	Electronic structure calculations of lead chalcogenides PbS, PbSe, PbTe. Journal of Physics and Chemistry of Solids, 2002, 63, 833-841.	1.9	143
1877	A simple theory of 40K superconductivity in MgB <sub>2</sub> : first-principles calculations of T <sub>c</sub> , its dependence on boron mass and pressure. Journal of Physics and Chemistry of Solids, 2002, 63, 2201-2206.	1.9	14
1878	Optical properties of cubic and tetragonal KTa <sub>0.5</sub> Nb <sub>0.5</sub> O <sub>3</sub> by density functional theory. Optics Communications, 2002, 201, 79-84.	1.0	12
1879	Chiral recognition in dimerization of adsorbed cysteine observed by scanning tunnelling microscopy. Nature, 2002, 415, 891-893.	13.7	569
1880	Ab initio calculations of the equation of state and elastic constants of aluminum in the region of negative pressures. JETP Letters, 2002, 75, 184-186.	0.4	26

#	ARTICLE	IF	CITATIONS
1881	First-principles study of metal-carbide/nitride adhesion: Al/VC vs. Al/VN. <i>Acta Materialia</i> , 2002, 50, 619-631.	3.8	127
1882	Iron-iron interaction through an ethanedithiolate ligand: a magnetic and theoretical study. <i>Inorganica Chimica Acta</i> , 2002, 329, 129-134.	1.2	7
1883	Observation of the photogenerated CO-loss intermediate from [CpFe(CO)] <sub>2</sub> ( $\mu$ -CO)( $\mu$ -CHCH <sub>3</sub> ) via time-resolved IR spectroscopy. <i>Inorganica Chimica Acta</i> , 2002, 334, 371-375.	1.2	0
1884	Syntheses and structures of tetrakis(1-methyluracilato)palladium complexes capturing alkali metal ions. A new type of metallo-podand. <i>Inorganica Chimica Acta</i> , 2002, 339, 543-550.	1.2	14
1885	Toward understanding nephelauxetism: interelectronic repulsion in gaseous dq ions computed by Kohn-Sham DFT. <i>Coordination Chemistry Reviews</i> , 2002, 226, 17-38.	9.5	24
1886	Quantum-chemical calculations of CO and OH interacting with bimetallic surfaces. <i>Electrochimica Acta</i> , 2002, 47, 3621-3628.	2.6	197
1887	First-principle calculations for mechanisms of semiconductor epitaxial growth. <i>Journal of Crystal Growth</i> , 2002, 237-239, 1-7.	0.7	4
1888	Comparison of GaN growth processes on GaAs(111)A and (111)B substrates studied by ab initio calculation. <i>Journal of Crystal Growth</i> , 2002, 237-239, 1084-1088.	0.7	5
1889	Tuning in on single molecular states: adsorption sites and STM images of maleic anhydride on Si(100). <i>Chemical Physics Letters</i> , 2002, 355, 347-354.	1.2	22
1890	Identifying structural building blocks in CuO <sub>6</sub> clusters: CuO <sub>2</sub> complexes vs CuO <sub>3</sub> ozonides. <i>Chemical Physics Letters</i> , 2002, 356, 469-475.	1.2	18
1891	Correlation of adsorption energy with surface structure: ethylene adsorption on Pd surfaces. <i>Chemical Physics Letters</i> , 2002, 358, 377-382.	1.2	63
1892	Time-dependent density functional study of the static second hyperpolarizability of BB-, NN- and BN-substituted C <sub>60</sub> . <i>Chemical Physics Letters</i> , 2002, 359, 524-529.	1.2	19
1893	Diatomic bond lengths and vibrational frequencies: assessment of recently developed exchange-correlation functionals. <i>Chemical Physics Letters</i> , 2002, 360, 38-46.	1.2	34
1894	Theoretical study of thiol-induced reconstructions on the Au(111) surface. <i>Chemical Physics Letters</i> , 2002, 360, 264-271.	1.2	161
1895	Introduction of the explicit long-range nonlocality as an alternative to the gradient expansion approximation for the kinetic-energy functional. <i>Chemical Physics Letters</i> , 2002, 360, 209-216.	1.2	9
1896	Six-dimensional quantum dynamics of scattering of ( $v=0, j=0$ ) H <sub>2</sub> and D <sub>2</sub> from Cu(111): test of two LEPS potential energy surfaces. <i>Chemical Physics Letters</i> , 2002, 360, 390-399.	1.2	47
1897	Topotactic valence manipulation to design strontium manganate: a first principle study. <i>Chemical Physics Letters</i> , 2002, 362, 151-158.	1.2	0
1898	Ground-state reconstruction of the Si(001) surface: symmetric versus buckled dimers. <i>Chemical Physics Letters</i> , 2002, 362, 559-566.	1.2	23



#	ARTICLE	IF	CITATIONS
1899	Oxidative addition of SiH <sub>4</sub> to Pt(PH <sub>3</sub> ) <sub>2</sub> : a dynamical density functional study. Chemical Physics Letters, 2002, 364, 87-92.	1.2	8
1900	M@Si <sub>16</sub> , M=Ti, Zr, Hf: $\pi$ conjugation, ionization potentials and electron affinities. Chemical Physics Letters, 2002, 363, 319-322.	1.2	67
1901	Electronic structure and STM images of self-assembled styrene lines on a Si(100) surface. Chemical Physics Letters, 2002, 365, 129-134.	1.2	34
1902	Studies of rhodium nanoparticles using the first principles density functional theory calculations. Chemical Physics Letters, 2002, 366, 368-376.	1.2	57
1903	Linear Hydrocarbons Adsorbed in the Acid Zeolite Gmelinite at 700 K ab Initio Molecular Dynamics Simulation of Hexane and Hexene. Journal of Catalysis, 2002, 205, 147-156.	3.1	21
1904	Shape and Edge Sites Modifications of MoS <sub>2</sub> Catalytic Nanoparticles Induced by Working Conditions: A Theoretical Study. Journal of Catalysis, 2002, 207, 76-87.	3.1	337
1905	Steam Reforming and Graphite Formation on Ni Catalysts. Journal of Catalysis, 2002, 209, 365-384.	3.1	980
1906	Reaction Paths in the Hydrogenolysis of Acetic Acid to Ethanol over Pd(111), Re(0001), and PdRe Alloys. Journal of Catalysis, 2002, 209, 289-305.	3.1	121
1907	Methanol Decomposition on Cu(111): A DFT Study. Journal of Catalysis, 2002, 208, 291-300.	3.1	190
1908	Extraframework Aluminum Species in Zeolites: Ab Initio Molecular Dynamics Simulation of Gmelinite. Journal of Catalysis, 2002, 209, 480-488.	3.1	42
1909	Analysis of a dinitro-based molecular device. Journal of Chemical Physics, 2002, 116, 1671-1683.	1.2	127
1910	Ab initio melting curve of the fcc phase of aluminum. Physical Review B, 2002, 65, .	1.1	124
1911	Ab Initio Molecular Dynamics Investigation of the Structure and the Noncollinear Magnetism in Liquid Oxygen: Occurrence of O <sub>4</sub> Molecular Units. Physical Review Letters, 2002, 89, 197204.	2.9	18
1912	Pentagonal nanowires: a first-principles study of the atomic and electronic structure. Physical Review B, 2002, 65, .	1.1	75
1913	Systematic ab initio study of curvature effects in carbon nanotubes. Physical Review B, 2002, 65, .	1.1	235
1914	Effects of hydrogen adsorption on single-wall carbon nanotubes: Metallic hydrogen decoration. Physical Review B, 2002, 66, .	1.1	104
1915	Metal nanoring and tube formation on carbon nanotubes. Physical Review B, 2002, 66, .	1.1	33
1916	Vacancy and interstitial defects in hafnia. Physical Review B, 2002, 65, .	1.1	560

#	ARTICLE	IF	CITATIONS
1917	First-principles simulation: ideas, illustrations and the CASTEP code. Journal of Physics Condensed Matter, 2002, 14, 2717-2744.	0.7	8,382
1918	Magnetic ground state of Cr in density-functional theory. Physical Review B, 2002, 65, .	1.1	129
1919	What density-functional theory can tell us about the spin-density wave in Cr. Journal of Physics Condensed Matter, 2002, 14, 3275-3283.	0.7	53
1920	Hydrogen Activation on Mo-Based Sulfide Catalysts, a Periodic DFT Study. Journal of the American Chemical Society, 2002, 124, 7084-7095.	6.6	181
1921	Phosphorus and sulphur doping of diamond. Physical Review B, 2002, 66, .	1.1	98
1922	Spin-polarization in half-metals (invited). Journal of Applied Physics, 2002, 91, 8340.	1.1	201
1923	Electronic structure and photoemission studies on Kondo semimetal U $\text{Ru}_{2}\text{Sn}$ . European Physical Journal B, 2003, 35, 349-355.	0.6	9
1924	LDA and GGA investigations of some ground state properties of aluminium with the all electron MAPW method. European Physical Journal B, 2003, 37, 405-411.	0.6	11
1925	Comparative assessment of a new nonempirical density functional: Molecules and hydrogen-bonded complexes. Journal of Chemical Physics, 2003, 119, 12129-12137.	1.2	2,157
1926	Vacancy Formation on MoS <sub>2</sub> Hydrodesulfurization Catalyst: DFT Study of the Mechanism. Journal of Physical Chemistry B, 2003, 107, 4057-4064.	1.2	142
1927	Lattice dynamics of CuAu-orderedCuInSe <sub>2</sub> . Physical Review B, 2003, 68, .	1.1	31
1928	Dynamical stability of the $\hat{\Gamma}$ and $\hat{L}$ phases of alumina. Physical Review B, 2003, 67, .	1.1	68
1929	CO on Pt(111): A puzzle revisited. Journal of Chemical Physics, 2003, 119, 4522-4528.	1.2	101
1930	Stress-induced defects inSb <sub>2</sub> Te <sub>3</sub> . Physical Review B, 2003, 68, .	1.1	77
1931	Surface properties of metastable alumina: A comparative study of $\hat{\Gamma}$ - and $\hat{L}$ - $\text{Al}_2\text{O}_3$ . Physical Review B, 2003, 67, .	1.1	104
1932	Systematic study of adsorption of single atoms on a carbon nanotube. Physical Review B, 2003, 67, .	1.1	305
1933	Van der Waals Density Functional for Layered Structures. Physical Review Letters, 2003, 91, 126402.	2.9	623
1934	General Model for Water Monomer Adsorption on Close-Packed Transition and Noble Metal Surfaces. Physical Review Letters, 2003, 90, 216102.	2.9	358

#	ARTICLE	IF	CITATIONS
1935	Density functional study of Ni bulk, surfaces and the adsorbate systems Ni(111)R30Å°â€“Cl, and Ni(111)(2Å—2)â€“K. Surface Science, 2003, 544, 103-120.	0.8	20
1936	Methanol at the waterâ€“platinum interface studied by ab initio molecular dynamics. Surface Science, 2003, 544, L697-L702.	0.8	30
1937	A microkinetic model of the methanol oxidation over silver. Surface Science, 2003, 544, 5-23.	0.8	55
1938	Function of subsurface boron on Si(001)-2Å—1: water adsorption. Surface Science, 2003, 547, L882-L886.	0.8	6
1939	Hydrogen bonding in mixed ligand copper organophosphonates. Chemical Physics Letters, 2003, 378, 400-405.	1.2	4
1940	Density functional calculation of a potential energy surface for alkane thiols on Au(111) as function of alkane chain length. Chemical Physics Letters, 2003, 381, 315-321.	1.2	65
1941	The self-consistent implementation of exchange-correlation functionals depending on the local kinetic energy density. Chemical Physics Letters, 2003, 381, 495-504.	1.2	55
1942	A DFT based ligand field model for magnetic exchange coupling in transition metal dimer complexes:. Chemical Physics Letters, 2003, 381, 584-591.	1.2	26
1943	Fragment molecular orbital method with density functional theory and DIIS convergence acceleration. Chemical Physics Letters, 2003, 382, 611-617.	1.2	60
1944	On the stability of rhenium up to 1 TPa pressure against transition to thebcc structure. Bulletin of Materials Science, 2003, 26, 183-187.	0.8	17
1945	Ab initio study of phenyl benzoate: structure, conformational analysis, dipole moment, IR and Raman vibrational spectra. Journal of Molecular Modeling, 2003, 9, 248-258.	0.8	43
1946	The influence of triaxial stress on the ideal tensile strength of iron. Scripta Materialia, 2003, 49, 1007-1011.	2.6	52
1947	Perspectives on the first principles elucidation and the design of active sites. Journal of Catalysis, 2003, 216, 73-88.	3.1	157
1948	Simulations of the azimuthal distribution of low-energy H atoms scattered off Ag() at grazing incidence: DFT many-body versus model pair potentials. Nuclear Instruments & Methods in Physics Research B, 2003, 203, 211-217.	0.6	3
1949	Ferromagnetic and antiferromagnetic couplings in Cr(0 0 1) thin films and TM monolayer/Cr(0 0 1) (TM) Tj ETQq0 0,0 rgBT /Overlock 10	2.0	10
1950	Structural relationship between V2O5 (001) surface and the bulk: cluster bulk termination models. Materials Chemistry and Physics, 2003, 81, 183-190.	2.0	7
1951	Theoretical studies of substoichiometric CuI. Materials Chemistry and Physics, 2003, 82, 597-601.	2.0	41
1952	Experimental and Quantum-Chemical Studies on the Thermochemical Stabilities of Mercury Carbodiimide and Mercury Cyanamide. ChemPhysChem, 2003, 4, 725-731.	1.0	23

#	ARTICLE	IF	CITATIONS
1953	Bonding and energetics in small clusters of gallium and arsenic. <i>Heteroatom Chemistry</i> , 2003, 14, 189-196.	0.4	40
1954	Ab Initio Structure/Reactivity Investigations of Illudin-Based Antitumor Agents: A Model for Reaction in vivo. <i>Helvetica Chimica Acta</i> , 2003, 86, 4133-4151.	1.0	7
1955	Electrostatic potentials and covalent radii. <i>Journal of Computational Chemistry</i> , 2003, 24, 505-511.	1.5	34
1956	Performance assessment of density-functional methods for study of charge-transfer complexes. <i>Journal of Computational Chemistry</i> , 2003, 24, 623-631.	1.5	79
1957	Hydrogen bonding in diols and binary diol-water systems investigated using DFT methods. II. Calculated infrared OH-stretch frequencies, force constants, and NMR chemical shifts correlate with hydrogen bond geometry and electron density topology. A reevaluation of geometrical criteria for hydrogen bonding. <i>Journal of Computational Chemistry</i> , 2003, 24, 1120-1131.	1.5	79
1958	Regional self-interaction correction of density functional theory. <i>Journal of Computational Chemistry</i> , 2003, 24, 1592-1598.	1.5	51
1959	An environmental pseudopotential approach to molecular interactions: Implementation in MOLPRO. <i>Journal of Computational Chemistry</i> , 2003, 24, 2075-2082.	1.5	13
1960	Ein mikroskopischer Beleg für eine erhöhte katalytische Reaktivität gedehnter Oberflächen. <i>Angewandte Chemie</i> , 2003, 115, 2956-2959.	1.6	8
1961	The Solution Structure of (Me <sub>3</sub> Si) <sub>3</sub> CSiBr: An Ab Initio/NMR Study. <i>Chemistry - A European Journal</i> , 2003, 9, 3320-3323.	1.7	17
1962	Bonding of Multiple Noble-Gas Atoms to CUO in Solid Neon: CUO(Ng) <sub>n</sub> (Ng=Ar, Kr, Xe; n=1, 2, 3, 4) Complexes and the Singlet-Triplet Crossover Point. <i>Chemistry - A European Journal</i> , 2003, 9, 4781-4788.	1.7	22
1963	DFT Study of the NMR Properties of Xenon in Covalent Compounds and van der Waals Complexes: Implications for the Use of <sup>129</sup> Xe as a Molecular Probe. <i>Chemistry - A European Journal</i> , 2003, 9, 1486-1495.	1.7	51
1964	Atomic-Scale Evidence for an Enhanced Catalytic Reactivity of Stretched Surfaces. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 2850-2853.	7.2	60
1965	On the anisotropic optical response of Al(110). <i>Progress in Surface Science</i> , 2003, 74, 283-291.	3.8	3
1966	Potentials in density functional theory and the importance of sum rules. <i>Journal of Solid State Chemistry</i> , 2003, 176, 652-670.	1.4	13
1967	Dramatic effect of homoallylic substitution on the rate of palladium-catalyzed diene cycloisomerization. <i>Journal of Organometallic Chemistry</i> , 2003, 687, 498-507.	0.8	15
1968	A comparative study of O <sub>2</sub> adsorbed carbon nanotubes. <i>Chemical Physics Letters</i> , 2003, 380, 1-5.	1.2	30
1969	Thermal excitation of CO on Pt on the (2 $\sqrt{3}$ -1) Pt {110} surface: a theoretical simulation of a variable-temperature STM contrast. <i>Chemical Physics Letters</i> , 2003, 382, 41-47.	1.2	0
1970	Quantum-chemical study on the supported precious metal catalyst. <i>Catalysis Today</i> , 2003, 87, 43-50.	2.2	21

#	ARTICLE	IF	CITATIONS
1971	DFT calculation of core-electron binding energies. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2003, 133, 69-76.	0.8	103
1972	A tilt-dependent diffusional potential energy landscape: benzyne on Ir{100}. <i>Chemical Physics Letters</i> , 2003, 367, 116-122.	1.2	9
1973	Elastic constants and electronic structure of alkaline-earth chalcogenides. Performances of various hamiltonians. <i>Chemical Physics Letters</i> , 2003, 367, 430-438.	1.2	80
1974	Time-dependent DFT study on the electronic states of BBr. <i>Chemical Physics Letters</i> , 2003, 369, 214-219.	1.2	9
1975	Adjustment of Perdew-Wang exchange functional for describing van der Waals and DNA base-stacking interactions. <i>Chemical Physics Letters</i> , 2003, 370, 161-169.	1.2	43
1976	Gradient expansions in density functional calculations of intermolecular potentials. <i>Chemical Physics Letters</i> , 2003, 370, 353-359.	1.2	3
1977	Adsorption dynamics of CO on Pd(110): energy dependence, structure insensitivity and the role of the surface electronic structure. <i>Chemical Physics Letters</i> , 2003, 370, 247-253.	1.2	3
1978	Theoretical prediction of the state-state correlation among doublet state SNO isomers. <i>Chemical Physics Letters</i> , 2003, 370, 616-624.	1.2	9
1979	A density functional theory study of sulphur dioxide adsorption on rutile TiO <sub>2</sub> (110). <i>Chemical Physics Letters</i> , 2003, 373, 15-21.	1.2	30
1980	Electron correlation and the lone pair effect in the phosphorous and arsenious acids: ab initio study of molecular structure and DFT calculations of <sup>31</sup> P NMR spectra. <i>Chemical Physics Letters</i> , 2003, 376, 364-369.	1.2	10
1981	Structure analysis of SiSO <sup>+</sup> and GeSO <sup>+</sup> systems in doublet state at density functional theory and wavefunction-correlated levels. <i>Chemical Physics Letters</i> , 2003, 377, 462-468.	1.2	0
1982	A DFT based ligand field model for magnetic exchange coupling in transition metal dimer complexes: (i) principles. <i>Chemical Physics Letters</i> , 2003, 379, 209-215.	1.2	24
1983	Molecular orbital analysis based on fragment molecular orbital scheme. <i>Chemical Physics Letters</i> , 2003, 378, 589-597.	1.2	37
1984	The isotypism of BeH <sub>2</sub> and SiO <sub>2</sub> : an ab initio study. <i>Chemical Physics Letters</i> , 2003, 378, 343-348.	1.2	14
1985	DFT study of electronic structure and geometry of neutral and anionic silver clusters. <i>Computational and Theoretical Chemistry</i> , 2003, 664-665, 291-308.	1.5	52
1986	Cyanide-isocyanide isomers in polynuclear complexes. Reactivity and theoretical studies. <i>Inorganica Chimica Acta</i> , 2003, 356, 297-307.	1.2	6
1987	Te <sup>II</sup> -Te interactions in inorganic rings with sulfur donors. <i>Inorganica Chimica Acta</i> , 2003, 356, 319-327.	1.2	8
1988	Structural characterisation and DFT studies of [Cr(cyclam)(O-dmsO)Cl] <sub>2</sub> <sup>2+</sup> : a new precursor complex towards potential DNA intercalators. <i>Inorganica Chimica Acta</i> , 2003, 356, 335-342.	1.2	12

#	ARTICLE	IF	CITATIONS
1989	Massively parallel linear-scaling algorithm in an ab initio local-orbital total-energy method. <i>Journal of Computational Physics</i> , 2003, 188, 1-15.	1.9	12
1990	Local reactivity of thin Pd overlayers on Au single crystals. <i>Journal of Electroanalytical Chemistry</i> , 2003, 548, 121-130.	1.9	129
1991	Geometry and energetics of Si <sub>6</sub> O isomers. <i>Science and Technology of Advanced Materials</i> , 2003, 4, 361-365.	2.8	7
1992	Atomic understanding of strong nanometer-thin metal/alumina interfaces. <i>Surface Science</i> , 2003, 544, L689-L696.	0.8	16
1993	First principles studies of chemisorbed O on Ni{111}. <i>Surface Science</i> , 2003, 543, 12-18.	0.8	41
1994	Reconstruction and de-reconstruction of the Ir(100) surface and ultrathin Fe/Ir(100) films. <i>Surface Science</i> , 2003, 546, 27-38.	0.8	22
1995	High-resolution electron spectroscopy of different adsorption states of ethylene on Pd(111). <i>Surface Science</i> , 2003, 545, 122-136.	0.8	56
1996	Characterization of adsorption trends of NO <sub>2</sub> , nitrite, and nitrate on MgO terraces. <i>Surface Science</i> , 2003, 546, 75-86.	0.8	20
1997	Re-evaluation of the adsorption mode of ethene on the {111} surface of palladium using density functional theory. <i>Surface Science</i> , 2003, 547, L853-L858.	0.8	6
1998	Adsorption and diffusion energetics of hydrogen atoms on Fe(110) from first principles. <i>Surface Science</i> , 2003, 547, 85-98.	0.8	161
1999	A DFT periodic study of the vanadyl pyrophosphate (100) surface. <i>Surface Science</i> , 2003, 547, 438-451.	0.8	11
2000	A first principles analysis of CO oxidation over Pt and Pt <sub>66.7%</sub> Ru <sub>33.3%</sub> (111) surfaces. <i>Electrochimica Acta</i> , 2003, 48, 3759-3773.	2.6	114
2001	Crystal chemistry of molybdenum phosphides from density functional theory calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2003, 64, 405-411.	1.9	19
2002	Ground- and excited-state properties of inorganic solids from full-potential density-functional calculations. <i>Journal of Solid State Chemistry</i> , 2003, 176, 338-374.	1.4	10
2003	Quantum chemical contributions on the reactivity of solids. <i>Journal of Solid State Chemistry</i> , 2003, 176, 575-586.	1.4	2
2004	Vibrational spectroscopy using ab initio density-functional techniques. <i>Journal of Molecular Structure</i> , 2003, 651-653, 3-17.	1.8	27
2005	Vibrational and structural analysis of (hydroxypyridin-3-yl-methyl)phosphonic acid. <i>Journal of Molecular Structure</i> , 2003, 658, 229-239.	1.8	1
2006	Crystal structures of curium compounds: an ab initio study. <i>Journal of Nuclear Materials</i> , 2003, 322, 165-179.	1.3	37

#	ARTICLE	IF	CITATIONS
2007	An experimental and theoretical study of the isomerization of mononuclear bis(arylselenolato)bis(triphenylphosphine)platinum complexes [Pt(SeR) <sub>2</sub> (PPh <sub>3</sub> ) <sub>2</sub> ]. <i>Journal of Organometallic Chemistry</i> , 2003, 666, 111-120.	0.8	26
2008	Density functional study of lanthanide complexes (̇-5-C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> LnẊ-OC <sub>4</sub> H <sub>8</sub> (Ln=Lȧ“Lu; X=F, Cl, Br and I). <i>Journal of Organometallic Chemistry</i> , 2003, 679, 84-92.	0.8	16
2009	Rhodium pincer complexes of 2,2-̇-bis(diphenylphosphino)diphenylamine. <i>Journal of Organometallic Chemistry</i> , 2003, 682, 149-154.	0.8	83
2010	Effect of the surface model on the theoretical description of the chemisorption of atomic hydrogen on Cu(). <i>Surface Science</i> , 2003, 522, 185-197.	0.8	26
2011	STM images of molecularly and atomically chemisorbed oxygen on silver. <i>Surface Science</i> , 2003, 522, L27-L35.	0.8	38
2012	Reactivity of a reduced metal oxide surface: hydrogen, water and carbon monoxide adsorption on oxygen defective rutile TiO <sub>2</sub> (). <i>Surface Science</i> , 2003, 524, 49-62.	0.8	162
2013	Dissociative adsorption of hydrogen on strained Cu surfaces. <i>Surface Science</i> , 2003, 525, 107-118.	0.8	147
2014	Adsorption of Pd and Pt atoms on ̇-Al <sub>2</sub> O <sub>3</sub> (̇): density functional study of cluster models embedded in an elastic polarizable environment. <i>Surface Science</i> , 2003, 525, 173-183.	0.8	40
2015	CO bonding on tin modified Pt(̇)-(1̇-2). <i>Surface Science</i> , 2003, 526, 184-192.	0.8	14
2016	A periodic model for the V <sub>2</sub> O <sub>5</sub> ̇-TiO <sub>2</sub> (anatase) catalyst. Stability of dimeric species. <i>Surface Science</i> , 2003, 526, 297-308.	0.8	56
2017	CO adsorption on Ni̇“̇“a density functional theory study. <i>Surface Science</i> , 2003, 526, 332-340.	0.8	74
2018	Interaction between electronic structure and strain in Bi nanolines on Si(001). <i>Surface Science</i> , 2003, 527, L177-L183.	0.8	36
2019	Chemisorption of pyrrole (C <sub>4</sub> H <sub>4</sub> NH) on Si(001) calculated from first-principles. <i>Surface Science</i> , 2003, 532-535, 988-992.	0.8	11
2020	The structure of water on the (̇) surface of graphite. <i>Surface Science</i> , 2003, 532-535, 166-172.	0.8	75
2021	The effects of doping a grain boundary in ZnO with various concentrations of Bi. <i>Surface Science</i> , 2003, 532-535, 351-358.	0.8	9
2022	Theory of NO/K phase mixing, separation and catalytic promoter action on Co{1 0 1̇, 0}. <i>Surface Science</i> , 2003, 529, 312-318.	0.8	4
2023	Oxidation of graphite by atomic oxygen: a first-principles approach. <i>Surface Science</i> , 2003, 537, 55-63.	0.8	76
2024	A combined ab initio and atomistic simulation study of the surface and interfacial structures and energies of hydrated scheelite: introducing a CaWO <sub>4</sub> potential model. <i>Surface Science</i> , 2003, 531, 159-176.	0.8	58



#	ARTICLE	IF	CITATIONS
2025	Oxygen vibrations in O <sup>2</sup> /Ag(001). Surface Science, 2003, 530, 26-36.	0.8	17
2026	A spin-polarised first principles study of short dangling bond wires on Si. Surface Science, 2003, 531, L351-L355.	0.8	24
2027	Effects of the kinetic energy on the hydrogen abstraction dynamics on Cu(). Surface Science, 2003, 532-535, 148-153.	0.8	2
2028	Calculation of magnetic and structural properties of small Co <sup>2+</sup> /Rh clusters. Surface Science, 2003, 532-535, 334-340.	0.8	37
2029	Ab initio density functional study of O on the Ag(001) surface. Surface Science, 2003, 531, 272-286.	0.8	56
2030	Electric field effects on surface dynamics: Si ad-dimer diffusion and rotation on Si(). Surface Science, 2003, 536, 121-129.	0.8	22
2031	Density functional study of Pd adsorbates at SnO <sub>2</sub> (110) surfaces. Surface Science, 2003, 537, 168-178.	0.8	17
2032	A comparative study of CO chemisorption on flat and stepped Ni surfaces using density functional theory. Surface Science, 2003, 537, 217-227.	0.8	51
2033	First-principles theory and microcalorimetry of CO adsorption on the { 211 } surfaces of Pt and Ni. Surface Science, 2003, 538, 171-183.	0.8	52
2034	Density functional study of alkali metals adsorption on the MgO( 111 ) surface. Surface Science, 2003, 538, 240-248.	0.8	11
2035	A density functional study of adsorption of sodium-chloride overlayers on a stepped and a flat copper surface. Surface Science, 2003, 540, 172-184.	0.8	41
2036	The adsorption and dissociation of O <sub>2</sub> molecular precursors on Cu: the effect of steps. Surface Science, 2003, 538, 219-232.	0.8	47
2037	A first-principles study of surface and subsurface H on and in Ni(111): diffusional properties and coverage-dependent behavior. Surface Science, 2003, 540, 215-229.	0.8	183
2038	Unified picture of the molecular adsorption process: O <sub>2</sub> /Pt(111). Surface Science, 2003, 539, L542-L548.	0.8	70
2039	DFT study of adsorption and dissociation of thiophene molecules on Ni(110). Surface Science, 2003, 540, 474-490.	0.8	37
2040	Adsorption of Au atoms on stoichiometric and reduced TiO <sub>2</sub> (110) rutile surfaces: a first principles study. Surface Science, 2003, 542, 72-80.	0.8	87
2041	Relaxation of the surface in binary Sc, Ti and V nitrides: a first principles density functional study. Surface Science, 2003, 541, 217-224.	0.8	15
2042	DFT calculations of (111) surfaces of Au, Cu, and Pt: stability and reconstruction. Vacuum, 2003, 71, 101-106.	1.6	22

#	ARTICLE	IF	CITATIONS
2043	A density functional study of some physical properties of carnosine (N- $\beta$ -alanyl-L-histidine). Computational and Theoretical Chemistry, 2003, 621, 245-251.	1.5	10
2044	Thermochemistry of the higher chlorine oxides ClO <sub>x</sub> (x=3, 4) and Cl <sub>2</sub> O <sub>x</sub> (x=3-7). Computational and Theoretical Chemistry, 2003, 620, 215-226.	1.5	21
2045	A density functional study on the Pt(0)-catalysed hydrosilylation of ethylene. Computational and Theoretical Chemistry, 2003, 623, 277-288.	1.5	11
2046	Chlorofluorocarbons adsorption structures and energetic over faujasite type zeolites—a first principle study. Computational and Theoretical Chemistry, 2003, 630, 233-242.	1.5	15
2047	Assessment of density functional theory for the prediction of the nature of the oxirene stationary point. Computational and Theoretical Chemistry, 2003, 629, 263-270.	1.5	15
2048	A theoretical study of the electronic structure of O <sub>2</sub> interstitial impurities in silica. Computational and Theoretical Chemistry, 2003, 631, 111-116.	1.5	2
2049	A density functional study of the adsorption of pyridine, 2-vinylpyridine, and 4-vinylpyridine onto a silica surface. Computational and Theoretical Chemistry, 2003, 634, 187-193.	1.5	6
2050	First-principle investigation of the hydroxylation of zirconia and hafnia surfaces. Microelectronic Engineering, 2003, 69, 587-593.	1.1	68
2051	First-principle theoretical study on the electronic properties of SiO <sub>2</sub> models with hydrogenated impurities and charges. Applied Surface Science, 2003, 216, 463-470.	3.1	8
2052	Theoretical study on the initial processes of nitridation of silicon thin film. Applied Surface Science, 2003, 216, 141-148.	3.1	6
2053	Reliable potential for small sulfuric acid-water clusters. Chemical Physics, 2003, 287, 7-19.	0.9	40
2054	Ab initio studies of ferromagnetic properties of galvinoxyl. Journal of Magnetism and Magnetic Materials, 2003, 257, 11-14.	1.0	12
2055	Lifetime of holes and electrons at metal surfaces; electron-phonon coupling. Journal of Electron Spectroscopy and Related Phenomena, 2003, 129, 97-104.	0.8	13
2056	Development of an all-atoms force field from ab initio calculations for alternative refrigerants. Fluid Phase Equilibria, 2003, 210, 105-116.	1.4	29
2057	Energies and stabilities of sodium chloride clusters based on inversion pair potentials. Physica B: Condensed Matter, 2003, 325, 172-183.	1.3	24
2058	First-principles study on the electronic structure and the ferromagnetic properties of the organic radical DTDA. Physica B: Condensed Matter, 2003, 325, 380-384.	1.3	9
2059	Ab initio calculations of the electronic structure of the silver palladium oxide Ag <sub>2</sub> PdO <sub>2</sub> . Physica B: Condensed Matter, 2003, 337, 102-110.	1.3	3
2060	Vibrational and quantum-chemical study of pH dependent molecular structures of (hydroxypyridin-4-yl-methyl)phosphonic acid. Vibrational Spectroscopy, 2003, 33, 83-92.	1.2	4

#	ARTICLE	IF	CITATIONS
2061	Competition between $\pi$ - and $f$ -based interactions in metal ion complexes of the phenyl radical. <i>International Journal of Mass Spectrometry</i> , 2003, 227, 33-46.	0.7	19
2062	The ideal strength of iron in tension and shear. <i>Acta Materialia</i> , 2003, 51, 2271-2283.	3.8	196
2063	A computational and experimental study of anhydrous phosphotungstic acid and its interaction with water molecules. <i>Applied Catalysis A: General</i> , 2003, 256, 51-68.	2.2	100
2064	Oxygen vacancies at Ni/c-ZrO <sub>2</sub> interfaces. <i>Journal of the European Ceramic Society</i> , 2003, 23, 2737-2740.	2.8	19
2065	Structure-property transition-state model for the copolymerization of ethene and 1-hexene with experimental and theoretical applications to novel disilylene-bridged zirconocenes. <i>Journal of Polymer Science Part A</i> , 2003, 41, 1622-1631.	2.5	13
2066	Diffusion, surface alloy formation, and spin alignment in Fe/Cr(001) systems and superlattices. <i>Physica Status Solidi (B): Basic Research</i> , 2003, 236, 166-172.	0.7	8
2067	Properties of the UFe <sub>5</sub> Sn compound: electronic structure and X-ray photoemission. <i>Physica Status Solidi (B): Basic Research</i> , 2003, 236, 548-551.	0.7	1
2068	Electronic structure of the uranium monostannide USn. <i>Physica Status Solidi (B): Basic Research</i> , 2003, 236, 552-555.	0.7	2
2069	Electronic study of FeTi, CoTi, and NiTi alloys: bulk, surfaces, and interfaces. <i>Physica Status Solidi (B): Basic Research</i> , 2003, 239, 389-398.	0.7	13
2070	Electronic structure calculations of magnesium chalcogenides MgS and MgSe. <i>Physica Status Solidi (B): Basic Research</i> , 2003, 240, 565-573.	0.7	56
2071	First-principle study on the structures and electronic properties of gallium nitride nanowires. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2003, 0, 2318-2322.	0.8	17
2072	Formation of C <sub>x</sub> clusters in Cu/ZnO nanocomposites studied by IR spectroscopy. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2003, 0, 2956-2960.	0.8	0
2073	Fractional occupation numbers and spin density functional calculations of degenerate systems. <i>International Journal of Quantum Chemistry</i> , 2003, 93, 317-323.	1.0	11
2074	DFT-based solution to the gap problem of antiferromagnetic transition metal oxides and parent compounds of high-T <sub>c</sub> superconductors. <i>International Journal of Quantum Chemistry</i> , 2003, 91, 216-223.	1.0	4
2075	Ab initio and DFT studies for accurate description of van der Waals interaction between rare-gas atoms. <i>International Journal of Quantum Chemistry</i> , 2003, 91, 355-362.	1.0	29
2076	Realizations of the noninteracting kinetic energy functional enhancement factor through local-scaling transformations: Atoms. <i>International Journal of Quantum Chemistry</i> , 2003, 91, 94-104.	1.0	7
2077	Generalized spin density functional study of radical reactions. <i>International Journal of Quantum Chemistry</i> , 2003, 91, 376-383.	1.0	18
2078	First principles calculations of the formation energy of Cr/Al vacancies in spinel-type MgCr <sub>2</sub> O <sub>4</sub> and MgAl <sub>2</sub> O <sub>4</sub> . <i>International Journal of Quantum Chemistry</i> , 2003, 91, 208-210.	1.0	3

#	ARTICLE	IF	CITATIONS
2079	Nonlocal WDA functional capable of describing the image potential of a metallic surface. International Journal of Quantum Chemistry, 2003, 91, 139-144.	1.0	6
2080	Ferromagnetic instabilities in atomically thin lithium and sodium wires. International Journal of Quantum Chemistry, 2003, 91, 239-244.	1.0	19
2081	DFT calculations of correlation energies for excited electronic states using MCSCF wave functions. International Journal of Quantum Chemistry, 2003, 91, 451-460.	1.0	12
2082	Magnetism and energetics of the 4d bimetallic cluster Pd <sub>6</sub> Ru <sub>6</sub> . International Journal of Quantum Chemistry, 2003, 91, 270-276.	1.0	7
2083	Benzonitriles: Survey of their importance and scaling of their vibrational frequencies. International Journal of Quantum Chemistry, 2003, 94, 189-204.	1.0	51
2084	Interaction of M <sub>2</sub> Sn (M=Ru, Rh, Pd) dimers with CH <sub>2</sub> and CF <sub>2</sub> : A density functional study. International Journal of Quantum Chemistry, 2003, 95, 164-176.	1.0	7
2085	First-principles study of metal/nitride polar interfaces: Ti/TiN. Surface and Interface Analysis, 2003, 35, 835-841.	0.8	35
2086	Electronic Structure and Bulk Properties of $\beta$ -SiAlONs. Journal of the American Ceramic Society, 2003, 86, 1162-1167.	1.9	13
2087	Crystal structures and shape-memory behaviour of NiTi. Nature Materials, 2003, 2, 307-311.	13.3	320
2088	Transport properties of magnetic atom bridges controlled by a scanning tunneling microscope. Applied Surface Science, 2003, 212-213, 829-832.	3.1	6
2089	Electron theory in materials modeling. Acta Materialia, 2003, 51, 5649-5673.	3.8	30
2090	Structure and Bonding in B <sub>6</sub> -and B <sub>6</sub> : $\Delta$ Planarity and Antiaromaticity. Journal of Physical Chemistry A, 2003, 107, 1359-1369.	1.1	193
2091	Photoelectron Spectroscopy and ab Initio Study of B <sub>3</sub> -and B <sub>4</sub> -Anions and Their Neutrals. Journal of Physical Chemistry A, 2003, 107, 9319-9328.	1.1	183
2092	Lattice dielectric response of CdCu <sub>3</sub> Ti <sub>4</sub> O <sub>12</sub> and CaCu <sub>3</sub> Ti <sub>4</sub> O <sub>12</sub> from first principles. Physical Review B, 2003, 67, .	1.1	93
2093	Basis-set limit binding energies of Be and Mg (n=2,3,4) clusters. Physical Review A, 2003, 68, .	1.0	19
2094	Ab initio calculations of dimensional and adsorbate effects on the workfunction of single-walled carbon nanotube. Diamond and Related Materials, 2003, 12, 565-571.	1.8	22
2095	Structural stability of Pu(1-x)Mx (M=Al, Ga, and In) compounds. Physical Review B, 2003, 68, .	1.1	44
2096	Molecular alligator clips: a theoretical study of adsorption of S, Se and S <sup>2-</sup> H on Au(111). Nanotechnology, 2003, 14, 849-858.	1.3	25

#	ARTICLE	IF	CITATIONS
2097	Instability of the rhodium magnetic moment as the origin of the metamagnetic phase transition in $\text{FeRh}$ . <i>Physical Review B</i> , 2003, 67, .	1.1	89
2098	Interatomic potentials for atomistic simulations of the Ti-Al system. <i>Physical Review B</i> , 2003, 68, .	1.1	527
2099	DFT Calculations and Spectral Measurements of Charge-Transfer Complexes Formed by Aromatic Amines and Nitrogen Heterocycles with Tetracyanoethylene and Chloranil. <i>Journal of Physical Chemistry A</i> , 2003, 107, 8939-8948.	1.1	66
2100	Predicting aqueous solubilities from aqueous free energies of solvation and experimental or calculated vapor pressures of pure substances. <i>Journal of Chemical Physics</i> , 2003, 119, 1661-1670.	1.2	97
2101	Towards reliable prediction of kinetics and mechanisms for elementary processes: Key combustion initiation reactions of ammonium perchlorate. <i>Theoretical and Computational Chemistry</i> , 2003, , 373-443.	0.2	5
2102	High Throughput Experimental and Theoretical Predictive Screening of Materials – A Comparative Study of Search Strategies for New Fuel Cell Anode Catalysts. <i>Journal of Physical Chemistry B</i> , 2003, 107, 11013-11021.	1.2	231
2103	Interaction of $\text{Li}^+$ , $\text{Na}^+$ , and $\text{K}^+$ with the Proline Amino Acid. Complexation Modes, Potential Energy Profiles, and Metal Ion Affinities. <i>Journal of Physical Chemistry B</i> , 2003, 107, 2588-2594.	1.2	103
2104	Magnetic Properties and Diffusion of Adatoms on a Graphene Sheet. <i>Physical Review Letters</i> , 2003, 91, 017202.	2.9	419
2105	Effective Pathway for Hydrogen Atom Adsorption on Graphene. <i>Journal of the Physical Society of Japan</i> , 2003, 72, 995-997.	0.7	69
2106	Initial stages in the oxidation and reduction of the $\sqrt{3}\times\sqrt{3}$ surface oxide phase on $\text{Ag}\{111\}$ : A combined density-functional theory and STM simulation study. <i>Physical Review B</i> , 2003, 68, .	1.1	17
2107	Theoretical calculations of positron annihilation characteristics in inorganic solids – Recent advances and problems. <i>Advances in Quantum Chemistry</i> , 2003, , 77-108.	0.4	12
2108	Local reactivity of metal overlayers: Density functional theory calculations of Pd on Au. <i>Physical Review B</i> , 2003, 67, .	1.1	130
2109	First principles studies for the dissociative adsorption of $\text{H}_2$ on graphene. <i>Journal of Applied Physics</i> , 2003, 93, 3395-3400.	1.1	145
2110	General Rules for Predicting Where a Catalytic Reaction Should Occur on Metal Surfaces: A Density Functional Theory Study of $\text{C-H}$ and $\text{C-O}$ Bond Breaking/Making on Flat, Stepped, and Kinked Metal Surfaces. <i>Journal of the American Chemical Society</i> , 2003, 125, 1958-1967.	6.6	534
2111	Surface Structures of $\text{SrTiO}_3(001)$ : A $\text{TiO}_2$ -rich Reconstruction with a $c(4\sqrt{2})$ Unit Cell. <i>Journal of the American Chemical Society</i> , 2003, 125, 10050-10056.	6.6	134
2112	Chemistry of one-dimensional metallic edge states in $\text{MoS}_2$ nanoclusters. <i>Nanotechnology</i> , 2003, 14, 385-389.	1.3	212
2113	Adhesion of metal-carbide/nitride interfaces: Al/TiC and Al/TiN. <i>Journal of Physics Condensed Matter</i> , 2003, 15, 8103-8114.	0.7	60
2114	Adatoms, dimers, and interstitials on group-IV(113) surfaces: First-principles studies of energetical, structural, and electronic properties. <i>Physical Review B</i> , 2003, 67, .	1.1	26

#	ARTICLE	IF	CITATIONS
2115	Structural and Electronic Properties of the Layered LiNi <sub>0.5</sub> Mn <sub>0.5</sub> O <sub>2</sub> Lithium Battery Material. <i>Chemistry of Materials</i> , 2003, 15, 4280-4286.	3.2	84
2116	Density functional calculations of hydrogen adsorption on palladium-silver alloy surfaces. <i>Journal of Chemical Physics</i> , 2003, 118, 3268-3276.	1.2	62
2117	Theoretical Study of the Adsorption of Acetylene on the (111) Surfaces of Pd, Pt, Ni, and Rh. <i>Journal of Physical Chemistry B</i> , 2003, 107, 217-223.	1.2	107
2118	Adsorption of Unsaturated Hydrocarbons on Pd(111) and Pt(111): A DFT Study. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12287-12295.	1.2	148
2119	Ab initio study of anthracene under high pressure. <i>Physical Review B</i> , 2003, 67, .	1.1	65
2120	Ab initio calculation of the ideal tensile and shear strength of cubic silicon nitride. <i>Physical Review B</i> , 2003, 67, .	1.1	41
2121	The role of the basis set: Assessing density functional theory. <i>Journal of Chemical Physics</i> , 2003, 119, 3005-3014.	1.2	181
2122	Ab initio elasticity of chalcopyrites. <i>Journal of Applied Physics</i> , 2003, 93, 3789-3795.	1.1	34
2123	A Quantum Molecular Dynamics Simulation Study of the Initial Hydrolysis Step in Sol-Gel Process. <i>Journal of Physical Chemistry B</i> , 2003, 107, 1518-1524.	1.2	115
2124	Density Functional Theory Study of the Direct Conversion of Methane to Acetic Acid by RhCl <sub>3</sub> . <i>Organometallics</i> , 2003, 22, 3513-3525.	1.1	32
2125	The Possible Role of SO <sub>3</sub> as an Oxidizing Agent in Methane Functionalization by the Catalytic Process. A Density Functional Theory Study. <i>Organometallics</i> , 2003, 22, 1668-1674.	1.1	29
2126	Mechanism of Cis-to-Trans Isomerization of Azobenzene: Direct MD Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4555-4562.	1.1	39
2127	Quantum mechanical predictions of nonscalar equations of state and nonmonotonic elastic stress-strain relations. <i>Applied Physics Letters</i> , 2003, 83, 1151-1153.	1.5	4
2128	Force-based many-body interatomic potential for ZrC. <i>Journal of Applied Physics</i> , 2003, 93, 9072-9085.	1.1	49
2129	Origin of Network Connectivity and Structural Units in Amorphous SiSe <sub>2</sub> . <i>Physical Review Letters</i> , 2003, 90, 125502.	2.9	25
2130	Different Surface Chemistries of Water on Ru{0001}: From Monomer Adsorption to Partially Dissociated Bilayers. <i>Journal of the American Chemical Society</i> , 2003, 125, 2746-2755.	6.6	228
2131	First-principles calculations of intrinsic defects in Al <sub>2</sub> O <sub>3</sub> . <i>Physical Review B</i> , 2003, 68, .	1.1	270
2132	Vacancy formation and O adsorption at the Al(111) surface. <i>Physical Review B</i> , 2003, 68, .	1.1	22

#	ARTICLE	IF	CITATIONS
2133	New Insights into Ethene Epoxidation on Two Oxidized Ag{111} Surfaces. Journal of the American Chemical Society, 2003, 125, 5620-5621.	6.6	108
2134	Non-local screened-exchange calculations for defects in semiconductors: vacancy in silicon. Journal of Physics Condensed Matter, 2003, 15, 4387-4395.	0.7	34
2135	Metal-Nonmetal Transition in the Boron Group Elements. Physical Review Letters, 2003, 90, 065701.	2.9	111
2136	Free energy of liquid water on the basis of quasichemical theory and ab initio molecular dynamics. Physical Review E, 2003, 68, 041505.	0.8	133
2137	Understanding the complex metallic element Mn. Geometric frustration in $\hat{\Gamma}^2$ -Mn, phase stability, and phase transitions. Physical Review B, 2003, 68, .	1.1	133
2138	First-Principles Characterization of NO <sub>x</sub> Adsorption on MgO. Journal of Physical Chemistry B, 2003, 107, 157-163.	1.2	44
2139	Accurate Calculations of Bond Dissociation Enthalpies with Density Functional Methods. Journal of Physical Chemistry A, 2003, 107, 9991-9996.	1.1	107
2140	Surface Strain versus Substrate Interaction in Heteroepitaxial Metal Layers: Pt on Ru(0001). Physical Review Letters, 2003, 91, 016101.	2.9	316
2141	Structural, Spectroscopic, and Redox Consequences of a Central Ligand in the FeMoco of Nitrogenase: A Density Functional Theoretical Study. Journal of the American Chemical Society, 2003, 125, 8377-8383.	6.6	146
2142	Unusual CO Adsorption Sites on Vanadium Oxide $\sim$ Pd(111) $\sim$ Inverse Model Catalyst $\sim$ Surfaces. Journal of Physical Chemistry B, 2003, 107, 4777-4785.	1.2	50
2143	Uracil Adsorbed on Si(001): Structure and Energetics. Journal of Physical Chemistry B, 2003, 107, 5031-5035.	1.2	27
2144	Physisorption and Chemisorption of Somen-Hydrocarbons at the Brønsted Acid Site in Zeolites 12-Membered Ring Main Channels: Ab Initio Study of the Gmelinite Structure. Journal of Physical Chemistry B, 2003, 107, 9756-9762.	1.2	46
2145	Study of the Mechanism of Electron-Transfer Quenching by Boron $\sim$ Nitrogen Adducts in Fluorescent Sensors. Journal of Physical Chemistry B, 2003, 107, 12942-12948.	1.2	122
2146	Insights into the Structure and Reactivity of Acylperoxy Complexes in the Kochi $\sim$ Jacobsen $\sim$ Katsuki Catalytic System. A Density Functional Study. Journal of the American Chemical Society, 2003, 125, 13879-13889.	6.6	38
2147	Bond formation at the Ni/ZrO <sub>2</sub> interface. Physical Review B, 2003, 68, .	1.1	69
2148	$\tilde{f}$ -Aromaticity and $\tilde{f}$ -Antiaromaticity in Alkali Metal and Alkaline Earth Metal Small Clusters. Journal of Physical Chemistry A, 2003, 107, 554-560.	1.1	193
2149	An Average-of-Configuration Method for Using Kohn $\sim$ Sham Density Functional Theory in Modeling Ligand-Field Theory. Inorganic Chemistry, 2003, 42, 4088-4097.	1.9	26
2150	Electronic and Structural Evolution of Monoiron Sulfur Clusters, FeSn- and FeSn (n = 1 $\sim$ 6), from Anion Photoelectron Spectroscopy. Journal of Physical Chemistry A, 2003, 107, 2821-2828.	1.1	40



#	ARTICLE	IF	CITATIONS
2151	Ethylene Adsorption and Coadsorption with H on Pd(110) from First Principles. <i>Journal of Physical Chemistry B</i> , 2003, 107, 1604-1615.	1.2	27
2152	Chemical termination of the CsCl-structure FeSi/Si(111) film surface and its multilayer relaxation. <i>Physical Review B</i> , 2003, 67, .	1.1	24
2153	Vibrational Band Assignments for the Chiral Modifier Cinchonidine: Implications for Surface Studies. <i>Journal of Physical Chemistry B</i> , 2003, 107, 14365-14373.	1.2	112
2154	Computational Evidence of Bubble ZnS Clusters. <i>Journal of Physical Chemistry B</i> , 2003, 107, 10337-10340.	1.2	82
2155	First-principles study of defect energetics in titanium-doped alumina. <i>Physical Review B</i> , 2003, 68, .	1.1	53
2156	Theoretical Study of CO Migratory Insertion Reactions with Group 10 Metal Alkyl and Alkoxide Bonds. <i>Organometallics</i> , 2003, 22, 4547-4556.	1.1	49
2157	A Programmable Molecular Diode Driven by Charge-Induced Conformational Changes. <i>Journal of the American Chemical Society</i> , 2003, 125, 14240-14241.	6.6	64
2158	Structural, electronic, and magnetic properties of a ferromagnetic semiconductor: Co-doped TiO <sub>2</sub> rutile. <i>Physical Review B</i> , 2003, 68, .	1.1	75
2159	Adsorption of HCl on Single-Crystal Al <sub>2</sub> O <sub>3</sub> (0001) Surface: A DFT Study. <i>Journal of Physical Chemistry B</i> , 2003, 107, 186-195.	1.2	36
2160	Adsorption and Desorption of Methanol on Pd (111) and on a Pd/V Surface Alloy. <i>Journal of Physical Chemistry B</i> , 2003, 107, 2552-2558.	1.2	68
2161	Atomic and electronic structure of MoS <sub>2</sub> nanoparticles. <i>Physical Review B</i> , 2003, 67, .	1.1	352
2162	Cl <sub>3</sub> V(1/4-S(CH <sub>3</sub> ) <sub>2</sub> ) <sub>3</sub> VOCl <sub>3</sub> : A First-Row, Face-Shared Biocahedral Complex with Multiple Metal-Metal Bonding. <i>Inorganic Chemistry</i> , 2003, 42, 4417-4424.	1.9	4
2163	An Infrared and Theoretical Study about the C-XCN Band Formation: Reactivity of HNCO with NH <sub>3</sub> Astrophysical Ice Laboratory Analogues and the Spontaneous Production of OCN-. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9335-9343.	1.1	29
2164	Luminescent Compounds fac- and mer-Aluminum Tris(quinolin-8-olate). A Pure and Hybrid Density Functional Theory and Time-Dependent Density Functional Theory Investigation of Their Electronic and Spectroscopic Properties. <i>Journal of Physical Chemistry A</i> , 2003, 107, 2560-2569.	1.1	67
2165	Adsorption of Small Palladium Clusters on the Relaxed Al <sub>2</sub> O <sub>3</sub> (0001) Surface. <i>Journal of Physical Chemistry B</i> , 2003, 107, 6411-6424.	1.2	39
2166	Carbon Monoxide Adsorption on Molybdenum Phosphides: Fourier Transform Infrared Spectroscopic and Density Functional Theory Studies. <i>Journal of Physical Chemistry B</i> , 2003, 107, 13698-13702.	1.2	26
2167	Combinatorial Computational Chemistry Approach to the High-Throughput Screening of Metal Sulfide Catalysts for CO Hydrogenation Process. <i>Energy &amp; Fuels</i> , 2003, 17, 857-861.	2.5	9
2168	Atomistic Simulation of the Dissociative Adsorption of Water on Calcite Surfaces. <i>Journal of Physical Chemistry B</i> , 2003, 107, 7676-7682.	1.2	141

#	ARTICLE	IF	CITATIONS
2169	DFT Calculations of Isomer Shifts and Quadrupole Splitting Parameters in Synthetic Iron <sup>VI</sup> Oxo Complexes: Applications to Methane Monooxygenase and Ribonucleotide Reductase. <i>Inorganic Chemistry</i> , 2003, 42, 5244-5251.	1.9	47
2170	Reaction of Pentadienyl Complexes with Metal Carbonyls: Synthetic, Structural, and Theoretical Studies of Metallabenzene $\eta^5$ -Complexes. <i>Organometallics</i> , 2003, 22, 264-274.	1.1	44
2171	Density Functional Theory Studies of Chemisorption and Diffusion Properties of Ni and Ni <sup>II</sup> Thiophene Complexes on the MoS <sub>2</sub> Basal Plane. <i>Journal of Physical Chemistry B</i> , 2003, 107, 1988-2000.	1.2	16
2172	$\eta^2$ -Sheet Preferences from First Principles. <i>Journal of the American Chemical Society</i> , 2003, 125, 16383-16386.	6.6	24
2173	The Heterolytic Dissociation of Neutral and Protonated Nitrous Acid. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11112-11119.	1.1	6
2174	Relativistic DFT Calculations of Copper Hyperfine Coupling Constants: Effect of Spin-Orbit Coupling. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5583-5587.	1.1	14
2175	Electronic correlation effects in transition-metal sulfides. <i>Journal of Physics Condensed Matter</i> , 2003, 15, 979-996.	0.7	231
2176	First-Principles Calculations of the Adsorption of Nitromethane and 1,1-Diamino-2,2-dinitroethylene (FOX-7) Molecules on the Al(111) Surface. <i>Journal of Physical Chemistry B</i> , 2003, 107, 8953-8964.	1.2	40
2177	Hydrogen Trioxide Anion: A Possible Atmospheric Intermediate and Path to Oxygen-Rich Molecules. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1203-1206.	1.1	10
2178	The particle-in-cell model for ab initio thermodynamics: implications for the elastic anisotropy of the Earth's inner core. <i>Physics of the Earth and Planetary Interiors</i> , 2003, 139, 243-253.	0.7	36
2179	Carbon dissolution and diffusion in ferrite and austenite from first principles. <i>Physical Review B</i> , 2003, 67, .	1.1	398
2180	An <i>ab initio</i> study of the ideal tensile and shear strength of single-crystal $\eta^3$ -Si <sub>3</sub> N <sub>4</sub> . <i>Journal of Materials Research</i> , 2003, 18, 1168-1172.	1.2	25
2181	The spin-flip approach within time-dependent density functional theory: Theory and applications to diradicals. <i>Journal of Chemical Physics</i> , 2003, 118, 4807-4818.	1.2	581
2182	Novel Stabilization Mechanism on Polar Surfaces: ZnO(0001)-Zn. <i>Physical Review Letters</i> , 2003, 90, 016102.	2.9	493
2183	A quantitative theory and computational approach for the vibrational Stark effect. <i>Journal of Chemical Physics</i> , 2003, 119, 851-858.	1.2	57
2184	The hydrolysis process of the cis-dichloro(ethylenediamine)platinum(II): A theoretical study. <i>Journal of Chemical Physics</i> , 2003, 118, 10584-10592.	1.2	67
2185	Theoretical characterization of several models of nanoporous carbon. <i>New Journal of Physics</i> , 2003, 5, 123-123.	1.2	32
2186	Theoretical Study of Atomic Oxygen Adsorption on the Chlorine-Modified Ag(111) Surface. <i>Journal of Physical Chemistry B</i> , 2003, 107, 3813-3819.	1.2	14

#	ARTICLE	IF	CITATIONS
2187	Theoretical study about adsorption of atomic oxygen on unmodified and I-modified Ag(100) surface. Journal of Chemical Physics, 2003, 118, 11210-11216.	1.2	6
2188	Electronic Structure of Transition Metals Fe, Ni and Cu in the GW Approximation. Journal of the Physical Society of Japan, 2003, 72, 607-610.	0.7	32
2189	Adsorption and Dissociation of O <sub>2</sub> on Gold Surfaces: A Effect of Steps and Strain. Journal of Physical Chemistry B, 2003, 107, 9298-9307.	1.2	322
2190	A Computer Modeling Study of Perfect and Defective Silver (111) Surfaces. Journal of Physical Chemistry B, 2003, 107, 3528-3534.	1.2	23
2191	Density-functional study of the structure and stability of ZnO surfaces. Physical Review B, 2003, 67, .	1.1	536
2192	Active Role of Oxide Support during CO Oxidation at Au/MgO. Physical Review Letters, 2003, 90, 206102.	2.9	431
2193	Adsorption energy and spin state of first-row transition metals adsorbed on MgO(100). Physical Review B, 2003, 67, .	1.1	67
2194	An ab initio approach to the calculation of current-voltage characteristics of programmable molecular devices. Proceedings of the IEEE, 2003, 9, 1958-1975.	16.4	65
2195	Structure effects on the energetic, electronic, and magnetic properties of palladium nanoparticles. Journal of Chemical Physics, 2003, 118, 5793-5801.	1.2	74
2196	Metal island growth and dynamics on molybdenite surfaces. Geochimica Et Cosmochimica Acta, 2003, 67, 923-934.	1.6	27
2197	Surface complexation of arsenic(V) to iron(III) (hydr)oxides: structural mechanism from ab initio molecular geometries and EXAFS spectroscopy. Geochimica Et Cosmochimica Acta, 2003, 67, 4223-4230.	1.6	624
2198	Anisotropy of the mobility of pentacene from frustration. Synthetic Metals, 2003, 139, 109-114.	2.1	125
2199	Magnetism of ultrathin wires suspended in free space and adsorbed on vicinal surfaces. Physical Review B, 2003, 67, .	1.1	47
2200	Identification of new adsorption sites of H and D on rhodium(100). Journal of Chemical Physics, 2003, 119, 5253-5266.	1.2	21
2201	Solvation Effects on Alternative Nucleophilic Substitution Reaction Paths for Chloride/Allyl Chloride and <sup>13</sup> C-Methylated Congeners. Journal of Organic Chemistry, 2003, 68, 6375-6386.	1.7	30
2202	Catalytic conversion of hydrocarbons over zeolites from first principles. Computational Materials Science, 2003, 27, 87-95.	1.4	8
2203	Magnetism of monoatomic wires on vicinal surfaces. Computational Materials Science, 2003, 27, 138-150.	1.4	11
2204	Efficient linear scaling geometry optimization and transition-state search for direct wavefunction optimization schemes in density functional theory using a plane-wave basis. Computational Materials Science, 2003, 27, 437-445.	1.4	172

#	ARTICLE	IF	CITATIONS
2205	The electronic and electrochemical properties of the TiFe-based alloys. Journal of Alloys and Compounds, 2003, 348, 285-292.	2.8	28
2206	Electronic structure of magnesium nitride-fluorides from first-principles calculations. Journal of Alloys and Compounds, 2003, 351, 72-76.	2.8	23
2207	Ab initio calculation of the crystal structure of the lanthanide Ln <sub>2</sub> O <sub>3</sub> sesquioxides. Journal of Alloys and Compounds, 2003, 351, 31-34.	2.8	137
2208	Electronic structure calculations for LaNi <sub>5</sub> and LaNi <sub>5</sub> H <sub>7</sub> : energetics and elastic properties. Journal of Alloys and Compounds, 2003, 353, 74-85.	2.8	103
2209	Electronic structures of semiconducting alkaline-earth metal silicides. Journal of Alloys and Compounds, 2003, 358, 257-263.	2.8	109
2210	Energetics, electric-field gradients and optical properties of YH <sub>3</sub> (YD <sub>3</sub> ) by first-principles calculations. Journal of Alloys and Compounds, 2003, 356-357, 73-79.	2.8	12
2211	First principles study of sodium-“aluminum”-hydrogen phases. Journal of Alloys and Compounds, 2003, 356-357, 486-489.	2.8	41
2212	An Interfacial Complex in ZnO and Its Influence on Charge Transport. Physical Review Letters, 2003, 91, 165506.	2.9	45
2213	DFT Study of Cysteine Adsorption on Au(111). Journal of Physical Chemistry B, 2003, 107, 1151-1156.	1.2	200
2214	Ternary Stannides LiT <sub>3</sub> Sn <sub>4</sub> (T = Ru, Rh, Ir) Chemical Bonding and Physical Properties. Journal of Physical Chemistry B, 2003, 107, 1943-1948.	1.2	21
2215	Co-phase penetration of WC(101̂0)/WC(101̂0) grain boundaries from first principles. Physical Review B, 2003, 67, .	1.1	85
2216	Description of the Ground State Wave Functions of Ni Dithiolenes Using Sulfur K-edge X-ray Absorption Spectroscopy. Journal of the American Chemical Society, 2003, 125, 9158-9169.	6.6	180
2217	Noble Gas-Actinide Complexes of the CUO Molecule with Multiple Ar, Kr, and Xe Atoms in Noble-Gas Matrices. Journal of the American Chemical Society, 2003, 125, 3126-3139.	6.6	124
2218	ReaxFFSiO Reactive Force Field for Silicon and Silicon Oxide Systems. Journal of Physical Chemistry A, 2003, 107, 3803-3811.	1.1	821
2219	Enhancement of electronic conductivity of LiFePO <sub>4</sub> by Cr doping and its identification by first-principles calculations. Physical Review B, 2003, 68, .	1.1	249
2220	Structural and thermal properties of silicon-doped fullerenes. Journal of Chemical Physics, 2003, 119, 1127-1135.	1.2	39
2221	Density functional theory studies of screw dislocation core structures in bcc metals. Philosophical Magazine, 2003, 83, 365-375.	0.7	197
2222	Theoretical Prediction of the Co-C Bond Strength in Cobalamins. Journal of Physical Chemistry A, 2003, 107, 7539-7545.	1.1	168

#	ARTICLE	IF	CITATIONS
2223	A First-Principles Analysis of Acetylene Hydrogenation over Pd(111). Journal of Physical Chemistry B, 2003, 107, 2009-2017.	1.2	124
2224	Effects of Microsolvation on the Structures and Reactions of Neutral and Zwitterion Alanine: A Computational Study. Journal of Physical Chemistry B, 2003, 107, 14109-14118.	1.2	76
2225	First-principles study of adhesion at Cu/SiO <sub>2</sub> interfaces. Physical Review B, 2003, 68, .	1.1	81
2226	Stability and clusterization of hydrogen-vacancy complexes in Fe: An ab initio study. Physical Review B, 2003, 67, .	1.1	296
2227	Vacancy concentration in Al from combined first-principles and model potential calculations. Physical Review B, 2003, 67, .	1.1	73
2228	Energetics, vibrational spectrum, and scanning tunneling microscopy images for the intermediate in water production reaction on Pt(111) from density functional calculations. Journal of Chemical Physics, 2003, 119, 4865-4872.	1.2	68
2229	The stability of the hydroxylated (0001) surface of $\alpha$ -Al <sub>2</sub> O <sub>3</sub> . Journal of Chemical Physics, 2003, 118, 11179-11188.	1.2	146
2230	Stabilization of Si <sub>60</sub> Cage Structure. Physical Review Letters, 2003, 90, 135503.	2.9	88
2231	Geometrical and Electronic Structures of Gold, Silver, and Gold-Silver Binary Clusters: Origins of Ductility of Gold and Gold-Silver Alloy Formation. Journal of Physical Chemistry B, 2003, 107, 9994-10005.	1.2	283
2232	Understanding the complex metallic element Mn. I. Crystalline and noncollinear magnetic structure of Mn. Physical Review B, 2003, 68, .	1.1	236
2233	First-principles studies of the geometry and energetics of the Si <sub>36</sub> cluster. Physical Review A, 2003, 67, .	1.0	38
2234	Effects of Basis Set Choice upon the Atomization Energy of the Second-Row Compounds SO <sub>2</sub> , CCl <sub>4</sub> , and ClO <sub>2</sub> for B3LYP and B3PW91. Journal of Physical Chemistry A, 2003, 107, 6720-6724.	1.1	50
2235	Derivation of the Density Functional Theory from the Cluster Expansion. Physical Review Letters, 2003, 91, 133001.	2.9	12
2236	Computer Modeling of Local Level Structures in (Ce, Zr) Mixed Oxide. Journal of Physical Chemistry B, 2003, 107, 8840-8853.	1.2	33
2237	Steric Effects on the Adsorption of Alkylthiolate Self-Assembled Monolayers on Au (111). Journal of Physical Chemistry B, 2003, 107, 3803-3807.	1.2	78
2238	Structure, Bonding, and Vibrational Frequencies of CH <sub>3</sub> CN-BF <sub>3</sub> : New Insight into Medium Effects and the Discrepancy between the Experimental and Theoretical Geometries. Journal of Physical Chemistry A, 2003, 107, 4009-4018.	1.1	56
2239	Theoretical Studies of Monosubstituted and Higher Phenyl-Substituted Octahydrosilsesquioxanes. Journal of Physical Chemistry B, 2003, 107, 13788-13792.	1.2	41
2240	Photolysis of Chiral 1-Pyrazolines to Cyclopropanes: Mechanism and Stereospecificity. Journal of Organic Chemistry, 2003, 68, 4906-4911.	1.7	19

#	ARTICLE	IF	CITATIONS
2241	Spin-orbit induced local band structure variations revealed by scanning tunnelling spectroscopy. Journal of Physics Condensed Matter, 2003, 15, S679-S692.	0.7	14
2242	CO adsorption on the CO-precovered Pt(111) surface characterized by density-functional theory. Physical Review B, 2003, 68, .	1.1	34
2243	First-principles calculations of the adsorption of nitromethane and 1,1-diamino 2,2-dinitroethylene (FOX-7) molecules on the Al[111] surface. , 0, , .		1
2244	A combined density functional theory and molecular mechanics (QM/MM) study of single site ethylene polymerization catalyzed by [Cp{NC(t-Bu) <sub>2</sub> TiR}]+ in the presence of the counterion (CH <sub>3</sub> B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> ) <sup>-1</sup> . Canadian Journal of Chemistry, 2003, 81, 1413-1429.	0.6	15
2245	Lattice inversion for interionic pair potentials. Journal of Chemical Physics, 2003, 118, 3974-3982.	1.2	17
2246	From ab initio quantum chemistry to molecular dynamics: The delicate case of hydrogen bonding in ammonia. Journal of Chemical Physics, 2003, 119, 5965-5980.	1.2	153
2247	Computational chemistry models leading to mediation of gun tube erosion. , 0, , .		0
2248	Density Functionals for Non-relativistic Coulomb Systems in the New Century. Lecture Notes in Physics, 2003, , 1-55.	0.3	96
2249	Atomic-scale investigation of the dielectric screening at the interface between silicon and its oxide. Materials Research Society Symposia Proceedings, 2003, 786, 511.	0.1	0
2250	Novel Method for the Activation of Acceptor Dopant in AlN Introducing Localized Band by Isoelectronic Dopant. Materials Research Society Symposia Proceedings, 2003, 798, 164.	0.1	0
2251	Ab-initio study on the $\beta$ -Al <sub>2</sub> O <sub>3</sub> surfaces and interfaces.. Materials Research Society Symposia Proceedings, 2003, 786, 521.	0.1	2
2252	Modeling the Polymorphism of Pentacene. Journal of the American Chemical Society, 2003, 125, 6323-6330.	6.6	214
2253	Density Functional Theory Study of the Interaction of Cl[ <sup>+</sup> ] with Passivated Nickel Surfaces. Electrochemical and Solid-State Letters, 2003, 6, B47.	2.2	36
2254	Influence of Stress on Thermoelectric Properties of Antimony Telluride. Materials Research Society Symposia Proceedings, 2003, 793, 38.	0.1	0
2255	Calculated thermodynamic properties of plutonium metal. Journal of Physics Condensed Matter, 2003, 15, 8377-8387.	0.7	39
2256	Cohesive Properties of PuGa Alloys. Materials Research Society Symposia Proceedings, 2003, 802, 203.	0.1	0
2257	Electronic structure of the organic half-metallic magnet 2-(4-nitrophenyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-1-oxyl 3-N-oxide. Physical Review B, 2003, 67, .	1.1	43
2258	Quantization condition of quantum-well states in Cu/Co(001). Physical Review B, 2003, 68, .	1.1	13

#	ARTICLE	IF	CITATIONS
2259	Structure, bonding, and adhesion at the TiC(100)/Fe(110) interface from first principles. Journal of Chemical Physics, 2003, 118, 8982-8996.	1.2	183
2260	First-principles study of the role of solvent in the dissociation of water over a Pt-Ru alloy. Physical Review B, 2003, 68, .	1.1	93
2261	Stability of gold nanowires at large Au-Au separations. Physical Review B, 2003, 67, .	1.1	72
2262	First-principles study of Peierls instability in infinite single row Al wires. Physical Review B, 2003, 68, .	1.1	14
2263	Tetragonal silver films on V(100): Experimental and ab initio studies. Physical Review B, 2003, 68, .	1.1	12
2264	First-principles studies of cation-doped spinel LiMn <sub>2</sub> O <sub>4</sub> for lithium ion batteries. Physical Review B, 2003, 67, .	1.1	51
2265	Hole dynamics in a quantum-well state at Na/Cu(111). Physical Review B, 2003, 68, .	1.1	86
2266	Oxygenation of carbon nanotubes: Atomic structure, energetics, and electronic structure. Physical Review B, 2003, 67, .	1.1	109
2267	Structural properties of Cu <sub>4</sub> O and Cu <sub>5</sub> O clusters: A density functional study. Journal of Chemical Physics, 2003, 119, 8305-8310.	1.2	20
2268	Electronic structure of the contact between carbon nanotube and metal electrodes. Applied Physics Letters, 2003, 83, 3180-3182.	1.5	61
2269	Covalent and Reversible Short-Range Electrostatic Imaging in Noncontact Atomic Force Microscopy. Physical Review Letters, 2003, 91, 216401.	2.9	25
2270	Supported Fe Nanoclusters: Evolution of Magnetic Properties with Cluster Size. Physical Review Letters, 2003, 90, 247202.	2.9	43
2271	Density functional study of the insertion mechanism for ethylene-styrene copolymerization with constrained geometry catalysts. Journal of Chemical Physics, 2003, 119, 1824-1837.	1.2	23
2272	The crystalline surfaces of PdH <sub>2</sub> {111}: Ideal surface terminations of a stoichiometric bulk compound relevant to heterogeneous catalysis. Journal of Chemical Physics, 2003, 118, 5623-5634.	1.2	21
2273	Mechanisms of Molecular Manipulation with the Scanning Tunneling Microscope at Room Temperature: Chlorobenzene/Si(111) (7Å <sup>2</sup> –7). Physical Review Letters, 2003, 91, 118301.	2.9	81
2274	Electronic structure and energetics of RCo <sub>5</sub> H <sub>4</sub> and RCo <sub>5</sub> (R=La,Pr). Applied Physics Letters, 2003, 82, 1042-1044.	1.5	10
2275	Reaction of H atoms with Cl adsorbed on Au(111): Quantum and quasiclassical studies. Journal of Chemical Physics, 2003, 118, 2357-2366.	1.2	27
2276	Structures and electronic properties of aluminum nanowires. Journal of Chemical Physics, 2003, 119, 538-546.	1.2	24



#	ARTICLE	IF	CITATIONS
2277	Surface structure and dynamics of $\text{KTaO}_3(001)$ . <i>Physical Review B</i> , 2003, 68, .	1.1	11
2278	Calculations of nuclear magnetic shielding in paramagnetic molecules. <i>Journal of Chemical Physics</i> , 2003, 118, 2550.	1.2	71
2279	Diffusion of an adsorbed Si atom on the $\text{Si}(111)\sqrt{7}\times\sqrt{7}$ surface. <i>Physical Review B</i> , 2003, 67, .	1.1	35
2280	Surface structure and stability of PdZn and PtZn alloys: $\rho$ -Density-functional slab model studies. <i>Physical Review B</i> , 2003, 68, .	1.1	108
2281	$\sqrt{3}\times\sqrt{2}$ reconstruction of the Sm/Si(111) interface. <i>Physical Review B</i> , 2003, 67, .	1.1	26
2282	Why are the 3d-5d compounds CuAu and NiPt stable, whereas the 3d-4d compounds CuAg and NiPd are not. <i>Physical Review B</i> , 2003, 67, .	1.1	32
2283	Dimensional change as a function of charge injection in graphite intercalation compounds: $\rho$ -Density functional theory study. <i>Physical Review B</i> , 2003, 68, .	1.1	24
2284	Structural stability and magnetic properties in $\text{X}_2\text{AlX}$ ( $\text{X}=\text{Fe}, \text{Co}, \text{Ni}; \text{X}=\text{Ti}, \text{Cr}$ ) Heusler alloys from quantum mechanical calculations. <i>Journal of Applied Physics</i> , 2003, 94, 3292-3298.	1.1	73
2285	Restricted density-functional linear response theory calculations of electronic g-tensors. <i>Journal of Chemical Physics</i> , 2003, 119, 10489-10496.	1.2	26
2286	Theoretical extension of the gold pressure calibration standard beyond 3 Mbars. <i>Physical Review B</i> , 2003, 67, .	1.1	29
2287	First-principle dynamical electronic characteristics of Al electromigration in the bulk, surface, and grain boundary. <i>Physical Review B</i> , 2003, 67, .	1.1	8
2288	Effect of dimensionality on the electronic structure of Cu, Ag, and Au. <i>Physical Review B</i> , 2003, 68, .	1.1	69
2289	A molecular picture of hydrophilic and hydrophobic interactions from ab initio density functional theory calculations. <i>Journal of Chemical Physics</i> , 2003, 119, 7617-7620.	1.2	59
2290	Ab initio study of Al-ceramic interfacial adhesion. <i>Physical Review B</i> , 2003, 67, .	1.1	127
2291	Formation of quantum structures on a single nanotube by modulating hydrogen adsorption. <i>Physical Review B</i> , 2003, 68, .	1.1	29
2292	A simple and realistic model system for studying hydrogen bonds in $\hat{\rho}^2$ -sheets. <i>Journal of Chemical Physics</i> , 2003, 118, 9783-9794.	1.2	19
2293	Density-functional theory applied to Rh(111) and CO/Rh(111) systems: $\rho$ -Geometries, energies, and chemical shifts. <i>Physical Review B</i> , 2003, 67, .	1.1	46
2294	Lattice dynamics of HgSe: Neutron scattering measurements and ab initio studies. <i>Physical Review B</i> , 2003, 67, .	1.1	21

#	ARTICLE	IF	CITATIONS
2295	First-principles study on the energetics and vibrational properties of the S <sub>2</sub> impurity in alkali-halide crystals. <i>Physical Review B</i> , 2003, 68, .	1.1	6
2296	First-principles study of the solubility, diffusion, and clustering of C in Ni. <i>Physical Review B</i> , 2003, 68, .	1.1	71
2297	Exchange-correlation energy and the phase diagram of Si. <i>Physical Review B</i> , 2003, 68, .	1.1	38
2298	Pressure dependence of electron-phonon coupling and superconductivity in hcp Fe: A linear response study. <i>Physical Review B</i> , 2003, 67, .	1.1	33
2299	Vibrations of a water adlayer on Ru(0001). <i>Physical Review B</i> , 2003, 67, .	1.1	56
2300	Interactions and structure of poly(dimethylsiloxane) at silicon dioxide surfaces: Electronic structure and molecular dynamics studies. <i>Journal of Chemical Physics</i> , 2003, 118, 5132-5142.	1.2	60
2301	Diffusion and vibration of CO molecules adsorbed on a Cu(100) surface: A periodic density functional theory study. <i>Journal of Chemical Physics</i> , 2003, 119, 509-514.	1.2	30
2302	Ab initio Simulations of Homoepitaxial SiC Growth. <i>Physical Review Letters</i> , 2003, 91, 136101.	2.9	15
2303	Four-Atom Period in the Conductance of Monatomic Al Wires. <i>Physical Review Letters</i> , 2003, 91, 146801.	2.9	82
2304	Formation of the c(1 $\sqrt{3}$ ×1)Cu monolayer on CaO(100): A theoretical study. <i>Physical Review B</i> , 2003, 68, .	1.1	6
2305	Resolution of an Ancient Surface Science Anomaly: Work Function Change Induced by N Adsorption on W{100}. <i>Physical Review Letters</i> , 2003, 90, 246103.	2.9	122
2306	When Scanning Tunneling Microscopy Gets the Wrong Adsorption Site: H on Rh(100). <i>Physical Review Letters</i> , 2003, 90, 176101.	2.9	21
2307	Modeling oxide-metal interfaces from density-functional theory: Platinum adsorption on tetragonal zirconia. <i>Physical Review B</i> , 2003, 68, .	1.1	16
2308	Ab initio study of adsorption and diffusion of Ag atoms on a Si(001) surface. <i>Physical Review B</i> , 2003, 67, .	1.1	26
2309	Linear monatomic wires stabilized by alloying: Ab initio density functional calculations. <i>Physical Review B</i> , 2003, 67, .	1.1	34
2310	Significance of single-electron energies for the description of CO on Pt(111). <i>Physical Review B</i> , 2003, 68, .	1.1	225
2311	Why Do Grain Boundaries Exhibit Finite Facet Lengths?. <i>Physical Review Letters</i> , 2003, 90, 246102.	2.9	34
2312	Competing stabilization mechanism for the polar ZnO(0001)-Zn surface. <i>Physical Review B</i> , 2003, 68, .	1.1	335

#	ARTICLE	IF	CITATIONS
2313	Dilute nonisovalent (II-VI)-(III-V) semiconductor alloys: Monodoping, codoping, and cluster doping in ZnSe-GaAs. <i>Physical Review B</i> , 2003, 68, .	1.1	20
2314	Uniaxial phase transition in Si:Ab initio calculations. <i>Physical Review B</i> , 2003, 67, .	1.1	16
2315	Assignment of the $(1\bar{1}2)$ surface of rutile $\text{TiO}_2(110)$ from first principles. <i>Physical Review B</i> , 2003, 67, .	1.1	23
2316	Performance of coupled cluster theory in thermochemical calculations of small halogenated compounds. <i>Journal of Chemical Physics</i> , 2003, 118, 3510-3522.	1.2	195
2317	Optical spectroscopy of jet-cooled NiSi. <i>Journal of Chemical Physics</i> , 2003, 118, 2190-2196.	1.2	24
2318	Local lattice relaxations in random metallic alloys: Effective tetrahedron model and supercell approach. <i>Physical Review B</i> , 2003, 67, .	1.1	97
2319	Embedded-atom-method tantalum potential developed by the force-matching method. <i>Physical Review B</i> , 2003, 67, .	1.1	93
2320	Surface theory moves into the real world. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2003, 21, S64-S70.	0.9	3
2321	Ab initio study of elastic properties of Ir and Ir <sub>3</sub> X compounds. <i>Journal of Applied Physics</i> , 2003, 93, 2414-2417.	1.1	128
2322	Electronic properties of metal-“molecule”-metal systems at zero bias: A periodic density functional study. <i>Journal of Chemical Physics</i> , 2003, 119, 6729-6735.	1.2	65
2323	Influence of sulfur on the adhesion of the nickel/alumina interface. <i>Physical Review B</i> , 2003, 67, .	1.1	83
2324	Reactive Wetting: H <sub>2</sub> O/Rh(111). <i>Physical Review Letters</i> , 2003, 90, 186103.	2.9	41
2325	Reconstruction and magnetic structure of ultrathin $\text{Fe}$ films on Cu(111). <i>Physical Review B</i> , 2003, 67, .	1.1	17
2326	Theoretical analysis of clock-reconstructed PdCu surface alloy. <i>Physical Review B</i> , 2003, 67, .	1.1	10
2327	Defect sites at the (001) surface of mordenite: An ab initio study. <i>Journal of Chemical Physics</i> , 2003, 118, 8437-8445.	1.2	22
2328	Structural transition in Ba <sub>n</sub> O <sub>m</sub> clusters. <i>Physical Review B</i> , 2003, 67, .	1.1	6
2329	Six low-strain zinc-blende half metals: An ab initio investigation. <i>Physical Review B</i> , 2003, 67, .	1.1	176
2330	Electronic structure of Te- and As-covered Si(211). <i>Physical Review B</i> , 2003, 68, .	1.1	12

#	ARTICLE	IF	CITATIONS
2331	Coexistence of ferromagnetic and antiferromagnetic order in Mn-doped Ni <sub>2</sub> MnGa. <i>Physical Review B</i> , 2003, 67, .	1.1	208
2332	Formation of clean dimers during gas-source growth of Si(001). <i>Physical Review B</i> , 2003, 67, .	1.1	12
2333	Hydrogen effect on adhesion and adhesive transfer at aluminum/diamond interfaces. <i>Physical Review B</i> , 2003, 68, .	1.1	46
2335	Quantum Mechanical Study of Clean and H-Covered $\hat{\pm}$ -MoO <sub>3</sub> (100) Surface. <i>Journal of Theoretical and Computational Chemistry</i> , 2003, 02, 245-256.	1.8	2
2336	Electronic structure calculations of $\hat{\pm}$ -Pu based alloys. <i>Materials Research Society Symposia Proceedings</i> , 2003, 802, 209.	0.1	0
2337	First-Principles Calculation of the Work Functions for the High-Index Copper Surfaces. <i>Surface Review and Letters</i> , 2003, 10, 207-211.	0.5	3
2338	The dependence of exchange constants and electronic structure of manganese ferrite on the scaling factor. <i>IEEE Transactions on Magnetics</i> , 2003, 39, 3133-3135.	1.2	2
2339	Pyrrole (C <sub>4</sub> H <sub>4</sub> NH) and Polypyrrole Functionalized Silicon Surfaces Calculated from First Principles. <i>Surface Review and Letters</i> , 2003, 10, 221-226.	0.5	2
2340	Elastic constants and chemical bonding of LaNi <sub>5</sub> and LaNi <sub>5</sub> H <sub>7</sub> by first principles calculations. <i>Journal of Physics Condensed Matter</i> , 2003, 15, 6549-6561.	0.7	23
2341	First Principles Studies on the Interaction of a Hydrogen Atom with a Single-Walled Carbon Nanotube. <i>Japanese Journal of Applied Physics</i> , 2003, 42, 4626-4629.	0.8	14
2342	Calculation of exchange integrals and electronic structure of manganese ferrite (MnFe <sub>2</sub> O <sub>4</sub> ). <i>Journal of Applied Physics</i> , 2003, 93, 8017-8019.	1.1	17
2343	Computational approaches to heats of formation. <i>Theoretical and Computational Chemistry</i> , 2003, 12, 247-277.	0.2	4
2344	Vacancy formation enthalpy at high pressures in tantalum. <i>Journal of Physics Condensed Matter</i> , 2003, 15, 855-861.	0.7	24
2345	A relationship between the weighted density approximation and the local-scaling transformation version of density functional theory. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2003, 36, 2881-2890.	0.6	2
2346	Electronic band structure of PuCoGa <sub>5</sub> . <i>Journal of Physics Condensed Matter</i> , 2003, 15, L155-L159.	0.7	8
2347	Comparison of density functional theory methods as applied to compound semiconductor-oxide interfaces: Slab versus cluster models. <i>Journal of Vacuum Science &amp; Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena</i> , 2003, 21, 1908.	1.6	10
2348	Structural and magnetic correlations in liquid oxygen: an ab initio molecular dynamics study. <i>Journal of Physics Condensed Matter</i> , 2003, 15, S89-S94.	0.7	2
2349	On the stability of Met-Car analogue clusters in the solid state. <i>Journal of Physics Condensed Matter</i> , 2003, 15, 4341-4348.	0.7	2

#	ARTICLE	IF	CITATIONS
2350	A coherent relation between structure and conduction of infinite atomic wires. <i>Nanotechnology</i> , 2003, 14, 299-303.	1.3	7
2351	Simple model for localization in $\hat{A}$ -Pu. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2003, 11, 851-858.	0.8	13
2352	An electron momentum spectroscopy and density functional theory study of the outer valence electronic structure of stella-2,6-dione. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2003, 36, 3155-3171.	0.6	18
2353	Evidence of concentration fluctuations in disordered network-forming systems: the case of GeSe <sub>4</sub> and SiSe <sub>2</sub> . <i>Journal of Physics Condensed Matter</i> , 2003, 15, S1537-S1546.	0.7	6
2354	Density Functional Theory Calculation of Semiconducting Carbon Nanotubes under an External Electric Field. <i>Journal of the Chinese Chemical Society</i> , 2003, 50, 627-629.	0.8	1
2355	Calculation of electronic structure and electronic density of dielectric BaTiO <sub>3</sub> . , 0, , .		0
2356	Density Functional Theory Studies of Adsorption and Vibrational Spectra of Hydrogen on the Rh(111) Surface. <i>Journal of the Chinese Chemical Society</i> , 2003, 50, 621-626.	0.8	3
2357	Stable Hydrogen Configurations between Graphite Layers. <i>Journal of the Physical Society of Japan</i> , 2003, 72, 1867-1870.	0.7	22
2358	Ab initio-Monte Carlo Studies on Magnetic Properties of Tetragonal L1 <sub>0</sub> Ordered 3d/Au Superlattices. <i>Materials Transactions</i> , 2003, 44, 1529-1534.	0.4	5
2359	Theory and Modeling of Catalytic and Electrocatalytic Reactions. , 2003, , .		0
2360	Dynamics of molecule-surface interactions from first principles. <i>Chemical Physics of Solid Surfaces</i> , 2003, 11, 1-26.	0.3	6
2361	Models of defects in wide-gap oxides. , 2003, , 151-222.		17
2362	Measurements of electron densities in solids: a real-space view of electronic structure and bonding in inorganic crystals. <i>Reports on Progress in Physics</i> , 2004, 67, 2053-2103.	8.1	54
2363	Oxidation- and organic-molecule-induced changes of the Si surface optical anisotropy: ab initio predictions. <i>Journal of Physics Condensed Matter</i> , 2004, 16, S4323-S4334.	0.7	13
2364	First principles force field for metallic tantalum. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2004, 12, S445-S459.	0.8	34
2365	Investigation on exchange and correlation holes in a strongly confined electron gas. <i>Journal of Physics Condensed Matter</i> , 2004, 16, 4833-4844.	0.7	4
2366	The effect of hydrogen adsorption on the magnetic properties of Fe adatoms on Si(001). <i>Journal of Physics Condensed Matter</i> , 2004, 16, S5763-S5767.	0.7	3
2367	Ab initio theory of magnetic interactions at surfaces. <i>Journal of Physics Condensed Matter</i> , 2004, 16, S2557-S2574.	0.7	11

#	ARTICLE	IF	CITATIONS
2368	First-principles study of binary transition-metal clusters and alloys. Journal of Physics Condensed Matter, 2004, 16, S2263-S2272.	0.7	24
2369	Structure and stability of non-molecular nitrogen at ambient pressure. Europhysics Letters, 2004, 65, 400-406.	0.7	20
2370	Ab initioelastic stiffness of nano-laminate (M <sub>x</sub> M <sup>2</sup> Al <sub>x</sub> ) (M and M <sup>2</sup> = Ti, V and Cr) solid solution. Journal of Physics Condensed Matter, 2004, 16, 2819-2827.	0.7	67
2371	The interstitial CiOi defect in bulk Si and Si <sub>1-x</sub> Ge <sub>x</sub> . Journal of Physics Condensed Matter, 2004, 16, 8545-8555.	0.7	5
2372	Atomic and Electronic Structures of Zr Atomic Chains. Chinese Physics Letters, 2004, 21, 1791-1794.	1.3	8
2373	First-principles-based study of transport properties of Fe thin films on Cu surfaces. Journal of Physics Condensed Matter, 2004, 16, S5791-S5795.	0.7	1
2374	The pressure induced phase transition of confined water from ab initio molecular dynamics simulation. Journal of Physics Condensed Matter, 2004, 16, 8851-8859.	0.7	4
2375	Reversible short-range electrostatic imaging in frequency modulation atomic force microscopy on metallic surfaces. Nanotechnology, 2004, 15, S55-S59.	1.3	6
2376	Ab initio melting curve of copper by the phase coexistence approach. Journal of Chemical Physics, 2004, 120, 2872-2878.	1.2	68
2377	The construction and application of a fully flexible computer simulation model for lithium oxide. Journal of Physics Condensed Matter, 2004, 16, S2795-S2810.	0.7	29
2378	Ga-Rich Limit of Surface Reconstructions on GaAs(001): Atomic Structure of the(4 $\times$ 6)Phase. Physical Review Letters, 2004, 93, 266101.	2.9	57
2379	Realistic kinetic Monte Carlo study of the surface phase reconstruction. Physical Review E, 2004, 69, 021606.	0.8	5
2380	Valence-electron distribution in MgB <sub>2</sub> by accurate diffraction measurements and first-principles calculations. Physical Review B, 2004, 69, .	1.1	44
2381	Dependence of elastic stiffness on electronic band structure of nanolaminate M <sub>2</sub> AlC (M=Ti,V,Nb). Tj ETQq1 1 0.784314 rgBT /Overlock 11301	1.1	301
2382	Charge-induced structural changes in Al <sub>12</sub> C clusters. Physical Review B, 2004, 70, .	1.1	33
2383	First-principles study of the origin of retarded diffusion of boron in silicon in the presence of germanium. Physical Review B, 2004, 70, .	1.1	17
2384	Stability of reduced V <sub>2</sub> O <sub>5</sub> (001) surfaces. Physical Review B, 2004, 70, .	1.1	119
2385	Electronic structure, magnetic, and transport studies of single-crystalline UCoGa <sub>5</sub> . Physical Review B, 2004, 70, .	1.1	22

#	ARTICLE	IF	CITATIONS
2386	First-principles calculations for the surface termination of pure and yttria-doped zirconia surfaces. <i>Physical Review B</i> , 2004, 69, .	1.1	73
2387	Density-functional study of the cycloaddition of acrylonitrile on the Si(100) surface. <i>Journal of Chemical Physics</i> , 2004, 120, 9793-9799.	1.2	10
2388	Electronic structures of rocksalt, litharge, and herzenbergite SnO by density functional theory. <i>Physical Review B</i> , 2004, 70, .	1.1	114
2389	First-principles study of the electric field gradient at the cubic-tetragonal phase transition in barium titanate. <i>Physical Review B</i> , 2004, 69, .	1.1	7
2390	Energies of isoelectronic atomic ions from a successful metageneralized gradient approximation and other density functionals. <i>Physical Review A</i> , 2004, 70, .	1.0	33
2391	Complexes, clustering, and native-defect-assisted diffusion of aluminum in silicon. <i>Physical Review B</i> , 2004, 70, .	1.1	10
2392	Potential-energy surfaces for excited states in extended systems. <i>Journal of Chemical Physics</i> , 2004, 120, 4593-4602.	1.2	103
2393	Saturated adsorption of CO and coadsorption of CO and O <sub>2</sub> on AuN <sup>+</sup> (N=2-7) clusters. <i>Journal of Chemical Physics</i> , 2004, 120, 6574-6584.	1.2	72
2394	First-principles simulations of STM images: From tunneling to the contact regime. <i>Physical Review B</i> , 2004, 70, .	1.1	87
2395	Structure of ultrathin crystalline SiO <sub>2</sub> films on Mo(112). <i>Physical Review B</i> , 2004, 69, .	1.1	29
2396	Magnetism of Fe <sup>2+</sup> nanostructures on flat and stepped W(110) surfaces: Effects of dimensionality and substrate. <i>Physical Review B</i> , 2004, 70, .	1.1	22
2397	Relationship between domain-boundary free energy and the temperature dependence of stress-domain patterns of Pb on Cu(111). <i>Physical Review B</i> , 2004, 70, .	1.1	18
2398	Adsorption and dissociation of NO on stepped Pt (533). <i>Journal of Chemical Physics</i> , 2004, 121, 7946.	1.2	44
2399	Effect of impurity incorporation on crystallization in AlN sublimation epitaxy. <i>Journal of Applied Physics</i> , 2004, 96, 5293-5297.	1.1	40
2400	Lateral interactions between oxygen atoms adsorbed on platinum (111) by first principles. <i>Molecular Physics</i> , 2004, 102, 273-279.	0.8	33
2401	A reactive force field simulation of liquid-liquid phase transitions in phosphorus. <i>Journal of Chemical Physics</i> , 2004, 121, 8147.	1.2	31
2402	Sodium Pyroxene NaTiSi <sub>2</sub> O <sub>6</sub> : Possible Haldane Spin-1 Chain System. <i>Physical Review Letters</i> , 2004, 93, 036401.	2.9	23
2403	Molecular Chemisorption as the Theoretically Preferred Pathway for Water Adsorption on Ideal Rutile TiO <sub>2</sub> (110). <i>Physical Review Letters</i> , 2004, 93, 086105.	2.9	156



#	ARTICLE	IF	CITATIONS
2404	When Langmuir Is Too Simple:H <sub>2</sub> Dissociation on Pd(111) at High Coverage. Physical Review Letters, 2004, 93, 146103.	2.9	81
2405	Nucleation of Pd Dimers at Defect Sites of the MgO(100) Surface. Physical Review Letters, 2004, 92, 096105.	2.9	101
2406	Fluctuating Lattice Constants of Indium under High Pressure. Physical Review Letters, 2004, 92, 195501.	2.9	22
2407	Experimental Evidence for a Partially Dissociated Water Bilayer on Ru{0001}. Physical Review Letters, 2004, 93, 196102.	2.9	130
2408	Vibronic coupling and double excitations in linear response time-dependent density functional calculations: Dipole-allowed states of N <sub>2</sub> . Journal of Chemical Physics, 2004, 121, 6155-6166.	1.2	80
2409	A first-principles potential energy surface and vibrational states for hydrogen on Cu(100). Journal of Chemical Physics, 2004, 121, 7434-7439.	1.2	15
2410	Vibrational coherence transfer characterized with Fourier-transform 2D IR spectroscopy. Journal of Chemical Physics, 2004, 121, 362.	1.2	175
2411	High-Coverage Oxygen Structures on Rh(111): Adsorbate Repulsion and Site Preference Is Not Enough. Physical Review Letters, 2004, 93, 266103.	2.9	46
2412	Energetics of Si(001) Surfaces Exposed to Electric Fields and Charge Injection. Physical Review Letters, 2004, 93, 036101.	2.9	59
2413	Ab initio transmission electron microscopy image simulations of coherent Ag/MgO interfaces. Physical Review B, 2004, 70, .	1.1	15
2414	Vibrational properties of hydrogen atom adsorbed on Cu(111) and on Ir(111) surfaces. Journal of Applied Physics, 2004, 96, 5020-5025.	1.1	20
2415	Structural and electronic properties of Si <sub>3</sub> P <sub>4</sub> . Physical Review B, 2004, 69, .	1.1	31
2416	Computational study of electron states in Au chains on NiAl(110). Physical Review B, 2004, 70, .	1.1	22
2417	Structural models and core-level shifts of the oxidation of the Si(001) surface. Physical Review B, 2004, 70, .	1.1	5
2418	Diffusion of Fe atoms on W surfaces and Fe/W films and along surface steps. Physical Review B, 2004, 70, .	1.1	41
2419	Energetics of Sr atom interactions on the Mo(112) surface. Physical Review B, 2004, 69, .	1.1	22
2420	Density functional theory study of H and H <sub>2</sub> interacting with NiAl(110). Journal of Chemical Physics, 2004, 121, 751-760.	1.2	44
2421	First-principles calculations for the adsorption of water molecules on the Cu(100) surface. Physical Review B, 2004, 70, .	1.1	39

#	ARTICLE	IF	CITATIONS
2422	O adsorption and incipient oxidation of the Mg(0001) surface. <i>Physical Review B</i> , 2004, 69, .	1.1	33
2423	Ab initio total energy study of ZnO adsorption on a sapphire (0001) surface. <i>Physical Review B</i> , 2004, 70, .	1.1	9
2424	Periodic density functional study on structural and vibrational properties of vanadium oxide aggregates. <i>Physical Review B</i> , 2004, 69, .	1.1	76
2425	First-principles study of low-index surfaces of lead. <i>Physical Review B</i> , 2004, 70, .	1.1	57
2426	Electronic structure of calcium hexaboride within the weighted density approximation. <i>Physical Review B</i> , 2004, 69, .	1.1	31
2427	Nanowires for spintronics: A study of transition-metal elements of groups 8–10. <i>Physical Review B</i> , 2004, 69, .	1.1	74
2428	Structure, energetics, and extrinsic levels of small self-interstitial clusters in silicon. <i>Physical Review B</i> , 2004, 69, .	1.1	48
2429	Anchoring the potential energy surface of the cyclic water trimer. <i>Journal of Chemical Physics</i> , 2004, 121, 11023.	1.2	68
2430	Chemical short-range-order effects on stability in $\hat{\text{r}}\text{-Pu-Ga}$ alloys. <i>Philosophical Magazine</i> , 2004, 84, 1877-1888.	0.7	8
2431	Phosphorus under pressure: A Ba-IV-type structure as a candidate for P-IV. <i>Physical Review B</i> , 2004, 69, .	1.1	19
2432	Contrast Reversal and Shape Changes of Atomic Adsorbates Measured with Scanning Tunneling Microscopy. <i>Physical Review Letters</i> , 2004, 92, 206101.	2.9	66
2433	On the zirconium oxide neutral cluster distribution in the gas phase: Detection through 118 nm single photon, and 193 and 355 nm multiphoton, ionization. <i>Journal of Chemical Physics</i> , 2004, 120, 4142-4149.	1.2	40
2434	Ab initio study of the magnetic structure of fcc Fe grown on a Cu(001) substrate. <i>Physical Review B</i> , 2004, 70, .	1.1	13
2435	Determining the adsorptive and catalytic properties of strained metal surfaces using adsorption-induced stress. <i>Journal of Chemical Physics</i> , 2004, 120, 7720-7724.	1.2	31
2436	Bayesian Ensemble Approach to Error Estimation of Interatomic Potentials. <i>Physical Review Letters</i> , 2004, 93, 165501.	2.9	95
2437	Novel Water Overlayer Growth on Pd(111) Characterized with Scanning Tunneling Microscopy and Density Functional Theory. <i>Physical Review Letters</i> , 2004, 93, 116101.	2.9	173
2438	Structure, electronic density of states and electric field gradients of icosahedral AlCuFe: An ab initio study of the original and a modified Cockayne model. <i>Physical Review B</i> , 2004, 69, .	1.1	15
2439	Ternary half-metallics and related binary compounds: A study of stoichiometry, surface states, and spin. <i>Physical Review B</i> , 2004, 70, .	1.1	41

#	ARTICLE	IF	CITATIONS
2440	Molecular adsorption on the surface of strongly correlated transition-metal oxides: A case study for CO/NiO(100). <i>Physical Review B</i> , 2004, 69, .	1.1	216
2441	Initial growth of Ba on Si(001). <i>Physical Review B</i> , 2004, 69, .	1.1	12
2442	Ab initio treatment of noncollinear magnets with the full-potential linearized augmented plane wave method. <i>Physical Review B</i> , 2004, 69, .	1.1	194
2443	Origin of Spontaneous Electric Dipoles in Homonuclear Niobium Clusters. <i>Physical Review Letters</i> , 2004, 93, 246105.	2.9	27
2444	Phonon Dispersion Curves of aBC <sub>3</sub> Honeycomb Epitaxial Sheet. <i>Physical Review Letters</i> , 2004, 93, 177003.	2.9	129
2445	Ab Initio Calculations to Model Anomalous Fluorine Behavior. <i>Physical Review Letters</i> , 2004, 93, 245901.	2.9	42
2446	Charge fluctuations and concentration fluctuations at intermediate-range distances in the disordered network-forming materials SiO <sub>2</sub> , SiSe <sub>2</sub> , and GeSe <sub>2</sub> . <i>Physical Review B</i> , 2004, 70, .	1.1	38
2447	Dimer-Anticorrelation-Induced Stabilization of Adsorbate Clustering on the Si(100) $\sqrt{2}\times\sqrt{2}$ Surface. <i>Physical Review Letters</i> , 2004, 92, 096103.	2.9	25
2448	Na <sub>3</sub> O(CN): Ab initio calculations on a multidomain structure. <i>Physical Review B</i> , 2004, 70, .	1.1	1
2449	Electronic and superconducting properties of oxygen-ordered MgB <sub>2</sub> compounds of the form Mg <sub>2</sub> B <sub>3</sub> O <sub>x</sub> . <i>Physical Review B</i> , 2004, 70, .	1.1	6
2450	Evidence from first principles calculations for a bent CO <sub>2</sub> intermediate in the oxidation of carbon monoxide on the Cu (110) surface. <i>Journal of Chemical Physics</i> , 2004, 121, 4339-4345.	1.2	8
2451	Green's function formalism coupled with Gaussian broadening of discrete states for quantum transport: Application to atomic and molecular wires. <i>Journal of Chemical Physics</i> , 2004, 121, 8050.	1.2	55
2452	Wetting of TiC and TiN by metals. <i>Physical Review B</i> , 2004, 69, .	1.1	98
2453	Analytic second variational derivative of the exchange-correlation functional. <i>Physical Review B</i> , 2004, 69, .	1.1	7
2454	Electron delocalization at the hybrid aromatic-thiol-Cu(100) interface. <i>Physical Review B</i> , 2004, 70, .	1.1	13
2455	Atomic-level growth study of vanadium oxide nanostructures on Rh(111). <i>Physical Review B</i> , 2004, 69, .	1.1	87
2456	Modifications of the electronic structure of GaSb surface by chalcogen atoms: S, Se, and Te. <i>Journal of Applied Physics</i> , 2004, 96, 4302-4307.	1.1	3
2457	Structural stability and magnetic properties of metastable Fe-Cu alloys studied by ab initio calculations and molecular dynamics simulations. <i>Physical Review B</i> , 2004, 69, .	1.1	17

#	ARTICLE	IF	CITATIONS
2458	First-principles study of C adsorption, O adsorption, and CO dissociation on flat and stepped Ni surfaces. <i>Journal of Chemical Physics</i> , 2004, 121, 10241-10249.	1.2	44
2459	First-principles extrapolation method for accurate CO adsorption energies on metal surfaces. <i>Physical Review B</i> , 2004, 69, .	1.1	204
2460	MgO $\hat{\wedge}$ Ag(001) interface structure and STM images from first principles. <i>Physical Review B</i> , 2004, 70, .	1.1	29
2461	Theoretical study of Ga-based nanowires and the interaction of Ga with single-wall carbon nanotubes. <i>Physical Review B</i> , 2004, 70, .	1.1	12
2462	SrTiO $\hat{\wedge}$ Si(001) epitaxial interface: A density functional theory study. <i>Physical Review B</i> , 2004, 70, .	1.1	32
2463	Periodic density functional theory study of the crystal morphology of FeZn <sub>13</sub> . <i>Physical Review B</i> , 2004, 70, .	1.1	9
2464	Correlation of magnetic moment versus spacing distance of metastable fcc structured iron. <i>Applied Physics Letters</i> , 2004, 84, 3627-3629.	1.5	46
2465	Reactive scattering of H <sub>2</sub> from Cu(100): Six-dimensional quantum dynamics results for reaction and scattering obtained with a new, accurately fitted potential-energy surface. <i>Journal of Chemical Physics</i> , 2004, 121, 11379.	1.2	26
2466	Ab initio study of cubyl chains and networks. <i>Journal of Chemical Physics</i> , 2004, 121, 9172-9177.	1.2	8
2467	Experimental and computational investigation of structure and magnetism in pyrite Co <sub>1-x</sub> Fe <sub>x</sub> S <sub>2</sub> : $\hat{\wedge}$ Chemical bonding and half-metallicity. <i>Physical Review B</i> , 2004, 70, .	1.1	70
2468	Optical reflectance anisotropy of Al(110): Experiment and ab initio calculation. <i>Physical Review B</i> , 2004, 69, .	1.1	9
2469	Carbon induced restructuring of the Si(111) surface. <i>Physical Review B</i> , 2004, 69, .	1.1	17
2470	Phase diagram of oxygen adsorbed on platinum (111) by first-principles investigation. <i>Physical Review B</i> , 2004, 70, .	1.1	103
2471	Acetonitrile adsorption on Si(001). <i>Physical Review B</i> , 2004, 69, .	1.1	14
2472	Structural and magnetic properties of Fe clusters at the Al(001) surface: Early transition from paramagnetic to ferromagnetic Fe. <i>Physical Review B</i> , 2004, 69, .	1.1	12
2473	Relativistic spin-orbit effects on hyperfine coupling tensors by density-functional theory. <i>Journal of Chemical Physics</i> , 2004, 120, 2127-2139.	1.2	89
2474	Organic modification of surface electronic properties: $\hat{\wedge}$ A first-principles study of uracil on Si(001). <i>Physical Review B</i> , 2004, 69, .	1.1	27
2475	First-principles study of adsorption of methanethiol on Co(0001). <i>Physical Review B</i> , 2004, 70, .	1.1	19

#	ARTICLE	IF	CITATIONS
2476	Density-functional theory calculations of the adsorption of Cl at perfect and defective Ag(111) surfaces. <i>Physical Review B</i> , 2004, 69, .	1.1	25
2477	Magnetic properties of $\text{Sm}_3\text{Fe}_{28.1-x}\text{Co}_x\text{Mo}_{0.9}$ ( $x=0,4,8,12,14,16$ ) compounds. <i>Physical Review B</i> , 2004, 69, .	1.1	18
2478	Adsorption, diffusion, and dissociation of molecular oxygen at defected $\text{TiO}_2(110)$ : A density functional theory study. <i>Journal of Chemical Physics</i> , 2004, 120, 988-997.	1.2	251
2479	The nonmetallicity of molybdenum clusters. <i>Journal of Chemical Physics</i> , 2004, 121, 7717.	1.2	48
2480	Vicinal fluorine-fluorine coupling constants: Fourier analysis. <i>Journal of Chemical Physics</i> , 2004, 121, 6268-6276.	1.2	14
2481	Adsorption and vibrational spectroscopy of ammonia at mordenite: Ab initio study. <i>Journal of Chemical Physics</i> , 2004, 120, 10263-10277.	1.2	39
2482	Hydrogen site energetics in $\text{LaNi}_5\text{H}_n$ and $\text{LaCo}_5\text{H}_n$ : Toward predicting hydrides. <i>Applied Physics Letters</i> , 2004, 85, 3465-3467.	1.5	8
2484	The mechanism of $\text{N}_2\text{O}$ formation via the $(\text{NO})_2$ dimer: A density functional theory study. <i>Journal of Chemical Physics</i> , 2004, 121, 2737.	1.2	36
2485	Ab Initio Study of Cyclohexane Dehydrogenation with a Transition Metal (Pt, Pd, Ni and Cu) Atom. <i>Journal of the Physical Society of Japan</i> , 2004, 73, 1281-1284.	0.7	12
2486	From The Cover: Hydration and mobility of $\text{HO}^-$ (aq). <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 7229-7233.	3.3	145
2487	Ab Initio Study of Magnetic Properties of SiC-Based Diluted Magnetic Semiconductors. <i>Key Engineering Materials</i> , 2004, 264-268, 1237-1240.	0.4	12
2488	Electron Binding to Nucleic Acid Bases. <i>Experimental and Theoretical Studies. A Review. Collection of Czechoslovak Chemical Communications</i> , 2004, 69, 1395-1428.	1.0	43
2489	Oscillation of Conductance in Molecular Junctions of Carbon Ladder Compounds. <i>Journal of the American Chemical Society</i> , 2004, 126, 14182-14189.	6.6	49
2490	Ab Initio Simulation of Lewis Sites in Mordenite and Comparative Study of the Strength of Active Sites via CO Adsorption. <i>Journal of Physical Chemistry B</i> , 2004, 108, 13656-13666.	1.2	57
2491	Carbon allotropes and strong nanotube bundles. <i>Journal of Physics Condensed Matter</i> , 2004, 16, 9083-9091.	0.7	19
2492	Effect of Magnesium Substitution in Lithium Nickel Oxide. <i>Journal of the Electrochemical Society</i> , 2004, 151, J91.	1.3	3
2493	Enthalpy of Formation of Various Phases and Formation Energy of Point Defects in Perovskite-Type $\text{NaNbO}_3$ by First-Principles Calculation. <i>Japanese Journal of Applied Physics</i> , 2004, 43, 6793-6798.	0.8	65
2494	Structure and stability of complex metal hydrides – theoretical approach. <i>Materials Research Society Symposia Proceedings</i> , 2004, 837, 13.	0.1	0

#	ARTICLE	IF	CITATIONS
2495	Methods and Implementation of Robust, High-Precision Gaussian Basis DFT Calculations for Periodic Systems: the GTOFF Code. <i>Theoretical and Computational Chemistry</i> , 2004, , 171-228.	0.2	9
2496	Spin-polarised surfaces: Current state of Density Functional Theory investigations. <i>Theoretical and Computational Chemistry</i> , 2004, 15, 261-295.	0.2	3
2497	Structure and stability of possible new alanates. <i>Europhysics Letters</i> , 2004, 67, 607-613.	0.7	41
2498	Atomic and electronic structures of the lattice mismatched metal-ceramic interface. <i>Journal of Physics Condensed Matter</i> , 2004, 16, 5781-5790.	0.7	13
2499	DENSITY-FUNCTIONAL STUDY OF THE SURFACE AND INTERFACE OF ZnO/Al <sub>2</sub> O <sub>3</sub> (0001). <i>Surface Review and Letters</i> , 2004, 11, 509-513.	0.5	3
2500	Analysis of shear deformations in Al and Cu: empirical potentials versus density functional theory. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2004, 12, 1017-1029.	0.8	36
2501	CO adsorption on close-packed transition and noble metal surfaces: trends from ab initio calculations. <i>Journal of Physics Condensed Matter</i> , 2004, 16, 1141-1164.	0.7	366
2502	Twinning pathway in BCC molybdenum. <i>Europhysics Letters</i> , 2004, 68, 405-411.	0.7	26
2503	On elasticity under pressure. <i>Journal of Physics Condensed Matter</i> , 2004, 16, 8101-8104.	0.7	45
2504	COMPLEX DONORS IN NITROGEN-DOPED DIAMOND. <i>International Journal of Nanoscience</i> , 2004, 03, 455-461.	0.4	1
2505	Phase stability of Pu alloys: a key role of chemical short range order. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2004, 12, 693-707.	0.8	11
2506	Grain Boundary Sliding of $\Sigma$ 5(001) Twist Grain Boundary in Aluminium Bicrystal from First-Principles Calculations. <i>Materials Science Forum</i> , 2004, 447-448, 27-32.	0.3	11
2507	Theoretical Prediction of Post-spinel Phases of Silicon Nitride. <i>Journal of the American Ceramic Society</i> , 2002, 85, 7-10.	1.9	29
2508	First-Principles Calculations of Anion Vacancies in Oxides and Nitrides. <i>Journal of the American Ceramic Society</i> , 2002, 85, 68-74.	1.9	51
2509	Effective Doping in Cubic Si <sub>3</sub> N <sub>4</sub> and Ge <sub>3</sub> N <sub>4</sub> : A First-Principles Study. <i>Journal of the American Ceramic Society</i> , 2002, 85, 97-100.	1.9	32
2510	A negative surface energy for alumina. <i>Nature Materials</i> , 2004, 3, 289-293.	13.3	191
2511	Tailoring ferromagnetic chalcopyrites. <i>Nature Materials</i> , 2004, 3, 410-414.	13.3	151
2512	Alloy catalysts designed from first principles. <i>Nature Materials</i> , 2004, 3, 810-815.	13.3	1,030

#	ARTICLE	IF	CITATIONS
2513	Theoretical Structure Determination of a Complex Material: $\text{Al}_2\text{O}_3$ . Journal of the American Ceramic Society, 1999, 82, 1365-1380.	1.9	82
2514	Anomalous behavior of a $\pm$ -iron zero-temperature isotherm in the region of negative pressures. JETP Letters, 2004, 79, 537-541.	0.4	3
2515	Equation of state in the quasi-classical approximation. Technical Physics, 2004, 49, 1546-1557.	0.2	1
2516	First principles search of hard materials within the $\text{Si}-\text{C}-\text{N}$ ternary system. Solid State Sciences, 2004, 6, 315-323.	1.5	18
2517	The structures of $\text{X}_2[(\text{Mo}_6\text{Cl}_8)\text{Cl}_6]\cdot n\text{H}_2\text{O}$ , $\text{X}=\text{NH}_4, \text{K}, \text{Rb}, \text{Cs}$ . Solid State Sciences, 2004, 6, 509-517.	1.5	5
2518	Solvothermal preparation of ferromagnetic sub-micron spinel $\text{CuCr}_2\text{Se}_4$ particles. Solid State Sciences, 2004, 6, 841-845.	1.5	20
2519	Structure of amorphous iron-based coatings processed by HVOF and APS thermally spraying. Materials Chemistry and Physics, 2004, 85, 113-119.	2.0	44
2520	Interaction of magic gold cluster with $\text{Si}_{60}$ cage. European Physical Journal D, 2004, 29, 231-234.	0.6	15
2521	Spin Splitting of $s$ and $p$ States in Single Atoms and Magnetic Coupling in Dimers on a Surface. Physical Review Letters, 2004, 92, 186802.	2.9	47
2522	Ab initio study of incorporation of $\text{O}_2$ molecules into $\text{Si}(001)$ surfaces: Oxidation by $\text{Si}$ ejection. Physical Review B, 2004, 70, .	1.1	23
2523	Development of an interatomic potential for phosphorus impurities in $\pm$ -iron. Journal of Physics Condensed Matter, 2004, 16, S2629-S2642.	0.7	502
2524	High-conducting magnetic nanowires obtained from uniform titanium-covered carbon nanotubes. Physical Review B, 2004, 69, .	1.1	51
2525	The behavior of density functionals with respect to basis set. I. The correlation consistent basis sets. Journal of Chemical Physics, 2004, 121, 7632.	1.2	98
2526	First Principles Analysis of the Stability and Diffusion of Oxygen Vacancies in Metal Oxides. Physical Review Letters, 2004, 93, 225502.	2.9	158
2527	Crystal structure and thermodynamic stability of the lithium aluminates $\text{LiAlH}_4$ and $\text{Li}_3\text{AlH}_6$ . Physical Review B, 2004, 69, .	1.1	114
2528	In situ x-ray photoelectron spectroscopic and density-functional studies of Si atoms adsorbed on a $\text{C}_{60}$ film. Journal of Chemical Physics, 2004, 121, 11351.	1.2	4
2529	Effects of additives in $\pm$ - and $\hat{\Gamma}$ -alumina: an ab initio study. Journal of Physics Condensed Matter, 2004, 16, 8971-8980.	0.7	32
2530	Active Sites for the Vapor Phase Beckmann Rearrangement over Mordenite: An ab Initio Study. Journal of Physical Chemistry A, 2004, 108, 11388-11397.	1.1	46



#	ARTICLE	IF	CITATIONS
2531	Adsorption and migration of carbon adatoms on carbon nanotubes: Density-functional ab initio and tight-binding studies. <i>Physical Review B</i> , 2004, 69, .	1.1	111
2532	Functionalized carbon nanotubes and device applications. <i>Journal of Physics Condensed Matter</i> , 2004, 16, R901-R960.	0.7	104
2533	Structural Stability of Complex Hydrides: LiBH <sub>4</sub> Revisited. <i>Physical Review Letters</i> , 2004, 93, 145501.	2.9	153
2534	Effects of Peripheral Substituents and Axial Ligands on the Electronic Structure and Properties of Iron Phthalocyanine. <i>Inorganic Chemistry</i> , 2004, 43, 7151-7161.	1.9	68
2535	Comparison of the accuracy of semiempirical and some DFT methods for predicting heats of formation. <i>Journal of Molecular Modeling</i> , 2004, 10, 6-12.	0.8	104
2536	First-principles studies of the adsorption of O <sub>2</sub> on Al (001). <i>Science Bulletin</i> , 2004, 49, 1768-1771.	1.7	6
2537	Theoretical study of ZnO adsorption and bonding on Al <sub>2</sub> O <sub>3</sub> (0001) surface. <i>Science in China Series G: Physics, Mechanics and Astronomy</i> , 2004, 47, 664-675.	0.2	0
2538	A comparative theoretical study of Au, Ag and Cu adsorption on TiO <sub>2</sub> (110) rutile surfaces. <i>Korean Journal of Chemical Engineering</i> , 2004, 21, 537-547.	1.2	20
2539	The simple cubic structure of Ir clusters and the element effect on cluster structures. <i>Chemical Physics Letters</i> , 2004, 383, 67-71.	1.2	72
2540	Density functional theory and tight-binding quantum chemical molecular dynamics calculations on Ce <sub>1-x</sub> Cu <sub>x</sub> O <sub>2</sub> catalyst and the adsorptions of CH <sub>3</sub> OH and CH <sub>3</sub> O on Ce <sub>1-x</sub> Cu <sub>x</sub> O <sub>2</sub> . <i>Chemical Physics Letters</i> , 2004, 384, 30-34.	1.2	18
2541	Competitive CN and N <sub>2</sub> formation on Rh(1 1 1): a case of entropic stabilization. <i>Chemical Physics Letters</i> , 2004, 385, 52-54.	1.2	16
2542	Nucleation and growth of epitaxial ZrB <sub>2</sub> (0001) on Si(111). <i>Journal of Crystal Growth</i> , 2004, 267, 554-563.	0.7	30
2543	Adsorption and migration of carbon adatoms on zigzag carbon nanotubes. <i>Carbon</i> , 2004, 42, 1021-1025.	5.4	52
2544	Modeling of high-pressure CO dissociation on Pt(100) and Pt(111). <i>Catalysis Today</i> , 2004, 89, 357-362.	2.2	5
2545	Interplay of local structure and magnetism in Co-doped TiO <sub>2</sub> anatase. <i>Solid State Communications</i> , 2004, 129, 741-746.	0.9	44
2546	Vibronic model for antiferroelectric phase transition in squaric acid, H <sub>2</sub> C <sub>4</sub> O <sub>4</sub> . <i>Solid State Communications</i> , 2004, 130, 729-733.	0.9	5
2547	Reflectance anisotropy of uracil covered Si(001) surfaces: Ab initio predictions. <i>Surface Science</i> , 2004, 548, 183-186.	0.8	18
2548	FS <sup>+</sup> and FS <sup>+</sup> (OH <sup>-</sup> ) defect centers at the MgO(100) surface: cluster and periodic calculations. <i>Surface Science</i> , 2004, 549, 294-304.	0.8	24

#	ARTICLE	IF	CITATIONS
2549	Adhesion and bonding of the Al/TiC interface. Surface Science, 2004, 550, 46-56.	0.8	69
2550	A DFT investigation of potential energy surface and vibrational properties of hydrogen adsorbed on the Rh(111) surface. Surface Science, 2004, 550, 15-20.	0.8	11
2551	Microkinetic analysis of the oxygen-silver system. Surface Science, 2004, 552, 260-272.	0.8	13
2552	A combined density functional theory and interatomic potential-based simulation study of the hydration of nano-particulate silicate surfaces. Surface Science, 2004, 554, 193-210.	0.8	63
2553	Structure and bonding mechanism of cyanide adsorbed on Pt(111). Surface Science, 2004, 558, 111-121.	0.8	34
2554	Molecular dynamics simulations of cinchonidine-modified platinum in ethanol: comparisons with surface studies. Surface Science, 2004, 563, 57-73.	0.8	22
2555	An off-lattice model for Br electrodeposition on Au(100): from DFT to experiment. Surface Science, 2004, 563, 169-182.	0.8	18
2556	H <sub>2</sub> O on Si(001): surface optical anisotropy from first-principles calculations. Surface Science, 2004, 571, 157-160.	0.8	11
2557	Structure and electronic properties of BEDT-TTF and its charge transfer salts. Journal of Physics and Chemistry of Solids, 2004, 65, 39-49.	1.9	12
2558	Surface Raman characterization of cinchonidine-modified platinum in ethanol: effects of liquid-phase concentration and co-adsorbed hydrogen. Journal of Molecular Catalysis A, 2004, 212, 277-289.	4.8	49
2559	Correlating the electronic properties and HDN reactivities of organonitrogen compounds: an ab initio DFT study. Journal of Molecular Catalysis A, 2004, 222, 243-251.	4.8	18
2560	FeNb and FeSi thermal spraying coatings: microstructure and first principle calculations. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2004, 107, 27-32.	1.7	5
2561	Investigation of the Magnetic Hyperfine Field at <sup>140</sup> Ce on Gd Sites in GdCo <sub>2</sub> Compound. Hyperfine Interactions, 2004, 158, 189-193.	0.2	5
2562	Modelling the Deposition of High-k Dielectric Films by First Principles. Journal of Electroceramics, 2004, 13, 117-120.	0.8	20
2563	Ab initio Study of the Si Adsorption on Mo(110). Journal of Electroceramics, 2004, 13, 327-330.	0.8	2
2564	Adsorption of d-metal atoms on the regular MgO(001) surface: Density functional study of cluster models embedded in an elastic polarizable environment. Applied Physics A: Materials Science and Processing, 2004, 78, 823-828.	1.1	84
2565	Concentrations of native and gold defects in HgCdTe from first principles calculations. Journal of Electronic Materials, 2004, 33, 737-741.	1.0	11
2566	Computational investigation of the vibrational and electronic states of S <sub>2</sub> N <sub>2</sub> . Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 471-480.	2.0	9

#	ARTICLE	IF	CITATIONS
2567	The effects of Ni on structural and electronic properties of BaTiO <sub>3</sub> ceramic. <i>Ceramics International</i> , 2004, 30, 81-85.	2.3	9
2568	First-principles periodic and semiempirical cyclic cluster calculations for single oxygen vacancies in crystalline Al <sub>2</sub> O <sub>3</sub> . <i>Physica Status Solidi (B): Basic Research</i> , 2004, 241, 1032-1040.	0.7	25
2569	Electronic and structural properties of strontium chalcogenides SrS, SrSe and SrTe. <i>Physica Status Solidi (B): Basic Research</i> , 2004, 241, 2529-2537.	0.7	43
2570	Proton transfer in nafion membrane by quantum chemistry calculation. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2004, 42, 1905-1914.	2.4	32
2571	Magnetism of Fe nanowires encapsulated in carbon nanotube. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2004, 1, 3264-3270.	0.8	4
2572	Density functional theory study of point defects in the Si/SiO <sub>2</sub> system and in substoichiometric titanium dioxide TiO <sub>2-x</sub> . <i>International Journal of Quantum Chemistry</i> , 2004, 99, 677-684.	1.0	12
2573	Tight-binding parameterization of transition and noble metal clusters. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 654-666.	1.0	9
2574	Application of accurate MP2 energies for closed-shell atoms in examinations of density functionals for 3d 10 electron ions. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 277-287.	1.0	7
2575	First-principles calculation of formation energy of neutral point defects in perovskite-type BaTiO <sub>3</sub> . <i>International Journal of Quantum Chemistry</i> , 2004, 99, 824-827.	1.0	35
2576	Studies on structure and conformational stability of free canonical 2'-deoxyribonucleosides: Approximate SCC-DFTB and LMP2 methods. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 28-38.	1.0	5
2577	Borderline cases in density functional theory. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 681-694.	1.0	4
2578	Separability between valence and conduction bands in transition metal clusters. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 277-287.	1.0	5
2579	Strain-Induced Formation of Subsurface Species in Transition Metals. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 4296-4300.	7.2	64
2581	Multiple Aromaticity and Antiaromaticity in Silicon Clusters. <i>ChemPhysChem</i> , 2004, 5, 1885-1891.	1.0	48
2582	Structure, Characterization, and Metal-Complexation Properties of a New Tetraazamacrocycle Containing Two Phenolic Pendant Arms. <i>Helvetica Chimica Acta</i> , 2004, 87, 2613-2628.	1.0	4
2583	Ground- and excited-state properties of DNA base molecules from plane-wave calculations using ultrasoft pseudopotentials. <i>Journal of Computational Chemistry</i> , 2004, 25, 112-122.	1.5	88
2584	QM/MM study of aqueous solvation of the uranyl fluoride [UO <sub>2</sub> F <sub>4</sub> ?] complex. <i>Journal of Computational Chemistry</i> , 2004, 25, 386-392.	1.5	35
2585	Retardation of setting of plaster of Paris by organic acids: Understanding the mechanism through molecular modeling. <i>Journal of Computational Chemistry</i> , 2004, 25, 1438-1448.	1.5	42

#	ARTICLE	IF	CITATIONS
2586	Energetic and topological analysis of the reaction of Mo and Mo <sub>2</sub> with NH <sub>3</sub> , C <sub>2</sub> H <sub>2</sub> , and C <sub>2</sub> H <sub>4</sub> molecules. <i>Journal of Computational Chemistry</i> , 2004, 25, 1647-1655.	1.5	15
2587	The performance of nonhybrid density functionals for calculating the structures and spin states of Fe(II) and Fe(III) complexes. <i>Journal of Computational Chemistry</i> , 2004, 25, 1840-1848.	1.5	86
2588	N,N'-Ethylenebis(pyridoxylideneiminato) and N,N'-Ethylenebis(pyridoxylaminato): Synthesis, Characterization, Potentiometric, Spectroscopic, and DFT Studies of Their Vanadium(IV) and Vanadium(V) Complexes. <i>Chemistry - A European Journal</i> , 2004, 10, 2301-2317.	1.7	127
2589	Solvent Effects on <sup>195</sup> Pt and <sup>205</sup> Tl NMR Chemical Shifts of the Complexes [(NC) <sub>5</sub> Pt(ξ;Ti(CN) <sub>n</sub> )] <sup>n+</sup> (n=0-3), and [(NC) <sub>5</sub> Pt(ξ;Ti(ξ;Pt(CN) <sub>5</sub> )] <sup>3+</sup> Studied by Relativistic Density Functional Theory. <i>Chemistry - A European Journal</i> , 2004, 10, 2581-2589.	1.7	45
2590	A theoretical study on the cyclopropane adsorption onto the copper surfaces by density functional theory and quantum chemical molecular dynamics methods. <i>Journal of Molecular Catalysis A</i> , 2004, 220, 189-198.	4.8	21
2591	Structural and energetic characterization of ylidenemalonodinitrile tautomers, precursors of fungicidal species. <i>Journal of Molecular Structure</i> , 2004, 689, 43-48.	1.8	19
2592	Nanocrystalline materials for Ni-MH batteries. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2004, 108, 67-75.	1.7	31
2593	Electronic structure of Ti <sub>2</sub> CAI and Ti <sub>2</sub> NAI. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2004, 110, 280-284.	1.7	7
2594	Ga-doping effects on electronic and structural properties of wurtzite ZnO. <i>Physica B: Condensed Matter</i> , 2004, 349, 136-142.	1.3	37
2595	A theoretical investigation of the Chalk-Harrod and modified Chalk-Harrod mechanisms involved in hybrid integrated circuit building. <i>Future Generation Computer Systems</i> , 2004, 20, 781-791.	4.9	5
2596	Nitrogen adsorption on a supported iron nanocluster. <i>Vacuum</i> , 2004, 74, 173-177.	1.6	2
2597	Structure analysis of [P,N,O] species in singlet and triplet states at density functional theory and wavefunction-correlated levels. <i>Computational and Theoretical Chemistry</i> , 2004, 668, 163-169.	1.5	1
2598	Spectroscopic constants of gallium monohalides: a DFT study. <i>Computational and Theoretical Chemistry</i> , 2004, 668, 209-215.	1.5	1
2599	Atomistic simulations of Cu deposition on the $\hat{\pm}$ -Al <sub>2</sub> O <sub>3</sub> (0001) surface. <i>Computational and Theoretical Chemistry</i> , 2004, 709, 79-85.	1.5	1
2600	DFT studies on tautomerism of C5-substituted 1,2,4-triazoles. <i>Computational and Theoretical Chemistry</i> , 2004, 680, 107-115.	1.5	59
2601	Theoretical study of UX <sub>6</sub> and UO <sub>2</sub> X <sub>2</sub> (X=F, Cl, Br, I). <i>Computational and Theoretical Chemistry</i> , 2004, 684, 35-42.	1.5	34
2602	A DFT study of the reactions of tetrameric and hexameric methyllithium with CO and CNMe. <i>Computational and Theoretical Chemistry</i> , 2004, 684, 211-215.	1.5	5
2603	The effectiveness of a primary aliphatic amino group as an internal Lewis base on the formation of a boron-oxygen-carbon linkage: a computational study. <i>Computational and Theoretical Chemistry</i> , 2004, 712, 9-19.	1.5	15

#	ARTICLE	IF	CITATIONS
2604	A density functional theory benchmark of the formation enthalpy and first CO dissociation enthalpy of hexacarbonyl complexes of chromium, molybdenum, and tungsten. Computational and Theoretical Chemistry, 2004, 711, 123-131.	1.5	10
2605	A theoretical study of the thermal fragmentation of ferrocene. Thin Solid Films, 2004, 458, 325-329.	0.8	35
2606	Density-functional calculations of self-capacitances of carbon nanostructures. Thin Solid Films, 2004, 464-465, 346-349.	0.8	2
2607	Field emission and electronic structures of carbon allotropes. Thin Solid Films, 2004, 464-465, 354-359.	0.8	4
2608	Electronic structure of solid C <sub>48</sub> N <sub>12</sub> aza-fullerene. Solid State Communications, 2004, 129, 379-383.	0.9	24
2609	Stabilization of monoatomic gold wires by carbon impurities. Solid State Communications, 2004, 130, 755-757.	0.9	14
2610	Electronic properties of Nd <sub>3</sub> Co <sub>13</sub> B <sub>2</sub> compound. Solid State Communications, 2004, 132, 225-228.	0.9	4
2611	H <sub>2</sub> dissociative adsorption at the armchair edges of graphite. Solid State Communications, 2004, 132, 713-718.	0.9	37
2612	The electronic structure and the ferromagnetic properties of the organic radical 4-methacryloyloxy-2,2,6,6-tetramethyl-1-piperidinyloxy (MOTMP). Solid State Communications, 2004, 132, 657-660.	0.9	7
2613	Theoretical study of defect structures in pure and titanium-doped alumina. Solid State Ionics, 2004, 172, 155-158.	1.3	20
2614	Modeling catalytic reduction of NO by ammonia over V <sub>2</sub> O <sub>5</sub> . Surface Science Reports, 2004, 55, 169-236.	3.8	75
2615	Revisit to the Ising model for order-disorder phase transition on Si(001). Surface Science, 2004, 554, 150-158.	0.8	7
2616	BaO/W(100) thermionic emitters and the effects of Sc, Y, La, and the density functional used in computations. Surface Science, 2004, 549, 115-120.	0.8	10
2617	Assessment of competing mechanisms of the abstraction of hydrogen from CH <sub>4</sub> on Li/MgO(001). Surface Science, 2004, 549, 217-226.	0.8	18
2618	The geometric and electronic properties of the PbS, PbSe and PbTe (001) surfaces. Surface Science, 2004, 551, 91-98.	0.8	36
2619	Conveying chirality onto the electronic structure of achiral metals: (R,R)-tartaric acid on nickel. Surface Science, 2004, 554, 141-149.	0.8	51
2620	Effect of relaxation on structure and reactivity of anatase (100) and (001) surfaces. Surface Science, 2004, 552, 169-179.	0.8	73
2621	V <sub>2</sub> O <sub>3</sub> (0001) surface terminations: a density functional study. Surface Science, 2004, 555, 118-134.	0.8	64

#	ARTICLE	IF	CITATIONS
2622	Accurate valence band maximum determination for SrTiO <sub>3</sub> (001). Surface Science, 2004, 554, 81-89.	0.8	78
2623	Interactions among adsorbates on metal surfaces. Surface Science, 2004, 558, 1-3.	0.8	9
2624	Predicting the metal growth mode and wetting of noble metals supported on c-ZrO <sub>2</sub> . Surface Science, 2004, 561, 43-56.	0.8	27
2625	A theoretical study of H surface and subsurface species on Pt(1 1 1). Surface Science, 2004, 559, 169-178.	0.8	53
2626	Structure, bonding, and adhesion at the ZrC(100)/Fe(110) interface from first principles. Surface Science, 2004, 560, 103-120.	0.8	108
2627	Local reactivity of supported metal clusters: Pd <sub>n</sub> on Au(1 1 1). Surface Science, 2004, 559, L180-L186.	0.8	75
2628	Surface-science approach to the study of mercaptobenzoxazole on Cu(100). Surface Science, 2004, 566-568, 579-584.	0.8	3
2629	H <sub>2</sub> dissociative adsorption on Mg, Ti, Ni, Pd and La Surfaces. Surface Science, 2004, 566-568, 703-707.	0.8	74
2630	A comparative study of the interaction of cyclopentene, cyclohexene, and 1,4-cyclohexadiene with the silicon (100) surface. Surface Science, 2004, 566-568, 713-718.	0.8	8
2631	STM, LEED, and DFT characterization of epitaxial ZrO <sub>2</sub> films on Pt(111). Surface Science, 2004, 562, 204-218.	0.8	44
2632	DFT plane-wave calculations of the Rh/MgO(001) interface. Surface Science, 2004, 566-568, 977-982.	0.8	10
2633	Water molecule dissociation at ice/MgO(100) interface. Surface Science, 2004, 562, 237-246.	0.8	8
2634	CO dissociation and O removal on Co(0001): a density functional theory study. Surface Science, 2004, 562, 247-256.	0.8	124
2635	Deuterium adsorption on W(100) studied by LEIS and DRS. Surface Science, 2004, 571, 31-40.	0.8	5
2636	Adsorption and dissociation of CO on Fe(110) from first principles. Surface Science, 2004, 570, 167-177.	0.8	118
2637	CO and hydrogen adsorption on Pd(210). Surface Science, 2004, 570, 227-236.	0.8	27
2638	The adsorption structure on Co{0001}: a combined Tensor LEED and DFT study. Surface Science, 2004, 572, 1-10.	0.8	13
2639	Dissociative chemisorption of H <sub>2</sub> on Pt(111): isotope effect and effects of the rotational distribution and energy dispersion. Surface Science, 2004, 573, 433-445.	0.8	42

#	ARTICLE	IF	CITATIONS
2640	TiO <sub>2</sub> -rich reconstructions of SrTiO <sub>3</sub> (001): a theoretical study of structural patterns. <i>Surface Science</i> , 2004, 573, 446-456.	0.8	56
2641	CO adsorption on the Pt(111) surface: a comparison of a gradient corrected functional and a hybrid functional. <i>Surface Science</i> , 2004, 573, 464-473.	0.8	86
2642	Magnetism and electronic structure for RMn <sub>2</sub> (R=Y and lanthanoids) with the cubic Laves phase (C15) structure. <i>Journal of Magnetism and Magnetic Materials</i> , 2004, 272-276, E223-E225.	1.0	0
2643	Screened full-potential KKR calculations for iron compounds, based on the generalized-gradient approximation. <i>Journal of Magnetism and Magnetic Materials</i> , 2004, 272-276, E231-E232.	1.0	4
2644	Electronic structure and magnetic moments of 3d transition metal-doped ZnO. <i>Journal of Magnetism and Magnetic Materials</i> , 2004, 282, 275-278.	1.0	114
2645	Electronic structure and X-ray photoemission spectra of the compounds APtSn I (A=Th, U). <i>Journal of Magnetism and Magnetic Materials</i> , 2004, 281, 281-289.	1.0	7
2646	The melting curve of iron from quantum mechanics calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2004, 65, 1573-1580.	1.9	28
2647	Cyanide adsorption on gold electrodes: a combined surface enhanced Raman spectroscopy and density functional theory study. <i>Journal of Electroanalytical Chemistry</i> , 2004, 563, 111-120.	1.9	55
2648	Hybrid iodoperfluoroalkane-ferrocene supramolecular arrays: the shortest contacts iodine forms with nitrogen atoms and unsaturated moieties. <i>Journal of Fluorine Chemistry</i> , 2004, 125, 629-640.	0.9	29
2649	First-principles studies on the conductive and ferromagnetic properties of MnII CuII bimetallic chains. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2004, 330, 286-290.	0.9	3
2650	Effect of dimerization on conductive and ferromagnetic properties of quasi-one-dimensional organic metallic-ferromagnet. <i>Physica B: Condensed Matter</i> , 2004, 353, 305-309.	1.3	2
2651	Ligand effect on the periodic properties of trivalent organolanthanide complexes: a density functional study. <i>Inorganic Chemistry Communication</i> , 2004, 7, 566-568.	1.8	6
2652	Molecular-level descriptions of surface chemistry in kinetic models using density functional theory. <i>Chemical Engineering Science</i> , 2004, 59, 4679-4691.	1.9	227
2653	The calculation of field shift effects in the rotational spectra of heavy metal-containing diatomic molecules using density functional theory: comparison with experiment for the Tl-halides and Pb-chalcogenides. <i>Chemical Physics</i> , 2004, 298, 205-212.	0.9	16
2654	Calculation of the electronic and optical properties of indium tin oxide by density functional theory. <i>Chemical Physics</i> , 2004, 300, 285-293.	0.9	114
2655	Rotational barriers in ammonium hexachlorometallates as studied by NMR, tunnelling spectroscopy and ab initio calculations. <i>Chemical Physics</i> , 2004, 299, 113-122.	0.9	13
2656	Quantum interference in polycyclic hydrocarbon molecular wires. <i>Chemical Physics</i> , 2004, 299, 139-145.	0.9	108
2657	A DFT study of asymmetric meso-substituted porphyrins and their zinc complexes. <i>Chemical Physics</i> , 2004, 305, 13-26.	0.9	20



#	ARTICLE	IF	CITATIONS
2658	A comparative ab initio study of the "ideal" strength of single crystal $\alpha$ - and $\beta$ -Si <sub>3</sub> N <sub>4</sub> . Acta Materialia, 2004, 52, 233-238.	3.8	67
2659	Effects of cobalt intergranular segregation on interface energetics in WC-Co. Acta Materialia, 2004, 52, 2199-2207.	3.8	91
2660	Energetics and electronic properties of vacancies, anti-sites, and atomic defects (B, C, and N) in B <sub>2</sub> -FeAl alloys. Acta Materialia, 2004, 52, 3263-3271.	3.8	43
2661	First-principles study of polar Al/TiN(1 1 1) interfaces. Acta Materialia, 2004, 52, 3681-3688.	3.8	191
2662	Simulations of intergranular fracture in nanocrystalline molybdenum. Acta Materialia, 2004, 52, 5019-5029.	3.8	69
2663	Structural and electronic properties of small Cu <sub>m</sub> clusters. Applied Surface Science, 2004, 226, 306-312.	3.1	11
2664	Methylchloride adsorbed on Si(001): an ab initio study. Applied Surface Science, 2004, 234, 155-161.	3.1	15
2665	First principles simulations of Cu and Au deposition on $\alpha$ -Al <sub>2</sub> O <sub>3</sub> (0001) surface. Applied Surface Science, 2004, 238, 228-232.	3.1	19
2666	First-principle study on structures and electronic properties of aluminum nanowire wrapped in carbon nanotube. Electrochimica Acta, 2004, 50, 739-744.	2.6	9
2667	All electron scalar relativistic calculations on adsorption of CO on Pt(111) with full-geometry optimization: a correct estimation for CO site-preference. Chemical Physics Letters, 2004, 384, 271-276.	1.2	105
2668	Location and role of exchangeable cations in zeolite catalysis: a first principle study. Chemical Physics Letters, 2004, 385, 20-24.	1.2	15
2669	Two-dimensional arrangement of CH <sub>3</sub> NH <sub>2</sub> adsorption on Si(0 0 1)-2 Å <sup>-1</sup> . Chemical Physics Letters, 2004, 385, 144-148.	1.2	8
2670	Construction of local hybrid exchange-correlation potentials and their evaluation for nuclear shielding constants. Chemical Physics Letters, 2004, 386, 8-16.	1.2	42
2671	Structure and conformational equilibrium of new thiacalix[4]arene derivatives. Chemical Physics Letters, 2004, 385, 368-373.	1.2	17
2672	The solvent effect on the aquation processes of the cis-dichloro(ethylenediamine)platinum(II) using continuum solvation models. Chemical Physics Letters, 2004, 387, 182-187.	1.2	43
2673	Structures and bonding character of cyclic AsO <sub>2</sub> and As <sub>2</sub> S <sub>2</sub> systems in the doublet state. Chemical Physics Letters, 2004, 387, 160-164.	1.2	2
2674	What the stretch frequency spectrum of D <sub>2</sub> O/Ru(0001) does and does not mean. Chemical Physics Letters, 2004, 389, 92-95.	1.2	26
2675	Dielectric susceptibility of dipolar molecular liquids by ab initio molecular dynamics: application to liquid HCl. Chemical Physics Letters, 2004, 390, 193-198.	1.2	24

#	ARTICLE	IF	CITATIONS
2676	Unrestricted open-shell Kohn-Sham scheme with local hybrid exchange-correlation potentials: improved calculation of electronic g-tensors for transition-metal complexes. <i>Chemical Physics Letters</i> , 2004, 391, 16-21.	1.2	33
2677	From planar to three-dimensional structural transition in gold clusters and the spin-orbit coupling effect. <i>Chemical Physics Letters</i> , 2004, 392, 452-455.	1.2	180
2679	Imidazopyridopyrimidine base pairing motifs consisting of four hydrogen bonds: a quantum chemical study. <i>Chemical Physics Letters</i> , 2004, 392, 508-513.	1.2	2
2680	Representing high-dimensional potential-energy surfaces for reactions at surfaces by neural networks. <i>Chemical Physics Letters</i> , 2004, 395, 210-215.	1.2	311
2681	Density functional study of onion-skin-like [As@Ni <sub>12</sub> As <sub>20</sub> ] <sup>3+</sup> and [Sb@Pd <sub>12</sub> Sb <sub>20</sub> ] <sup>3+</sup> cluster ions. <i>Chemical Physics Letters</i> , 2004, 396, 161-166.	1.2	13
2682	Strong and weak adsorption of CO on CeO <sub>2</sub> surfaces from first principles calculations. <i>Chemical Physics Letters</i> , 2004, 396, 384-392.	1.2	108
2683	Efficient calculation of the structural and electronic properties of mixed valence materials: application to Prussian Blue analogues. <i>Chemical Physics Letters</i> , 2004, 397, 154-159.	1.2	23
2684	The role of surface elasticity in giant corrugations observed by scanning tunneling microscopes. <i>Chemical Physics Letters</i> , 2004, 397, 354-359.	1.2	28
2685	Theoretical study of propene adsorbed on sulphated Pt(111). <i>Chemical Physics Letters</i> , 2004, 399, 295-299.	1.2	4
2686	The calculation of ESR parameters by density functional theory: the g- and A-tensors of Co(acacen). <i>Chemical Physics Letters</i> , 2004, 399, 433-439.	1.2	47
2687	A systematic study of the effect of correlation, DFT functional and basis set on the structure of Roesky's ketone. <i>Chemical Physics Letters</i> , 2004, 399, 516-521.	1.2	10
2688	Atomic and electronic structure dependence of surface chemical reactivity. <i>Catalysis Today</i> , 2004, 89, 363-368.	2.2	2
2689	Electronic structure of the extended vanadyl pyrophosphate (1 0 0) surface. <i>Catalysis Today</i> , 2004, 91-92, 177-180.	2.2	9
2690	Field penetration induced charge redistribution effects on the field emission properties of carbon nanotubes—a first-principle study. <i>Applied Surface Science</i> , 2004, 228, 143-150.	3.1	24
2691	Adsorption and decomposition of acetone on Si(001). <i>Applied Surface Science</i> , 2004, 234, 185-189.	3.1	7
2692	Adsorption of Pd atoms on $\gamma$ -Al <sub>2</sub> O <sub>3</sub> : a density functional study of metal-support interactions. <i>Applied Surface Science</i> , 2004, 238, 82-85.	3.1	23
2693	Ab initio study of field emission from hydrogen defects in diamond subsurfaces. <i>Applied Surface Science</i> , 2004, 237, 483-488.	3.1	7
2694	Noble gas-uranium coordination and intersystem crossing for the ClU(Ne) <sub>x</sub> (Ng) <sub>n</sub> (Ng = Ar, Kr, Xe) complexes in solid neon. <i>New Journal of Chemistry</i> , 2004, 28, 289-294.	1.4	17

#	ARTICLE	IF	CITATIONS
2695	Organogermanium Reactive Intermediates. The Direct Detection and Characterization of Transient Germylenes and Digermenes in Solution. <i>Journal of the American Chemical Society</i> , 2004, 126, 16105-16116.	6.6	73
2696	C6F5-Group Transfer from [MeB(C6F5)3]-to the Metal Center of L2MMe+(M = Ti, Zr) as a Deactivation Pathway in Olefin Polymerization Catalysis: A Combined Density Functional Theory and Molecular Mechanics Investigation. <i>Organometallics</i> , 2004, 23, 3847-3852.	1.1	40
2697	Effects of Ag and Ni Additives on Zn Diffusion in Steel Hot-Dip Galvanizing: An ab Initio Molecular Dynamics Simulation. <i>Chemistry of Materials</i> , 2004, 16, 5567-5573.	3.2	7
2698	Car Exhaust Catalysis from First Principles: Selective NO Reduction under Excess O2 Conditions on Ir. <i>Journal of the American Chemical Society</i> , 2004, 126, 10746-10756.	6.6	101
2699	A density functional theory study on the water formation at high coverages and the water effect in the Fischer-Tropsch synthesis. <i>Molecular Physics</i> , 2004, 102, 993-1000.	0.8	21
2700	Geometrical and Electronic Structure of the Pt7 Cluster: A Density Functional Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3806-3812.	1.1	51
2701	The triplet excited state of ruthenium(ii) bis(2,2',6',2''-terpyridine): Comparison between experiment and theory. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 1157-1164.	1.3	63
2702	2-(2-Pyridyl)pyrroles: Part I. Structure and energetics of pyridylpyrroles, their dimers, complexes and excited states. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 3938-3947.	1.3	16
2703	Experimental and theoretical study of the recombination reaction $F + FC(O)O + M \rightarrow F + FC(O)O + M$ . <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 747-755.	1.3	14
2704	LiSr2(NCN)13: the first empty tetrahedral strontium(ii) entity coordinated by carbodiimide units but without strontium-strontium bonding. <i>Chemical Communications</i> , 2004, , 2302-2303.	2.2	9
2705	Multiscale modeling of oxygen diffusion through the oxide during silicon oxidation. <i>Physical Review B</i> , 2004, 70, .	1.1	86
2706	First principles calculations of electronic structures and metal mobility of NaxSi46 and NaxSi34 clathrates. <i>Journal of Chemical Physics</i> , 2004, 120, 6142-6151.	1.2	25
2707	Effectiveness of BaZrO3 buffer layer in SmBa2Cu3Oy epitaxial growth on MgO substrate: A first-principles study. <i>Journal of Applied Physics</i> , 2004, 95, 2309-2318.	1.1	6
2708	Evidence for interstitial hydrogen as the dominant electronic defect in nanometer alumina films. <i>Physical Review B</i> , 2004, 69, .	1.1	48
2709	Density Functional Theory Study of Silica Zeolite Structures: Stabilities and Mechanical Properties of SOD, LTA, CHA, MOR, and MFI. <i>Journal of Physical Chemistry B</i> , 2004, 108, 9208-9215.	1.2	89
2710	Calculating Cumulene/Poly-yne Isomerization Energies. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4030-4035.	1.1	12
2711	Oxygen vacancies on TiO2 (110) from first principles calculations. <i>Journal of Chemical Physics</i> , 2004, 121, 7427-7433.	1.2	75
2712	Conformational Flexibility of Corey Lactone Derivatives Indicated by Absorption and Vibrational Circular Dichroism Spectra. <i>Journal of Organic Chemistry</i> , 2004, 69, 26-32.	1.7	9

#	ARTICLE	IF	CITATIONS
2713	Reduced SnO <sub>2</sub> surfaces by first-principles calculations. Applied Physics Letters, 2004, 84, 909-911.	1.5	88
2714	First principles calculations of the chemisorption properties of nitro-containing molecules on the Al/sub 2/O/sub 3/(0001) surface. , 2004, , .		0
2715	Comparative study of ab initio and tight-binding electronic structure calculations applied to platinum surfaces. Physical Review B, 2004, 70, .	1.1	40
2716	Density-Functional Based Modeling of the Intermediate in the Water Production Reaction on Pt(111). Physical Review Letters, 2004, 92, 136103.	2.9	70
2717	Density-Functional Calculations of f <sub>1/2</sub> , f <sub>3/2</sub> , f <sub>5/2</sub> , and μ Plutonium. Physical Review Letters, 2004, 92, 185702.	2.9	168
2718	Polymorphism of Ti <sub>3</sub> SiC <sub>2</sub> ceramic: First-principles investigations. Physical Review B, 2004, 69, .	1.1	114
2719	Importance of Shear in the bcc-to-hcp Transformation in Iron. Physical Review Letters, 2004, 93, 115501.	2.9	133
2720	Theoretical study of nitric oxide adsorption on Au clusters. Journal of Chemical Physics, 2004, 121, 2558.	1.2	78
2721	Electronic and magnetic properties of bulk and (100) and (111) surfaces of MnPt <sub>3</sub> : An ab initio study. Physical Review B, 2004, 70, .	1.1	2
2722	Adhesion and adhesive transfer at aluminum/diamond interfaces: A first-principles study. Physical Review B, 2004, 69, .	1.1	118
2723	General Insight into CO Oxidation: A Density Functional Theory Study of the Reaction Mechanism on Platinum Oxides. Physical Review Letters, 2004, 93, 106104.	2.9	47
2724	Ab Initio Calculations of the Structures and Vibrational Spectra of Ethene Complexes. Journal of Physical Chemistry A, 2004, 108, 146-156.	1.1	25
2725	Water-Assisting Proton Transfer Isomerization of the HNO/HON System in the Singlet State: On the Number of the Effective Water Molecules. Journal of Physical Chemistry B, 2004, 108, 11732-11743.	1.2	4
2726	Distribution of Cations in FeSbO <sub>4</sub> : A Computer Modeling Study. Chemistry of Materials, 2004, 16, 1954-1960.	3.2	37
2727	Atomic and Molecular Adsorption on Ir(111). Journal of Physical Chemistry B, 2004, 108, 987-994.	1.2	145
2728	Band-resolved analysis of nonlinear optical properties of crystalline and molecular materials. Physical Review B, 2004, 70, .	1.1	263
2729	Influence of the Counterion MeB(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> <sup>-</sup> and Solvent Effects on Ethylene Polymerization Catalyzed by [(CpSiMe <sub>2</sub> NR)TiMe] <sup>+</sup> : A Combined Density Functional Theory and Molecular Mechanism Study. Organometallics, 2004, 23, 104-116.	1.1	75
2730	Sulfuric Acid and Sulfuric Acid Hydrates in the Gas Phase: A DFT Investigation. Journal of Physical Chemistry A, 2004, 108, 8914-8929.	1.1	78

#	ARTICLE	IF	CITATIONS
2731	On the Noble-Gas-Induced Intersystem Crossing for the CUO Molecule:Â Experimental and Theoretical Investigations of CUO(Ng) <sub>n</sub> (Ng = Ar, Kr, Xe;n= 1, 2, 3, 4) Complexes in Solid Neon. <i>Inorganic Chemistry</i> , 2004, 43, 882-894.	1.9	54
2732	Arachno, Nido, and Closo Aromatic Isomers of the Li <sub>6</sub> B <sub>6</sub> H <sub>6</sub> Molecule. <i>Inorganic Chemistry</i> , 2004, 43, 3588-3592.	1.9	28
2733	Reactivity of the Oxygen Sites in the V <sub>2</sub> O <sub>5</sub> /TiO <sub>2</sub> Anatase Catalyst. <i>Journal of Physical Chemistry B</i> , 2004, 108, 15679-15685.	1.2	40
2735	Reactivity Extrapolation from Small to Large Molecular Systems via Isodesmic Reactions for Transition States. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10714-10722.	1.1	9
2736	Density-functional band-structure calculations for La-, Y-, and Sc-filledCoP <sub>3</sub> -based skutterudite structures. <i>Physical Review B</i> , 2004, 70, .	1.1	27
2737	Performance of Density Functionals for Calculating Barrier Heights of Chemical Reactions Relevant to Astrophysics. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7621-7636.	1.1	80
2738	Adsorption of CO <sub>2</sub> on Model Surfaces of Cesium Oxides Determined from First Principles. <i>Journal of Physical Chemistry B</i> , 2004, 108, 16798-16805.	1.2	25
2739	Internal Ceramic Reconstruction Weakens MetalâZrO <sub>2</sub> Adhesion. <i>Journal of Physical Chemistry B</i> , 2004, 108, 15439-15442.	1.2	9
2740	The Nature of the Complex Counterion of the Chromophore in Rhodopsin. <i>Journal of Physical Chemistry B</i> , 2004, 108, 3673-3680.	1.2	30
2741	The Simple Cubic Structure of Ruthenium Clusters. <i>Journal of Physical Chemistry B</i> , 2004, 108, 2140-2147.	1.2	70
2742	A First Principles Analysis of the Location and Affinity of Protons in the Secondary Structure of Phosphotungstic Acid. <i>Journal of Physical Chemistry B</i> , 2004, 108, 12292-12300.	1.2	36
2743	Substitution Effect of Carbon with Group 13, 14, and 15 Elements on Lithium Intercalation in Graphite. <i>Journal of the Electrochemical Society</i> , 2004, 151, A1696.	1.3	5
2744	Methyl Chloride Adsorption on Si(001)âElectronic Structure. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7809-7813.	1.2	20
2745	A Combined Density Functional Theory and Molecular Mechanics (QM/MM) Study of Single-Site Ethylene Polymerization Catalyzed by [(C <sub>6</sub> H <sub>5</sub> NCH)C <sub>4</sub> H <sub>3</sub> N] <sub>2</sub> -RM+{M = Ti, Zr} in the Presence of the Counterion CH <sub>3</sub> B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> -. <i>Organometallics</i> , 2004, 23, 2900-2910.	1.1	32
2746	Trends in the Chemisorption of Aromatic Molecules on a Pt(111) Surface:â Benzene, Naphthalene, and Anthracene from First Principles Calculations. <i>Journal of Physical Chemistry B</i> , 2004, 108, 12084-12091.	1.2	104
2747	Improved Description of Chemical Barriers with Generalized Gradient Approximations (GGAs) and Meta-GGAs. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4459-4469.	1.1	48
2748	Atomistic mechanism of proton conduction in solidCsHSO <sub>4</sub> by a first-principles study. <i>Physical Review B</i> , 2004, 69, .	1.1	22
2749	First-principles-based kinetic Monte Carlo simulation of nitric oxide decomposition over Pt and Rh surfaces under lean-burn conditions. <i>Molecular Physics</i> , 2004, 102, 361-369.	0.8	50

#	ARTICLE	IF	CITATIONS
2750	Driving Forces for Self-Organized Coadsorption: $C_6H_6/2O$ and $C_6H_6/2CO$ on Ni{111}. Journal of the American Chemical Society, 2004, 126, 10962-10971.	6.6	12
2751	First-Principles Quantum Chemical Study of Thermal Decomposition Routes for the Cationic Catalyst $L_2TiMe^+$ . Organometallics, 2004, 23, 5737-5743.	1.1	2
2752	Isomerizations of Bicyclo[2.1.0]pent-2-ene and Tricyclo[2.1.0.0.2,5]pentane into Cyclopenta-1,3-diene: A Computational Study by DFT and High-Level ab Initio Methods. Journal of Physical Chemistry A, 2004, 108, 507-514.	1.1	42
2753	Experimental determination of valence band maxima for $SrTiO_3$ , $TiO_2$ , and $SrO$ and the associated valence band offsets with $Si(001)$ . Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2004, 22, 2205.	1.6	251
2754	Theory of Methane Dehydrogenation on $Pt\{110\}(1 \text{ \AA}^{-2})$ . Part I: Chemisorption of $CH_x$ ( $x = 0 \text{ \AA}^{-3}$ ). Journal of Physical Chemistry B, 2004, 108, 5909-5919.	1.2	61
2755	Crystalline Effects on the Properties of the Dative Bond: A Computational Study of $HCN \sim BF_3$ . Journal of Physical Chemistry A, 2004, 108, 8378-8384.	1.1	16
2756	Axial Ligand and Solvent Effects on the $O \text{ \AA}^{-1} O$ Bond Activation in Acylperoxy Complexes of [(Salen)Mn(III)]: A Mn(IV) versus Mn(V) Species. Journal of Physical Chemistry B, 2004, 108, 3845-3854.	1.2	19
2757	Density Functional Theory Study of Co, Rh, and Ir Atoms Deposited on the $\pm Al_2O_3(0001)$ Surface. Journal of Physical Chemistry B, 2004, 108, 15671-15678.	1.2	30
2758	Effect of Sn on the Reactivity of Cu Surfaces. Journal of Physical Chemistry B, 2004, 108, 14062-14073.	1.2	13
2759	Ethylene Decomposition on $Rh(100)$ : Theory and Experiment. Journal of Physical Chemistry B, 2004, 108, 14541-14548.	1.2	23
2760	Theory of Methane Dehydrogenation on $Pt\{110\}(1 \text{ \AA}^{-2})$ . Part II: Microscopic Reaction Pathways for $CH_x \text{ \AA}^{-1} CH_{x-1}$ ( $x = 1 \text{ \AA}^{-3}$ ). Journal of Physical Chemistry B, 2004, 108, 5920-5929.	1.2	26
2761	A Combined Computational and Experimental Study of Polynuclear $Ru \text{ \AA}^{-1} TPPZ$ Complexes: Insight into the Electronic and Optical Properties of Coordination Polymers. Journal of the American Chemical Society, 2004, 126, 9715-9723.	6.6	78
2762	Structural and Spectroelectrochemical Study of Carbonate and Bicarbonate Adsorbed on $Pt(111)$ and $Pd/Pt(111)$ Electrodes. Journal of Physical Chemistry B, 2004, 108, 17928-17939.	1.2	39
2763	Effects of Subsurface Boron and Phosphorus on Surface Reactivity of $Si(001)$ : Water and Ammonia Adsorption. Journal of Physical Chemistry B, 2004, 108, 16147-16153.	1.2	3
2764	Theoretical Studies of $N_2O$ Adsorption and Reactivity to $N_2$ and $NO$ on $Rh(111)$ . Journal of Physical Chemistry B, 2004, 108, 17921-17927.	1.2	38
2765	Hydrogen Transfer from $[MeB(C_6F_5)_3]$ - to the Methyl Group of $L_2MMe^+$ ( $M = Ti, Zr$ ) as a Deactivation Pathway in Olefin Polymerization Catalysis: A Combined Quantum Mechanics and Molecular Mechanics Investigation. Organometallics, 2004, 23, 2651-2657.	1.1	19
2766	Time-Dependent Density Functional Calculations on the Electronic Absorption Spectra of an Asymmetric Meso-Substituted Porphyrin and Its Zinc Complex. Journal of Physical Chemistry A, 2004, 108, 9435-9441.	1.1	15
2767	Chemisorption of Benzene on $Pt(111)$ , $Pd(111)$ , and $Rh(111)$ Metal Surfaces: A Structural and Vibrational Comparison from First Principles. Journal of Physical Chemistry B, 2004, 108, 5653-5665.	1.2	158



#	ARTICLE	IF	CITATIONS
2768	Density Functional Theory Studies of the Interaction of H, S, Ni <sup>+</sup> H, and Ni <sup>+</sup> S Complexes with the MoS <sub>2</sub> Basal Plane. <i>Journal of Physical Chemistry B</i> , 2004, 108, 239-249.	1.2	29
2769	Competing Pathways in the [2 + 2] Cycloadditions of Cyclopentyne and Benzyne. A DFT and ab Initio Study. <i>Journal of Organic Chemistry</i> , 2004, 69, 5390-5394.	1.7	23
2770	Kinetics and Thermochemistry of the Reaction of 2-Chloroallyl Radicals with Molecular Oxygen. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11339-11344.	1.1	2
2771	Qualitative Differences in the Adsorption Chemistry of Acidic (CO <sub>2</sub> , SO <sub>x</sub> ) and Amphiphilic (NO <sub>x</sub> ) Species on the Alkaline Earth Oxides. <i>Journal of Physical Chemistry B</i> , 2004, 108, 273-282.	1.2	147
2772	Electronic Structure, Isomerism, and Chemical Bonding in B <sub>7</sub> - and B <sub>7</sub> . <i>Journal of Physical Chemistry A</i> , 2004, 108, 3509-3517.	1.1	201
2773	Gas molecule effects on field emission properties of single-walled carbon nanotube. <i>Diamond and Related Materials</i> , 2004, 13, 1306-1313.	1.8	24
2774	Influence of hydrogen on the stability of iron phases under pressure. <i>Geophysical Research Letters</i> , 2004, 31, .	1.5	14
2775	Ab-initio high-pressure alloying of iron and potassium: Implications for the Earth's core. <i>Geophysical Research Letters</i> , 2004, 31, n/a-n/a.	1.5	33
2776	First-principles study of H <sub>2</sub> O diffusion on a metal surface: $\epsilon_f$ H <sub>2</sub> O on Al{100}. <i>Physical Review B</i> , 2004, 69, .	1.1	39
2777	Theoretical study of crossed and parallel carbon nanotube junctions and three-dimensional grid structures. <i>Physical Review B</i> , 2004, 70, .	1.1	34
2778	Ab initio study of the (0001) surfaces of hematite and chromia: Influence of strong electronic correlations. <i>Physical Review B</i> , 2004, 70, .	1.1	357
2779	Binding of propene on small gold clusters and on Au(111): Simple rules for binding sites and relative binding energies. <i>Journal of Chemical Physics</i> , 2004, 121, 3756-3766.	1.2	94
2780	Adsorption energies of molecular oxygen on Au clusters. <i>Journal of Chemical Physics</i> , 2004, 120, 9594-9600.	1.2	159
2781	Electronic Structures of Metal Sites in Proteins and Models: Contributions to Function in Blue Copper Proteins. <i>Chemical Reviews</i> , 2004, 104, 419-458.	23.0	782
2782	Adsorption of C <sub>60</sub> on the Si(001) surface calculated within the generalized gradient approximation. <i>Nanotechnology</i> , 2004, 15, S1-S4.	1.3	26
2783	Interstitial oxygen in Si and Si <sup>1-x</sup> G <sub>x</sub> . <i>Physical Review B</i> , 2004, 69, .	1.1	25
2784	DFT and Metal-Metal Bonding: A Dys-Functional Treatment for Multiply Charged Complexes?. <i>Inorganic Chemistry</i> , 2004, 43, 2597-2610.	1.9	50
2785	Raman under nitrogen. The high-resolution Raman spectroscopy of crystalline uranocene, thorocene, and ferrocene. <i>Journal of Chemical Physics</i> , 2004, 120, 2708-2718.	1.2	32



#	ARTICLE	IF	CITATIONS
2786	Adsorption of a carbon atom on the Ni <sub>38</sub> magic cluster and three low-index nickel surfaces: A comparative first-principles study. <i>Physical Review B</i> , 2004, 69, .	1.1	40
2787	Structure Dependence of NO Adsorption and Dissociation on Platinum Surfaces. <i>Journal of the American Chemical Society</i> , 2004, 126, 1551-1559.	6.6	112
2788	First-principles study of the polar O-terminated ZnO surface in thermodynamic equilibrium with oxygen and hydrogen. <i>Physical Review B</i> , 2004, 69, .	1.1	245
2789	Charge Transport in DNA-Based Devices. <i>Topics in Current Chemistry</i> , 2004, , 183-228.	4.0	227
2790	Hybrid Meta Density Functional Theory Methods for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions: The MPW1B95 and MPWB1K Models and Comparative Assessments for Hydrogen Bonding and van der Waals Interactions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6908-6918.	1.1	1,497
2791	Theoretical prediction of electronic structures of fully $\pi$ -conjugated zinc oligoporphyrins with curved surface structures. <i>Journal of Chemical Physics</i> , 2004, 120, 7963-7970.	1.2	24
2792	A semiempirical generalized gradient approximation exchange-correlation functional. <i>Journal of Chemical Physics</i> , 2004, 121, 5654-5660.	1.2	211
2793	Ground and Low-Lying States of Cu <sub>2</sub> +H <sub>2</sub> O. A Difficult Case for Density Functional Methods. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6072-6078.	1.1	85
2794	Molecular Wheel B82- as a New Inorganic Ligand. Photoelectron Spectroscopy and ab Initio Characterization of LiB8-. <i>Inorganic Chemistry</i> , 2004, 43, 3552-3554.	1.9	150
2795	Noncollinear magnetism in liquid oxygen: A first-principles molecular dynamics study. <i>Physical Review B</i> , 2004, 70, .	1.1	28
2796	Structures of Platinum Clusters: Planar or Spherical? <i>Journal of Physical Chemistry A</i> , 2004, 108, 8605-8614.	1.1	254
2797	Comparing the weighted density approximation with the LDA and GGA for ground-state properties of ferroelectric perovskites. <i>Physical Review B</i> , 2004, 70, .	1.1	139
2798	Structure and magnetic properties of adatoms on carbon nanotubes. <i>Physical Review B</i> , 2004, 69, .	1.1	82
2799	Experimental Evidence for a High-Pressure Isostructural Phase Transition in Osmium. <i>Physical Review Letters</i> , 2004, 93, 095502.	2.9	119
2800	Early chemistry in hot and dense nitromethane: Molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2004, 120, 10146-10153.	1.2	103
2801	A Systematic Study of CO Oxidation on Metals and Metal Oxides: Density Functional Theory Calculations. <i>Journal of the American Chemical Society</i> , 2004, 126, 8-9.	6.6	267
2802	Structure and Energetics of LiBH <sub>4</sub> and Its Surfaces: A First-Principles Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 8682-8690.	1.1	66
2803	Structure and Magnetism of Anion Iron Oxide Clusters. <i>Molecular Simulation</i> , 2004, 30, 911-915.	0.9	16

#	ARTICLE	IF	CITATIONS
2804	Adsorption of O <sub>2</sub> and oxidation of CO at Au nanoparticles supported by TiO <sub>2</sub> (110). Journal of Chemical Physics, 2004, 120, 7673-7680.	1.2	294
2805	Atomic and magnetic configurational energetics by the generalized perturbation method. Physical Review B, 2004, 70, .	1.1	128
2806	Water adsorption on metal surfaces: A general picture from density functional theory studies. Physical Review B, 2004, 69, .	1.1	448
2807	Insight into H <sub>2</sub> O-ice adsorption and dissociation on metal surfaces from first-principles simulations. Physical Review B, 2004, 69, .	1.1	161
2808	Performance of the OPBE exchange-correlation functional. Molecular Physics, 2004, 102, 2467-2474.	0.8	378
2809	Computational Study of Model Pd <sup>+</sup> Zn Nanoclusters and Their Adsorption Complexes with CO Molecules. Journal of Physical Chemistry B, 2004, 108, 5424-5430.	1.2	59
2810	First-principles study of binary bcc alloys using special quasirandom structures. Physical Review B, 2004, 69, .	1.1	266
2811	Density functional study of the adsorption of propene on silver clusters, Ag <sub>m</sub> q (m=1-5; q=0, +1). Journal of Chemical Physics, 2004, 121, 9925-9930.	1.2	41
2812	Ab initio calculations of structure and lattice dynamics in Ni <sup>+</sup> Mn <sup>+</sup> Al shape memory alloys. Physical Review B, 2004, 70, .	1.1	55
2813	Dependence of workfunction on the geometries of single-walled carbon nanotubes. Nanotechnology, 2004, 15, 480-484.	1.3	58
2814	Nitroacetylene: Computed Heats of Formation and Analysis of Reaction Mechanisms with Vinyl Ethers. Journal of Physical Chemistry A, 2004, 108, 3493-3498.	1.1	2
2815	The Interaction of Water with the Pt(533) Surface. Journal of Physical Chemistry B, 2004, 108, 12575-12582.	1.2	59
2816	Ab initio study of $\alpha$ -Al <sub>2</sub> O <sub>3</sub> surfaces. Physical Review B, 2004, 70, .	1.1	197
2817	Transistors and Atoms. Springer Series in Materials Science, 2004, , 1-38.	0.4	1
2818	Development of density functionals for thermochemical kinetics. Journal of Chemical Physics, 2004, 121, 3405-3416.	1.2	1,380
2819	Arene-perfluoroarene interactions in crystal engineering: structural preferences in polyfluorinated toluenes. Journal of Materials Chemistry, 2004, 14, 413-420.	6.7	101
2820	Oxygen stoichiometry, crystal structure, and magnetism of La <sub>0.5</sub> Sr <sub>0.5</sub> CoO <sub>3</sub> . Journal of Physics Condensed Matter, 2004, 16, 6477-6484.	0.7	30
2821	Density functional theory study of the interaction of monomeric water with the Ag{111} surface. Physical Review B, 2004, 69, .	1.1	53

#	ARTICLE	IF	CITATIONS
2822	Density-functional electronic structure of PuCoGa5. <i>Physical Review B</i> , 2004, 70, .	1.1	9
2823	Chemistry of Sulfur Oxides on Transition Metals. III. Oxidation of SO <sub>2</sub> and Self-Diffusion of O, SO <sub>2</sub> , and SO <sub>3</sub> on Pt(111). <i>Journal of Physical Chemistry B</i> , 2004, 108, 13329-13340.	1.2	40
2824	Ab initio thermodynamics of oxide surfaces: O <sub>2</sub> on Fe <sub>2</sub> O <sub>3</sub> (0001). <i>Physical Review B</i> , 2004, 69, .	1.1	147
2825	Coordination and Haptotropic Rearrangement of Cr(CO) <sub>3</sub> on (n,0) Nanotube Sidewalls: A Dynamical Density Functional Study. <i>Journal of Physical Chemistry B</i> , 2004, 108, 5243-5249.	1.2	25
2826	Energetics and Electronic Structures of Individual Atoms Adsorbed on Carbon Nanotubes. <i>Journal of Physical Chemistry B</i> , 2004, 108, 575-582.	1.2	116
2827	Band gap modification of single-walled carbon nanotube and boron nitride nanotube under a transverse electric field. <i>Nanotechnology</i> , 2004, 15, 1837-1843.	1.3	159
2828	Optical and Electrical Properties of Three-Dimensional Interlinked Gold Nanoparticle Assemblies. <i>Journal of the American Chemical Society</i> , 2004, 126, 3349-3356.	6.6	232
2829	Adsorption and Dissociation of O <sub>2</sub> on Pt <sup>*</sup> Co and Pt <sup>*</sup> Fe Alloys. <i>Journal of the American Chemical Society</i> , 2004, 126, 4717-4725.	6.6	615
2830	First-principles electronic structure of spinel LiCr <sub>2</sub> O <sub>4</sub> : A possible half-metal. <i>Physical Review B</i> , 2004, 69, .	1.1	20
2831	A computer modelling study of the uptake and segregation of fluoride ions at the hydrated hydroxyapatite (0001) surface: introducing a Ca <sub>10</sub> (PO <sub>4</sub> ) <sub>6</sub> (OH) <sub>2</sub> potential model. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 1860-1866.	1.3	94
2832	Intrinsic hole localization mechanism in magnetic semiconductors. <i>Journal of Physics Condensed Matter</i> , 2004, 16, L457-L462.	0.7	64
2833	A Density Functional Study on the Stereoselectivity of Styrene Polymerization with a $\sigma$ -Metalloocene Catalyst. <i>Macromolecules</i> , 2004, 37, 5741-5751.	2.2	25
2834	Understanding the High Activity of a Nanostructured Catalyst Obtained by a Deposit of Pd on Ni: First Principle Calculations. <i>Journal of the American Chemical Society</i> , 2004, 126, 3228-3233.	6.6	30
2835	Investigating the M <sup>*</sup> He exciplexes, M={Li,Na,K,Rb,Cs,Fr}: Density functional approach. <i>Journal of Chemical Physics</i> , 2004, 121, 11625-11628.	1.2	27
2836	Basic Density-Functional Theory an Overview. <i>Physica Scripta</i> , 2004, T109, 9.	1.2	87
2837	Ab initio molecular dynamics of metal surfaces. <i>Journal of Physics Condensed Matter</i> , 2004, 16, S2575-S2596.	0.7	18
2838	High-Pressure Melting of Molybdenum. <i>Physical Review Letters</i> , 2004, 92, 195701.	2.9	86
2839	Electronic structures of tungsten surfaces and total-energy distributions of the field-emission current. <i>Physical Review B</i> , 2004, 70, .	1.1	6

#	ARTICLE	IF	CITATIONS
2840	Towards M/metalated DNA-based structures. <i>Nanotechnology</i> , 2004, 15, 1256-1263.	1.3	46
2841	Free Energy of Adsorption of Water and Metal Ions on the {101̄},4} Calcite Surface. <i>Journal of the American Chemical Society</i> , 2004, 126, 10152-10161.	6.6	276
2842	Adsorption of O, OH, and H <sub>2</sub> O on Pt-Based Bimetallic Clusters Alloyed with Co, Cr, and Ni. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6378-6384.	1.1	80
2843	Icosahedral gold cage clusters: M@Au[sub 12][sup ̄] (M=V, Nb, and Ta). <i>Journal of Chemical Physics</i> , 2004, 121, 8369.	1.2	137
2844	Water Dimer Diffusion on Pd{111} Assisted by an H-Bond Donor-Acceptor Tunneling Exchange. <i>Physical Review Letters</i> , 2004, 92, 136104.	2.9	114
2845	The Formation and Stability of Adsorbed Formyl as a Possible Intermediate in Fischer-Tropsch Chemistry on Ruthenium. <i>Journal of Physical Chemistry B</i> , 2004, 108, 3614-3624.	1.2	49
2846	Supported metal species and adsorption complexes on metal oxides and in zeolites: Density functional cluster model studies. <i>Theoretical and Computational Chemistry</i> , 2004, , 367-450.	0.2	5
2847	First-principle molecular dynamics with ultrasoft pseudopotentials: Parallel implementation and application to extended bioinorganic systems. <i>Journal of Chemical Physics</i> , 2004, 120, 5903-5915.	1.2	95
2848	Atomic strings of group IV, III-V, and II-VI elements. <i>Applied Physics Letters</i> , 2004, 85, 6179-6181.	1.5	30
2849	Structure of the Na <sub>x</sub> Cl <sub>x+1</sub> (x=1-4) clusters via ab initio genetic algorithm and photoelectron spectroscopy. <i>Journal of Chemical Physics</i> , 2004, 121, 5709-5719.	1.2	261
2850	Comparative study of defect energetics in HfO <sub>2</sub> and SiO <sub>2</sub> . <i>Applied Physics Letters</i> , 2004, 84, 1492-1494.	1.5	113
2851	Possible structures of nonstoichiometric tin oxide: the composition Sn <sub>2</sub> O <sub>3</sub> . <i>Modelling and Simulation in Materials Science and Engineering</i> , 2004, 12, 33-41.	0.8	57
2852	Self-Limited Growth of a Thin Oxide Layer on Rh(111). <i>Physical Review Letters</i> , 2004, 92, 126102.	2.9	198
2853	Modification of the Monkhorst-Pack special points meshes in the Brillouin zone for density functional theory and Hartree-Fock calculations. <i>Physical Review B</i> , 2004, 70, .	1.1	103
2854	Interaction of benzene thiol and thiolate with small gold clusters. <i>Journal of Chemical Physics</i> , 2004, 120, 10062-10068.	1.2	41
2855	First-principles study of Li ion diffusion in LiFePO <sub>4</sub> . <i>Physical Review B</i> , 2004, 69, .	1.1	250
2856	Ab initio Monte Carlo simulations for finite-temperature properties: application to lithium clusters and bulk liquid lithium. <i>Computational Materials Science</i> , 2004, 29, 145-151.	1.4	16
2857	Magnetism of ultrathin nanowires: ab initio study. <i>Computational Materials Science</i> , 2004, 30, 278-282.	1.4	4

#	ARTICLE	IF	CITATIONS
2858	Electronic structure of bulk and (001) surface layers of pyrite FeS <sub>2</sub> . Computational Materials Science, 2004, 30, 358-363.	1.4	38
2859	Density functional study of the ionization potentials and electron affinities of small Ni <sub>n</sub> clusters with n=2-6 and 8. Computational Materials Science, 2004, 31, 292-298.	1.4	16
2860	Vanadium(V) adsorption onto goethite (α-FeOOH) at pH 1.5 to 12: a surface complexation model based on ab initio molecular geometries and EXAFS spectroscopy. Geochimica Et Cosmochimica Acta, 2004, 68, 1723-1733.	1.6	240
2861	Copper(II) sorption onto goethite, hematite and lepidocrocite: a surface complexation model based on ab initio molecular geometries and EXAFS spectroscopy. Geochimica Et Cosmochimica Acta, 2004, 68, 2623-2637.	1.6	194
2862	First-principles calculations of stability of Pu-Am alloys. Journal of Alloys and Compounds, 2004, 376, 62-67.	2.8	11
2863	Electronic and elastic properties of RCo <sub>5</sub> and RCo <sub>5</sub> H (R = La, Ce, Pr). Journal of Alloys and Compounds, 2004, 379, 41-53.	2.8	23
2864	First-principles investigation of L10-disorder phase equilibria of Fe-Ni, Ni-Pd, and Ni-Pt binary alloy systems. Journal of Alloys and Compounds, 2004, 383, 23-31.	2.8	77
2865	Characterization of the electronic properties of YB <sub>4</sub> and YB <sub>6</sub> using <sup>11</sup> B NMR and first-principles calculations. Journal of Alloys and Compounds, 2004, 383, 232-238.	2.8	57
2866	HVOF-sprayed Triballoy Ti-400: microstructure and first principle calculations. Materials Letters, 2004, 58, 2433-2436.	1.3	25
2867	Calculation of elastic constants of 4d transition metals. Materials Letters, 2004, 58, 2975-2978.	1.3	98
2868	DFT Computation of Relative Spin-State Energetics of Transition Metal Compounds. Structure and Bonding, 2004, , 151-184.	1.0	224
2869	Direct Observation of Charge Transfer at a MgO(111) Surface. Physical Review Letters, 2004, 92, 026101.	2.9	36
2870	Magnetic properties of vacancies in graphene and single-walled carbon nanotubes. New Journal of Physics, 2004, 6, 68-68.	1.2	370
2871	Ab Initio Study of Chemisorption Reactions for Carboxylic Acids on Hydrogenated Silicon Surfaces. Journal of Physical Chemistry B, 2004, 108, 17278-17280.	1.2	21
2872	Unoccupied electronic states in CaB <sub>6</sub> studied by density functional theory and EELS measurements. Physical Review B, 2004, 69, .	1.1	19
2873	Computational Insights into the Acceptor Chemistry of Phosphonium Cations. Inorganic Chemistry, 2004, 43, 7857-7867.	1.9	57
2874	Melting curve of materials: theory versus experiments. Journal of Physics Condensed Matter, 2004, 16, S973-S982.	0.7	59
2875	ZnS bubble clusters with onion-like structures. Chemical Communications, 2004, , 864-865.	2.2	51

#	ARTICLE	IF	CITATIONS
2876	Alternative Low-Symmetry Structure for 13-Atom Metal Clusters. <i>Physical Review Letters</i> , 2004, 93, 133401.	2.9	195
2877	Theoretical study of CO oxidation on Au nanoparticles supported by MgO(100). <i>Physical Review B</i> , 2004, 69, .	1.1	246
2878	Amorphization Mechanism of Icosahedral Metal Nanoclusters. <i>Physical Review Letters</i> , 2004, 93, 065502.	2.9	113
2879	Ab Initio Quantum-Chemical Calculations in Electrochemistry. , 2004, , 51-130.		3
2880	Adsorption modes of cysteine on Au(111): Thiolate, amino-thiolate, disulfide. <i>Journal of Chemical Physics</i> , 2004, 120, 4906-4914.	1.2	190
2881	Ab Initio Calculations of Intermediates of Oxygen Reduction on Low-Index Platinum Surfaces. <i>Journal of the Electrochemical Society</i> , 2004, 151, A2016.	1.3	169
2882	The importance of spin-orbit coupling and electron correlation in the rationalization of the ground state of the CUO molecule. <i>Journal of Chemical Physics</i> , 2004, 121, 5783-5788.	1.2	32
2883	Quasiharmonic approach to a second-order phase transition. <i>Physical Review B</i> , 2004, 70, .	1.1	17
2884	Predicting Adsorption Coefficients at Air~Water Interfaces Using Universal Solvation and Surface Area Models. <i>Journal of Physical Chemistry B</i> , 2004, 108, 12882-12897.	1.2	34
2885	Theoretical Study of Stable Intermolecular Complexes of Furan with Hydrogen Halides. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11375-11380.	1.1	16
2886	CePt3Si:An unconventional superconductor without inversion center. <i>Physical Review B</i> , 2004, 69, .	1.1	232
2887	Atomic and electronic structure of unreduced and reduced CeO2 surfaces: A first-principles study. <i>Journal of Chemical Physics</i> , 2004, 120, 7741-7749.	1.2	338
2888	Metastability of a gold nanoring: Density-functional calculations. <i>Physical Review B</i> , 2004, 70, .	1.1	16
2889	Surface properties ofCeO2from first principles. <i>Physical Review B</i> , 2004, 69, .	1.1	299
2890	Chemistry of Sulfur Oxides on Transition Metals. II. Thermodynamics of Sulfur Oxides on Platinum(111). <i>Journal of Physical Chemistry B</i> , 2004, 108, 250-264.	1.2	43
2891	Growth of Unidirectional Molecular Rows of Cysteine onAu(110)~(1Å–2)Driven by Adsorbate-Induced Surface Rearrangements. <i>Physical Review Letters</i> , 2004, 93, 086101.	2.9	112
2892	Quantum-Chemical and Force-Field Investigations of Ice Ih:~Computation of Proton-Ordered Structures and Prediction of Their Lattice Energies. <i>Journal of Physical Chemistry B</i> , 2004, 108, 15856-15864.	1.2	97
2893	Full-potential KKR calculations for vacancies inAl: Screening effect and many-body interactions. <i>Physical Review B</i> , 2004, 70, .	1.1	26

#	ARTICLE	IF	CITATIONS
2894	Field emission mechanisms of graphitic nanostructures. <i>Physical Review B</i> , 2004, 70, .	1.1	59
2895	Effect of Molecular Structure and Hydration on the Uptake of Gas-Phase Sulfuric Acid by Charged Clusters/Ultrafine Particles. <i>Aerosol Science and Technology</i> , 2004, 38, 349-353.	1.5	20
2896	Theory of elastic and inelastic tunnelling microscopy and spectroscopy: CO on Cu revisited. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2004, 362, 1173-1183.	1.6	33
2897	Ab Initio Extended Density Functional Theory for Strongly Correlated Electron Systems: Fundamental Aspects of the Broken-Symmetry Approach and Possible Applications for Molecular Material Design. <i>Bulletin of the Chemical Society of Japan</i> , 2004, 77, 1269-1286.	2.0	26
2898	Interaction between Substitutional and Interstitial Elements in $\alpha$ -Fe Studied by First-Principles Calculation. <i>Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals</i> , 2004, 68, 977-982.	0.2	8
2899	First-Principles Calculation of $L_{10}$ -Disorder Phase Boundary in Fe-Pd System. <i>Materials Transactions</i> , 2004, 45, 1478-1484.	0.4	29
2900	Thermodynamic Analysis of the Ni-Si-Ti System Using Thermochemical Properties Determined from Ab Initio Calculations. <i>Materials Transactions</i> , 2004, 45, 1507-1514.	0.4	53
2901	Atomic and Electronic Structures of Hydrated Polymolybdates by First Principles Calculations. <i>Materials Transactions</i> , 2004, 45, 1982-1986.	0.4	5
2902	Ab initio Modeling of the Stress-Strain Response of SiAlON ( $Si_6Al_2O_8N_8$ ) Tj ETQq0 00rgBT /Qverlock 10		
2903	Dynamics of water and methanol in h-mordenite. <i>Studies in Surface Science and Catalysis</i> , 2004, 154, 2143-2150.	1.5	0
2904	An accelerated quantum molecular dynamics study of NH <sub>3</sub> interaction with the Brønsted acid in periodic zeolite models. <i>Studies in Surface Science and Catalysis</i> , 2004, , 1763-1768.	1.5	1
2905	A DFT study of the adsorption of butane in MOR and activation on the Lewis center. <i>Studies in Surface Science and Catalysis</i> , 2005, 158, 939-946.	1.5	0
2907	Theoretical modeling of the isopropyl cation: Exploring nonclassical carbonyl behavior. <i>Journal of Coordination Chemistry</i> , 2005, 58, 595-603.	0.8	0
2908	Methylchloride Adsorption on Si(001) $\alpha$ Electronic Properties. , 2005, , 115-127.		0
2909	Elastic Constants of AlLi from First Principles. <i>Materials Transactions</i> , 2005, 46, 1117-1121.	0.4	32
2910	Interaction between Substitutional and Interstitial Elements in $\alpha$ iron Studied by First-principles Calculation. <i>Materials Transactions</i> , 2005, 46, 1140-1147.	0.4	13
2911	Hydrogen-Promoted Grain Boundary Embrittlement and Vacancy Activity in Metals: Insights from Ab Initio Total Energy Calculatons. <i>Materials Transactions</i> , 2005, 46, 756-760.	0.4	39
2912	Analysis of <sup>13</sup> C NMR Chemical Shielding and XPS for Cellulose and Chitosan by DFT Calculations Using the Model Molecules. <i>Polymer Journal</i> , 2005, 37, 21-29.	1.3	19



#	ARTICLE	IF	CITATIONS
2913	Ab initio vibrational spectroscopy of molecular adsorbates in mordenite. <i>Studies in Surface Science and Catalysis</i> , 2005, 158, 601-608.	1.5	3
2914	Origin of visible-light-driven photocatalysis: A comparative study on N/F-doped and Nâ€F-codoped TiO <sub>2</sub> powders by means of experimental characterizations and theoretical calculations. <i>Journal of Solid State Chemistry</i> , 2005, 178, 3293-3302.	1.4	327
2915	Structural and magnetic properties of clean and methylthiolate-adsorbed Co(0001) surfaces: a first-principles study. <i>Journal of Magnetism and Magnetic Materials</i> , 2005, 286, 119-123.	1.0	7
2916	Calculation of enthalpies of formation of actinide nitrides. <i>Journal of Nuclear Materials</i> , 2005, 344, 40-44.	1.3	49
2917	Structure instability of A <sub>2</sub> Al <sub>2</sub> B <sub>2</sub> O <sub>7</sub> (A=K, Na) crystals. <i>Journal of Physics and Chemistry of Solids</i> , 2005, 66, 1655-1659.	1.9	18
2918	First-principles calculation of defect formation energy in chalcopyrite-type CuInSe <sub>2</sub> , CuGaSe <sub>2</sub> and CuAlSe <sub>2</sub> . <i>Journal of Physics and Chemistry of Solids</i> , 2005, 66, 1924-1927.	1.9	47
2919	Lithium insertion and mobility in the TiO <sub>2</sub> -anatase/titanate structure: A periodic DFT study. <i>Journal of Electroanalytical Chemistry</i> , 2005, 581, 216-223.	1.9	52
2920	Ab initio modeling of structure and defects at the HfO <sub>2</sub> /Si interface. <i>Microelectronic Engineering</i> , 2005, 80, 412-415.	1.1	51
2921	An investigation of enhanced secondary ion emission under Au <sup>n+</sup> (n=1â€7) bombardment. <i>Journal of the American Society for Mass Spectrometry</i> , 2005, 16, 733-742.	1.2	26
2922	GaN growth process using GaP(111)A and (111)B surfaces as an initial substrate. <i>Journal of Crystal Growth</i> , 2005, 275, e1631-e1636.	0.7	1
2923	Epitaxial film growth of zirconium diboride on Si(001). <i>Journal of Crystal Growth</i> , 2005, 277, 364-371.	0.7	15
2924	Tailor-made ionic liquids. <i>Journal of Chemical Thermodynamics</i> , 2005, 37, 537-558.	1.0	180
2925	Properties of charge and magnetic impurities in a spin-polarized electron gas: A semiclassical approach. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2005, 28, 313-322.	1.3	1
2926	Stability and electronic structure of single-walled InN nanotubes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2005, 30, 81-85.	1.3	51
2927	Structural stabilities and electronic structures of Ti atomic chains. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2005, 30, 138-142.	1.3	14
2928	First principles study of wurtzite and zinc blende GaN: a comparison of the electronic and optical properties. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2005, 336, 145-151.	0.9	30
2929	Ab initio investigation of the surface properties of Cu(111) and Li diffusion in Cu thin film. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2005, 337, 247-255.	0.9	45
2930	Theoretical investigation of the exciplexes. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2005, 341, 170-176.	0.9	5

#	ARTICLE	IF	CITATIONS
2931	Structure and magnetism of anion iron oxide clusters., Polyhedron, 2005, 24, 2472-2476.	1.0	25
2932	Electronic structure and magnetism at the active site in ferredoxin: Ab initio approach to (Fe <sub>2</sub> S <sub>2</sub> ) <sub>2</sub> + complex with the 1st peptide shell. Polyhedron, 2005, 24, 2550-2556.	1.0	1
2933	The role of the hydrogen bonding network for the shear modulus of PIPD. Polymer, 2005, 46, 9144-9154.	1.8	18
2934	Ab initio study of charged states of H in amorphous SiO <sub>2</sub> . Microelectronic Engineering, 2005, 80, 288-291.	1.1	25
2935	A simple correlation between average T-O-T angles and 27Al NMR chemical shifts does not hold in high-silica zeolites. Microporous and Mesoporous Materials, 2005, 85, 279-283.	2.2	29
2936	Orientation of ethoxy, mono-, di-, and tri-fluoroethoxy on Cu(111): a DFT study. Journal of Molecular Catalysis A, 2005, 228, 77-82.	4.8	16
2937	Theory and experiments on the structure of 7Å... alumina films grown on Ni3Al. Journal of Molecular Catalysis A, 2005, 228, 83-87.	4.8	9
2938	First-principles calculations and thermodynamic modeling of the Ni-Mo system. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2005, 397, 288-296.	2.6	67
2939	van der Waals interactions of the benzene dimer: Towards treatment of polycyclic aromatic hydrocarbon dimers. Materials Science and Engineering C, 2005, 25, 787-792.	3.8	16
2940	Modeling rhenium metallization of a silicon-rich (001) 6H-SiC surface. Materials Science in Semiconductor Processing, 2005, 8, 497-501.	1.9	0
2941	Threshold displacement energies in rutile TiO <sub>2</sub> : A molecular dynamics simulation study. Nuclear Instruments & Methods in Physics Research B, 2005, 239, 191-201.	0.6	53
2942	Diastereoselective synthesis of 3,4-disubstituted 5-(p-tolylsulfinyl)-5,6-dehydropiperidin-2-ones: chirality transfer in the enantioselective synthesis of ethyl (+)-(3S,4aS,7aS)-1-oxo-octahydro-1H-cyclopenta[c]pyridine-3-carboxylate. Tetrahedron: Asymmetry, 2005, 16, 4034-4044.	1.8	4
2943	DFT study of the thermochemistry of gas-phase 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (Î <sup>2</sup> -HMX). Computational and Theoretical Chemistry, 2005, 714, 147-152.	1.5	26
2944	First-principles calculations on the surface electronic and reactive properties of M/SnO <sub>2</sub> (M=Ge, Mn) (110). Computational and Theoretical Chemistry, 2005, 714, 221-233.	1.5	17
2945	Theoretical study of hydrated sulfuric acid: clusters and periodic modeling. Computational and Theoretical Chemistry, 2005, 718, 71-76.	1.5	21
2946	Theoretical study of molecular nitrogen adsorption on Au clusters. Computational and Theoretical Chemistry, 2005, 755, 9-17.	1.5	30
2947	Insight into the structure and intrinsic stability of the Keggin and Wells-Dawson neutral cages. Computational and Theoretical Chemistry, 2005, 755, 119-126.	1.5	9
2948	On the Î <sup>2</sup> -[AlW <sub>12</sub> O <sub>40</sub> ] <sup>5-</sup> stability: Revisited. Computational and Theoretical Chemistry, 2005, 755, 113-117.	1.5	9

#	ARTICLE	IF	CITATIONS
2949	Electronic and magnetic structure studies of double perovskite Sr <sub>2</sub> CrReO <sub>6</sub> by first-principles calculations. <i>Solid State Communications</i> , 2005, 133, 219-222.	0.9	45
2950	First-principles study on the structure instability and electronic structure of cubic Ba <sub>0.5</sub> Sr <sub>0.5</sub> TiO <sub>3</sub> . <i>Solid State Communications</i> , 2005, 135, 290-293.	0.9	14
2951	Structural study of iron-based microstructured and nanostructured powders sprayed by HVOF thermal spraying. <i>Surface and Coatings Technology</i> , 2005, 192, 19-26.	2.2	42
2952	Hydrogen adsorption energies on bimetallic overlayer systems at the solid-vacuum and the solid-liquid interface. <i>Surface Science</i> , 2005, 597, 42-50.	0.8	50
2953	Ab initio studies of the cubic boron nitride (110) surface. <i>Surface Science</i> , 2005, 574, 269-286.	0.8	33
2954	Oscillatory interaction between O impurities and Al adatoms on Al(111) and its effect on nucleation and growth. <i>Surface Science</i> , 2005, 575, 89-102.	0.8	9
2955	Cu, Ag and Au atoms deposited on the $\hat{1}\hat{1}\hat{1}$ -Al <sub>2</sub> O <sub>3</sub> (0001) surface: a comparative density functional study. <i>Surface Science</i> , 2005, 575, 189-196.	0.8	63
2956	Computational study of charge accumulation at SnO <sub>2</sub> (110) surface. <i>Surface Science</i> , 2005, 577, 127-138.	0.8	36
2957	DFT study of oxygen adsorption on W(112) surface. <i>Surface Science</i> , 2005, 577, 229-235.	0.8	17
2958	Adsorption and reaction of N <sub>2</sub> H <sub>4</sub> on Si(100)-2 $\times$ 1: A computational study with single- and double-dimer cluster models. <i>Surface Science</i> , 2005, 579, 197-214.	0.8	8
2959	Interaction of oxygen with the Pt(111) surface in wide conditions range. A DFT-based thermodynamical simulation. <i>Surface Science</i> , 2005, 580, 137-144.	0.8	40
2960	On-surface and sub-surface oxygen on ideal and reconstructed Cu(100). <i>Surface Science</i> , 2005, 584, 62-69.	0.8	36
2961	First-principles investigation of the electronic properties of niobium and molybdenum mononitride surfaces. <i>Surface Science</i> , 2005, 583, 69-79.	0.8	13
2962	Surface segregation in palladium based alloys from density-functional calculations. <i>Surface Science</i> , 2005, 583, 100-106.	0.8	113
2963	Comparison of the reduction of metal oxide surfaces: TiO <sub>2</sub> -anatase, TiO <sub>2</sub> -rutile and SnO <sub>2</sub> -rutile. <i>Surface Science</i> , 2005, 583, 107-117.	0.8	110
2964	The first-principle study on chlorine-modified silver surfaces. <i>Surface Science</i> , 2005, 584, 187-198.	0.8	23
2965	Structure and vibrational spectra of crystalline SiO <sub>2</sub> ultra-thin films on Mo(112). <i>Surface Science</i> , 2005, 584, 225-236.	0.8	65
2966	Interaction of condensed water molecules with hydroxyl and hydrogen groups on Si(001). <i>Surface Science</i> , 2005, 587, 34-40.	0.8	19

#	ARTICLE	IF	CITATIONS
2967	CO adsorption on Cu(111) and Cu(001) surfaces: Improving site preference in DFT calculations. <i>Surface Science</i> , 2005, 590, 117-126.	0.8	116
2968	Electronic and dielectric properties of a suboxide interlayer at the silicon-oxide interface in MOS devices. <i>Surface Science</i> , 2005, 586, 183-191.	0.8	46
2969	Catalyst-induced changes in a substituted aromatic: A combined approach via experiment and theory. <i>Surface Science</i> , 2005, 589, 173-183.	0.8	23
2970	Excitation mechanism and ultrafast vibrational wavepacket dynamics of alkali-metal atoms on Pt(111). <i>Surface Science</i> , 2005, 593, 110-115.	0.8	7
2971	Two-electron processes of desorption of a single ammonia molecule from Cu(100). <i>Surface Science</i> , 2005, 593, 122-132.	0.8	8
2972	A simple chemical view of relaxations at stoichiometric (110) surfaces of rutile-structure type oxides: A first-principles study of stishovite, SiO <sub>2</sub> . <i>Surface Science</i> , 2005, 594, 70-82.	0.8	10
2973	Atomic structure of O/Ir(210) nanofacets. <i>Surface Science</i> , 2005, 596, 89-97.	0.8	21
2974	Effects of hydrogen on electronic properties of doped diamond. <i>Carbon</i> , 2005, 43, 1009-1014.	5.4	16
2975	Adsorption and decomposition of H <sub>2</sub> S on Pd(111) surface: a first-principles study. <i>Catalysis Today</i> , 2005, 99, 315-322.	2.2	89
2976	First principles calculations of the adsorption and diffusion of hydrogen on Fe(100) surface and in the bulk. <i>Catalysis Today</i> , 2005, 105, 44-65.	2.2	90
2977	A density functional theory study of the adsorption of acetone to the (111) surface of Pt: Implications for hydrogenation catalysis. <i>Catalysis Today</i> , 2005, 105, 85-92.	2.2	43
2978	Surface processes and phase transitions from ab initio atomistic thermodynamics and statistical mechanics. <i>Catalysis Today</i> , 2005, 105, 17-35.	2.2	108
2979	Nucleation and growth of 1B metal clusters on rutile TiO <sub>2</sub> (110): Atomic level understanding from first principles studies. <i>Catalysis Today</i> , 2005, 105, 78-84.	2.2	22
2980	DFT calculations of EPR parameters of transition metal complexes: Implications for catalysis. <i>Catalysis Today</i> , 2005, 105, 122-133.	2.2	66
2981	Computational study of carbon segregation and diffusion within a nickel grain boundary. <i>Acta Materialia</i> , 2005, 53, 87-96.	3.8	36
2982	A combined first-principles and experimental study of the lattice site preference of Pt in B <sub>2</sub> NiAl. <i>Acta Materialia</i> , 2005, 53, 2101-2109.	3.8	71
2983	First-principles study of constitutional point defects in B <sub>2</sub> NiAl using special quasirandom structures. <i>Acta Materialia</i> , 2005, 53, 2643-2652.	3.8	42
2984	First-principles study on the crystal, electronic structure and stability of LaNi <sub>5-x</sub> Al <sub>x</sub> (x=0, 0.25, 0.5). <i>J. Phys.: Condens. Matter</i> , 2005, 17, 3843-3852.	0.784314	39

#	ARTICLE	IF	CITATIONS
2985	Phase stability in the Fe–Ni system: Investigation by first-principles calculations and atomistic simulations. <i>Acta Materialia</i> , 2005, 53, 4029-4041.	3.8	262
2986	Influence of La on electronic structure of $\gamma$ -Al <sub>2</sub> O <sub>3</sub> high k-gate from first principles. <i>Ceramics International</i> , 2005, 31, 671-675.	2.3	17
2987	Computational study of calix[4]arene derivatives and complexation with Zn <sup>2+</sup> . <i>Chemical Physics</i> , 2005, 310, 109-122.	0.9	31
2988	Investigation of the electrical and optical properties of iridium oxide by reflectance FTIR spectroscopy and density functional theory calculations. <i>Chemical Physics</i> , 2005, 313, 25-31.	0.9	34
2989	DFT benchmark study for the oxidative addition of CH <sub>4</sub> to Pd. Performance of various density functionals. <i>Chemical Physics</i> , 2005, 313, 261-270.	0.9	94
2990	First-principles calculations on the role of CN precursors for the formation of fullerene-like carbon nitride. <i>Chemical Physics Letters</i> , 2005, 401, 288-295.	1.2	67
2991	The effect of different density functional methods on basis set parameters. <i>Chemical Physics Letters</i> , 2005, 402, 510-513.	1.2	30
2992	Electronic structure and geometry optimization of nanoparticles Fe <sub>2</sub> C, FeC <sub>2</sub> , Fe <sub>3</sub> C, FeC <sub>3</sub> and Fe <sub>2</sub> C <sub>2</sub> . <i>Chemical Physics Letters</i> , 2005, 404, 400-408.	1.2	34
2993	Theoretical calculation of the energy of formation of LiBH <sub>4</sub> . <i>Chemical Physics Letters</i> , 2005, 405, 73-78.	1.2	85
2994	Role of surface geometry and electronic structure in STM images of O/Ru(0001). <i>Chemical Physics Letters</i> , 2005, 405, 131-135.	1.2	21
2995	Tautomerism of 1,3-diphospholes. <i>Chemical Physics Letters</i> , 2005, 406, 173-178.	1.2	7
2996	The magnitude of pseudo-potential errors for density functional calculations. <i>Chemical Physics Letters</i> , 2005, 406, 501-503.	1.2	6
2997	Structure and stability of thiophene–hydrogen halide complexes: An ab initio molecular orbital study. <i>Chemical Physics Letters</i> , 2005, 407, 222-226.	1.2	10
2998	Simulating temperature programmed desorption directly from density functional calculations: How adsorbate configurations relate to desorption features. <i>Chemical Physics Letters</i> , 2005, 407, 227-231.	1.2	9
2999	Density functional molecular orbital calculations on the stability of hydrogen-bonded 4-hydroxyazobenzene dimers. <i>Chemical Physics Letters</i> , 2005, 408, 197-204.	1.2	14
3000	Reactivity of a gas/metal/metal-oxide three-phase boundary: CO oxidation at the Pt(111)–c(4 $\times$ 2)-2CO/l $\pm$ -PtO <sub>2</sub> phase boundary. <i>Chemical Physics Letters</i> , 2005, 409, 1-7.	1.2	52
3001	Proton ordered cubic and hexagonal periodic models of ordinary ice. <i>Chemical Physics Letters</i> , 2005, 409, 110-117.	1.2	50
3002	Water bilayer on the Pd/Au(111) overlayer system: Coadsorption and electric field effects. <i>Chemical Physics Letters</i> , 2005, 409, 157-162.	1.2	110

#	ARTICLE	IF	CITATIONS
3003	First-principles calculations on the curvature evolution and cross-linkage in carbon nitride. Chemical Physics Letters, 2005, 410, 228-234.	1.2	57
3004	A wetting layer breaks the ice rules. Chemical Physics Letters, 2005, 410, 120-124.	1.2	19
3005	Density functional theory study of adsorption of OOH on Pt-based bimetallic clusters alloyed with Cr, Co, and Ni. Chemical Physics Letters, 2005, 410, 275-281.	1.2	60
3006	The magnitude of pseudo-potential errors for bond distances and vibrational frequencies. Chemical Physics Letters, 2005, 412, 12-15.	1.2	5
3007	The surface oxide as a source of oxygen on Rh(111). Journal of Electron Spectroscopy and Related Phenomena, 2005, 144-147, 367-372.	0.8	62
3008	A density functional study of molecular oxygen adsorption and reaction barrier on Pu (100) surface. European Physical Journal B, 2005, 43, 131-141.	0.6	21
3009	First-principles study of the optical properties of pure $\gamma$ -Al <sub>2</sub> O <sub>3</sub> and La aluminates. European Physical Journal B, 2005, 43, 439-444.	0.6	31
3010	Relaxation of the Mo(112) and W(112) surfaces. European Physical Journal B, 2005, 44, 551-555.	0.6	15
3011	Quantum dynamics of the dissociation of H <sub>2</sub> on Rh(111). European Physical Journal B, 2005, 45, 425-432.	0.6	9
3012	First-principles study of the optical properties of PbTiO <sub>3</sub> . European Physical Journal B, 2005, 46, 463-469.	0.6	21
3013	Structural properties of AlN from first principles calculations. European Physical Journal B, 2005, 47, 379-383.	0.6	50
3014	From antiferromagnetic to ferromagnetic coupling for V adatoms on Co(001) substrates. European Physical Journal B, 2005, 48, 249-254.	0.6	12
3015	CO dynamics induced by tunneling electrons: differences on Cu(110) and Ag(110). European Physical Journal D, 2005, 35, 341-348.	0.6	25
3016	Electronic properties of single-walled silicon nanotubes compared to carbon nanotubes. Physical Review B, 2005, 72, .	1.1	145
3017	Adsorption of Ar atoms on the relaxed defect-free TiO <sub>2</sub> (110) surface. Physical Review B, 2005, 71, .	1.1	17
3018	Adsorption and Vibrational Spectroscopy of CO on Mordenite: An Ab initio Density-Functional Study. Journal of Physical Chemistry B, 2005, 109, 7345-7357.	1.2	32
3019	Computational DFT Study of ZrSiO <sub>4</sub> Polymorphs: Microelectronic, Nuclear Safety and Geological Implications. Materials Research Society Symposia Proceedings, 2005, 894, 1.	0.1	1
3020	Assessment of Gaussian-3 and density-functional theories on the G3/05 test set of experimental energies. Journal of Chemical Physics, 2005, 123, 124107.	1.2	320

#	ARTICLE	IF	CITATIONS
3021	Effect of Subsurface Oxygen on the Reactivity of the Ag(111) Surface. <i>Journal of the American Chemical Society</i> , 2005, 127, 12823-12827.	6.6	151
3022	Behaviour of density functionals with respect to basis set: II. Polarization consistent basis sets. <i>Molecular Physics</i> , 2005, 103, 345-358.	0.8	32
3023	Hydrogen Storage in Novel Organometallic Buckyballs. <i>Physical Review Letters</i> , 2005, 94, 155504.	2.9	629
3024	Crystal structure of Ca(AlH <sub>4</sub> ) <sub>2</sub> predicted from density-functional band-structure calculations. <i>Physical Review B</i> , 2005, 71, .	1.1	58
3025	The electronic structure of liquid water within density-functional theory. <i>Journal of Chemical Physics</i> , 2005, 123, 014501.	1.2	98
3026	Energy landscape of deformation twinning in bcc and fcc metals. <i>Physical Review B</i> , 2005, 71, .	1.1	215
3027	Highly controlled acetylene accommodation in a metal-organic microporous material. <i>Nature</i> , 2005, 436, 238-241.	13.7	1,386
3028	Geometry of {001} Surfaces of Spinel (MgAl <sub>2</sub> O <sub>4</sub> ): First-Principles Simulations and Experimental Measurements. <i>Journal of the American Ceramic Society</i> , 2005, 88, 1544-1548.	1.9	34
3029	First principles calculations on Ni impurities in Cu clusters. <i>Journal of Magnetism and Magnetic Materials</i> , 2005, 294, 122-126.	1.0	6
3030	Magnetic and half-metallic properties of Cr-doped $\beta$ -SiC. <i>IEEE Transactions on Magnetics</i> , 2005, 41, 2733-2735.	1.2	15
3031	Accuracy and efficiency of atomic basis set methods versus plane wave calculations with ultrasoft pseudopotentials for DNA base molecules. <i>Journal of Computational Chemistry</i> , 2005, 26, 599-605.	1.5	15
3032	Development of a force field for Li <sub>2</sub> SiF <sub>6</sub> . <i>Journal of Computational Chemistry</i> , 2005, 26, 716-724.	1.5	7
3033	Oxidative addition of the ethane C-H bond to Pd. An ab initio benchmark and DFT validation study. <i>Journal of Computational Chemistry</i> , 2005, 26, 1006-1020.	1.5	69
3034	Energetic and topological analyses of the oxidation reaction between Mon (n = 1, 2) and N <sub>2</sub> O. <i>Journal of Computational Chemistry</i> , 2005, 26, 1284-1293.	1.5	29
3035	Benchmarking approximate density functional theory. I.s/d excitation energies in 3d transition metal cations. <i>Journal of Computational Chemistry</i> , 2005, 26, 1505-1518.	1.5	57
3036	Solid-State Structure, Quantum Calculations and Spectroscopic Characterization of the Hydrogen-Bonded Complex [Os(bpy) <sub>2</sub> (CO)(EtO- $\dot{A}$ -H-DMAP)] [PF <sub>6</sub> ] <sub>2</sub> . <i>European Journal of Inorganic Chemistry</i> , 2005, 2005, 606-614.	1.0	7
3037	Ab Initio Study of Free-Radical Polymerizations: Cost-Effective Methods to Determine the Reaction Rates. <i>ChemPhysChem</i> , 2005, 6, 180-189.	1.0	45
3038	Testing the Pairwise Additive Potential Approximation Using DFT: Coadsorption of CO and N on Rh(100). <i>ChemPhysChem</i> , 2005, 6, 473-480.	1.0	14



#	ARTICLE	IF	CITATIONS
3039	A DFT Study of the Adsorption and Dissociation of CO on Fe(100): Influence of Surface Coverage on the Nature of Accessible Adsorption States. <i>ChemPhysChem</i> , 2005, 6, 254-260.	1.0	106
3040	Assessment of Density Functionals for the High-Spin/Low-Spin Energy Difference in the Low-Spin Iron(II) Tris(2,2'-bipyridine) Complex. <i>ChemPhysChem</i> , 2005, 6, 1393-1410.	1.0	162
3041	Generalized Hybrid-Orbital Method for Combining Density Functional Theory with Molecular Mechanicals. <i>ChemPhysChem</i> , 2005, 6, 1853-1865.	1.0	67
3042	The Influence of Promoters and Poisons on Carbon Monoxide Adsorption on Rh(100): A DFT Study. <i>ChemPhysChem</i> , 2005, 6, 1293-1298.	1.0	15
3043	Pressure Dependence in the Methyl Vinyl Ketone+OH and Methacrolein+OH Oxidation Reactions: An Electronic Structure Study. <i>ChemPhysChem</i> , 2005, 6, 1567-1573.	1.0	7
3044	Oxidation of Formic Acid and Carbon Monoxide on Gold Electrodes Studied by Surface-Enhanced Raman Spectroscopy and DFT. <i>ChemPhysChem</i> , 2005, 6, 2597-2606.	1.0	99
3045	Influence of Coadsorbates on the NO Dissociation on a Rhodium(311) Surface. <i>ChemPhysChem</i> , 2005, 6, 2513-2521.	1.0	15
3046	Guanine Quartet Networks Stabilized by Cooperative Hydrogen Bonds. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 2270-2275.	7.2	275
3047	Tuning Reaction Rates by Lateral Strain in a Palladium Monolayer. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 2080-2084.	7.2	523
3048	Structures of Nonheme Oxoiron(IV) Complexes from X-ray Crystallography, NMR Spectroscopy, and DFT Calculations. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 3690-3694.	7.2	247
3049	Heterolytic Splitting of Hydrogen with Rhodium(I) Amides. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 6318-6323.	7.2	122
3050	Elucidation of the Reaction Mechanism for the Palladium-Catalyzed Synthesis of Vinyl Acetate. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 4572-4574.	7.2	63
3051	Guanine Quartet Networks Stabilized by Cooperative Hydrogen Bonds. <i>Angewandte Chemie</i> , 2005, 117, 2310-2315.	1.6	64
3056	Analysis and calculation of the $^{31}\text{P}$ and $^{19}\text{F}$ NMR spectra of hexafluorocyclotriphosphazene. <i>Magnetic Resonance in Chemistry</i> , 2005, 43, 294-301.	1.1	13
3057	Vibrational and electronic circular dichroism of $\hat{\Gamma}^{\nu}$ -TRISPHAT [tris(tetrachlorobenzenediolato)phosphate(V)] anion. <i>Chirality</i> , 2005, 17, S143-S148.	1.3	19
3058	The 'Invisible' $^{13}\text{C}$ NMR Chemical Shift of the Central Carbon Atom in $[(\text{Ph}_3\text{PAu})_6\text{C}]^{2+}$ : A Theoretical Investigation. <i>Chemistry - A European Journal</i> , 2005, 11, 1677-1686.	1.7	15
3059	Nanocap-Shaped Tin Phthalocyanines: Synthesis, Characterization, and Corrosion Inhibition Activity. <i>Chemistry - A European Journal</i> , 2005, 11, 2705-2715.	1.7	25
3060	Understanding the Conformational Dependence of Spin-Spin Coupling Constants: Through-Bond and Through-Space( $^{31}\text{P}$ , $^{31}\text{P}$ ) Coupling in Tetraphosphane-1,4-diides $[\text{M}(\text{L})_x]_2[\text{P}_4\text{R}_4]$ . <i>Chemistry - A European Journal</i> , 2005, 11, 2773-2782.	1.7	29

#	ARTICLE	IF	CITATIONS
3061	Triple-Bond Covalent Radii. Chemistry - A European Journal, 2005, 11, 3511-3520.	1.7	370
3062	Structure and Bonding of Zinc Antimonides: Complex Frameworks and Narrow Band Gaps. Chemistry - A European Journal, 2005, 11, 4912-4920.	1.7	88
3063	Crystal morphology and surface structures of orthorhombic MgSiO <sub>3</sub> perovskite. Physics and Chemistry of Minerals, 2005, 31, 671-682.	0.3	17
3064	On local structural changes in lizardite-1T: {Si <sup>4+</sup> /Al <sup>3+</sup> }, {Si <sup>4+</sup> /Fe <sup>3+</sup> }, [Mg <sup>2+</sup> /Al <sup>3+</sup> ], [Mg <sup>2+</sup> /Fe <sup>3+</sup> ] substitutions. Physics and Chemistry of Minerals, 2005, 32, 362-373.	0.3	9
3065	Electronic and optical properties of Fe, Zn and Pb sulfides. Physics and Chemistry of Minerals, 2005, 32, 255-268.	0.3	44
3066	A DFT study on the hydrated V <sub>2</sub> O <sub>5</sub> -TiO <sub>2</sub> -anatase catalyst: stability of monomeric species. Theoretical Chemistry Accounts, 2005, 114, 29-37.	0.5	26
3067	The epitaxial ZrO <sub>2</sub> on silicon as alternative gate dielectric: film growth, characterization and electronic structure calculations. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2005, 118, 122-126.	1.7	8
3068	Some recent theoretical advances in the understanding of the catalytic activity of Au. Applied Catalysis A: General, 2005, 291, 21-31.	2.2	240
3069	The relationship between adsorption and solid acidity of heteropolyacids. Catalysis Today, 2005, 105, 134-143.	2.2	34
3070	The influence of the counterion B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> CH <sub>3</sub> <sup>-</sup> and solvent effects on the propagation and termination steps of ethylene polymerization catalyzed by Cp <sub>2</sub> ZrR <sup>+</sup> (R=Me,Pr). A density functional study. Comptes Rendus Chimie, 2005, 8, 1552-1565.	0.2	19
3071	Band structure and optical electron spectra of (TrMA)CoCl <sub>3</sub> ·2H <sub>2</sub> O crystal. Physica B: Condensed Matter, 2005, 367, 216-222.	1.3	2
3072	Elastic properties of tantalum carbide (TaC). Solid State Communications, 2005, 134, 245-250.	0.9	101
3073	Methanol adsorption on silicon (001). Surface Science, 2005, 575, 287-299.	0.8	29
3074	Half-sandwich metal atom complexes with benzene: a model for adsorption onto graphite. Surface Science, 2005, 577, 167-174.	0.8	18
3075	Diffusion mechanisms for iron on tungsten. Surface Science, 2005, 584, 55-61.	0.8	17
3076	Density-functional study of oxidation at the Mn-Co interface. Surface Science, 2005, 584, 146-152.	0.8	8
3077	Atomic and molecular adsorption on Pt(111). Surface Science, 2005, 587, 159-174.	0.8	247
3078	Conformation-selective adsorption of 2,3-butanediol on Si(001). Surface Science, 2005, 585, 191-196.	0.8	9

#	ARTICLE	IF	CITATIONS
3079	A DFT investigation of methane molecular adsorption on Pt(100). <i>Surface Science</i> , 2005, 594, 231-239.	0.8	29
3080	First-principles study of sulfur overlayers on Pd(111) surface. <i>Surface Science</i> , 2005, 596, 229-241.	0.8	38
3081	Surface atomic structure and energetics of tantalum. <i>Surface Science</i> , 2005, 598, 276-284.	0.8	29
3082	From cluster calculations to molecular materials: a mixed pseudopotential approach to modeling mixed-valence systems. <i>Journal of Molecular Modeling</i> , 2005, 11, 288-292.	0.8	6
3083	Linking first-principles energetics to CALPHAD: An application to thermodynamic modeling of the Al-Ca binary system. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2005, 36, 5-13.	1.1	41
3084	Interconverting WW Triple Bonds and W4 Clusters: Structures of W <sub>4</sub> (OPrn) <sub>16</sub> and [Li <sub>2</sub> W <sub>2</sub> (OPrn) <sub>8</sub> (DME)] <sub>2</sub> <sup>*</sup> . <i>Journal of Cluster Science</i> , 2005, 16, 231-249.	1.7	1
3085	Structure of irradiated polytetrafluoroethylene according to DFT calculations of NMR chemical shifts. <i>Journal of Structural Chemistry</i> , 2005, 46, 87-92.	0.3	3
3086	Correlation between structure and spectral characteristics of rhodium(I) chelate dicarbonyl complexes and their electron. <i>Journal of Structural Chemistry</i> , 2005, 46, 220-229.	0.3	15
3087	Protonation-induced stereoisomerism in nicotine: Conformational studies using classical (AMBER) and ab initio (CaracParrinello) molecular dynamics. <i>Journal of Computer-Aided Molecular Design</i> , 2005, 19, 1-15.	1.3	14
3088	Trichloropalladate(II) Complexes with Pyridine Ligands - Molecular Structure and Conformational Analysis of [K(18C6)][PdCl <sub>3</sub> (py)]. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2005, 631, 1456-1462.	0.6	6
3089	Soft cohesive forces. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 579-598.	1.0	82
3090	Van der Waals density functional theory with applications. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 599-610.	1.0	304
3091	DFT study of mixed-valent Mn(II/III) hexacyanide clusters. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 753-760.	1.0	9
3092	Theoretical study of neutral and cationic complexes involving phenol. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 854-859.	1.0	9
3093	Role of the electronic properties of azurin active site in the electron-transfer process. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 328-342.	1.0	24
3094	Ab initio analysis of electron currents in thioalkanes. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 711-723.	1.0	79
3095	Chemical reaction dynamics of PeCB and TCDD decomposition: A tight-binding quantum chemical molecular dynamics study with first-principles parameterization. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 318-327.	1.0	21
3096	Model density approach to the Kohn-Sham problem: Efficient extension of the density fitting technique. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 743-761.	1.0	26

#	ARTICLE	IF	CITATIONS
3097	Localized hybrid exchange-correlation potentials for Kohn-Sham DFT calculations of NMR and EPR parameters. <i>International Journal of Quantum Chemistry</i> , 2005, 104, 261-271.	1.0	30
3098	Ab initio study of molecular oxygen adsorption on Pu (111) surface. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 280-291.	1.0	19
3099	Computational prediction of standard gas, liquid, and solid-phase heats of formation and heats of vaporization and sublimation. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 341-347.	1.0	119
3100	Adsorption of 1-propanol on the Si(100) surface. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 359-367.	1.0	8
3101	Density functional theory study of the relative energies and structures of the chair, twist, and boat conformations of stannacyclohexane, 1-methylstannacyclohexane, and 1,1-dimethylstannacyclohexane. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 416-428.	1.0	5
3102	Chemical bonding, less screening, and Hund's rule revisited. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 687-700.	1.0	9
3103	Spin-polarized XANES: theoretical analysis of the Ni K-edge of NiF <sub>2</sub> . <i>Physica Status Solidi (B): Basic Research</i> , 2005, 242, 3117-3122.	0.7	0
3104	Field electron energy spectroscopy of alumina-supported platinum adatoms. <i>Physica Status Solidi (B): Basic Research</i> , 2005, 242, 2462-2467.	0.7	3
3105	Effect of solvent on cis-to-trans isomerization of 4-hydroxyazobenzene aggregated through intermolecular hydrogen bonds. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 994-1000.	0.9	49
3106	First Principles Studies for the Interaction of Hydrogen with a Li(100) Surface. <i>Journal of the Physical Society of Japan</i> , 2005, 74, 478-482.	0.7	13
3107	Ab initio calculations of the ferromagnetic shape memory alloy Ni <sub>49</sub> Mn <sub>41</sub> Al. <i>Phase Transitions</i> , 2005, 78, 267-276.	0.6	3
3108	Composition Dependence of the Energy Barrier for Lithium Diffusion in Amorphous WO <sub>3</sub> . <i>Electrochemical and Solid-State Letters</i> , 2005, 8, J21.	2.2	13
3109	Ligand chemistry of alkylselenolates: an experimental and DFT study of the formation and structural characterization of [PtCl <sub>2</sub> (SR) <sub>2</sub> ](SeR)(PPH <sub>3</sub> ) <sub>2</sub> (SR = <i>i</i> -Bu, <i>n</i> -Bu). <i>Main Group Chemistry</i> , 2005, 4, 49-68.	0.4	10
3110	Evaluations of Phases and Vacancy Formation Energies in KNbO <sub>3</sub> by First-Principles Calculation. <i>Japanese Journal of Applied Physics</i> , 2005, 44, 8048-8054.	0.8	51
3111	TiO <sub>2</sub> (rutile) doped with double impurities for fabricating spintronic devices—a combinatorial computational approach. <i>Measurement Science and Technology</i> , 2005, 16, 242-247.	1.4	5
3112	Applied density functional theory and the deMon codes 1964–2004. , 2005, , 1079-1097.		4
3113	Towards the First-Principles Investigation of Ordering Dynamics. <i>Materials Science Forum</i> , 2005, 475-479, 3075-3080.	0.3	6
3114	Segregation Effects on the Metal-Carbide Interface. <i>Materials Science Forum</i> , 2005, 475-479, 4251-4254.	0.3	2

#	ARTICLE	IF	CITATIONS
3115	Electronic Structure of AgPbmSbTem+2 Compounds – Implications on Thermoelectric Properties. Materials Research Society Symposia Proceedings, 2005, 886, 1.	0.1	1
3116	Half-metallic ferromagnetism in transition-metal encapsulated boron nitride nanotubes. New Journal of Physics, 2005, 7, 39-39.	1.2	54
3117	First-principles study of the effect of hydrogen on the metal–ceramic interface. Journal of Physics Condensed Matter, 2005, 17, 5335-5348.	0.7	29
3118	First-principles Studies of Phase Stability and the Neutral Atomic Vacancies in LiNbO <sub>3</sub> , NaNbO <sub>3</sub> and KNbO <sub>3</sub> . Materials Research Society Symposia Proceedings, 2005, 902, 1.	0.1	2
3119	A First Principles Study of Ultra-Thin (AlO) <sub>n</sub> Nanorods: Mechanical Behaviour Under Tension and Compression. Proceedings of the Institution of Mechanical Engineers, Part N: Journal of Nanoengineering and Nanosystems, 2005, 219, 123-130.	0.1	0
3120	Symmetry reduction of $\hat{\Gamma}$ -plutonium: an electronic-structure effect. Materials Research Society Symposia Proceedings, 2005, 893, 1.	0.1	0
3121	Orientation and Composition Dependences of the Surface Energy and Work Function Observed by First-Principles Calculation for the Mo–Hf System. Journal of the Physical Society of Japan, 2005, 74, 1766-1771.	0.7	9
3122	Ab Initio Calculation of Work Functions of ZrO/W(100) and YO/W(100) Surfaces. Japanese Journal of Applied Physics, 2005, 44, 7518-7520.	0.8	3
3123	27Al NMR chemical shifts do not correlate with average T-O-T angles: Theoretical study of MCM-58 zeolite. Studies in Surface Science and Catalysis, 2005, 158, 917-924.	1.5	2
3124	First-Principles Study of Structural and Magnetic Properties for Ultrathin Cr Films on W(100) and W(110). Chinese Physics Letters, 2005, 22, 1232-1235.	1.3	5
3125	Computational Study on Stable Structures, Formation Energies, and Conductance of Single Benzene-dithiolate between Two Au Electrodes. Japanese Journal of Applied Physics, 2005, 44, 7729-7731.	0.8	9
3126	Stability of the Metastable Phases in the Co–Ta System Studied by ab initio and Thermodynamic Calculations Together with Ion-Beam-Mixing Experiment. Journal of the Physical Society of Japan, 2005, 74, 2501-2505.	0.7	11
3127	Atomic-scale modelling of kinetic processes occurring during silicon oxidation. Journal of Physics Condensed Matter, 2005, 17, S2051-S2063.	0.7	19
3128	First-principles investigation of Mg segregation at $\hat{\Gamma} = 11(113)$ grain boundaries in Al. Journal of Physics Condensed Matter, 2005, 17, 4301-4308.	0.7	44
3129	Layered growth modelling of epitaxial growth processes for SiC polytypes. Journal of Physics Condensed Matter, 2005, 17, 5355-5366.	0.7	7
3130	An ab initio study of electron transport through nitrobenzene: the influence of leads and contacts. Nanotechnology, 2005, 16, S155-S160.	1.3	23
3131	Stability and properties of the cluster assembled solid phases of X <sub>8</sub> C <sub>12</sub> and YX <sub>7</sub> C <sub>12</sub> . Journal of Physics Condensed Matter, 2005, 17, 2571-2584.	0.7	4
3132	Orbital Hybridization of the Ferroelectric Rb <sub>2</sub> Cd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> : Origin of Domain Walls. Chinese Physics Letters, 2005, 22, 439-441.	1.3	2

#	ARTICLE	IF	CITATIONS
3133	Generalized stacking fault energies, ductilities, and twinnabilities of Ni and selected Ni alloys. Applied Physics Letters, 2005, 87, 121901.	1.5	167
3134	Thermodynamically complete equations of state for nickel-titanium alloy. Journal of Applied Physics, 2005, 98, 093512.	1.1	12
3135	Ab initio multireference configuration-interaction theoretical study on the low-lying spin states in binuclear transition-metal complex: Magnetic exchange of $[(\text{NH}_3)_5\text{Cr}(\frac{1}{4}\text{-OH})\text{Cr}(\text{NH}_3)_5]^{5+}$ and $[\text{Cl}_3\text{FeOFeCl}_3]^{2-}$ . Journal of Chemical Physics, 2005, 122, 204310.	1.2	15
3136	Hybrid approach for ab initio molecular dynamics simulation combining energy density analysis and short-time Fourier transform: Energy transfer spectrogram. Journal of Chemical Physics, 2005, 123, 034101.	1.2	26
3137	Away from generalized gradient approximation: Orbital-dependent exchange-correlation functionals. Journal of Chemical Physics, 2005, 123, 062202.	1.2	55
3138	When seeing is not believing: Oxygen on Ag(111), a simple adsorption system?. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2005, 23, 1487-1497.	0.9	108
3139	Geometric, electronic, and bonding properties of Au <sub>N</sub> M (N=1-7, M=Ni, Pd, Pt) clusters. Journal of Chemical Physics, 2005, 122, 114310.	1.2	159
3140	Coverage and strain dependent magnetization of titanium-coated carbon nanotubes. Physical Review B, 2005, 71, .	1.1	14
3141	Ab initio study of disorder broadening of core photoemission spectra in random Cu <sup>~</sup> Pd and Ag <sup>~</sup> Pd alloys. Physical Review B, 2005, 72, .	1.1	25
3142	Trends in sticking and adsorption of diatomic molecules on the Al(111) surface. Physical Review B, 2005, 71, .	1.1	35
3143	Thermal decomposition mechanisms of hafnium and zirconium silicates at the atomic scale. Journal of Applied Physics, 2005, 97, 114911.	1.1	22
3144	Ab initio calculation of electron effective masses in solid pentacene. Journal of Applied Physics, 2005, 98, 113709.	1.1	39
3145	Shock wave propagation in dissociating low-Z liquids: D <sub>2</sub> . Journal of Chemical Physics, 2005, 122, 124503.	1.2	11
3146	Ab initio calculation of the elastic properties of Al <sub>1-x</sub> Li <sub>x</sub> (x=0.20) random alloys. Physical Review B, 2005, 71, .	1.1	89
3147	Supported metal electronic structure: Implications for molecular adsorption. Physical Review B, 2005, 72, .	1.1	26
3148	Binding of the N interstitial with neutral MgH in p-type GaN investigated with density functional theory. Physical Review B, 2005, 72, .	1.1	4
3149	P-assisted growth of molecular wires on Si(001)-2x1. Applied Physics Letters, 2005, 86, 023108.	1.5	7
3150	Surface states and resonances on Al(110): Ultraviolet photoemission spectroscopy and ab initio calculations. Physical Review B, 2005, 72, .	1.1	6

#	ARTICLE	IF	CITATIONS
3151	Metal-semiconductor and semiconductor-semiconductor transitions in carbon nanotubes induced by intercalating alkali atoms. <i>Physical Review B</i> , 2005, 71, .	1.1	15
3152	Ab initio characterization of the mechanical and electronic properties of $\text{Si}_2\text{AlON}$ ( $\text{Si}_6\text{Al}_z\text{O}_z\text{N}_8$ ; $z=0-5$ ). <i>Physical Review B</i> , 2005, 71, .	1.1	16
3153	Critical examination of the supermolecule density functional theory calculations of intermolecular interactions. <i>Journal of Chemical Physics</i> , 2005, 122, 014117.	1.2	47
3154	Reduction of vanadium-oxide monolayer structures. <i>Physical Review B</i> , 2005, 71, .	1.1	76
3155	Difference in formation of hydrogen and helium clusters in tungsten. <i>Applied Physics Letters</i> , 2005, 87, 163113.	1.5	145
3156	Hydrogen-induced magnetism in carbon nanotubes. <i>Physical Review B</i> , 2005, 72, .	1.1	53
3157	Nitric acid monohydrates at high pressure: An experimental and computational study. <i>Physical Review B</i> , 2005, 72, .	1.1	7
3158	Gradient-corrected density-functional potential with correct asymptotic behavior: Application to interconfigurational energies in transition-metal atoms. <i>Journal of Chemical Physics</i> , 2005, 122, 244109.	1.2	4
3159	Chemisorption and diffusion of hydrogen on surface and subsurface sites of flat and stepped nickel surfaces. <i>Journal of Chemical Physics</i> , 2005, 122, 204707.	1.2	84
3160	Chemical characterization of a zirconia-supported Pt cluster. <i>Physical Review B</i> , 2005, 71, .	1.1	19
3161	Origin of nonlocal interactions in adsorption of polar molecules on $\text{Si}(001)-2\times 1$ . <i>Journal of Chemical Physics</i> , 2005, 122, 164706.	1.2	26
3162	Accurate molecular energies by extrapolation of atomic energies using an analytic quantum mechanical model. <i>Physical Review B</i> , 2005, 71, .	1.1	14
3163	Length dependence of the electronic and structural properties of monoatomic gold wires. <i>Physical Review B</i> , 2005, 72, .	1.1	26
3164	Electronic structure of Li with emphasis on the momentum density and the Compton profile. <i>Physical Review B</i> , 2005, 72, .	1.1	14
3165	Structures and magnetic properties of iron chains encapsulated in tubal carbon nanocapsules. <i>Physical Review B</i> , 2005, 71, .	1.1	26
3166	Fluorine in Si: Native-defect complexes and the suppression of impurity diffusion. <i>Physical Review B</i> , 2005, 72, .	1.1	53
3167	Density functional calculations of the influence of hydrogen adsorption on the surface relaxation of Ti (0001). <i>Physical Review B</i> , 2005, 71, .	1.1	29
3168	Atomic structures and magnetism in small $\text{MoS}_2$ and $\text{WS}_2$ clusters. <i>Physical Review A</i> , 2005, 71, .	1.0	47



#	ARTICLE	IF	CITATIONS
3169	Polymerization of Formic Acid under High Pressure. <i>Physical Review Letters</i> , 2005, 94, 065505.	2.9	62
3170	Quasiparticle bands and optical spectra of highly ionic crystals: AlN and NaCl. <i>Physical Review B</i> , 2005, 72, .	1.1	65
3171	Using Ar adsorption to estimate the van der Waals contribution to the wetting of Ru(0001). <i>Physical Review B</i> , 2005, 72, .	1.1	20
3172	Structural, thermal, and electronic properties of $\text{Fe}_2\text{VSi}_{1-x}\text{Al}_x$ . <i>Physical Review B</i> , 2005, 71, .	1.1	22
3173	Optical response of $\pi$ -conjugated molecular monolayer adsorbed on the semiconductor Si(001) surface: A first-principles study. <i>Physical Review B</i> , 2005, 71, .	1.1	21
3174	Coverage dependence of oxygen decomposition and surface diffusion on rhodium (111): A DFT study. <i>Journal of Chemical Physics</i> , 2005, 122, 034710.	1.2	56
3175	Conversion between two binding states of benzene on Si(001). <i>Physical Review B</i> , 2005, 72, .	1.1	22
3176	High-resolution infrared spectroscopy of the charge-transfer complex $[\text{Ar}^{\oplus}\text{N}_2]^{\oplus\text{TM}}$ : A combined experimental/theoretical study. <i>Journal of Chemical Physics</i> , 2005, 123, 144305.	1.2	8
3177	On the convergence of isolated neutral oxygen vacancy and divacancy properties in metal oxides using supercell models. <i>Journal of Chemical Physics</i> , 2005, 122, 224705.	1.2	27
3178	Ab initio study of the adsorption of Fe atoms on a defective MgO(001) surface: Blind adsorption. <i>Physical Review B</i> , 2005, 71, .	1.1	15
3179	Xe adsorption on metal surfaces: First-principles investigations. <i>Physical Review B</i> , 2005, 72, .	1.1	94
3180	Surface electronic structure of Cr(001): Experiment and theory. <i>Physical Review B</i> , 2005, 72, .	1.1	31
3181	Decomposition reactions for $\text{NaAlH}_4$ , $\text{Na}_3\text{AlH}_6$ , and $\text{NaH}$ : First-principles study. <i>Physical Review B</i> , 2005, 71, .	1.1	97
3182	Growth and structure of small gold particles on rutile $\text{TiO}_2(110)$ . <i>Physical Review B</i> , 2005, 72, .	1.1	62
3183	CO adsorption on a Cu(211) surface: First-principle calculation and STM study. <i>Physical Review B</i> , 2005, 71, .	1.1	27
3184	Biferroic $\text{YCrO}_3$ . <i>Physical Review B</i> , 2005, 72, .	1.1	209
3185	Trapping hydrogen with a bimetallic interface. <i>Physical Review B</i> , 2005, 71, .	1.1	17
3186	B and N ion implantation into carbon nanotubes: Insight from atomistic simulations. <i>Physical Review B</i> , 2005, 71, .	1.1	88

#	ARTICLE	IF	CITATIONS
3187	Atomic Structure of a Thin Silica Film on a Mo(112) Substrate: A Two-Dimensional Network of SiO <sub>4</sub> Tetrahedra. <i>Physical Review Letters</i> , 2005, 95, 076103.	2.9	201
3188	Comparison of density functionals for differences between the high- ( $T_{2g}$ ) and low- ( $A_{1g}$ ) spin states of iron(II) compounds. IV. Results for the ferrous complexes [Fe(L)( $\eta^5$ -NHS <sub>4)]<sup>2+</sup>. <i>Journal of Chemical Physics</i>, 2005, 122, 234321.</sub>	1.2	127
3189	An interaction model for OH+H <sub>2</sub> O-mixed and pure H <sub>2</sub> O overlayers adsorbed on Pt(111). <i>Journal of Chemical Physics</i> , 2005, 122, 194705.	1.2	53
3190	Six-dimensional quantum dynamics of ( $v=0, j=0$ ) D <sub>2</sub> and of ( $v=1, j=0$ ) H <sub>2</sub> scattering from Cu(111). <i>Journal of Chemical Physics</i> , 2005, 122, 214709.	1.2	27
3191	Density functional calculations of Ti-enhanced NaAlH <sub>4</sub> . <i>Physical Review B</i> , 2005, 71, .	1.1	107
3192	van der Waals interaction of simple, parallel polymers. <i>Journal of Chemical Physics</i> , 2005, 122, 164902.	1.2	24
3193	Evolution of the electronic structure of Be clusters. <i>Journal of Chemical Physics</i> , 2005, 123, 074329.	1.2	29
3194	Ab initio molecular dynamics of liquid hydrogen chloride. <i>Journal of Chemical Physics</i> , 2005, 122, 114512.	1.2	6
3195	Photoelectron spectroscopy and ab initio study of the doubly antiaromatic B <sub>6</sub> <sup>2-</sup> dianion in the LiB <sub>6</sub> <sup>+</sup> cluster. <i>Journal of Chemical Physics</i> , 2005, 122, 054313.	1.2	103
3196	Interaction potentials from periodic density-functional theory calculations: Molecular-dynamics simulations of Au clusters deposited on the TiN (001) surface. <i>Journal of Chemical Physics</i> , 2005, 123, 244706.	1.2	9
3197	Comment on "Molecular Chemisorption as the Theoretically Preferred Pathway for Water Adsorption on Ideal Rutile TiO <sub>2</sub> (110)". <i>Physical Review Letters</i> , 2005, 95, 029601.	2.9	23
3198	Fraction of Boroxol Rings in Vitreous Boron Oxide from a First-Principles Analysis of Raman and NMR Spectra. <i>Physical Review Letters</i> , 2005, 95, 137401.	2.9	63
3199	Coulombic Amino Group-Metal Bonding: Adsorption of Adenine on Cu(110). <i>Physical Review Letters</i> , 2005, 94, 236102.	2.9	131
3200	Melting Curve of MgO from First-Principles Simulations. <i>Physical Review Letters</i> , 2005, 94, 235701.	2.9	158
3201	Surface and Interface Studies of GaN Epitaxy on Si(111) via ZrB <sub>2</sub> Buffer Layers. <i>Physical Review Letters</i> , 2005, 95, 266105.	2.9	53
3202	Adsorption of carbon on Pd clusters of nanometer size: A first-principles theoretical study. <i>Journal of Chemical Physics</i> , 2005, 122, 174705.	1.2	33
3203	Medium-Range Structural Properties of Vitreous Germania Obtained through First-Principles Analysis of Vibrational Spectra. <i>Physical Review Letters</i> , 2005, 95, 075505.	2.9	57
3204	Mapping Out Electron-Electron Interactions at Surfaces. <i>Physical Review Letters</i> , 2005, 95, 117601.	2.9	41

#	ARTICLE	IF	CITATIONS
3205	Influence of initial oxygen coverage and magnetic moment on the NO decomposition on rhodium (111). Journal of Chemical Physics, 2005, 122, 154702.	1.2	29
3206	N interstitial and its interaction with substitutional Mg in p-type GaN. Journal of Applied Physics, 2005, 98, 033704.	1.1	3
3207	Polycubanes linked with C <sub>2</sub> N <sub>2</sub> , NO, and NS: From insulating to metallic behavior. Physical Review B, 2005, 71, .	1.1	3
3208	First-principles study of phonon modes in PuCoGa <sub>5</sub> superconductor. Physical Review B, 2005, 72, .	1.1	39
3209	First-principles study of phase stability in pseudobinary (Ni <sub>1-x</sub> Pt <sub>x</sub> ) <sub>3</sub> Al alloys. Physical Review B, 2005, 72, .	1.1	38
3210	Cubic and orthorhombic structures of aluminum hydride AlH <sub>3</sub> predicted by a first-principles study. Physical Review B, 2005, 71, .	1.1	67
3211	Supported nanoclusters: Pre-adsorbates tuning catalytic activity. Physical Review B, 2005, 71, .	1.1	5
3212	Top-gated field-effect transistor and rectifying diode operation of core-shell structured GaP nanowire devices. Physical Review B, 2005, 71, .	1.1	39
3213	Interaction of oxygen with ZrC(001) and VC(001): Photoemission and first-principles studies. Physical Review B, 2005, 72, .	1.1	50
3214	First-principles investigation on chemical bonding and bulk modulus of the ternary carbide Zr <sub>2</sub> Al <sub>3</sub> C <sub>5</sub> . Physical Review B, 2005, 72, .	1.1	14
3215	First-principles studies on the reactions of O <sub>2</sub> with silicon clusters. Journal of Chemical Physics, 2005, 122, 174311.	1.2	20
3216	Magnetic doping of 4d transition-metal surfaces: A first-principles study. Physical Review B, 2005, 71, .	1.1	19
3217	Interrupted chain-assisted Al atomic wires on Si(211): Density functional calculations. Physical Review B, 2005, 72, .	1.1	1
3218	Ab initio density-functional study of the bridging addition of acrylonitrile on the Si(100) surface. Journal of Chemical Physics, 2005, 123, 174705.	1.2	7
3219	Crystal stability and equation of state for Am: Theory. Physical Review B, 2005, 72, .	1.1	46
3220	Origin of the different color of ruby and emerald. Physical Review B, 2005, 72, .	1.1	45
3221	Quantum effects on the structure of pure and binary metallic nanoclusters. Physical Review B, 2005, 72, .	1.1	174
3222	Dependence of oxygen dissociative adsorption on platinum surface structures. Physical Review B, 2005, 72, .	1.1	23

#	ARTICLE	IF	CITATIONS
3223	Simple model for the spherically and system-averaged pair density: Results for two-electron atoms. Physical Review A, 2005, 71, .	1.0	38
3224	Structure of a thin oxide film on Rh(100). Physical Review B, 2005, 71, .	1.1	101
3225	Density-functional study of structural and electronic properties of Al <sub>n</sub> N (n=2–12) clusters. Physical Review A, 2005, 72, .	1.0	26
3226	Silicon-carbon fullerene-like nanostructures: An ab initio study on the stability of Si <sub>60</sub> C <sub>2n</sub> (n=1, 2) clusters. Physical Review A, 2005, 72, .	1.0	11
3227	First-principles study of the onset of noncollinearity in Mn clusters: Magnetic arrangements in Mn <sub>5</sub> and Mn <sub>6</sub> . Physical Review B, 2005, 72, .	1.1	36
3228	Tailoring the electronic properties of silicon with cysteine: A first-principles study. Physical Review B, 2005, 72, .	1.1	5
3229	Ab initio investigation of the magnetism of tetragonal Mn: Bulk, surface, ultrathin films, and multilayers. Physical Review B, 2005, 72, .	1.1	69
3230	Atomic and electronic structures of N interstitials in GaAs. Physical Review B, 2005, 72, .	1.1	27
3231	Molecular hydrogen adsorption and dissociation on the plutonium (111) surface. Physical Review B, 2005, 72, .	1.1	32
3232	Chemisorption of C <sub>28</sub> fullerene on a (4×4) reconstructed GaAs(001) surface: A density functional theory study. Physical Review B, 2005, 71, .	1.1	5
3233	Coadsorption phases of CO and oxygen on Pd(111) studied by scanning tunneling microscopy. Physical Review B, 2005, 71, .	1.1	37
3234	Ab initio investigation of magnetism in two-dimensional uranium systems. Physical Review B, 2005, 71, .	1.1	2
3235	Ab initio studies on the stability and electronic structure of LiCoO <sub>2</sub> (003) surfaces. Physical Review B, 2005, 71, .	1.1	29
3236	Oxygen adsorption at anionic free and supported Au clusters. Journal of Chemical Physics, 2005, 123, 161104.	1.2	76
3237	BeB <sub>2</sub> nanostructures: A density functional study. Physical Review B, 2005, 72, .	1.1	6
3238	Structure of GaSb digitally doped with Mn. Physical Review B, 2005, 71, .	1.1	10
3239	Differential tunneling spectroscopy simulations: Imaging surface states. Physical Review B, 2005, 71, .	1.1	32
3240	Structures of Mo <sub>2</sub> O <sub>y</sub> and Mo <sub>2</sub> O <sub>y</sub> (y=2, 3, and 4) studied by anion photoelectron spectroscopy and density functional theory calculations. Journal of Chemical Physics, 2005, 122, 094313.	1.2	75

#	ARTICLE	IF	CITATIONS
3241	Ab initio study of Mg(AlH <sub>4</sub> ) <sub>2</sub> . Physical Review B, 2005, 72, .	1.1	49
3242	First-principles study of ZrO <sub>2</sub> /Si interfaces: Energetics and band offsets. Physical Review B, 2005, 72, .	1.1	58
3243	Growth of Te on As-exposed Si(211): Electronic structure calculations. Physical Review B, 2005, 71, .	1.1	12
3244	Structure-dependent ferroelectricity of niobium clusters (Nb <sub>N</sub> , N=2-52). Physical Review B, 2005, 71, .	1.1	21
3245	High-pressure structural study of the scheelite tungstates CaWO <sub>4</sub> and SrWO <sub>4</sub> . Physical Review B, 2005, 72, .	1.1	159
3246	Adsorption-induced constraint on delocalization of electron states in an Au chain on NiAl(110). Physical Review B, 2005, 72, .	1.1	4
3247	Second-order Kohn-Sham perturbation theory: Correlation potential for atoms in a cavity. Journal of Chemical Physics, 2005, 123, 224102.	1.2	61
3248	First-principles studies of GaN(0001) heteroepitaxy on ZrB <sub>2</sub> (0001). Physical Review B, 2005, 72, .	1.1	34
3249	Ab initio molecular dynamics and quasichemical study of H <sup>+</sup> (aq). Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6704-6708.	3.3	94
3250	The structure and spin-states of some Fe(III) mimics of nitrile hydratase, studied by DFT and ONIOM(DFT:PM3) calculations. Molecular Physics, 2005, 103, 905-923.	0.8	12
3251	Effects of fluorination on electronic and excited states of fused zinc oligoporphyrins. Journal of Chemical Physics, 2005, 122, 184702.	1.2	15
3252	Applications of quantum chemical methods in zeolite science. Studies in Surface Science and Catalysis, 2005, , 243-262.	1.5	7
3253	Enhancement factors in semi-empirical exchange-correlation functionals. Molecular Physics, 2005, 103, 2397-2405.	0.8	4
3254	Density-functional band-structure calculations of magnesium alanate Mg(AlH <sub>4</sub> ) <sub>2</sub> . Physical Review B, 2005, 72, .	1.1	27
3255	Physical Origin of Hydrogen-Adsorption-Induced Metallization of the SiC Surface: n-Type Doping via Formation of Hydrogen Bridge Bond. Physical Review Letters, 2005, 95, 196803.	2.9	30
3256	Analytic energy gradients of the optimized effective potential method. Journal of Chemical Physics, 2005, 123, 134111.	1.2	12
3257	First-principles study of ultrathin magnetic Mn films on W surfaces.. Physical Review B, 2005, 72, .	1.1	19
3258	Charging of Metal Atoms on Ultrathin MgO/Mo(100) Films. Physical Review Letters, 2005, 94, 226104.	2.9	338

#	ARTICLE	IF	CITATIONS
3259	Six-dimensional quantum dynamics of dissociative chemisorption of H <sub>2</sub> on Ru(0001). Journal of Chemical Physics, 2005, 122, 044701.	1.2	60
3260	Electronic structure of the C(111) surface: Solution by self-consistent many-body calculations. Physical Review B, 2005, 72, .	1.1	26
3261	Stretching dependence of the vibration modes of a single-molecule Pt-H <sub>2</sub> -Pt bridge. Physical Review B, 2005, 71, .	1.1	142
3262	Scanning tunneling microscopy and spectroscopy of NaCl overlayers on the stepped Cu(311) surface: Experimental and theoretical study. Physical Review B, 2005, 71, .	1.1	50
3263	Mechanism of Cu Deposition on the Al <sub>2</sub> O <sub>3</sub> (0001) Surface. Physical Review Letters, 2005, 94, 016104.	2.9	37
3264	Band-gap modification of defective carbon nanotubes under a transverse electric field. Physical Review B, 2005, 72, .	1.1	33
3265	Conduction Mechanism in a Molecular Hydrogen Contact. Physical Review Letters, 2005, 94, 036807.	2.9	63
3266	Maleic anhydride adsorption on silicon (001). Journal of Chemical Physics, 2005, 123, 074708.	1.2	2
3267	Water adsorption at metal surfaces: A first-principles study of the p(3×3)R30°H <sub>2</sub> O bilayer on Ru(0001). Physical Review B, 2005, 71, .	1.1	60
3268	Random conductivity of Bi <sub>2</sub> O <sub>3</sub> films. Applied Physics Letters, 2005, 86, 241910.	1.5	30
3269	SIX-DIMENSIONAL DYNAMICS OF DISSOCIATIVE CHEMISORPTION OF H <sub>2</sub> ON METAL SURFACES. Journal of Theoretical and Computational Chemistry, 2005, 04, 493-581.	1.8	82
3270	Effect of electronic topological transitions on the calculations of some Zn and Fe properties. Journal of Physics Condensed Matter, 2005, 17, 559-569.	0.7	30
3271	STUDY OF THE ELECTRONIC STRUCTURE AND PHYSICAL PROPERTIES OF THE IRIDIUM BASED INTERMETALLIC COMPOUNDS UNDER PRESSURE. International Journal of Modern Physics B, 2005, 19, 4587-4604.	1.0	12
3272	Theoretical electron energy-loss spectroscopy and its application in materials research. Microscopy (Oxford, England), 2005, 54, 293-298.	0.7	5
3273	Effects of vibrational entropy on the Al-Si phase diagram. Journal of Physics Condensed Matter, 2005, 17, 2197-2210.	0.7	37
3274	A theoretical approach to the energetic stability and geometry of hydrogen and oxygen terminated diamond (100) surfaces. Materials Research Society Symposia Proceedings, 2005, 890, 1.	0.1	1
3275	DNA Base Properties from First Principles Plane-Wave Calculations. , 2005, , 349-361.		0
3276	CORRELATION BETWEEN ELECTRONIC STRUCTURES OF METAL-INTERCALATED SINGLE WALL CARBON NANOTUBES WITH THEIR FIELD EMISSION PROPERTIES. Journal of Theoretical and Computational Chemistry, 2005, 04, 657-668.	1.8	0

#	ARTICLE	IF	CITATIONS
3277	Modern Electronic Structure Theory for Complex Properties of Magnetic Materials. , 2005, , 1-43.		1
3278	Total energy calculation for high pressure selenium: the origin of incommensurate modulations in Se IV and the instability of proposed Se II. Journal of Physics Condensed Matter, 2005, 17, 1851-1859.	0.7	12
3279	Abnormal Lattice Expansion and Double Periodicity in La <sub>0.7</sub> Sr <sub>0.3</sub> MnO <sub>3</sub> Thin Films Under Electron Irradiation. Journal of Materials Research, 2005, 20, 1778-1784.	1.2	4
3280	Study on the Filling Fraction Limit of Impurities in CoSb <sub>3</sub> . Materials Research Society Symposia Proceedings, 2005, 886, 1.	0.1	0
3281	Phase Stability in heavy f-Electron Metals from First-Principles Theory. Materials Research Society Symposia Proceedings, 2005, 893, 1.	0.1	1
3282	First Principles Study on Electronic Structure of PbFe <sub>0.5</sub> Nb <sub>0.5</sub> O <sub>3</sub> . Chinese Physics Letters, 2005, 22, 469-471.	1.3	8
3283	<i>De novo</i> prediction of the ground state structure of transition metal complexes using semiempirical and <i>ab initio</i> quantum mechanics. Coordination isomerism. Journal of Coordination Chemistry, 2005, 58, 575-585.	0.8	9
3284	Crystal Structure of Cs <sub>2</sub> Zn(NO <sub>2</sub> ) <sub>4</sub> : Influence of Steric Crowding on Nitrite Coordination. Australian Journal of Chemistry, 2005, 58, 224.	0.5	1
3285	First-principles equations of state and elastic properties of seven metals. Physical Review B, 2005, 72, .	1.1	112
3286	Structural properties of nanoclusters: Energetic, thermodynamic, and kinetic effects. Reviews of Modern Physics, 2005, 77, 371-423.	16.4	1,609
3287	Adsorption and Reaction of Methanol on Stoichiometric and Defective SrTiO <sub>3</sub> (100) Surfaces. Journal of Physical Chemistry B, 2005, 109, 4507-4513.	1.2	27
3288	Orbital-free embedding applied to the calculation of induced dipole moments in CO <sub>2</sub> @X (X=He, Ne, Ar, Kr,) Tj ETQq <sub>1,2</sub> 1 0.784314 rgB <sub>01</sub>		
3289	Diffusion of Palladium Clusters on Magnesium Oxide. Physical Review Letters, 2005, 95, 246103.	2.9	62
3290	Progress in the development of exchange-correlation functionals. , 2005, , 669-724.		108
3291	Relative stability and elastic properties of hcp, bcc, and fcc beryllium under pressure. Physical Review B, 2005, 71, .	1.1	71
3292	Influence of the Anion on Lone Pair Formation in Sn(II) Monochalcogenides: A DFT Study. Journal of Physical Chemistry B, 2005, 109, 18868-18875.	1.2	182
3293	Hole localization in [AlO <sub>4</sub> ] defects in silica materials. Journal of Chemical Physics, 2005, 122, 144704.	1.2	74
3294	Electronic structure of highly ordered Sr <sub>2</sub> FeMoO <sub>6</sub> : XPS and XES studies. Journal of Physics Condensed Matter, 2005, 17, 4309-4317.	0.7	23



#	ARTICLE	IF	CITATIONS
3295	Adsorption and diffusion of Pt and Au on the stoichiometric and reduced TiO <sub>2</sub> rutile (110) surfaces. <i>Physical Review B</i> , 2005, 72, .	1.1	92
3296	MX <sub>3</sub> -Superhalogens (M = Be, Mg, Ca; X = Cl, Br): A Photoelectron Spectroscopic and ab Initio Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11560-11567.	1.1	150
3297	A Comparative Study of Unrelaxed Surfaces on Quartz and Kaolinite, Using the Periodic Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2005, 109, 10835-10841.	1.2	32
3298	Magnetism and half-metallicity at the O surfaces of ceramic oxides. <i>Journal of Physics Condensed Matter</i> , 2005, 17, L451-L457.	0.7	61
3299	Accurate ab Initio Binding Energies of Alkaline Earth Metal Clusters. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11927-11932.	1.1	36
3300	Theoretical Investigation of CO Interaction with Copper Sites in Zeolites: A Periodic DFT and Hybrid Quantum Mechanical/Interatomic Potential Function Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 9631-9638.	1.2	77
3301	Vacancy formation in $\delta$ -plutonium: A density-functional study in the generalized gradient approximation. <i>Europhysics Letters</i> , 2005, 71, 412-417.	0.7	21
3302	AB INITIO STUDY OF MAGNETISM IN PALLADIUM CLUSTERS SUPPORTED ON (110) SURFACE OF TiO <sub>2</sub> RUTILE. <i>International Journal of Modern Physics B</i> , 2005, 19, 2544-2549.	1.0	3
3303	NO Chemisorption on Pt(111), Rh/Pt(111), and Pd/Pt(111). <i>Journal of Physical Chemistry B</i> , 2005, 109, 17630-17634.	1.2	48
3304	Dielectric properties and long-wavelength optical modes of the high- $\epsilon$ oxide LaAlO <sub>3</sub> . <i>Physical Review B</i> , 2005, 71, .	1.1	65
3305	Dynamics of circular hydrogen bond array in calix[4]arene in a nonpolar solvent: A nuclear magnetic resonance study. <i>Journal of Chemical Physics</i> , 2005, 122, 044506.	1.2	21
3306	Calculation of ferromagnetic states in metastable bcc and hcp Ni by projector-augmented wave method. <i>Journal of Applied Physics</i> , 2005, 97, 106107.	1.1	27
3307	Equivalent oxide thickness of a thin oxide interlayer in gate insulator stacks on silicon. <i>Applied Physics Letters</i> , 2005, 86, 192901.	1.5	23
3308	Impact of interface structure on Schottky-barrier height for Ni $\alpha$ -ZrO <sub>2</sub> (001) interfaces. <i>Applied Physics Letters</i> , 2005, 86, 132103.	1.5	43
3309	Pinning mass-selected Ag <sub>n</sub> clusters on the TiO <sub>2</sub> (110) $\sqrt{1\times 1}$ surface via deposition at high kinetic energy. <i>Journal of Chemical Physics</i> , 2005, 123, 204701.	1.2	28
3310	Density-functional calculation of CeO <sub>2</sub> surfaces and prediction of effects of oxygen partial pressure and temperature on stabilities. <i>Journal of Chemical Physics</i> , 2005, 123, 064701.	1.2	198
3311	Structure and stability of binary transition-metal clusters (NbCo) <sub>n</sub> (n = 1-5): A relativistic density-functional study. <i>Journal of Chemical Physics</i> , 2005, 123, 064315.	1.2	11
3312	The role of nitrogen-related defects in high-k dielectric oxides: Density-functional studies. <i>Journal of Applied Physics</i> , 2005, 97, 053704.	1.1	138

#	ARTICLE	IF	CITATIONS
3313	Short-range exchange and correlation energy density functionals: Beyond the local-density approximation. <i>Journal of Chemical Physics</i> , 2005, 122, 014110.	1.2	120
3314	Assessment of theoretical prediction of the NMR shielding tensor of $^{195}\text{PtCl}_x\text{Br}_{6-x}$ complexes by DFT calculations: experimental and computational results. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 1732-1738.	1.3	34
3315	The molecular structure of $[\text{Sn}(\text{P}2\text{C}2\text{But}2)]$ using gas-phase electron diffraction and DFT calculations. <i>Dalton Transactions</i> , 2005, , 1972.	1.6	11
3316	Linear Response Properties Required to Simulate Vibrational Spectra of Biomolecules in Various Media: (R)-Phenyloxirane (A Comparative Theoretical and Spectroscopic Vibrational Study). <i>Advances in Quantum Chemistry</i> , 2005, , 91-124.	0.4	13
3317	Electronic and structural properties of SnO under pressure. <i>Physical Review B</i> , 2005, 72, .	1.1	53
3318	First Principle Study on Origin of Ferroelectricity of $\text{PbFe}_{0.5}\text{Nb}_{0.5}\text{O}_3$ . <i>Ferroelectrics</i> , 2005, 323, 11-15.	0.3	4
3319	Level of theory study of magnetic resonance parameters of chalcogen $\text{XY}_2$ (X, Y = O, S and Se) defects in alkali halides. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 240-249.	1.3	7
3320	The interaction of $\text{CO}_2$ with sodium-promoted $\text{W}(011)$ . <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3866.	1.3	17
3321	Effect of Solvent Polarity on the Initiation and the Propagation of Ethylene Polymerization with Constrained Geometry Catalyst/MAO Catalytic System: A Density Functional Study with the Conductor-Like Screening Model. <i>Macromolecules</i> , 2005, 38, 1402-1409.	2.2	24
3322	Hydrogen sites occupation in $\text{LaNi}_4\text{Al}$ hydride. <i>Molecular Simulation</i> , 2005, 31, 1101-1106.	0.9	1
3323	Structures and Electronic States of Gadolinium Oxide Clusters. <i>Japanese Journal of Applied Physics</i> , 2005, 44, 6115-6123.	0.8	8
3324	Energetics of hydrogen coverage on group VIII transition metal surfaces and a kinetic model for adsorption/desorption. <i>Journal of Chemical Physics</i> , 2005, 122, 014704.	1.2	38
3325	Understanding the optical anisotropy of oxidized $\text{Si}(001)$ surfaces. <i>Physical Review B</i> , 2005, 72, .	1.1	26
3326	Density functional studies of the $\text{COCu}_{18}$ system. <i>Molecular Physics</i> , 2005, 103, 1075-1082.	0.8	2
3327	Bayesian Error Estimation in Density-Functional Theory. <i>Physical Review Letters</i> , 2005, 95, 216401.	2.9	163
3328	Investigation of the humidity effect on the electrical properties of single-walled carbon nanotube transistors. <i>Applied Physics Letters</i> , 2005, 87, 093101.	1.5	120
3329	Molecular simulations for the conformational assessment of a porphyrin-fullerene dyad in different environments. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3126.	1.3	10
3330	A geometric switching approach toward thermal activation of metalloenediynes. <i>Chemical Communications</i> , 2005, , 5295.	2.2	10

#	ARTICLE	IF	CITATIONS
3331	Atomic and electronic structures of neutral and cation $S_n$ ( $n=2-20$ ) clusters: A comparative theoretical study with different exchange-correlation functionals. <i>Physical Review B</i> , 2005, 71, .	1.1	40
3332	Theory of Nanoscale Atomic Lithography. An ab Initio Study of the Interaction of $^{133}\text{Cs}$ Atoms with Organothiols Self-assembled Monolayers on Au(111). <i>Journal of Physical Chemistry B</i> , 2005, 109, 1815-1821.	1.2	5
3333	Density Functional Theory and the Correlation Consistent Basis Sets: The Tight d Effect on HSO and HOS. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7187-7196.	1.1	43
3334	DFT Study of Oxygen Adsorption on Modified Nanostructured Gold Pyramids. <i>Journal of Physical Chemistry B</i> , 2005, 109, 7624-7630.	1.2	44
3335	Structural and electronic properties of the (100) surface and bulk of alkaline-earth metal oxides. <i>Physical Review B</i> , 2005, 72, .	1.1	65
3336	Molecular adsorption of NO on NiO(100): DFT and DFT+U calculations. <i>Physical Review B</i> , 2005, 71, .	1.1	61
3337	Unprecedented $\pi$ - $\pi$ coordination mode in a terpyridine ligand. <i>Chemical Communications</i> , 2005, , 3355.	2.2	24
3338	Density Functional Theory Predicts the Barriers for Radical Fragmentation in Solution. <i>Journal of Organic Chemistry</i> , 2005, 70, 2014-2020.	1.7	19
3339	Roles of $\text{CH}\cdots\text{O}$ and $\pi$ -Stacking Interactions in the 2-Bromoacrolein Complex with N-Tosyl-(S)-tryptophan-Derived Oxazaborolidinone Catalyst. <i>Journal of Organic Chemistry</i> , 2005, 70, 5487-5493.	1.7	14
3340	The Exploration of Neutral Azoligand-Based Grubbs Type Palladium(II) Complex as Potential Catalyst for the Copolymerization of Ethylene with Acrylonitrile: A Theoretical Study Based on Density Functional Theory. <i>Organometallics</i> , 2005, 24, 1242-1251.	1.1	21
3341	Reduction of the (001) Surface of $\text{V}_2\text{O}_5$ Compared to $\text{V}_2\text{O}_5$ . <i>Journal of Physical Chemistry B</i> , 2005, 109, 374-380.	1.2	19
3342	First-principles investigation of the structural, magnetic, and electronic properties of olivine $\text{LiFePO}_4$ . <i>Physical Review B</i> , 2005, 71, .	1.1	57
3343	Electrostatic DFT Map for the Complete Vibrational Amide Band of NMA. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9747-9759.	1.1	180
3344	Structure, energetics, and mechanical stability of Fe-Cu bcc alloys from first-principles calculations. <i>Physical Review B</i> , 2005, 72, .	1.1	120
3345	Low-temperature polymorphs of $\text{ZrO}_2$ and $\text{HfO}_2$ : A density-functional theory study. <i>Physical Review B</i> , 2005, 72, .	1.1	194
3346	Ammonia Synthesis from First-Principles Calculations. <i>Science</i> , 2005, 307, 555-558.	6.0	1,109
3347	Adsorption and dissociation of hydrogen molecules on bare and functionalized carbon nanotubes. <i>Physical Review B</i> , 2005, 72, .	1.1	255
3348	A Density Functional Theory Study of Molecular and Dissociative Adsorption of $\text{H}_2$ on Active Sites in Mordenite. <i>Journal of Physical Chemistry B</i> , 2005, 109, 22491-22501.	1.2	45

#	ARTICLE	IF	CITATIONS
3349	Single d-Metal Atoms on Fsand Fs+Defects of MgO(001):Â A Theoretical Study across the Periodic Table. Journal of the American Chemical Society, 2005, 127, 11652-11660.	6.6	80
3350	High-Pressure Melting ofMgSiO3. Physical Review Letters, 2005, 94, 195701.	2.9	54
3351	Cooperative Pull and Push Effects on the OâˆO Bond Cleavage in Acylperoxo Complexes of [(Salen)Mn(III)]:Â Ensuring Formation of Manganese(V) Oxo Species. Inorganic Chemistry, 2005, 44, 306-315.	1.9	22
3352	Identification, Structure, and Spectroscopy of Neutral Vanadium Oxide Clusters. Journal of Physical Chemistry A, 2005, 109, 3803-3811.	1.1	86
3353	Electron-Transfer Doping on a (001) Surface of Diamond:Â Quantum Mechanical Study. Journal of Physical Chemistry B, 2005, 109, 22426-22431.	1.2	17
3354	MetalâˆOlefin Interactions in M(CO)5(cycloolefin) (M = Cr, Mo, W; Cycloolefin = Cyclopropene to Tj ETQq1 1 0.784314 rgBTj /Overlock	1.1	21
3355	Reactions of Hydrazoic Acid on TiO2 Nanoparticles:â€‰ an Experimental and Computational Study. Journal of Physical Chemistry B, 2005, 109, 5133-5142.	1.2	14
3356	Combined Charge and Spin Density Experimental Study of the Yttrium(III) Semiquinonato Complex Y(HBPz3)2(DTBSQ) and DFT Calculations. Journal of Physical Chemistry B, 2005, 109, 2723-2732.	1.2	25
3357	Electronic CompositionâˆProperty Relationship Applied to SO2Chemisorption on Pt(111) Surfaces, Alloys, and Overlayers. Journal of Physical Chemistry B, 2005, 109, 6948-6951.	1.2	13
3358	Possible Thermal Decomposition Routes in [MeB(C6F5)3]-[L2TiMe+] as Deactivation Pathways in Olefin Polymerization Catalysis:Â A Combined Density Functional Theory and Molecular Mechanics Investigation. Organometallics, 2005, 24, 2076-2085.	1.1	20
3359	Vanadium Oxides on Aluminum Oxide Supports. 2. Structure, Vibrational Properties, and Reducibility of V2O5 Clusters on Î±-Al2O3(0001). Journal of Physical Chemistry B, 2005, 109, 23532-23542.	1.2	27
3360	Intramolecular Nitro-Assisted Proton Transfer in Photoirradiated 2-(2â€ˆ,4â€ˆ-Dinitrobenzyl)pyridine:â€‰ Polarized Optical Spectroscopic Study and Electronic Structure Calculations. Journal of Physical Chemistry A, 2005, 109, 7264-7275.	1.1	20
3361	Periodic DFT Calculations of the Stability of Al/Si Substitutions and Extraframework Zn2+Cations in Mordeinite and Reaction Pathway for the Dissociation of H2and CH4. Journal of Physical Chemistry B, 2005, 109, 20361-20369.	1.2	56
3362	Diamond Surface Conductivity under Atmospheric Conditions:Â Theoretical Approach. Journal of Physical Chemistry B, 2005, 109, 10304-10311.	1.2	31
3363	A Quantitative Curve-Crossing Model for Radical Fragmentation. Journal of Physical Chemistry A, 2005, 109, 2912-2919.	1.1	10
3364	Cu3C4:Â A New Sandwich Molecule with Two Revolving C22-Units. Journal of Physical Chemistry A, 2005, 109, 562-570.	1.1	32
3365	Simulation of the Embryonic Stage of ZnS Formation from Aqueous Solution. Journal of the American Chemical Society, 2005, 127, 2580-2590.	6.6	38
3366	Direct Detection of Dimethylstannylene and Tetramethyldistannene in Solution and the Gas Phase by Laser Flash Photolysis of 1,1-Dimethylstannacyclopent-3-enes. Journal of the American Chemical Society, 2005, 127, 17469-17478.	6.6	31

#	ARTICLE	IF	CITATIONS
3367	Structures and Energies of Coadsorbed CO and H <sub>2</sub> on Fe <sub>5</sub> C <sub>2</sub> (001), Fe <sub>5</sub> C <sub>2</sub> (110), and Fe <sub>5</sub> C <sub>2</sub> (100). <i>Journal of Physical Chemistry B</i> , 2005, 109, 10922-10935.	1.2	46
3368	Slater's Exchange Parameters $\hat{I}_{\pm}$ for Analytic and Variational $\hat{X}_{\pm}$ Calculations. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 1193-1200.	2.3	19
3369	Vanadium Oxides on Aluminum Oxide Supports. 1. Surface Termination and Reducibility of Vanadia Films on $\hat{I}_{\pm}$ -Al <sub>2</sub> O <sub>3</sub> (0001). <i>Journal of Physical Chemistry B</i> , 2005, 109, 23523-23531.	1.2	42
3370	Ground States, Excited States, and Metal-Ligand Bonding in Rare Earth Hexachloro Complexes: A DFT-Based Ligand Field Study. <i>Inorganic Chemistry</i> , 2005, 44, 2954-2963.	1.9	74
3371	Screening by Kinetic Monte Carlo Simulation of Pt-Au(100) Surfaces for the Steady-State Decomposition of Nitric Oxide in Excess Dioxygen. <i>Journal of Physical Chemistry B</i> , 2005, 109, 2234-2244.	1.2	49
3372	First-Principles Calculations of the Adsorption of Nitromethane and 1,1-Diamino-2,2-dinitroethylene (FOX-7) Molecules on the $\hat{I}_{\pm}$ -Al <sub>2</sub> O <sub>3</sub> (0001) Surface. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1451-1463.	1.2	48
3373	Coexistence of ionic and metallic bonding in noble-metal oxides. <i>Physical Review B</i> , 2005, 72, .	1.1	64
3374	Dopant Sources Choice for Formation of p-Type ZnO: Phosphorus Compound Sources. <i>Chemistry of Materials</i> , 2005, 17, 852-855.	3.2	39
3375	Ab Initio Probing of the Aromatic Oxygen Cluster O <sub>42</sub> <sup>+</sup> . <i>Journal of Physical Chemistry A</i> , 2005, 109, 236-239.	1.1	22
3376	Solvatochromism of a Novel Betaine Dye Derived from Purine. <i>Journal of Physical Chemistry A</i> , 2005, 109, 759-766.	1.1	80
3377	Reactions of Trimethylindium on TiO <sub>2</sub> Nanoparticles: An Experimental and Computational Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 20858-20867.	1.2	15
3378	Cluster and Periodic DFT Calculations of MgO/Pd(CO) and MgO/Pd(CO) <sub>2</sub> Surface Complexes. <i>Journal of Physical Chemistry B</i> , 2005, 109, 3416-3422.	1.2	16
3379	Synthetic Applications of (Me <sub>3</sub> SiNSN) <sub>2</sub> E (E = S, Se) in Chalcogen-Nitrogen Chemistry: Formation and Structural Characterization of Cl <sub>2</sub> TeSN <sub>2</sub> (E = S, Se) and [PPh <sub>4</sub> ] <sub>2</sub> [Pd <sub>2</sub> ( $\frac{1}{4}$ -Se <sub>2</sub> N <sub>2</sub> S) <sub>X</sub> ] <sub>4</sub> (X = Cl, Br). <i>Inorganic Chemistry</i> , 2005, 44, 4992-5000.	1.9	9
3380	Intramolecular Coupling of $\hat{I}$ -2-Iminoacyls on Zirconium Bis(aryloxides) and Calix[4]arenes: A Revised Mechanism by DFT Calculations and Car-Parrinello Molecular Dynamics Simulations. <i>Organometallics</i> , 2005, 24, 1867-1875.	1.1	10
3381	Extraordinary Cluster Formation and Intramolecular Ligand-Ligand Interactions in Cyanoacetylene Mediated by Mg: Implications for the Atmospheric Chemistry of Titan and for Circumstellar Chemistry. <i>Journal of the American Chemical Society</i> , 2005, 127, 13070-13078.	6.6	12
3382	Orbital-Free Density Functional Theory Applied to NaAlH <sub>4</sub> . <i>Journal of Physical Chemistry B</i> , 2005, 109, 16554-16562.	1.2	12
3383	The Oxygen-Rich Carboxide Series: A CO <sub>n</sub> (n = 3, 4, 5, 6, 7, or 8). <i>Journal of Physical Chemistry A</i> , 2005, 109, 3722-3727.	1.1	14
3384	The Structure of the Chiral Pt{531} Surface: A Combined LEED and DFT Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 22456-22462.	1.2	24

#	ARTICLE	IF	CITATIONS
3385	Geometric, electronic, and magnetic structure of Co <sub>2</sub> FeSi: Curie temperature and magnetic moment measurements and calculations. <i>Physical Review B</i> , 2005, 72, .	1.1	513
3386	Oxalate-Bridged Dinuclear M <sub>2</sub> Units: Å Dimers of Dimers, Cyclotetramers, and Extended Sheets (M = Mo,) <i>Tj ETQq1 1 0.784314 rgBT /Ov</i>	1.9	18
3387	Multiple scattering in a vacuum barrier obtained from real-space wavefunctions. <i>Journal of Physics Condensed Matter</i> , 2005, 17, 2705-2713.	0.7	92
3388	NMR Relaxation Study of the Protonated Form of 1,8-Bis(dimethylamino)naphthalene in Isotropic Solution: Anisotropic Motion outside of Extreme Narrowing and Ultrafast Proton Transfer. <i>Journal of Physical Chemistry A</i> , 2005, 109, 57-63.	1.1	23
3389	Theoretical study of the structure and optical properties of carbon-doped rutile and anatase titanium oxides. <i>Journal of Chemical Physics</i> , 2005, 123, 084704.	1.2	140
3390	A systematic density functional theory study of the electronic structure of bulk and (001) surface of transition-metals carbides. <i>Journal of Chemical Physics</i> , 2005, 122, 174709.	1.2	180
3391	Bimetallic Clusters Pt <sub>6</sub> Au: Geometric and Electronic Structures within Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9860-9866.	1.1	15
3392	ReaxFFMgH Reactive Force Field for Magnesium Hydride Systems. <i>Journal of Physical Chemistry A</i> , 2005, 109, 851-859.	1.1	234
3393	Structures of Glycine, Enantiopure Alanine, and Racemic Alanine Adlayers on Cu(110) and Cu(100) Surfaces. <i>Journal of Physical Chemistry B</i> , 2005, 109, 16764-16773.	1.2	101
3394	Probing Enantiospecific Interactions between Proline and anl-Glutathione Self-Assembled Monolayer by Modulation Excitation ATR-IR Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2005, 109, 10243-10250.	1.2	33
3395	N <sub>2</sub> O Decomposition on TiO <sub>2</sub> (110) from Dynamic First-Principles Calculations. <i>Journal of Physical Chemistry B</i> , 2005, 109, 16223-16226.	1.2	38
3396	Combined Density Functional Theory and Molecular Mechanics (QM/MM) Study of Single-Site Ethylene Polymerization and Chain Termination for the Catalysts [(C <sub>6</sub> R <sub>5</sub> NCH) <sub>2</sub> C <sub>4</sub> H <sub>3</sub> N]PrTi+(R = F, H) and [bis( <i>i</i> -5-1-indenyl)dimethylsilane]PrZr+in the Presence of the Counterion CH <sub>3</sub> B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> -. <i>Organometallics</i> , 2005, 24, 419-430.	1.1	19
3397	Density Functional Theory Study of the Jahn-Teller Effect and Spin-Orbit Coupling for Copper and Gold Trimers. <i>Journal of Physical Chemistry A</i> , 2005, 109, 512-519.	1.1	22
3398	Binding Energy Curves from Nonempirical Density Functionals. I. Covalent Bonds in Closed-Shell and Radical Molecules. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11006-11014.	1.1	57
3399	Oxidative Addition of the Fluoromethane C-F Bond to Pd. An ab Initio Benchmark and DFT Validation Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9685-9699.	1.1	61
3400	Density Functional Study on Dihydrogen Activation at the H Cluster in Fe-Only Hydrogenases. <i>Inorganic Chemistry</i> , 2005, 44, 4941-4946.	1.9	29
3401	Theoretical Study of M(PH <sub>3</sub> ) <sub>2</sub> Complexes of C <sub>60</sub> , Corannulene (C <sub>20</sub> H <sub>10</sub> ), and Sumanene (C <sub>21</sub> H <sub>12</sub> ) (M = Pd) <i>Tj ETQq0 0 0 rgBT /Overloc</i>	1.1	56
3402	Reactions of Laser-Ablated Uranium Atoms with H <sub>2</sub> O in Excess Argon: A Matrix Infrared and Relativistic DFT Investigation of Uranium Oxyhydrides. <i>Inorganic Chemistry</i> , 2005, 44, 2159-2168.	1.9	51



#	ARTICLE	IF	CITATIONS
3403	Reconstruction of Pristine and Hydrolyzed Quartz Surfaces. <i>Journal of Physical Chemistry B</i> , 2005, 109, 4144-4151.	1.2	72
3404	Modeling alkali alanates for hydrogen storage by density-functional band-structure calculations. <i>Journal of Materials Research</i> , 2005, 20, 3199-3213.	1.2	41
3405	Ab initio calculations on the effects of additives on alumina phase stability. <i>Physical Review B</i> , 2005, 71, .	1.1	25
3406	Silica glass structure generation for ab initio calculations using small samples of amorphous silica. <i>Physical Review B</i> , 2005, 71, .	1.1	134
3407	Strength, elasticity, and equation of state of the nanocrystalline cubic silicon nitride $\beta$ -Si <sub>3</sub> N <sub>4</sub> to 68 GPa. <i>Physical Review B</i> , 2005, 72, .	1.1	43
3408	Studies of Iridium Nanoparticles Using Density Functional Theory Calculations. <i>Journal of Physical Chemistry B</i> , 2005, 109, 20817-20823.	1.2	87
3409	Water adsorption on hydroxylated silica surfaces studied using the density functional theory. <i>Physical Review B</i> , 2005, 71, .	1.1	105
3410	Introducing ONETEP: Linear-scaling density functional simulations on parallel computers. <i>Journal of Chemical Physics</i> , 2005, 122, 084119.	1.2	550
3411	X-ray photoemission spectra and electronic band structure of the ternary compounds U <sub>3</sub> M <sub>2</sub> M <sub>3</sub> Å <sup>2</sup> , M = Al, Ga, MÅ <sup>2</sup> = Si, Ge. <i>Journal of Alloys and Compounds</i> , 2005, 386, 75-81.	2.8	7
3412	Magnetic states of MgCo <sub>2</sub> and CaCo <sub>2</sub> with the cubic and hexagonal Laves phase structures. <i>Journal of Alloys and Compounds</i> , 2005, 388, 15-18.	2.8	6
3413	Crystal structures and electronic structures of alkali aluminohexahydrides from density functional calculations. <i>Journal of Alloys and Compounds</i> , 2005, 404-406, 757-761.	2.8	16
3414	Atom relaxations around hydrogen defects in lanthanum hydride. <i>Journal of Alloys and Compounds</i> , 2005, 404-406, 55-59.	2.8	16
3415	State of the art simulations in electronic structure and total energy for the high temperature superconductor YBa <sub>2</sub> Cu <sub>3</sub> O <sub>7</sub> . <i>Journal of Alloys and Compounds</i> , 2005, 403, 1-14.	2.8	8
3416	The magnetic structure of TiCrTe <sub>2</sub> . <i>Journal of Alloys and Compounds</i> , 2005, 403, 71-75.	2.8	9
3417	Surface complexation model for multisite adsorption of copper(II) onto kaolinite. <i>Geochimica Et Cosmochimica Acta</i> , 2005, 69, 3733-3745.	1.6	81
3418	Calculated optical spectra of IVÅ <sup>VI</sup> semiconductors PbS, PbSe and PbTe. <i>Computational Materials Science</i> , 2005, 32, 85-95.	1.4	65
3419	Predictive process design: a theoretical model of atomic layer deposition. <i>Computational Materials Science</i> , 2005, 33, 20-25.	1.4	29
3420	First principles modeling of intermediate range order in amorphous SiSe <sub>2</sub> . <i>Computational Materials Science</i> , 2005, 33, 106-111.	1.4	1



#	ARTICLE	IF	CITATIONS
3421	Spin polarization and band alignments at NiMnSb/GaAs interface. <i>Computational Materials Science</i> , 2005, 33, 263-268.	1.4	15
3422	Phase diagram calculations in the Co-Mo and Fe-Mo systems using first-principles results for the sigma phase. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2005, 29, 133-139.	0.7	47
3423	Contribution of first-principles energetics to Al-Mg thermodynamic modeling. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2005, 29, 303-311.	0.7	106
3424	The effect of temperature on the seismic anisotropy of the perovskite and post-perovskite polymorphs of MgSiO <sub>3</sub> . <i>Earth and Planetary Science Letters</i> , 2005, 230, 1-10.	1.8	137
3425	Bonding of Pd, Ag, and Au atoms on MgO(100) surfaces and MgO-Mo(100) ultra-thin films: A comparative DFT study. <i>Physical Review B</i> , 2005, 72, .	1.1	82
3426	Validation of intermolecular transfer integral and bandwidth calculations for organic molecular materials. <i>Journal of Chemical Physics</i> , 2005, 122, 234707.	1.2	76
3427	Experimental and DFT Studies of the Conversion of Ethanol and Acetic Acid on PtSn-Based Catalysts. <i>Journal of Physical Chemistry B</i> , 2005, 109, 2074-2085.	1.2	161
3428	Electron-concentration and pressure-induced structural changes in the alloys In <sub>1-x</sub> X <sub>x</sub> (X=Cd,Sn). <i>Physical Review B</i> , 2005, 72, .	1.1	17
3429	Designing meaningful density functional theory calculations in materials science—a primer. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2005, 13, R1-R31.	0.8	342
3430	Structural and Electronic Properties of Li <sub>2</sub> B <sub>4</sub> O <sub>7</sub> . <i>Journal of Physical Chemistry B</i> , 2005, 109, 13597-13604.	1.2	61
3431	Au Atoms and Dimers on the MgO(100) Surface: A DFT Study of Nucleation at Defects. <i>Journal of Physical Chemistry B</i> , 2005, 109, 8040-8048.	1.2	149
3432	Appraisal of the performance of nonhybrid density functional methods in characterization of the Al <sub>4</sub> C molecule. <i>Journal of Chemical Physics</i> , 2005, 122, 144322.	1.2	16
3433	Where Does the Planar-to-Nonplanar Turnover Occur in Small Gold Clusters?. <i>Journal of the American Chemical Society</i> , 2005, 127, 1049-1052.	6.6	207
3434	Design of magnetic materials: the electronic structure of the ordered, doped Heusler compound Co <sub>2</sub> Cr <sub>1-x</sub> Fe <sub>x</sub> Al. <i>Journal of Physics Condensed Matter</i> , 2005, 17, 7237-7252.	0.7	95
3435	Surface and Subsurface Hydrogen Adsorption Properties on Transition Metals and Near-Surface Alloys. <i>Journal of Physical Chemistry B</i> , 2005, 109, 3460-3471.	1.2	343
3436	Carbon-based nanotechnology on a supercomputer. <i>Journal of Physics Condensed Matter</i> , 2005, 17, R413-R459.	0.7	18
3437	DFT and In Situ EXAFS Investigation of Gold/Ceria-Zirconia Low-Temperature Water Gas Shift Catalysts: Identification of the Nature of the Active Form of Gold. <i>Journal of Physical Chemistry B</i> , 2005, 109, 22553-22559.	1.2	197
3438	First-principles study of the adsorption of cesium on Si(001)(2 $\times$ 1) surface. <i>Journal of Chemical Physics</i> , 2005, 122, 174704.	1.2	28

#	ARTICLE	IF	CITATIONS
3439	Functional designed to include surface effects in self-consistent density functional theory. Physical Review B, 2005, 72, .	1.1	533
3440	Sphalerite $\leftrightarrow$ Chalcopyrite Polymorphism in Semimetallic ZnSnSb <sub>2</sub> . Chemistry of Materials, 2005, 17, 6080-6085.	3.2	21
3441	Predicting ionic conductivity of solid oxide fuel cell electrolyte from first principles. Journal of Applied Physics, 2005, 98, 103513.	1.1	162
3442	A Density Functional Study of the Chemical Differences between Type I and Type II MoS <sub>2</sub> -Based Structures in Hydrotreating Catalysts $\epsilon$ . Journal of Physical Chemistry B, 2005, 109, 2245-2253.	1.2	170
3443	Forces and conductances in a single-molecule bipyridine junction. Physical Review B, 2005, 72, .	1.1	65
3444	Electronic spin state of ferric iron in Al-bearing perovskite in the lower mantle. Geophysical Research Letters, 2005, 32, .	1.5	47
3445	High temperature elastic anisotropy of the perovskite and post-perovskite polymorphs of Al <sub>2</sub> O <sub>3</sub> . Geophysical Research Letters, 2005, 32, .	1.5	37
3446	First-Principles Analysis of the Effects of Alloying Pd with Ag for the Catalytic Hydrogenation of Acetylene $\leftrightarrow$ Ethylene Mixtures. Journal of Physical Chemistry B, 2005, 109, 12449-12466.	1.2	172
3447	Adsorption Kinetics, Orientation, and Self-Assembling of N-Acetyl-L-cysteine on Gold: A Combined ATR-IR, PM-IRRAS, and QCM Study. Journal of Physical Chemistry B, 2005, 109, 22476-22485.	1.2	51
3448	Theoretical Study of the Adsorption and Dissociation of Oxygen on Pt(111) in the Presence of Homogeneous Electric Fields. Journal of Physical Chemistry B, 2005, 109, 6304-6310.	1.2	127
3449	Properties of the CdSe(0001), (0001 $\bar{1}$ ), and (112 $\bar{1}$ ,0) Single Crystal Surfaces: A Relaxation, Reconstruction, and Adatom and Admolecule Adsorption. Journal of Physical Chemistry B, 2005, 109, 19320-19328.	1.2	71
3450	Geometrical, electronic, and magnetic properties of Na <sub>0.5</sub> CoO <sub>2</sub> from first principles. Physical Review B, 2005, 71, .	1.1	18
3451	Structure and magnetic properties of the Fe <sub>3</sub> O <sub>4</sub> (001) surface: $\epsilon$ Ab initio studies. Physical Review B, 2005, 71, .	1.1	47
3452	Quasiclassical study of Eley $\leftrightarrow$ Rideal and hot atom reactions of H atoms with Cl adsorbed on a Au(111) surface. Journal of Chemical Physics, 2005, 122, 074705.	1.2	24
3453	Magnetic Interactions Influence the Properties of Helium Defects in Iron. Physical Review Letters, 2005, 94, 046403.	2.9	163
3454	Charging of Au Atoms on TiO <sub>2</sub> Thin Films from CO Vibrational Spectroscopy and DFT Calculations. Journal of Physical Chemistry B, 2005, 109, 18418-18426.	1.2	126
3455	Structure and Properties of ZnS Nanoclusters. Journal of Physical Chemistry B, 2005, 109, 2703-2709.	1.2	102
3456	All-Metal Aromaticity and Antiaromaticity. Chemical Reviews, 2005, 105, 3716-3757.	23.0	529

#	ARTICLE	IF	CITATIONS
3457	Adsorption of Atomic Oxygen and Nitrogen at $\hat{1}^2$ -Cristobalite (100): A Density Functional Theory Study. Journal of Physical Chemistry B, 2005, 109, 14954-14964.	1.2	49
3458	Theoretical study of the adsorption of H <sub>2</sub> on (3,3) carbon nanotubes. Physical Review B, 2005, 72, .	1.1	40
3459	DFT Studies of Pt/Au Bimetallic Clusters and Their Interactions with the CO Molecule. Journal of Physical Chemistry B, 2005, 109, 22341-22350.	1.2	128
3460	Role of vacancies in the structural stability of $\hat{1}^2$ -TiO: A first-principles study based on density-functional calculations. Physical Review B, 2005, 72, .	1.1	50
3461	L-Glutathione Chemisorption on Gold and Acid/Base Induced Structural Changes: A PM-IRRAS and Time-Resolved in Situ ATR-IR Spectroscopic Study. Langmuir, 2005, 21, 1354-1363.	1.6	76
3462	van der Waals interactions of polycyclic aromatic hydrocarbon dimers. Journal of Chemical Physics, 2005, 122, 054102.	1.2	46
3463	Simulations on the Thermal Decomposition of a Poly(dimethylsiloxane) Polymer Using the ReaxFF Reactive Force Field. Journal of the American Chemical Society, 2005, 127, 7192-7202.	6.6	395
3464	Size-dependent charge-separation reaction for hydrated sulfate dianion cluster, SO <sub>4</sub> <sup>2-</sup> (H <sub>2</sub> O) <sub>n</sub> , with n = 3-7. Journal of Chemical Physics, 2005, 123, 224302.	1.2	28
3465	Mechanisms of Methanol Decomposition on Platinum: A Combined Experimental and ab Initio Approach. Journal of Physical Chemistry B, 2005, 109, 11622-11633.	1.2	248
3466	Real-Time Observation of Molecular Motion on a Surface. Science, 2005, 310, 1790-1793.	6.0	167
3467	Iron-oxygen vacancy defect centers in PbTiO <sub>3</sub> : Newman superposition model analysis and density functional calculations. Physical Review B, 2005, 71, .	1.1	146
3468	First-principles studies of Au(100)-hex reconstruction in an electrochemical environment. Physical Review B, 2005, 72, .	1.1	28
3469	Why Copper Is Intrinsically More Selective than Silver in Alkene Epoxidation: Ethylene Oxidation on Cu(111) versus Ag(111). Journal of the American Chemical Society, 2005, 127, 10774-10775.	6.6	124
3470	Search for the Li <sub>n</sub> O <sup>+1/-1</sup> (n = 5-7) Lowest-Energy Structures Using the ab Initio Gradient Embedded Genetic Algorithm (GEGA). Elucidation of the Chemical Bonding in the Lithium Clusters. Journal of Chemical Theory and Computation, 2005, 1, 566-580.	2.3	198
3471	Theoretical study of environmental dependence of oxygen vacancy formation in CeO <sub>2</sub> . Applied Physics Letters, 2005, 87, 141917.	1.5	56
3472	Relativistic two-component calculations of electronic g-tensors that include spin polarization. Journal of Chemical Physics, 2005, 123, 244103.	1.2	72
3473	Enhancement of hydrogen physisorption on graphene and carbon nanotubes by Li doping. Journal of Chemical Physics, 2005, 123, 204721.	1.2	247
3474	Density-functional calculations of relativistic spin-orbit effects on nuclear magnetic shielding in paramagnetic molecules. Journal of Chemical Physics, 2005, 123, 174102.	1.2	50

#	ARTICLE	IF	CITATIONS
3475	Density functional study of the interaction of chlorine atom with small neutral and charged silver clusters. <i>Journal of Chemical Physics</i> , 2005, 122, 144701.	1.2	42
3476	Size-dependent martensitic transformation path causing atomic-scale twinning of nanocrystalline NiTi shape memory alloys. <i>Europhysics Letters</i> , 2005, 71, 98-103.	0.7	92
3477	Structure and energetics of small gold nanoclusters and their positive ions. <i>Journal of Chemical Physics</i> , 2005, 122, 094310.	1.2	142
3478	Possible Side Reactions Due to Water in Emulsion Polymerization by Late Transition Metal Complexes II: Deactivation of the Catalyst by a Wacker-Type Reaction. <i>Organometallics</i> , 2005, 24, 2679-2687.	1.1	30
3479	On the Extent of Intramolecular Hydrogen Bonding in Gas-Phase and Hydrated 1,2-Ethanediol. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2971-2977.	1.1	49
3480	Half-metallic properties of atomic chains of carbon-transition-metal compounds. <i>Physical Review B</i> , 2005, 72, .	1.1	35
3481	Attracted by Long-Range Electron Correlation: Adenine on Graphite. <i>Physical Review Letters</i> , 2005, 95, 186101.	2.9	275
3482	Surface core-level shift and electronic structure on transition-metal diboride (0001) surfaces. <i>Physical Review B</i> , 2005, 71, .	1.1	56
3483	Quantitative Analysis of WC Grain Shape in Sintered WC-Co Cemented Carbides. <i>Physical Review Letters</i> , 2005, 94, 066105.	2.9	48
3484	Chemical Bonding in Si <sub>52</sub> - and NaSi <sub>5</sub> -via Photoelectron Spectroscopy and ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11385-11394.	1.1	26
3485	Migration of the subsurface impurity in Pd(111). <i>Physical Review B</i> , 2005, 71, .	1.1	43
3486	Energetics of the Li amide/Li imide hydrogen storage reaction. <i>Physical Review B</i> , 2005, 72, .	1.1	110
3487	Energy Ranking of Molecular Crystals Using Density Functional Theory Calculations and an Empirical van der Waals Correction. <i>Journal of Physical Chemistry B</i> , 2005, 109, 15531-15541.	1.2	266
3488	Nitrogen in graphite and carbon nanotubes: Magnetism and mobility. <i>Physical Review B</i> , 2005, 72, .	1.1	117
3489	Density Functional Energetics of $\alpha$ -Quartz for Calibration of SiO <sub>2</sub> Interatomic Potentials. <i>Journal of Physical Chemistry B</i> , 2005, 109, 4168-4171.	1.2	8
3490	Silicon and III-V compound nanotubes: Structural and electronic properties. <i>Physical Review B</i> , 2005, 72, .	1.1	250
3491	Prescription for the design and selection of density functional approximations: More constraint satisfaction with fewer fits. <i>Journal of Chemical Physics</i> , 2005, 123, 062201.	1.2	769
3492	Electronic structure calculations of potassium-intercalated single-walled carbon nanotubes. <i>Physical Review B</i> , 2005, 72, .	1.1	11

#	ARTICLE	IF	CITATIONS
3493	Near-edge electronic structure in NbS <sub>2</sub> . Journal of Chemical Physics, 2005, 123, 244705.	1.2	6
3494	Nonequivalence of the generalized gradient approximations PBE and PW91. Physical Review B, 2006, 73, .	1.1	129
3495	Two-Dimensional Ir Cluster Lattice on a Graphene Moiré on Ir(111). Physical Review Letters, 2006, 97, 215501.	2.9	533
3496	Electronic Structure and Reactivity of Isomeric Oxo-Mn(V) Porphyrins: Effects of Spin-State Crossing and pKa Modulation. Inorganic Chemistry, 2006, 45, 4268-4276.	1.9	107
3497	A density functional theory study of the dissociation of H <sub>2</sub> on gold clusters: Importance of fluxionality and ensemble effects. Journal of Chemical Physics, 2006, 125, 164715.	1.2	114
3498	Adsorption and Activation of CO over Flat and Stepped Co Surfaces: A First Principles Analysis. Journal of Physical Chemistry B, 2006, 110, 15368-15380.	1.2	147
3499	Solid-State Modeling of the Terahertz Spectrum of the High Explosive HMX. Journal of Physical Chemistry A, 2006, 110, 1951-1959.	1.1	166
3500	First-Principles Investigation of Hydroxylated Monoclinic HfO <sub>2</sub> Surfaces. Chemistry of Materials, 2006, 18, 3397-3403.	3.2	30
3501	Acidity of Mesoporous MoO <sub>x</sub> /ZrO <sub>2</sub> and WO <sub>x</sub> /ZrO <sub>2</sub> Materials: A Combined Solid-State NMR and Theoretical Calculation Study. Journal of Physical Chemistry B, 2006, 110, 10662-10671.	1.2	70
3502	Ab initio thermodynamic properties of point defects and O-vacancy diffusion in Mg spinels. Physical Review B, 2006, 74, .	1.1	16
3503	Density functional calculations of hydrogen adsorption on boron nanotubes and boron sheets. Nanotechnology, 2006, 17, 778-785.	1.3	83
3504	First-principles calculations of impurity diffusion activation energies in Al. Physical Review B, 2006, 73, .	1.1	37
3505	First-principles study of the adsorption of methanol at the $\sqrt{3}\times\sqrt{3}$ -Al <sub>2</sub> O <sub>3</sub> (0001) surface. Journal of Physics Condensed Matter, 2006, 18, 1-12.	0.7	65
3506	Selective Nontemplated Adsorption of Organic Molecules on Nanofacets and the Role of Bonding Patterns. Physical Review Letters, 2006, 97, 156105.	2.9	65
3507	First principles reaction modeling of the electrochemical interface: Consideration and calculation of a tunable surface potential from atomic and electronic structure. Physical Review B, 2006, 73, .	1.1	394
3508	CO Adsorption on CoMo and NiMo Sulfide Catalysts: A Combined IR and DFT Study. Journal of Physical Chemistry B, 2006, 110, 1261-1270.	1.2	135
3509	Methanethiolate Adsorption Site on Au(111): A Combined STM/DFT Study at the Single-Molecule Level. Journal of Physical Chemistry B, 2006, 110, 21161-21167.	1.2	75
3510	Magnetism and origin of non-monotonous concentration dependence of the bulk modulus in Fe-rich alloys with Si, Ge and Sn: a first-principles study. Journal of Physics Condensed Matter, 2006, 18, 6677-6689.	0.7	25

#	ARTICLE	IF	CITATIONS
3511	Computational study of Met-Car analogue heterofullerenes. Modelling and Simulation in Materials Science and Engineering, 2006, 14, 637-646.	0.8	2
3512	Magnetic and Electronic Properties of Transition Metal Doped $\hat{I}^2$ -SiC - A Diluted Magnetic Semiconductor. Key Engineering Materials, 2006, 317-318, 889-892.	0.4	1
3513	Relativistic DFT Studies of Dehydrogenation of Methane by Pt Cationic Clusters: Cooperative Effect of Bimetallic Clusters. Journal of Physical Chemistry A, 2006, 110, 10078-10083.	1.1	42
3514	First-principles modeling of nonlinear optical properties of C <sub>3</sub> N <sub>4</sub> polymorphs. Applied Physics Letters, 2006, 89, 261117.	1.5	36
3515	Optical properties of Cr <sup>3+</sup> -doped oxides: Different behavior of two centers in alexandrite. Physical Review B, 2006, 74, .	1.1	33
3516	First-principles thermoelasticity of transition metals at high pressure: Tantalum prototype in the quasiharmonic limit. Physical Review B, 2006, 74, .	1.1	53
3517	Ab initio study of ultrathin MgO films on Fe(001): Influence of interfacial structures. Physical Review B, 2006, 73, .	1.1	57
3518	Thermodynamic properties of binary hcp solution phases from special quasirandom structures. Physical Review B, 2006, 74, .	1.1	122
3519	Adsorption trends for water, hydroxyl, oxygen, and hydrogen on transition-metal and platinum-skin surfaces. Physical Review B, 2006, 74, .	1.1	106
3520	Group 11 complexes with the bis(3,5-dimethylpyrazol-1-yl)methane ligand. How secondary bonds can influence the coordination environment of Ag(i): the role of coordinated water in [Ag <sub>2</sub> ( $\mu$ -L) <sub>2</sub> (OH) <sub>2</sub> ](OTf) <sub>2</sub> . Dalton Transactions, 2006, , 4104-4113.	1.6	33
3521	Adsorption of oxygen molecules on individual single-wall carbon nanotubes. Journal of Applied Physics, 2006, 99, 034306.	1.1	48
3522	Structural properties of hexagonal boron nitride. Modelling and Simulation in Materials Science and Engineering, 2006, 14, 515-535.	0.8	75
3523	Reactive and Nonreactive Scattering of H <sub>2</sub> from a Metal Surface Is Electronically Adiabatic. Science, 2006, 312, 86-89.	6.0	180
3524	Density-functional global optimization of gold nanoclusters. Physical Review B, 2006, 73, .	1.1	106
3525	Interaction of Pt Clusters with the Anatase TiO <sub>2</sub> (101) Surface: A First Principles Study. Journal of Physical Chemistry B, 2006, 110, 7463-7472.	1.2	95
3526	Computational design of Si $\hat{\alpha}$ -SiO <sub>2</sub> interfaces: Stress and strain on the atomic scale. Physical Review B, 2006, 73, .	1.1	36
3527	Vibrational spectra of vitreous germania from first-principles. Physical Review B, 2006, 74, .	1.1	56
3528	Density functional investigation of the adsorption of a methane monolayer on an MgO(100) surface. Physical Review B, 2006, 73, .	1.1	16

#	ARTICLE	IF	CITATIONS
3529	Electronic structure of an ordered Pb <sup>+</sup> Ag(111) surface alloy: Theory and experiment. Physical Review B, 2006, 73, .	1.1	92
3530	Structure, dynamics, and electronic properties of lithium disilicate melt and glass. Journal of Chemical Physics, 2006, 125, 114702.	1.2	73
3531	Hydrogen adsorption and dissociation on small platinum clusters: An electronic structure density functional study. Physical Review B, 2006, 74, .	1.1	26
3532	First-principles density-functional theory calculations of electron-transfer rates in azurin dimers. Journal of Chemical Physics, 2006, 124, 064501.	1.2	42
3533	First principles study on the structural, electronic and optical properties of diluted magnetic semiconductors Zn 1 <sup>+</sup> x Co x X ( X =S, Se, Te). Chinese Physics B, 2006, 15, 1585-1590.	1.3	18
3534	First principles calculations on martensitic transformation and phase instability of Ni <sup>+</sup> Mn <sup>+</sup> Ga high temperature shape memory alloys. Applied Physics Letters, 2006, 89, 231921.	1.5	54
3535	Structural studies of phosphorus induced dimers on Si(001). Physical Review B, 2006, 73, .	1.1	11
3536	Molecular studies of the structural properties of hydrogen gas in bulk water. Molecular Simulation, 2006, 32, 269-278.	0.9	23
3537	Local-property analysis for modeling of gate insulator materials. , 2006, , .		1
3538	Scalar relativistic calculations of hyperfine coupling tensors using the Douglas <sup>+</sup> Kroll <sup>+</sup> Hess method with a finite-size nucleus model. Physical Chemistry Chemical Physics, 2006, 8, 4079-4085.	1.3	52
3539	A structural analysis of lead hydroxyvanadinite. Physical Chemistry Chemical Physics, 2006, 8, 1845.	1.3	16
3540	Magnetostructural correlations in the cyano-bridged CrNi, Cr <sub>2</sub> Ni and CrNi <sub>6</sub> complexes: density functional theory calculations. Journal of Materials Chemistry, 2006, 16, 4657.	6.7	11
3541	Comparison of frozen-density embedding and discrete reaction field solvent models for molecular properties. Physical Chemistry Chemical Physics, 2006, 8, 2349.	1.3	87
3542	The influence of carbon on the adsorption of CO on a Rh(100) single crystal. Physical Chemistry Chemical Physics, 2006, 8, 624-632.	1.3	23
3543	Water desorption from an oxygen covered Pt(111) surface: Multichannel desorption. Journal of Chemical Physics, 2006, 124, 204712.	1.2	21
3544	Ab initio based tight-binding molecular dynamics simulation of the sticking and scattering of O <sub>2</sub> <sup>+</sup> Pt(111). Journal of Chemical Physics, 2006, 124, 174713.	1.2	29
3545	MOLECULAR DYNAMICS SIMULATION OF GAS ADSORPTION AND ABSORPTION IN NANOTUBES. , 2006, , 187-207.		2
3546	Transition-metal-doping-enhanced hydrogen storage in boron nitride systems. Applied Physics Letters, 2006, 89, 153104.	1.5	75



#	ARTICLE	IF	CITATIONS
3547	Electronic structure and energetics of the quaternary hydride Li <sub>4</sub> BN <sub>3</sub> H <sub>10</sub> . Applied Physics Letters, 2006, 88, 231904.	1.5	42
3548	Electronic and magnetic properties of double-impurities-doped TiO <sub>2</sub> (rutile): First-principles calculations. Journal of Applied Physics, 2006, 99, 08M105.	1.1	10
3549	Thickness dependence of the atomic and electronic structures of TiO <sub>2</sub> rutile (110) slabs and the effects on the electronic and magnetic properties of supported clusters of Pd and Rh. Physical Review B, 2006, 73, .	1.1	18
3550	Six-dimensional potential energy surface for H <sub>2</sub> at Ru(0001). Physical Chemistry Chemical Physics, 2006, 8, 688-696.	1.3	40
3551	The Ni + O <sub>2</sub> reaction: A combined IR matrix isolation and theoretical study of the formation and structure of NiO <sub>2</sub> . Physical Chemistry Chemical Physics, 2006, 8, 448-455.	1.3	25
3552	Structural and magnetic properties of betaine adducts with transition metals: I. ((CH <sub>3</sub> ) <sub>3</sub> NCH <sub>2</sub> COO) <sub>3</sub> MnMCl <sub>4</sub> with M = Mn <sup>2+</sup> , Co <sup>2+</sup> , Zn <sup>2+</sup> . Journal of Physics Condensed Matter, 2006, 18, 11067-11079.	0.7	5
3553	A combined Raman, DFT and MD study of the solvation dynamics and the adsorption process of pyridine in silver hydrosols. Physical Chemistry Chemical Physics, 2006, 8, 171-178.	1.3	38
3554	Electronic properties and reactivity of Pt-doped carbon nanotubes. Physical Chemistry Chemical Physics, 2006, 8, 3528.	1.3	28
3555	Gold as intermolecular glue: a predicted planar triaurotriazine, C <sub>3</sub> Au <sub>3</sub> N <sub>3</sub> , isomer of gold cyanide. Chemical Communications, 2006, , 2890.	2.2	14
3556	Dynamics of an [Fe <sub>4</sub> S <sub>4</sub> (SPh) <sub>4</sub> ] <sup>2+</sup> cluster explored via IR, Raman, and nuclear resonance vibrational spectroscopy (NRVS)-analysis using <sup>36</sup> S substitution, DFT calculations, and empirical force fields. Dalton Transactions, 2006, , 2192.	1.6	33
3557	<sup>195</sup> Pt NMR and DFT computational methods as tools towards the understanding of speciation and hydration/solvation of [PtX <sub>6</sub> ] <sup>2-</sup> (X = Cl <sup>-</sup> , Br <sup>-</sup> ) anions in solution. Dalton Transactions, 2006, , 3277-3284.	1.6	42
3558	Density functional theory investigation of the geometric and electronic structures of [UO <sub>2</sub> (H <sub>2</sub> O) <sub>m</sub> (OH) <sub>n</sub> ] <sup>2+</sup> (n + m = 5). Dalton Transactions, 2006, , 2403-2414.	1.6	60
3559	The effect of cation coordination on the properties of oxygen vacancies in FeSbO <sub>4</sub> . Journal of Materials Chemistry, 2006, 16, 1943.	6.7	19
3560	Photochemistry of Methyltrioxorhenium Revisited: A DFT/TD-DFT and CASSCF/MS-CASPT2 Theoretical Study. Organometallics, 2006, 25, 5235-5241.	1.1	12
3561	Energy Correctors for Accurate Prediction of Molecular Energies. Journal of Physical Chemistry A, 2006, 110, 1060-1064.	1.1	16
3562	Role of Pr Segregation in Acceptor-State Formation at ZnO Grain Boundaries. Physical Review Letters, 2006, 97, 106802.	2.9	109
3563	Interaction of SO <sub>3</sub> with c-ZrO <sub>2</sub> (111) films on Pt(111). Physical Chemistry Chemical Physics, 2006, 8, 1593.	1.3	12
3564	A precursor state for formation of TiAl <sub>3</sub> complex in reversible hydrogen desorption/adsorption from Ti-doped NaAlH <sub>4</sub> . Chemical Communications, 2006, , 1822.	2.2	40

#	ARTICLE	IF	CITATIONS
3565	Photochemical synthesis of benzoyl spiro[2.2]pentanes. <i>Photochemical and Photobiological Sciences</i> , 2006, 5, 1000.	1.6	8
3566	Nature of Point Defects on SiO <sub>2</sub> /Mo(112) Thin Films and Their Interaction with Au Atoms. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17015-17023.	1.2	28
3567	Charge transfers at metal/oxide interfaces: a DFT study of formation of K <sup>+</sup> and Au <sup>+</sup> species on MgO/Ag(100) ultra-thin films from deposition of neutral atoms. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3335-3341.	1.3	82
3568	Hydrogen Dissociation over Au Nanowires and the Fractional Conductance Quantum. <i>Physical Review Letters</i> , 2006, 96, 046803.	2.9	56
3569	Ag-like Au <sub>32</sub> detected in relativistic density-functional calculations of optical spectroscopy. <i>Physical Review B</i> , 2006, 73, .	1.1	20
3570	Interplay between hydrogen bonding and electron solvation on hydrated TiO <sub>2</sub> (110). <i>Physical Review B</i> , 2006, 73, .	1.1	50
3571	Density Functional Theory Study of Ligand Binding on CdSe (0001), (0001 $\bar{1}$ ), and (112 $\bar{1}$ ,0) Single Crystal Relaxed and Reconstructed Surfaces: A Implications for Nanocrystalline Growth. <i>Journal of Physical Chemistry B</i> , 2006, 110, 18007-18016.	1.2	152
3572	Is the uniform electron gas limit important for small Ag clusters? Assessment of different density functionals for Ag <sub>n</sub> (n $\leq$ 24). <i>Journal of Chemical Physics</i> , 2006, 124, 184102.	1.2	124
3573	Effect of spin-orbit coupling on small platinum nanoclusters. <i>Physical Review A</i> , 2006, 73, .	1.0	83
3574	Toward Computational Materials Design: The Impact of Density Functional Theory on Materials Research. <i>MRS Bulletin</i> , 2006, 31, 659-668.	1.7	265
3575	Phase stability and structural distortion of NiO under high pressure. <i>Transactions of Nonferrous Metals Society of China</i> , 2006, 16, s52-s58.	1.7	2
3576	Adsorption of atomic S and C on Mg(0001) surface. <i>Transactions of Nonferrous Metals Society of China</i> , 2006, 16, s253-s256.	1.7	1
3577	Influence of crystal structure and formation energies of impurities (Mg, Zn and Ca) in zinc blende GaN. <i>Transactions of Nonferrous Metals Society of China</i> , 2006, 16, s854-s857.	1.7	6
3578	Transition pressures and enthalpy barriers for the cubic diamond $\rightarrow$ tin transition in Si and Ge under nonhydrostatic conditions. <i>Physical Review B</i> , 2006, 73, .	1.1	26
3579	Vibrational and electron paramagnetic resonance properties of free and MgO supported AuCO complexes. <i>Journal of Chemical Physics</i> , 2006, 124, 174709.	1.2	25
3580	A theoretical and experimental study of lead substitution in calcium hydroxyapatite. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 967.	1.3	73
3581	Au and Pd atoms adsorbed on pure and Ti-doped SiO <sub>2</sub> /Mo(112) films. <i>Journal of Chemical Physics</i> , 2006, 124, 034701.	1.2	41
3582	Influence of the Hydroxylation of $\beta$ -Al <sub>2</sub> O <sub>3</sub> Surfaces on the Stability and Diffusion of Single Pd Atoms: A DFT Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 1759-1767.	1.2	103

#	ARTICLE	IF	CITATIONS
3583	Semiempirical van der Waals correction to the density functional description of solids and molecular structures. <i>Physical Review B</i> , 2006, 73, .	1.1	707
3584	High-pressure melting of lead. <i>Physical Review B</i> , 2006, 73, .	1.1	30
3585	Lattice strain effects on CO oxidation on Pt(111). <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3369.	1.3	96
3586	Ab Initio Study of Energetic Solids: Cupric Azide, Mercuric Azide, and Lead Azide. <i>Journal of Physical Chemistry B</i> , 2006, 110, 18196-18203.	1.2	56
3587	Static ionic displacements in Fe-Ni alloys from first principles. <i>Journal of Applied Physics</i> , 2006, 99, 08P906.	1.1	7
3588	Water adsorption on hydroxylated quartz (0001) surfaces: From monomer to flat bilayer. <i>Physical Review B</i> , 2006, 73, .	1.1	117
3589	Insight into the solvent effect: A density functional theory study of cisplatin hydrolysis. <i>Journal of Chemical Physics</i> , 2006, 125, 091101.	1.2	21
3590	Structural study of gold clusters. <i>Journal of Chemical Physics</i> , 2006, 124, 114309.	1.2	220
3591	Explicit density-functional exchange potential with correct asymptotic behavior. <i>Physical Review A</i> , 2006, 74, .	1.0	24
3592	Surface Dipoles and Work Functions of Alkylthiolates and Fluorinated Alkylthiolates on Au(111). <i>Journal of Physical Chemistry B</i> , 2006, 110, 22628-22634.	1.2	161
3593	Intramolecular Electron Transfer through the 20-Position of a Chlorophylla Derivative: An Unexpectedly Efficient Conduit for Charge Transport. <i>Journal of the American Chemical Society</i> , 2006, 128, 4779-4791.	6.6	95
3594	Interactions Study between the Copper II Ion and Constitutive Elements of Chitosan Structure by DFT Calculation. <i>Biomacromolecules</i> , 2006, 7, 31-37.	2.6	56
3595	Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides. <i>Physical Review B</i> , 2006, 74, .	1.1	309
3596	Tuning the chemical functionality of a gas sensitive material: Water adsorption on SnO <sub>2</sub> (101). <i>Surface Science</i> , 2006, 600, 29-32.	0.8	45
3597	Bonding in metal carbonyls: A comparison with experiment and calculations on adsorbed CO. <i>Computational and Theoretical Chemistry</i> , 2006, 762, 123-132.	1.5	20
3598	First-principles study of H adsorption on and absorption in Cu(111) surface. <i>Chemical Physics</i> , 2006, 321, 48-54.	0.9	30
3599	Density functional study of diamond epitaxy on the (111) and (100) surfaces of copper. <i>Diamond and Related Materials</i> , 2006, 15, 1201-1205.	1.8	3
3600	Structure and bonding of Au <sub>5</sub> M (M=Na, Mg, Al, Si, P, and S) clusters. <i>Physical Review B</i> , 2006, 74, .	1.1	113

#	ARTICLE	IF	CITATIONS
3601	A Small Paramagnetic Platinum Cluster in an NaY Zeolite: Characterization and Hydrogen Adsorption and Desorption. <i>Journal of Physical Chemistry B</i> , 2006, 110, 1213-1223.	1.2	55
3602	Phonon dispersion curves of stable and metastable BC <sub>3</sub> honeycomb epitaxial sheets and their chemical bonding: Experiment and theory. <i>Physical Review B</i> , 2006, 73, .	1.1	70
3603	First-principles calculations of structural and electronic properties of monoclinic hafnia surfaces. <i>Physical Review B</i> , 2006, 73, .	1.1	71
3604	Cu <sub>4</sub> Mo <sub>6</sub> Se <sub>8</sub> : Synthesis, Crystal Structure, and Electronic Structure of a New Chevrel Phase Structure Type. <i>Inorganic Chemistry</i> , 2006, 45, 2718-2726.	1.9	7
3605	Water adsorption on a NaCl (001) surface: A density functional theory study. <i>Physical Review B</i> , 2006, 74, .	1.1	43
3606	Energetics, structure, and long-range interaction of vacancy-type defects in carbon nanotubes: Atomistic simulations. <i>Physical Review B</i> , 2006, 74, .	1.1	202
3607	First-principles calculations of native defects in tin monoxide. <i>Physical Review B</i> , 2006, 74, .	1.1	276
3608	Elastic anisotropy of FeSiO <sub>3</sub> end-members of the perovskite and post-perovskite phases. <i>Geophysical Research Letters</i> , 2006, 33, n/a-n/a.	1.5	59
3609	Electronic spin transitions and the seismic properties of ferrous iron-bearing MgSiO <sub>3</sub> post-perovskite. <i>Geophysical Research Letters</i> , 2006, 33, .	1.5	50
3610	High-pressure alloying of iron and xenon: $\epsilon$ -Xe in the Earth's core?. <i>Journal of Geophysical Research</i> , 2006, 111, n/a-n/a.	3.3	25
3611	Bulk and surface oxygen vacancy formation and diffusion in single crystals, ultrathin films, and metal grown oxide structures. <i>Journal of Chemical Physics</i> , 2006, 125, 074711.	1.2	61
3612	Theoretical Study of the Relationship between the Nearest-Neighbor Exchange Coupling Interactions and the Number of Peripheral Complexes in the Cyano-Bridged CrMn <sub>6</sub> (CN) <sub>6</sub> and CrMn <sub>2</sub> (CN) <sub>2</sub> Clusters. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5096-5101.	1.1	12
3613	Theoretical models of directional proton molecular transport. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 3096.	1.5	15
3614	Structure of Ag(111)-p(4 $\times$ 4)-O: No Silver Oxide. <i>Physical Review Letters</i> , 2006, 96, 146102.	2.9	141
3615	More accurate generalized gradient approximation for solids. <i>Physical Review B</i> , 2006, 73, .	1.1	1,785
3616	Band-gap bowing coefficients in large size-mismatched II-VI alloys: first-principles calculations. <i>Physical Review B</i> , 2006, 74, .	1.1	78
3617	Properties of the quaternary half-metal-type Heusler alloy Co <sub>2</sub> Mn <sub>1-x</sub> Fe <sub>x</sub> Si. <i>Physical Review B</i> , 2006, 74, .	1.1	274
3618	On the accuracy of density functional theory in transition metal chemistry. <i>Annual Reports on the Progress of Chemistry Section C</i> , 2006, 102, 203.	4.4	285

#	ARTICLE	IF	CITATIONS
3619	A Quantum Chemical Study of Comparison of Various Propylene Epoxidation Mechanisms Using H <sub>2</sub> O <sub>2</sub> and TS-1 Catalyst. Journal of Physical Chemistry B, 2006, 110, 14627-14639.	1.2	76
3620	Energy storage capacity of polymeric nitrogen. Molecular Physics, 2006, 104, 745-749.	0.8	42
3621	Determination of the high-pressure crystal structure of BaWO <sub>4</sub> and PbWO <sub>4</sub> . Physical Review B, 2006, 73, .	1.1	95
3622	Electronic and Structural Shell Closure in AgCu and AuCu Nanoclusters. Journal of Physical Chemistry B, 2006, 110, 23197-23203.	1.2	90
3623	EFFECT OF RELAXATION ON THE ENERGETICS AND STRUCTURE OF ANATASE TiO <sub>2</sub> (101) SURFACE. Surface Review and Letters, 2006, 13, 825-831.	0.5	7
3624	Adsorption of phenol on graphite(0001) and $\gamma$ -Al <sub>2</sub> O <sub>3</sub> (0001): Nature of van der Waals bonds from first-principles calculations. Physical Review B, 2006, 74, .	1.1	89
3625	First-principles study of interaction of cluster Au <sub>32</sub> with CO, H <sub>2</sub> , and O <sub>2</sub> . Journal of Chemical Physics, 2006, 125, 124703.	1.2	60
3626	Methane Oxidation Mechanism on Pt(111): A Cluster Model DFT Study. Journal of Physical Chemistry B, 2006, 110, 24593-24605.	1.2	118
3627	Electronic Structures and Absorption Spectra of Linkage Isomers of Trithiocyanato (4,4'-bis(4-mercapto-2,2,6,6-tetracarboxy-2,2',6,2'-terpyridine) Ruthenium(II) Complexes: A DFT Study. Inorganic Chemistry, 2006, 45, 7600-7611.	1.2	108
3628	Reactive and nonreactive scattering of N <sub>2</sub> from Ru(0001): A six-dimensional adiabatic study. Journal of Chemical Physics, 2006, 125, 114706.	1.2	43
3629	Ab initio study of the critical thickness for ferroelectricity in ultrathin Pt/PbTiO <sub>3</sub> /Pt films. Physical Review B, 2006, 74, .	1.1	66
3630	Relativistic effective core potential calculations of Hg and eka-Hg (E112) interactions with gold: Spin-orbit density functional theory modeling of Hg-Au and E112-Au systems. Journal of Chemical Physics, 2006, 125, 241102.	1.2	24
3631	MAGNETIC EXCHANGE IN POLYNUCLEAR TRANSITION METAL SYSTEM: AB INITIO CASPT2 AND DENSITY FUNCTIONAL THEORY STUDY ON TRIANGULAR COPPER(II) COMPLEXES. Journal of Theoretical and Computational Chemistry, 2006, 05, 501-514.	1.8	3
3632	Density Functional Study of the Interaction of Carbon Monoxide with Small Neutral and Charged Silver Clusters. Journal of Physical Chemistry A, 2006, 110, 7167-7172.	1.1	57
3633	Olefin Adsorption on Silica-Supported Silver Salts: A DFT Study. Langmuir, 2006, 22, 5716-5722.	1.6	21
3634	Structure and activity of oxidized Pt(110) and PtO <sub>2</sub> . Physical Chemistry Chemical Physics, 2006, 8, 1566.	1.3	71
3635	Structural, electronic and magnetic properties of Gd investigated by DFT+U methods: bulk, clean and H-covered (0001) surfaces. Journal of Physics Condensed Matter, 2006, 18, 7021-7043.	0.7	64
3636	Theoretical Study of N-Doped TiO <sub>2</sub> Rutile Crystals. Journal of Physical Chemistry B, 2006, 110, 24011-24014.	1.2	140

#	ARTICLE	IF	CITATIONS
3637	Migration Energy of He in W Revisited by <i>Ab Initio</i> Calculations. <i>Physical Review Letters</i> , 2006, 97, 196402.	2.9	283
3638	d-Penicillamine Adsorption on Gold: An <i>In Situ</i> ATR-IR Spectroscopic and QCM Study. <i>Langmuir</i> , 2006, 22, 8379-8386.	1.6	38
3639	Ultrafast Vibrationally-Induced Dephasing of Electronic Excitations in PbSe Quantum Dots. <i>Nano Letters</i> , 2006, 6, 2295-2300.	4.5	88
3640	Comparative First-Principles Study of Structural and Optical Properties of Alkali Metal Azides. <i>Journal of Physical Chemistry B</i> , 2006, 110, 9856-9862.	1.2	48
3641	Electrochemical Oxidation of $\text{CoCp}(\text{CO})_2$ Radical-Substrate Reaction of a 17 e-/18 e-Pair and Production of a Unique Dimer Radical. <i>Journal of the American Chemical Society</i> , 2006, 128, 16587-16599.	6.6	57
3642	Competitive Adsorption of NO, NO <sub>2</sub> , CO <sub>2</sub> , and H <sub>2</sub> O on BaO(100): A Quantum Chemical Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17484-17492.	1.2	63
3643	Unsaturated Cyclopentadienyl-Molybdenum and Tungsten Carbonyl Cluster Complexes Containing Pd- and Pt(PBu <sub>3</sub> ) Groups. <i>Organometallics</i> , 2006, 25, 2673-2682.	1.1	6
3644	One-Dimensional Transition Metal-Benzene Sandwich Polymers: Possible Ideal Conductors for Spin Transport. <i>Journal of the American Chemical Society</i> , 2006, 128, 2310-2314.	6.6	202
3645	Reaction of Hydrogen with Ag(111): Binding States, Minimum Energy Paths, and Kinetics. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17145-17154.	1.2	51
3646	Hybrid Density Functional Theory with Specific Reaction Parameter: Hydrogen Abstraction Reaction of Fluoromethane by the Hydroxyl Radical. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7663-7671.	1.1	14
3647	Mechanistic Insights into NO <sub>3</sub> -Induced Self-Terminating Radical Oxygenations, Part 1: A Computational Study on NO <sub>3</sub> and Its Addition to Alkynes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2195-2203.	1.1	27
3648	Relativistic DFT Study on the Reaction Mechanism of Second-Row Transition Metal Ru with CO <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2006, 110, 3552-3558.	1.1	10
3649	Dissociative Adsorption of Carbon Monoxide on Mo(110): First-Principles Theory. <i>Journal of Physical Chemistry B</i> , 2006, 110, 18363-18367.	1.2	15
3650	Silapropargyl/Silaallenyl and Silylene Acetylide Complexes of $[\text{Cp}(\text{CO})_2\text{W}]^+$ . Theoretical Study of Their Interesting Bonding Nature and Formation Reaction. <i>Journal of the American Chemical Society</i> , 2006, 128, 11927-11939.	6.6	28
3651	Theoretical Analysis of Structural, Energetic, Electronic, and Defect Properties of Li <sub>2</sub> O. <i>Journal of Physical Chemistry B</i> , 2006, 110, 9413-9420.	1.2	66
3652	Anisotropic and Passivation-Dependent Quantum Confinement Effects in Germanium Nanowires: A Comparison with Silicon Nanowires. <i>Journal of Physical Chemistry B</i> , 2006, 110, 18332-18337.	1.2	28
3653	Fundamental Studies of P(GeH <sub>3</sub> ) <sub>3</sub> , As(GeH <sub>3</sub> ) <sub>3</sub> , and Sb(GeH <sub>3</sub> ) <sub>3</sub> : Practical n-Dopants for New Group IV Semiconductors. <i>Chemistry of Materials</i> , 2006, 18, 6266-6277.	3.2	51
3654	Electronic structure and bonding in hexagonal boron nitride. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 97-115.	0.7	137



#	ARTICLE	IF	CITATIONS
3655	Effect of Pre-covered Oxygen on the Dehydrogenation Reactions over Copper Surface: A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 26045-26054.	1.2	23
3656	Theoretical Investigation of the Binding Energies of the Iodide Ion and Xenon Atom with Decaborane. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12528-12534.	1.1	8
3657	Unravelling the Origin of the High-Catalytic Activity of Supported Au: A Density-Functional Theory-Based Interpretation. <i>Journal of the American Chemical Society</i> , 2006, 128, 15600-15601.	6.6	65
3658	First-Principles Calculations within Periodic Boundary Conditions of the NMR Shielding Tensor for a Transition Metal Nucleus in a Solid State System: The Example of $^{51}\text{V}$ in $\text{AlVO}_4$ . <i>Journal of Physical Chemistry B</i> , 2006, 110, 21403-21407.	1.2	27
3659	Molecular Electrostatic Potential Devices on Graphite and Silicon Surfaces. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12298-12302.	1.1	11
3660	Growth of Ultrathin Films of Amorphous Ruthenium-Phosphorus Alloys Using a Single Source CVD Precursor. <i>Journal of the American Chemical Society</i> , 2006, 128, 16510-16511.	6.6	25
3661	Nitric acid dihydrate at ambient and high pressure: An experimental and computational study. <i>Physical Review B</i> , 2006, 73, .	1.1	13
3662	Reactions of Hydrazoic Acid and Trimethylindium on $\text{TiO}_2$ Rutile (110) Surface: A Computational Study on the Formation of the First Monolayer $\text{InN}$ . <i>Journal of Physical Chemistry B</i> , 2006, 110, 2263-2270.	1.2	13
3663	Ionic Conductivity of $\text{Li}_2\text{B}_4\text{O}_7$ . <i>Journal of Physical Chemistry B</i> , 2006, 110, 17518-17523.	1.2	25
3664	Unusual Process of Water Formation on $\text{RuO}_2(110)$ by Hydrogen Exposure at Room Temperature. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14007-14010.	1.2	35
3665	Synthesis and Structures of Oxo-Bridged Distannyl- and Digermyl-dirhenium Complexes. <i>Organometallics</i> , 2006, 25, 3848-3855.	1.1	29
3666	Electronic structure of $\text{NiO}/\text{Ag}(100)$ thin films from DFT+U and hybrid functional DFT approaches. <i>Physical Review B</i> , 2006, 74, .	1.1	68
3667	Oxidative Addition of the Chloromethane $\text{C}-\text{Cl}$ Bond to Pd, an ab Initio Benchmark and DFT Validation Study. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 322-335.	2.3	81
3668	First-Principles Study of K and Cs Adsorbed on $\text{Pd}(111)$ . <i>Journal of Physical Chemistry B</i> , 2006, 110, 23904-23910.	1.2	10
3669	Molecular Understanding of Alumina Supported Single-Site Catalysts by a Combination of Experiment and Theory. <i>Journal of the American Chemical Society</i> , 2006, 128, 9157-9169.	6.6	125
3670	Density Functional Study of Small Neutral and Charged Silver Cluster Hydrides. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11537-11542.	1.1	33
3671	Water Adsorption and Diffusion on $\text{NaCl}(100)$ . <i>Journal of Physical Chemistry B</i> , 2006, 110, 24559-24564.	1.2	24
3672	Inelastic Electron Tunneling Spectroscopy and Vibrational Coupling. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13249-13252.	1.1	11



#	ARTICLE	IF	CITATIONS
3673	Local Structure and Chemical Bonding of Protonated $\text{Li}_x\text{Mn}_2\text{O}_4$ Spinels from First Principles. <i>Chemistry of Materials</i> , 2006, 18, 1169-1173.	3.2	20
3674	Reactions of Gadolinium Atoms and Dimers with CO: $\hat{\text{A}}$ Formation of Gadolinium Carbonyls and Photoconversion to CO Activated Molecules. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12585-12591.	1.1	35
3675	Native point defects in yttria and relevance to its use as a high-dielectric-constant gate oxide material: First-principles study. <i>Physical Review B</i> , 2006, 73, .	1.1	84
3676	Ridge-Bridge Adsorption of Molecular Oxygen on $\text{Pt}\{110\}(1 \hat{\text{A}} - 2)$ from First Principles. <i>Journal of Physical Chemistry B</i> , 2006, 110, 11962-11970.	1.2	13
3677	Characterization of the Structural and Electronic Properties of Crystalline Lithium Silicates. <i>Journal of Physical Chemistry B</i> , 2006, 110, 22346-22352.	1.2	56
3678	Simulating Temperature Programmed Desorption of Water on Hydrated $\hat{\text{I}}^3$ -Alumina from First-Principles Calculations. <i>Journal of Physical Chemistry B</i> , 2006, 110, 7392-7395.	1.2	27
3679	First-Principles Study on Proton Dissociation Properties of Fluorocarbon- and Hydrocarbon-Based Membranes in Low Humidity Conditions. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17872-17877.	1.2	18
3680	Role of the Fermi Surface in Adsorbate $\hat{\text{A}}$ Metal Interactions: $\hat{\text{A}}$ An Energy Decomposition Analysis. <i>Journal of Physical Chemistry B</i> , 2006, 110, 12470-12479.	1.2	14
3681	Periodic Density Functional Theory Study of Propane Oxidative Dehydrogenation over $\text{V}_2\text{O}_5(001)$ Surface. <i>Journal of the American Chemical Society</i> , 2006, 128, 11114-11123.	6.6	134
3682	First Principles Study of Adsorption and Dissociation of CO on $\text{W}(111)$ . <i>Journal of Physical Chemistry B</i> , 2006, 110, 1344-1349.	1.2	21
3683	Periodic DFT Study of the Structural and Electronic Properties of Bulk $\text{CoAl}_2\text{O}_4$ Spinel. <i>Journal of Physical Chemistry B</i> , 2006, 110, 988-995.	1.2	80
3684	Theory and Application of Dissociative Electron Capture in Molecular Identification. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4413-4418.	1.1	17
3685	Unusual $\text{Mn}\hat{\text{A}}\text{Mn}$ Spin Coupling in the Polar Intermetallic Compounds $\text{CaMn}_2\text{Sb}_2$ and $\text{SrMn}_2\text{Sb}_2$ . <i>Inorganic Chemistry</i> , 2006, 45, 4047-4054.	1.9	58
3686	$\text{CuNO}_2$ and $\text{Cu}^+\text{NO}_2$ Revisited: $\hat{\text{A}}$ Comparative ab Initio and DFT Study. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 997-1008.	2.3	4
3687	Computational Study of Multiple-Decker Sandwich and Rice-Ball Structures of Neutral Titanium $\hat{\text{A}}$ Benzene Clusters. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11988-11994.	1.1	55
3688	Stability of the body-centered-tetragonal phase of Fe at high pressure: Ground-state energies, phonon spectra, and molecular dynamics simulations. <i>Physical Review B</i> , 2006, 74, .	1.1	21
3689	First-principles calculations of the band gap and optical properties of germanium sulfide. <i>Physical Review B</i> , 2006, 74, .	1.1	91
3690	Nonlinear magnetoelastic behavior of the bcc phases of Co and Ni: Importance of third-order contributions for bcc Ni. <i>Physical Review B</i> , 2006, 73, .	1.1	8

#	ARTICLE	IF	CITATIONS
3691	Synthesis, Structural Characterization, and Theoretical Studies of Gold(I) and Gold(I) $\rightarrow$ Gold(III) Thiolate Complexes: Quenching of Gold(I) Thiolate Luminescence. <i>Inorganic Chemistry</i> , 2006, 45, 1059-1068.	1.9	61
3692	TD-DFT Description of Photoabsorption and Electron Transfer in a Covalently Bonded Porphyrin $\rightarrow$ Fullerene Dyad. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12470-12476.	1.1	35
3693	Effect of Particle Size on the Oxidizability of Platinum Clusters. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5839-5846.	1.1	75
3694	Density Functional Theory (DFT) Calculations of the Infrared Absorption Spectra of Acetaminophen Complexes Formed with Ethanol and Acetone Species. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8986-9001.	1.1	17
3695	V@Au <sub>12</sub> : An Improved Novel Catalyst for CO Oxidation?. <i>Journal of Physical Chemistry B</i> , 2006, 110, 11600-11603.	1.2	61
3696	DFT Studies on the Magnetic Exchange Across the Cyanide Bridge. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13332-13340.	1.1	55
3697	A density-functional theory study of the adsorption of CO molecules on Au/Ni(111). <i>Journal of Physics Condensed Matter</i> , 2006, 18, 10825-10835.	0.7	8
3698	Ba Adsorption on the Stoichiometric and Defective TiO <sub>2</sub> (110) Surface from First-Principles Calculations. <i>Journal of Physical Chemistry B</i> , 2006, 110, 19552-19556.	1.2	5
3699	Effect of Adsorption Site, Size, and Composition of Pt/Au Bimetallic Clusters on the CO Frequency: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 14036-14042.	1.1	46
3700	Thermodynamic Equilibrium Compositions, Structures, and Reaction Energies of Pt <sub>x</sub> O <sub>y</sub> (x= 1 $\rightarrow$ 3) Clusters Predicted from First Principles. <i>Journal of Physical Chemistry B</i> , 2006, 110, 16591-16599.	1.2	51
3701	Adsorption of Small Au <sub>n</sub> (n= 1 $\rightarrow$ 5) and Au $\rightarrow$ Pd Clusters Inside the TS-1 and S-1 Pores. <i>Journal of Physical Chemistry B</i> , 2006, 110, 16439-16451.	1.2	28
3702	Photoelectron Spectroscopy and DFT Calculations of Easily Ionized Quadruply Bonded Mo <sub>2</sub> <sup>4+</sup> Compounds and Their Bicyclic Guanidinate Precursors. <i>Journal of Physical Chemistry B</i> , 2006, 110, 19793-19798.	1.2	24
3703	Theoretical Calculation of the Dehydrogenation of Ethanol on a Rh/CeO <sub>2</sub> (111) Surface. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14816-14823.	1.2	55
3704	Identification of Destabilized Metal Hydrides for Hydrogen Storage Using First Principles Calculations. <i>Journal of Physical Chemistry B</i> , 2006, 110, 8769-8776.	1.2	273
3705	How Nitrogenase Shakes $\rightarrow$ Initial Information about P $\rightarrow$ Cluster and FeMo-cofactor Normal Modes from Nuclear Resonance Vibrational Spectroscopy (NRVS). <i>Journal of the American Chemical Society</i> , 2006, 128, 7608-7612.	6.6	73
3706	Density Function Theory Study of CO Adsorption on Fe <sub>3</sub> O <sub>4</sub> (111) Surface. <i>Journal of Physical Chemistry B</i> , 2006, 110, 13920-13925.	1.2	73
3707	Mono-, Di-, Tri-, and Tetra-Substituted Fluorotyrosines: New Probes for Enzymes That Use Tyrosyl Radicals in Catalysis. <i>Journal of the American Chemical Society</i> , 2006, 128, 1569-1579.	6.6	126
3708	Structure Determination of the 4d Metal Diborides: A Quantum Mechanical Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 5367-5371.	1.2	19

#	ARTICLE	IF	CITATIONS
3709	The Crystal Structure and Surface Energy of NaAlH <sub>4</sub> : A Comparison of DFT Methodologies. <i>Journal of Physical Chemistry B</i> , 2006, 110, 622-630.	1.2	43
3710	First Crystal Structure Studies of CaAlH <sub>5</sub> . <i>Inorganic Chemistry</i> , 2006, 45, 3849-3851.	1.9	46
3711	Binary Clusters AuPt and Au <sub>6</sub> Pt: A Structure and Reactivity within Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6285-6293.	1.1	64
3712	Structures and Potential Superconductivity in SiH <sub>4</sub> at High Pressure: En Route to a Metallic Hydrogen. <i>Physical Review Letters</i> , 2006, 96, 017006.	2.9	187
3713	Mechanistic Study of the Electrochemical Oxygen Reduction Reaction on Pt(111) Using Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2006, 110, 15338-15344.	1.2	91
3714	Ab initio studies of Al, O, and O <sub>2</sub> adsorption on $\gamma$ -Al <sub>2</sub> O <sub>3</sub> (0001) surfaces. <i>Physical Review B</i> , 2006, 74, .	1.1	42
3715	Rational Design of Selective, Sulfur-Resistant Oxidation Emissions Catalysts. <i>Journal of Physical Chemistry B</i> , 2006, 110, 6856-6863.	1.2	6
3716	Do Methanethiol Adsorbates on the Au(111) Surface Dissociate?. <i>Physical Review Letters</i> , 2006, 97, 045505.	2.9	57
3717	Perturbation of Adsorbed CO by Amine Derivatives Coadsorbed on the $\gamma$ -Al <sub>2</sub> O <sub>3</sub> Surface: A FTIR and First Principles Studies. <i>Journal of Physical Chemistry B</i> , 2006, 110, 4742-4750.	1.2	13
3718	Structure and Bonding of Alkanethiols on Cu(111) and Cu(100). <i>Journal of Physical Chemistry B</i> , 2006, 110, 17050-17062.	1.2	40
3719	Computational Studies of the Coordination Stereochemistry, Bonding, and Metal Selectivity of Mercury. <i>Journal of Physical Chemistry A</i> , 2006, 110, 452-462.	1.1	43
3720	Density Functional Study on the Regioselectivity of Styrene Polymerization with anansa-Metallocene Catalyst. <i>Organometallics</i> , 2006, 25, 1144-1150.	1.1	24
3721	Competition between Metal-Amido and Metal-Imido Chemistries in the Alkaline Earth Series: An Experimental and Theoretical Study of BaNH. <i>Journal of the American Chemical Society</i> , 2006, 128, 1109-1118.	6.6	14
3722	Meta-generalized gradient approximation for the exchange-correlation hole with an application to the jellium surface energy. <i>Physical Review B</i> , 2006, 73, .	1.1	71
3723	Ab initio study of the effect of nitrogen on carbon nanotube growth. <i>Nanotechnology</i> , 2006, 17, 909-912.	1.3	13
3724	Theoretical Probing of Deltahedral closo-Auroboranes B <sub>x</sub> Au <sub>2-x</sub> (x = 5-12). <i>Inorganic Chemistry</i> , 2006, 45, 5269-5271.	1.9	30
3725	A DFT Study of the Adsorption and Dissociation of CO on Sulfur-Precovered Fe(100). <i>Journal of Physical Chemistry B</i> , 2006, 110, 13897-13904.	1.2	46
3726	Density Functional Investigation of High-Spin XY (X = Cr, Mo, W and Y = C, N, O) Molecules. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4846-4853.	1.1	21

#	ARTICLE	IF	CITATIONS
3727	From periodic DFT calculations to classical molecular dynamics simulations. Computational Materials Science, 2006, 35, 183-186.	1.4	8
3728	Structural properties of small copper clusters with a nickel impurity. Computational Materials Science, 2006, 35, 311-315.	1.4	8
3729	Ab initio simulation of diamond epitaxial growth on copper. Computational Materials Science, 2006, 36, 139-142.	1.4	4
3730	A density functional theory study of CO adsorption on PtAu nanoparticles. Computational Materials Science, 2006, 35, 247-253.	1.4	56
3731	Assessment of the thermodynamic properties and phase diagram of the BiPd system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2006, 30, 14-17.	0.7	7
3732	Thermodynamic modeling of the HfSiO system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2006, 30, 375-386.	0.7	98
3733	First principles study of electronic and mechanical properties of molybdenum selenide type nanowires. Physical Review B, 2006, 74, .	1.1	26
3734	Mechanism of the Verwey transition in magnetite: JahnTeller distortion and charge ordering patterns. Journal of Physics Condensed Matter, 2006, 18, 10427-10436.	0.7	53
3735	First-principles modelling of Earth and planetary materials at high pressures and temperatures. Reports on Progress in Physics, 2006, 69, 2365-2441.	8.1	152
3736	Electronic Structure of Metal/Molecule/Metal Junctions: A Density Functional Theory Study of the Influence of the Molecular Terminal Group. Journal of Physical Chemistry B, 2006, 110, 3493-3498.	1.2	36
3737	Density Functional Theory Based Ab Initio Molecular Dynamics Using the Car-Parrinello Approach. , 2006, , 223-285.		9
3738	Calculation of zero-field splitting parameters: Comparison of a two-component noncolinear spin-density-functional method and a one-component perturbational approach. Journal of Chemical Physics, 2006, 125, 054110.	1.2	66
3739	Electronic structures of platinum group elements silicides calculated by a first-principle pseudopotential method using plane-wave basis. Journal of Alloys and Compounds, 2006, 417, 173-179.	2.8	23
3740	Distinct magnetic states of metastable fcc structured Fe and FeCu alloys studied by ab initio calculations. Journal of Alloys and Compounds, 2006, 414, 36-41.	2.8	25
3741	Thermodynamics modeling of the MgSr and CaMgSr systems. Journal of Alloys and Compounds, 2006, 421, 172-178.	2.8	41
3742	Contribution of first-principles energetics to the CaMg thermodynamic modeling. Journal of Alloys and Compounds, 2006, 420, 98-106.	2.8	36
3743	Comparative behavior of vacancy and C, B, N, O atoms single defect on hardening the B2-FeAl structure: An atomistic study. Intermetallics, 2006, 14, 142-148.	1.8	27
3744	Calculation of electronic properties of SrSi2 within the framework of a band theory. Intermetallics, 2006, 14, 666-671.	1.8	24

#	ARTICLE	IF	CITATIONS
3745	Electronic structures of semiconducting FeGa <sub>3</sub> , RuGa <sub>3</sub> , OsGa <sub>3</sub> , and RuIn <sub>3</sub> with the CoGa <sub>3</sub> - or the FeGa <sub>3</sub> -type structure. <i>Intermetallics</i> , 2006, 14, 722-728.	1.8	46
3746	Lattice stability of Ca, Sr and Yb disilicides. <i>Intermetallics</i> , 2006, 14, 1472-1486.	1.8	34
3747	Characterization of exciton self-trapping in amorphous silica. <i>Journal of Non-Crystalline Solids</i> , 2006, 352, 2589-2595.	1.5	29
3748	Elasticity of CaSiO <sub>3</sub> perovskite at high pressure and high temperature. <i>Physics of the Earth and Planetary Interiors</i> , 2006, 155, 249-259.	0.7	84
3749	Phase stability of CaSiO <sub>3</sub> perovskite at high pressure and temperature: Insights from ab initio molecular dynamics. <i>Physics of the Earth and Planetary Interiors</i> , 2006, 155, 260-268.	0.7	46
3750	First-principles electronic structure of light-emitting and transport materials: Zinc(II)2-(2-hydroxyphenyl)benzothiazolate. <i>Synthetic Metals</i> , 2006, 156, 1287-1291.	2.1	5
3751	Electronic structure of DNA derivatives and mimics by density functional theory. , 2006, , 485-507.		2
3752	3.4.1 Adsorbate properties of hydrogen on solid surfaces. , 0, , 1-130.		0
3753	Submatrix inversion approach to the ab initio Green's function method for electrical transport. <i>E-Journal of Surface Science and Nanotechnology</i> , 2006, 4, 484-489.	0.1	2
3755	Vibrational Analyses of Di- $\mu$ -oxo-Bridged Manganese Dimers Based on Density Functional Theory Calculations. Theoretical Evaluation of Mn <sup>IV</sup> -O Vibrations of the Mn-Cluster Core for Photosynthetic Oxygen-Evolving Complex. <i>Bulletin of the Chemical Society of Japan</i> , 2006, 79, 1025-1031.	2.0	7
3756	Growth of intact water ice on Ru(0001) between 140 and 160K: Experiment and density-functional theory calculations. <i>Physical Review B</i> , 2006, 73, .	1.1	125
3758	The Magnetic Nature of Intrinsic and Irradiation-induced Defects in Carbon Systems. , 2006, , 371-396.		5
3759	Density Functional Study of Catalytic Oxygen Reduction Reaction (ORR) on Cathode Electrode for Fuel Cell System. <i>Chemistry Letters</i> , 2006, 35, 1406-1407.	0.7	2
3760	The Depths of Hydrogen and Helium Bubbles in Tungsten: A Comparison. <i>Fusion Science and Technology</i> , 2006, 50, 43-57.	0.6	54
3761	Unexpected magnetism in low dimensional systems: the role of symmetry. <i>Journal of Physics: Conference Series</i> , 2006, 30, 215-223.	0.3	0
3762	Does Lung Surfactant Promote Disaggregation of Nanostructured Titanium Dioxide?. <i>Journal of Occupational and Environmental Medicine</i> , 2006, 48, 1314-1320.	0.9	43
3763	Superior mechanical properties of Nb <sub>2</sub> AsC to those of other layered ternary carbides: a first-principles study. <i>Journal of Physics Condensed Matter</i> , 2006, 18, L527-L533.	0.7	33
3764	Activation Barriers of CO Oxidation on Pt-M(M=Ru, Sn) Alloys. <i>Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals</i> , 2006, 70, 495-499.	0.2	5

#	ARTICLE	IF	CITATIONS
3765	Hybrid density functional theory study of fragment ions generated during mass spectrometry of 1,3-dioxane derivatives. <i>Rapid Communications in Mass Spectrometry</i> , 2006, 20, 1871-1876.	0.7	1
3766	Room-Temperature Ferromagnetism in Doped Face-Centered Cubic Fe Nanoparticles. <i>Small</i> , 2006, 2, 804-809.	5.2	41
3767	Electronic structure calculations and electrical resistivity of Dy(Co <sub>1-x</sub> Mx) <sub>2</sub> (M = Ni, Cu). <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2006, 3, 183-186.	0.8	2
3768	Ab-initio electronic structure calculations for Pr <sub>3</sub> Co <sub>13</sub> B <sub>2</sub> and Pr <sub>5</sub> Co <sub>19</sub> B <sub>6</sub> compounds. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2006, 3, 238-242.	0.8	1
3769	Spin polarized transport of iron nitride Fe <sub>4</sub> N: Analysis using a combination of first principles calculation and model calculation. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2006, 3, 3303-3306.	0.8	6
3770	On the magnetic properties and hyperfine fields in Fe-containing alloys: A theoretical study. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2006, 3, 3285-3291.	0.8	3
3771	First-principles studies of various crystallographic phases and neutral atomic vacancies in KNbO <sub>3</sub> and KTaO <sub>3</sub> . <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2006, 3, 2862-2866.	0.8	10
3772	Ab initio modeling of electron-phonon coupling in high-k dielectrics. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2006, 3, 3382-3385.	0.8	13
3773	Reactions of methyllithium with CO and CNMe: Theoretical study. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 692-696.	1.0	3
3774	Theoretical study of the magnetic exchange coupling behavior substituting Cr(III) with Mo(III) in cyano-bridged transition metal complexes. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1551-1560.	1.0	12
3775	Moletronics modeling toward molecular potentials. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1964-1969.	1.0	16
3776	Aromaticity-induced changes in electronic properties of size-expanded DNA bases: Case of xC. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2339-2346.	1.0	17
3777	Kinetics and structural aspects of the cisplatin interactions with guanine: A quantum mechanical description. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2129-2144.	1.0	35
3778	Orbital interactions and charge redistribution in weak hydrogen bonds: Watson-Crick GC mimic involving C $\delta^+$ H proton donor and F proton acceptor groups. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2428-2443.	1.0	8
3779	Optimization of strong and weak coordinates. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2536-2544.	1.0	101
3780	DFT study of bare and dye-sensitized TiO <sub>2</sub> clusters and nanocrystals. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 3214-3234.	1.0	230
3781	Structure of D-ribonic acid-dimethyltin(IV) in coordinating solvents: an experimental and DFT <sup>119</sup> Sn NMR study. <i>Journal of Physical Organic Chemistry</i> , 2006, 19, 874-883.	0.9	9
3782	Buckling in boron sheets and nanotubes. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2006, 203, 1105-1110.	0.8	22



#	ARTICLE	IF	CITATIONS
3783	Systematic studies on electronic structures of CuInSe <sub>2</sub> and the other chalcopyrite related compounds by first principles calculations. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2006, 203, 2634-2638.	0.8	57
3784	Theoretical study of cation doping effect on the electronic conductivity of Li <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> . <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 1835-1841.	0.7	83
3785	Plain DFT and hybrid HF-DFT LCAO calculations of SnO <sub>2</sub> (110) and (100) bare and hydroxylated surfaces. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 1823-1834.	0.7	30
3786	Electronic structure studies of DyNi <sub>4</sub> Cu. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 309-312.	0.7	0
3787	Interstitial Oxygen in Tin-Doped Indium Oxide Transparent Conductors. <i>Journal of the American Ceramic Society</i> , 2006, 89, 616-619.	1.9	30
3788	Photocatalytic Activity of Ni 8 wt%-Doped TiO <sub>2</sub> Photocatalyst Synthesized by Mechanical Alloying Under Visible Light. <i>Journal of the American Ceramic Society</i> , 2006, 89, 515-518.	1.9	87
3789	Microstructures and Theoretical Bulk Modulus of Layered Ternary Tantalum Aluminum Carbides. <i>Journal of the American Ceramic Society</i> , 2006, 89, 3765-3769.	1.9	118
3790	Switching the electrical resistance of individual dislocations in single-crystalline SrTiO <sub>3</sub> . <i>Nature Materials</i> , 2006, 5, 312-320.	13.3	1,581
3791	Current status of ab initio quantum chemistry study for oxygen electroreduction on fuel cell catalysts. <i>Electrochimica Acta</i> , 2006, 51, 1905-1916.	2.6	136
3792	Si(001) c(4Å <sup>2</sup> )â€“p(2Å <sup>2</sup> ) surface phase transitions induced by electric fields and doping. <i>Current Applied Physics</i> , 2006, 6, 331-333.	1.1	3
3793	Si(001) surface optical anisotropies induced by Î€-conjugated overlayers and oxidation. <i>Current Applied Physics</i> , 2006, 6, 525-530.	1.1	2
3794	Density functional study of graphite bulk and surface properties. <i>Carbon</i> , 2006, 44, 231-242.	5.4	192
3795	Pressure induced reactivity change on the side-wall of a carbon nanotube: A case study on the addition of singlet O <sub>2</sub> . <i>Carbon</i> , 2006, 44, 928-938.	5.4	10
3796	Near-surface alloys for hydrogen fuel cell applications. <i>Catalysis Today</i> , 2006, 111, 52-58.	2.2	148
3797	A density functional study of inhibition of the HDS hydrogenation pathway by pyridine, benzene, and H <sub>2</sub> S on MoS <sub>2</sub> -based catalysts. <i>Catalysis Today</i> , 2006, 111, 44-51.	2.2	93
3798	First-principles calculations of LaNi <sub>4</sub> Alâ€“H solid solution and hydrides. <i>Acta Materialia</i> , 2006, 54, 465-472.	3.8	28
3799	Phase equilibria and thermodynamic limits for partitionless crystallization in the Alâ€“La binary system. <i>Acta Materialia</i> , 2006, 54, 831-840.	3.8	53
3800	Site preference of ternary alloying elements in Ni <sub>3</sub> Al: A first-principles study. <i>Acta Materialia</i> , 2006, 54, 1147-1154.	3.8	130



#	ARTICLE	IF	CITATIONS
3801	Effects of Pt on the elastic properties of B2 NiAl: A combined first-principles and experimental study. <i>Acta Materialia</i> , 2006, 54, 2361-2369.	3.8	30
3802	Interfacial properties of ZrO <sub>2</sub> supported precious metal catalysts: A density functional study. <i>Applied Catalysis A: General</i> , 2006, 305, 102-109.	2.2	24
3803	Spin localization for NO adsorption on surface O atoms of metal oxides. <i>Catalysis Today</i> , 2006, 113, 201-207.	2.2	13
3804	A quantum chemical study of tertiary carbenium ions in acid catalyzed hydrocarbon conversions over phosphotungstic acid. <i>Catalysis Today</i> , 2006, 116, 90-98.	2.2	16
3805	Ab initio molecular dynamics simulations of organometallic reactivity. <i>Coordination Chemistry Reviews</i> , 2006, 250, 1497-1513.	9.5	27
3806	All-boron aromatic clusters as potential new inorganic ligands and building blocks in chemistry. <i>Coordination Chemistry Reviews</i> , 2006, 250, 2811-2866.	9.5	588
3807	Atomic and electronic structures of rubidium adsorption on Si(001)(2 $\times$ 1) surface: Comparison with Cs/Si(001) surface. <i>Chemical Physics</i> , 2006, 323, 383-390.	0.9	3
3808	Sb adsorption on Cu(110), (100), and (111) surfaces. <i>Chemical Physics</i> , 2006, 325, 519-524.	0.9	17
3809	Free tetra- and hexa-coordinated platinum-cyanide dianions, and : A combined photodetachment photoelectron spectroscopic and theoretical study. <i>Chemical Physics</i> , 2006, 329, 230-238.	0.9	22
3810	Adsorption of alkali metals on Ge(001)(2 $\times$ 1) surface. <i>Chemical Physics Letters</i> , 2006, 417, 6-10.	1.2	21
3811	A correlation functional for use with exact exchange in Kohn-Sham density functional theory. <i>Chemical Physics Letters</i> , 2006, 418, 126-131.	1.2	10
3812	Bending the rules: Contrasting vacancy energetics and migration in graphite and carbon nanotubes. <i>Chemical Physics Letters</i> , 2006, 418, 132-136.	1.2	302
3813	Density-functional calculations on DNA-DNA, PNA-DNA and PNA-PNA double strands. <i>Chemical Physics Letters</i> , 2006, 418, 239-244.	1.2	8
3814	Relativistic density-functional study on the dehydrogenation reactivity of PtMCH <sub>2</sub> +(M=Cu,Ag,Au,Pt) toward NH <sub>3</sub> . <i>Chemical Physics Letters</i> , 2006, 418, 386-391.	1.2	22
3815	Comparison of trigonal B <sub>2</sub> O <sub>3</sub> structures with high and low space-group symmetry. <i>Chemical Physics Letters</i> , 2006, 418, 565-568.	1.2	25
3816	Pople versus Dunning basis-sets for group IA metal hydrides and some other second row hydrides: The case against a De Facto standard. <i>Chemical Physics Letters</i> , 2006, 419, 254-258.	1.2	24
3817	Molecular oxygen adsorption on electropositive nano gold tips. <i>Chemical Physics Letters</i> , 2006, 421, 433-438.	1.2	36
3818	Density functional theory study of the structural and optical properties of lithium azide. <i>Chemical Physics Letters</i> , 2006, 422, 117-121.	1.2	39

#	ARTICLE	IF	CITATIONS
3819	The H <sup>2</sup> D isotope effect in the stability of lithium alanate. <i>Chemical Physics Letters</i> , 2006, 423, 102-105.	1.2	21
3820	Bonding nature and magnetism in small MoX <sub>2</sub> (X=O and S) clusters – A comparative study by first principles calculations. <i>Chemical Physics Letters</i> , 2006, 423, 202-207.	1.2	9
3821	The molecular structure of Roesky's sulfoxide – Another computational challenge. <i>Chemical Physics Letters</i> , 2006, 423, 422-426.	1.2	8
3822	Density functional study of CO oxidation on Pt and PtMo. <i>Chemical Physics Letters</i> , 2006, 424, 111-114.	1.2	18
3823	Interplay between theory and experiment in the quest for silica with reduced dimensionality grown on a Mo(112) surface. <i>Chemical Physics Letters</i> , 2006, 424, 115-119.	1.2	27
3824	Computational analysis of the conformations of a doubly linked porphyrin–fullerene dyad. <i>Chemical Physics Letters</i> , 2006, 424, 156-161.	1.2	5
3825	Self-catalyzed hydrogenation and dihydrogen adsorption on titanium carbide nanoparticles. <i>Chemical Physics Letters</i> , 2006, 425, 273-277.	1.2	60
3826	A density functional theory study of Ti-doped NaAlH <sub>4</sub> clusters. <i>Chemical Physics Letters</i> , 2006, 426, 180-186.	1.2	25
3827	Performance of various density functionals for the hydrogen bonds in DNA base pairs. <i>Chemical Physics Letters</i> , 2006, 426, 415-421.	1.2	149
3828	Effects of energetic stability in transport measurements of single benzene-dithiolate by the STM break junction technique. <i>Chemical Physics Letters</i> , 2006, 428, 367-370.	1.2	3
3829	A DFT based ligand field study of the EPR spectra of Co(II) and Cu(II) porphyrins. <i>Chemical Physics Letters</i> , 2006, 427, 449-454.	1.2	18
3830	First-principles study of pentaerythritol tetranitrate single crystals under high pressure: Vibrational properties. <i>Chemical Physics Letters</i> , 2006, 428, 394-399.	1.2	41
3831	The structure of protonated HCP: A classical or non-classical ion?. <i>Chemical Physics Letters</i> , 2006, 429, 23-26.	1.2	7
3832	Density functional theory study of single-wall platinum nanotubes. <i>Chemical Physics Letters</i> , 2006, 430, 319-322.	1.2	9
3833	Double H atom adsorption on a cluster model of a graphite surface. <i>Chemical Physics Letters</i> , 2006, 431, 135-138.	1.2	78
3834	AlGaInN metal-organic-chemical-vapor-deposition gas-phase chemistry in hydrogen and nitrogen diluents: First-principles calculations. <i>Chemical Physics Letters</i> , 2006, 431, 346-351.	1.2	42
3835	Structures of undecagold clusters: Ligand effect. <i>Chemical Physics Letters</i> , 2006, 432, 163-166.	1.2	36
3836	Oxygen influence on the dissociative chemisorption of methane on nickel: A quantum chemical cluster model study. <i>Chemical Physics Letters</i> , 2006, 432, 94-99.	1.2	3

#	ARTICLE	IF	CITATIONS
3837	Parity-violating effects in electron spin resonance g-tensors. <i>Chemical Physics Letters</i> , 2006, 433, 37-42.	1.2	4
3838	Combined EPR and DFT study of the copper(II) complexes with N-phosphoryl thioureas. <i>Chemical Physics</i> , 2006, 320, 59-74.	0.9	19
3839	First principles calculations on Na and K-adsorbed diamond(100) surface. <i>Chemical Physics</i> , 2006, 326, 308-314.	0.9	21
3840	The electronic structure of the dizincocene core. <i>Chemical Physics</i> , 2006, 327, 283-290.	0.9	38
3841	A density functional study of bare and hydrogenated platinum clusters. <i>Chemical Physics</i> , 2006, 331, 9-18.	0.9	39
3842	Density functional theory calculation of 2p core-electron binding energies of Si, P, S, Cl, and Ar in gas-phase molecules. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2006, 151, 9-13.	0.8	28
3843	Asymmetric $\frac{1}{2}$ -1,1-azido bridged copper(II) complex: Synthesis, X-ray structure, magnetic study and DFT calculations. <i>Inorganica Chimica Acta</i> , 2006, 359, 1193-1199.	1.2	66
3844	A DFT and MP2 study of luminescence of gold(I) complexes. <i>Inorganica Chimica Acta</i> , 2006, 359, 3617-3624.	1.2	18
3845	Accurate predictions of the EPR parameters in planar cobalt(II) complexes by hybrid density functional theory. <i>Inorganica Chimica Acta</i> , 2006, 359, 3865-3870.	1.2	6
3846	Adsorption of Na on Ge(001)( $2\times 1$ ) surface. <i>Physica B: Condensed Matter</i> , 2006, 371, 50-55.	1.3	5
3847	Atomic and electronic structures of the Rb-C(100) chemisorption system. <i>Physica B: Condensed Matter</i> , 2006, 383, 219-225.	1.3	5
3848	Electronic structure and half-metallic property of Mn-doped $\beta$ -SiC diluted magnetic semiconductor. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2006, 126, 194-196.	1.7	34
3849	Charged point defects in semiconductors. <i>Materials Science and Engineering Reports</i> , 2006, 55, 57-149.	14.8	115
3850	Ab initio study of point defects in dielectrics based on Pr oxides. <i>Materials Science in Semiconductor Processing</i> , 2006, 9, 897-903.	1.9	1
3851	Thionin adsorption on silicon (1 $\times$ 1): Structural analysis. <i>Applied Surface Science</i> , 2006, 253, 1978-1982.3.1		4
3852	Atomically sharp domain walls of Rb <sub>2</sub> Cd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> langbeinites: 4d electron effects. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2006, 350, 278-282.	0.9	3
3853	First-principles studies on the adsorption of molecular oxygen on Ba(110) surface. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2006, 352, 526-530.	0.9	8
3854	Vibrational properties of molecule and crystal of TATB: A comparative density functional study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2006, 358, 63-69.	0.9	46

#	ARTICLE	IF	CITATIONS
3855	Structural, magnetic and electronic properties of Fe encapsulated by silicon clusters. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2006, 360, 384-389.	0.9	12
3856	Crystal and molecular structure of W <sub>2</sub> (OBut) <sub>6</sub> and electronic structure calculations on various conformers of W <sub>2</sub> (OMe) <sub>6</sub> . <i>Polyhedron</i> , 2006, 25, 827-833.	1.0	4
3857	Theoretical studies of f-d loading and structural diversity in Cp <sub>3</sub> MX (M=Zr, Hf; X=H, CH <sub>3</sub> , OR, NR <sub>2</sub> ) compounds. <i>Polyhedron</i> , 2006, 25, 575-584.	1.0	11
3858	Quantum mechanics based multiscale modeling of stress-induced phase transformations in iron. <i>Journal of the Mechanics and Physics of Solids</i> , 2006, 54, 1276-1303.	2.3	30
3859	Calculation of helium defect clustering properties in iron using a multi-scale approach. <i>Journal of Nuclear Materials</i> , 2006, 351, 109-118.	1.3	83
3860	Formation of pyridine from acetylenes and nitriles catalyzed by RuCpCl, CoCp, and RhCp derivatives – A computational mechanistic study. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4434-4445.	0.8	62
3861	Synthesis and ligand properties towards gold and silver of the ferrocenylamidobenzimidazole ligand. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4181-4188.	0.8	10
3862	Electronic properties and elastic constants of wurtzite, zinc-blende and rocksalt AlN. <i>Journal of Physics and Chemistry of Solids</i> , 2006, 67, 1888-1892.	1.9	49
3863	Theoretical and experimental study of CaWO <sub>4</sub> and SrWO <sub>4</sub> under pressure. <i>Journal of Physics and Chemistry of Solids</i> , 2006, 67, 2164-2171.	1.9	24
3864	The role of orthorhombic distortions in gallium under high hydrostatic pressure. <i>Journal of Physics and Chemistry of Solids</i> , 2006, 67, 2132-2135.	1.9	11
3865	Theoretical study of the scheelite-to-fergusonite phase transition in YLiF <sub>4</sub> under pressure. <i>Journal of Physics and Chemistry of Solids</i> , 2006, 67, 2077-2082.	1.9	3
3866	Pressure induced metallization of Germane. <i>Journal of Physics and Chemistry of Solids</i> , 2006, 67, 2095-2099.	1.9	59
3867	First-principles calculations on the Jahn-Teller distortion in layered LiMnO <sub>2</sub> . <i>Journal of Power Sources</i> , 2006, 158, 1394-1400.	4.0	27
3868	First-principles investigation of Mg(AlH <sub>4</sub> ) <sub>2</sub> complex hydride. <i>Journal of Power Sources</i> , 2006, 159, 111-115.	4.0	30
3869	Synthesis, characterization, and photocatalytic properties of InVO <sub>4</sub> nanoparticles. <i>Journal of Solid State Chemistry</i> , 2006, 179, 804-811.	1.4	86
3870	IR and quantum-chemical studies of carboxylic acid and glycine adsorption on rutile TiO <sub>2</sub> nanoparticles. <i>Journal of Colloid and Interface Science</i> , 2006, 296, 71-78.	5.0	199
3871	Lattice dynamics and electrical properties of wurtzite ZnO determined by a density functional theory method. <i>Journal of Crystal Growth</i> , 2006, 287, 199-203.	0.7	37
3872	Computational study of the relative stabilities of ZnS clusters, for sizes between 1 and 4nm. <i>Journal of Crystal Growth</i> , 2006, 294, 2-8.	0.7	51

#	ARTICLE	IF	CITATIONS
3873	Low-temperature fluorination of fluoro-containing polymers. <i>Journal of Fluorine Chemistry</i> , 2006, 127, 1294-1301.	0.9	16
3874	A DFT overview of high-valent iron, cobalt and nickel tetraamidomacrocyclic ligand (TAML) complexes: The end of innocence?. <i>Journal of Inorganic Biochemistry</i> , 2006, 100, 620-626.	1.5	12
3875	A combined first-principles calculation and thermodynamic modeling of the Fâ€“Kâ€“Na system. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2006, 418, 161-171.	2.6	13
3876	Electronic and structural properties of cementite-type M <sub>3</sub> X (M=Fe, Co, Ni; X=C or B) by first principles calculations. <i>Physica B: Condensed Matter</i> , 2006, 371, 126-132.	1.3	130
3877	Band structure and UV optical spectra of TGS crystals in the range of 4â€“10eV. <i>Physica B: Condensed Matter</i> , 2006, 373, 328-333.	1.3	19
3878	Density functional studies on the ferromagnetic properties of (Zn,Cr)Te. <i>Solid State Communications</i> , 2006, 138, 275-278.	0.9	5
3879	Ab initio calculation of the properties and pressure induced transition of Sn. <i>Solid State Communications</i> , 2006, 140, 538-543.	0.9	37
3880	Growth and decay of the Pd(111)â€“Pd <sub>5</sub> O <sub>4</sub> surface oxide: Pressure-dependent kinetics and structural aspects. <i>Surface Science</i> , 2006, 600, 205-218.	0.8	57
3881	DFT study of the water/MgO(100) interface in acidic and basic media. <i>Surface Science</i> , 2006, 600, 357-365.	0.8	22
3882	Combined STM, LEED and DFT study of Ag(100) exposed to oxygen near atmospheric pressures. <i>Surface Science</i> , 2006, 600, 617-624.	0.8	29
3883	Using $\hat{I}^2$ -hydride elimination to test propositions for characterizing surface catalyzed reactions. <i>Surface Science</i> , 2006, 600, L25-L28.	0.8	12
3884	CO adsorption on the Cu(111) surface: A density functional study. <i>Surface Science</i> , 2006, 600, 1085-1092.	0.8	42
3885	Self-assembled molecular corrals on a semiconductor surface. <i>Surface Science</i> , 2006, 600, 43-47.	0.8	26
3886	Dissociative adsorption and adsorbate-induced reconstruction on Fe{211}. <i>Surface Science</i> , 2006, 600, 1431-1438.	0.8	27
3887	Quantum states of hydrogen (H,D,T) atoms on Cu(100) and (110) surfaces. <i>Surface Science</i> , 2006, 600, 3550-3554.	0.8	11
3888	Adsorption and reactions of HN <sub>3</sub> on Si(100)-2 $\times$ 1: A computational study. <i>Surface Science</i> , 2006, 600, 1113-1124.	0.8	3
3889	First-principles investigation of functionalization-defects on silicon surfaces. <i>Surface Science</i> , 2006, 600, 3892-3897.	0.8	6
3890	Oxygen induced segregation of copper to Ag/Cu(100) surface. <i>Surface Science</i> , 2006, 600, 4103-4107.	0.8	9

#	ARTICLE	IF	CITATIONS
3891	The local adsorption geometry and electronic structure of alanine on Cu{110}. Surface Science, 2006, 600, 1924-1935.	0.8	94
3892	Atomic and electronic structure of Sr/Si(001)-(2 $\times$ 2). Surface Science, 2006, 600, 3614-3618.	0.8	5
3893	NO adsorption and diffusion on unreconstructed Pt{100} surface. A density functional theory investigation. Surface Science, 2006, 600, 2663-2669.	0.8	12
3894	Formation of one-dimensional crystalline silica on a metal substrate. Surface Science, 2006, 600, L164-L168.	0.8	19
3895	Atmospheric effects on the adhesion and friction between non-hydrogenated diamond-like carbon (DLC) coating and aluminum $\hat{\epsilon}$ A first principles investigation. Surface Science, 2006, 600, 2955-2965.	0.8	155
3896	Experimental and theoretical studies of adsorption of on $\hat{\pm}$ -Fe <sub>2</sub> O <sub>3</sub> (0001) surfaces. Surface Science, 2006, 600, 2874-2885.	0.8	17
3897	Hydrogen bonds at metal surfaces: Universal scaling and quantification of substrate effects. Surface Science, 2006, 600, 224-228.	0.8	51
3898	Density functional theory study of hydrogen sulfide dissociation on bi-metallic Ni $\hat{\epsilon}$ Mo catalysts. Surface Science, 2006, 600, 3202-3216.	0.8	28
3899	Kinetic Monte Carlo simulations of the partial oxidation of methanol on oxygen-covered Cu(110). Surface Science, 2006, 600, 3258-3265.	0.8	32
3900	Binding sites for SiH <sub>2</sub> /Si(001): A combined ab initio, tight-binding, and classical investigation. Surface Science, 2006, 600, 4445-4453.	0.8	7
3901	Theoretical studies on the adsorption and decomposition of H <sub>2</sub> O on Pd(111) surface. Surface Science, 2006, 600, 4572-4583.	0.8	85
3902	Initial incorporation of sulfur into the Pd(111) surface: A theoretical study. Surface Science, 2006, 600, 4508-4516.	0.8	13
3903	Thermal regimes of passivative oxide film formation on Al surface: Theoretical and experimental study. Surface Science, 2006, 600, 4796-4800.	0.8	1
3904	The chemisorption of pentacene on Si(001)-2 $\hat{\times}$ 1. Surface Science, 2006, 600, 5092-5103.	0.8	25
3905	Normalization of the effective exchange hole in Becke's nondynamical correlation model: Closed-form analytic representation. Computational and Theoretical Chemistry, 2006, 762, 151-158.	1.5	11
3906	Multiplets of free d- and f-metal ions: A systematic DFT study. Computational and Theoretical Chemistry, 2006, 762, 93-107.	1.5	8
3907	A DFT study of the optical properties of substituted Zn(II)TPP complexes. Computational and Theoretical Chemistry, 2006, 759, 17-24.	1.5	71
3908	Ab initio predictions of the spectroscopic parameters of the germanium halomethylidyne (Ge=C-X; X=F,) Tj ETQq1 1.5 0.784314 rgBT /Ov	1.5	10

#	ARTICLE	IF	CITATIONS
3909	Quantum computations of the UV-visible spectra of uric acid and its anions. Computational and Theoretical Chemistry, 2006, 761, 203-207.	1.5	11
3910	Structure of small $Au_n$ , $Ag_n$ , and $Cu_n$ clusters ( $n=2\text{--}4$ ) on rutile $TiO_2(110)$ : A density functional theory study. Computational and Theoretical Chemistry, 2006, 771, 129-133.	1.5	31
3911	A systematic assessment of density functionals and ONIOM schemes for the study of hydrogen bonding between water and the side chains of serine, threonine, asparagine, and glutamine. Computational and Theoretical Chemistry, 2006, 771, 65-71.	1.5	9
3912	Partial oxidation of methanol on Cu(110): Energetics and kinetics. Computational and Theoretical Chemistry, 2006, 771, 117-122.	1.5	22
3913	Ba adsorption on the $TiO_2(110)$ surface. A density functional study. Computational and Theoretical Chemistry, 2006, 769, 237-242.	1.5	4
3914	Density functional study of closed-shell attractions of (X=N, O, P, S, As, Se) systems. Computational and Theoretical Chemistry, 2006, 773, 15-20.	1.5	5
3915	What is the best theoretical method to study molybdenum dithiolene complexes?. Computational and Theoretical Chemistry, 2006, 773, 59-70.	1.5	20
3916	Electronic structure of dimetalocene molecules: Dizincocene $Zn_2(\eta^5-C_5Me_5)_2$ . Computational and Theoretical Chemistry, 2006, 773, 43-52.	1.5	20
3917	Evolution of the dizincocene metal-metal bond in the series $Zn_2L_2$ where $L=H, CH_3, F, \eta^5-C_5H_5$ . Computational and Theoretical Chemistry, 2006, 776, 113-123.	1.5	17
3918	Glycine adsorption on single-walled carbon nanotubes. Thin Solid Films, 2006, 509, 218-222.	0.8	35
3919	Silicon-metal clusters: Nano-templates for cluster assembled materials. Thin Solid Films, 2006, 515, 1192-1196.	0.8	38
3920	Strongly bonded water monomers on the ice Ih basal plane: Density-functional calculations. Physical Review B, 2006, 74, .	1.1	64
3921	Hydrogen storage capacity of titanium met-cars. Journal of Physics Condensed Matter, 2006, 18, 9509-9517.	0.7	32
3922	Nondissociative Adsorption of $H_2$ Molecules in Light-Element-Doped Fullerenes. Physical Review Letters, 2006, 96, 016102.	2.9	305
3923	Quasiharmonic approximation applied to $LiBH_4$ and its decomposition products. Physical Review B, 2006, 73, .	1.1	51
3924	Structures of 13-atom clusters of fcc transition metals by ab initio and semiempirical calculations. Physical Review B, 2006, 74, .	1.1	64
3925	Heterolytic Splitting of $H_2$ and $CH_4$ on $\gamma$ -Alumina as a Structural Probe for Defect Sites. Journal of Physical Chemistry B, 2006, 110, 23944-23950.	1.2	141
3926	Tetragonal $I41\bar{a}$ crystal structure of $Li_3BN_2$ from dehydrogenated $Li^+Na^+H^-$ . Journal of Applied Physics, 2006, 99, 113523.	1.1	25



#	ARTICLE	IF	CITATIONS
3927	Ab initio calculation of the phase stability in Au-Pd and Ag-Pt alloys. <i>Physical Review B</i> , 2006, 73, .	1.1	116
3928	Hybrid density functional theory investigation of a series of alloxan-based thiosemicarbazones and semicarbazones. <i>Open Chemistry</i> , 2006, 4, .	1.0	3
3929	Unoccupied electronic states in quaterphenyl oligomer films and at the film-gold and film-oxidized silicon interfaces. <i>Technical Physics</i> , 2006, 51, 362-366.	0.2	2
3930	First-principles calculations of phase equilibria and transformation dynamics of Fe-based alloys. <i>Journal of Phase Equilibria and Diffusion</i> , 2006, 27, 47-53.	0.5	20
3931	Amino acid adsorption on single-walled carbon nanotubes. <i>European Physical Journal D</i> , 2006, 38, 117-120.	0.6	62
3932	Ab initio thermodynamics and phase diagram of solid magnesium: A comparison of the LDA and GGA. <i>Journal of Chemical Physics</i> , 2006, 125, 194507.	1.2	38
3934	Acid-based Catalysis in Zeolites Investigated by Density-Functional Methods. <i>Topics in Catalysis</i> , 2006, 37, 41-54.	1.3	46
3935	Special Sites at Noble and Late Transition Metal Catalysts. <i>Topics in Catalysis</i> , 2006, 37, 3-16.	1.3	274
3936	Reactivity of Bimetallic Systems Studied from First Principles. <i>Topics in Catalysis</i> , 2006, 37, 29-39.	1.3	189
3937	Reactivity of the V <sub>2</sub> O <sub>5</sub> /TiO <sub>2</sub> -anatase catalyst: role of the oxygen sites. <i>Topics in Catalysis</i> , 2006, 41, 17-26.	1.3	35
3938	Density Functional Study of the CO Oxidation on a Doped Rutile TiO <sub>2</sub> (110): Effect of Ionic Au in Catalysis. <i>Catalysis Letters</i> , 2006, 107, 143-147.	1.4	107
3939	Modeling of carbon combustion in molecular and atomic oxygen. <i>Combustion, Explosion and Shock Waves</i> , 2006, 42, 247-253.	0.3	3
3940	Computational Design of Silicon Suboxides: Chemical and Mechanical Forces on the Atomic Scale. <i>Journal of Computer-Aided Materials Design</i> , 2006, 13, 185-200.	0.7	4
3941	The electronic structure of Ni doped rutile TiO <sub>2</sub> . <i>Journal of Electroceramics</i> , 2006, 17, 951-953.	0.8	14
3942	The interface electronic structure of thiol terminated molecules on cobalt and gold surfaces. <i>Journal of Materials Science</i> , 2006, 41, 6198-6206.	1.7	22
3943	Nanocrystalline ruthenium oxide and ruthenium in sensing applications – an experimental and theoretical study. <i>Journal of Nanoparticle Research</i> , 2006, 8, 899-910.	0.8	43
3944	Theoretical study of hydrogenation of the doubly aromatic B <sub>7</sub> cluster. <i>Journal of Molecular Modeling</i> , 2006, 12, 569-576.	0.8	49
3945	Density functional study of closed-shell attraction on X(ML) <sub>3</sub> + (X = O, S, Se; M = Au, Ag, Cu) systems. <i>Journal of Molecular Modeling</i> , 2006, 13, 255-265.	0.8	8

#	ARTICLE	IF	CITATIONS
3946	Adsorption of dimers and trimers of Cu, Ag, and Au on regular sites and oxygen vacancies of the MgO(001) surface: a density functional study using embedded cluster models. <i>Applied Physics A: Materials Science and Processing</i> , 2006, 82, 181-189.	1.1	52
3947	Density functional theory simulations of water-metal interfaces: waltzing waters, a novel 2D ice phase, and more. <i>Applied Physics A: Materials Science and Processing</i> , 2006, 85, 415-425.	1.1	150
3948	Structure and Dynamics of Methyl-substituted Beryllocene: [Be(C5Me5)2]. <i>Theoretical Chemistry Accounts</i> , 2006, 116, 480-485.	0.5	6
3949	Adhesion at metal-ZrO2 interfaces. <i>Surface Science Reports</i> , 2006, 61, 303-344.	3.8	173
3950	Converged properties of clean metal surfaces by all-electron first-principles calculations. <i>Surface Science</i> , 2006, 600, 703-715.	0.8	252
3951	Intermediates in the hydrogenation of benzene to cyclohexene on Pt(111) and Pd(111): A comparison from DFT calculations. <i>Surface Science</i> , 2006, 600, 1339-1350.	0.8	79
3952	Methylthiolate adsorption on Au(111): Energetics, vibrational modes and STM imaging. <i>Surface Science</i> , 2006, 600, 4039-4043.	0.8	11
3953	First-principles investigation of Co wires at Pt(111) step-edges. <i>Surface Science</i> , 2006, 600, 4301-4304.	0.8	9
3954	Low temperature adsorption of oxygen on reduced V2O3(0001) surfaces. <i>Surface Science</i> , 2006, 600, 1497-1503.	0.8	55
3955	Studies of growth behavior of tetracene on at submonolayer coverage. <i>Surface Science</i> , 2006, 600, 2002-2006.	0.8	2
3956	EPR properties of Au atoms adsorbed on various sites of the MgO(100) surface from relativistic DFT calculations. <i>Surface Science</i> , 2006, 600, 2434-2442.	0.8	24
3957	Theoretical simulation of butane isomers adsorption on a Pt(100) surface. <i>Surface Science</i> , 2006, 600, 2938-2942.	0.8	5
3958	The self-assembly of metallic nanowires. <i>Surface Science</i> , 2006, 600, L274-L280.	0.8	26
3959	Periodic density functional and tight-binding quantum chemical molecular dynamics study of catalytic properties on $\gamma$ -Al2O3 supported Pt catalysts. <i>Applied Catalysis A: General</i> , 2006, 305, 64-69.	2.2	28
3960	Different support effect of M/ZrO2 and M/CeO2 (M=Pt and Pd) catalysts on CO adsorption: A periodic density functional study. <i>Catalysis Today</i> , 2006, 111, 322-327.	2.2	38
3961	Electron gas-density functional calculations of the repulsive potentials between noble gas atoms and noble metal surfaces. <i>Chemical Physics</i> , 2006, 321, 285-292.	0.9	6
3962	First-principles study of lithium adsorption on Si(100)2 $\times$ 1 and Ge(100)2 $\times$ 1 surface at 1.0 monolayer coverage. <i>Chemical Physics</i> , 2006, 325, 525-530.	0.9	4
3963	First-principles study of Sb adsorption on Ag(110)(2 $\times$ 2). <i>Chemical Physics</i> , 2006, 326, 583-588.	0.9	7

#	ARTICLE	IF	CITATIONS
3964	Absorption spectra of small silver clusters Ag <sub>n</sub> (n=4, 6, 8): A TDDFT study. <i>Chemical Physics</i> , 2006, 327, 261-268.	0.9	40
3965	Avoiding self-repulsion in density functional description of biased molecular junctions. <i>Chemical Physics</i> , 2006, 329, 266-275.	0.9	31
3966	Broken symmetry approach and density functional theory calculations for heterospin system consisting of copper(II) and aminoxyl radicals. <i>Chemical Physics</i> , 2006, 330, 82-89.	0.9	20
3967	Seven clues to the origin and structure of class-I ribonucleotide reductase intermediate X. <i>Journal of Inorganic Biochemistry</i> , 2006, 100, 771-779.	1.5	29
3968	Magnetic properties and electronic structure of GdNi <sub>4</sub> Si compound. <i>Journal of Magnetism and Magnetic Materials</i> , 2006, 305, 348-351.	1.0	12
3969	First-principle molecular-dynamics study of hydrogen adsorption on an aluminum-doped carbon nanotube. <i>Journal of Power Sources</i> , 2006, 163, 125-134.	4.0	19
3970	Effects of Al-doping on the stabilization of monoclinic LiMnO <sub>2</sub> . <i>Journal of Solid State Chemistry</i> , 2006, 179, 1602-1609.	1.4	16
3971	H-MOR: Density functional investigation for the relative strength of Brønsted acid sites and dynamics simulation of NH <sub>3</sub> protonation/deprotonation. <i>Journal of Molecular Catalysis A</i> , 2006, 243, 1-7.	4.8	16
3972	Adsorption on the carbon nanotubes. <i>Frontiers of Physics in China</i> , 2006, 1, 317-322.	1.0	9
3973	Mechanisms of plastic deformation of WC-Co and Ti(C, N)-WC-Co. <i>International Journal of Refractory Metals and Hard Materials</i> , 2006, 24, 135-144.	1.7	93
3974	Strength and reinforcement of interfaces in cemented carbides. <i>International Journal of Refractory Metals and Hard Materials</i> , 2006, 24, 80-88.	1.7	30
3975	A theoretical study of coverage effects for ethylene epoxidation on Cu(111) under low oxygen pressure. <i>Journal of Catalysis</i> , 2006, 243, 404-409.	3.1	41
3976	A density functional theory study of the alkylation of isobutane with butene over phosphotungstic acid. <i>Journal of Catalysis</i> , 2006, 244, 65-77.	3.1	51
3977	Magnetic Properties and Electronic Structure of Cr-Diffused SiC. <i>IEEE Transactions on Magnetics</i> , 2006, 42, 2709-2711.	1.2	2
3978	Al <sub>2</sub> (Mg,Ca) phases in Mg-Al-Ca ternary system: First-principles prediction and experimental identification. <i>Scripta Materialia</i> , 2006, 55, 573-576.	2.6	53
3979	Site preference of transition metal elements in Ni <sub>3</sub> Al. <i>Scripta Materialia</i> , 2006, 55, 433-436.	2.6	133
3980	Effects of Cr on the elastic properties of B <sub>2</sub> NiAl: A first-principles study. <i>Scripta Materialia</i> , 2006, 55, 759-762.	2.6	18
3981	Ab initio study of pressure-induced electronic band structure transition in Ge <sub>50</sub> Sn <sub>50</sub> ordered alloy. <i>Materials Letters</i> , 2006, 60, 1144-1146.	1.3	3

#	ARTICLE	IF	CITATIONS
3982	Electronic structure of some mono-, semi-titanium boride and diboride. <i>Materials Letters</i> , 2006, 60, 1433-1436.	1.3	19
3983	Elastic properties of InAs under pressure up to 18 GPa. <i>Materials Letters</i> , 2006, 60, 3269-3271.	1.3	9
3984	Paramagnetic susceptibility of ferrite and cementite obtained from ab initio calculations. <i>Journal of Magnetism and Magnetic Materials</i> , 2006, 299, 64-69.	1.0	9
3985	First principles study of magnetism in AlPdMn approximant. <i>Journal of Magnetism and Magnetic Materials</i> , 2006, 300, e567-e569.	1.0	2
3986	Reactions of Th and U Atoms with C <sub>2</sub> H <sub>2</sub> : Infrared Spectra and Relativistic Calculations of the Metallacyclopentene, Actinide Insertion, and Ethynyl Products. <i>Chemistry - A European Journal</i> , 2006, 12, 8324-8335.	1.7	37
3987	Computational Modeling of Polyoxotungstates by Relativistic DFT Calculations of <sup>183</sup> W NMR Chemical Shifts. <i>Chemistry - A European Journal</i> , 2006, 12, 8460-8471.	1.7	53
3988	Synthesis and Structure of Ultrathin Aluminosilicate Films. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 7636-7639.	7.2	45
3989	Relationship Between the Nearest-Neighbor Exchange Coupling Constants and the Number of Exchange Interactions in the Cyano-Bridged MnMo <sub>6</sub> (CN) <sub>18</sub> Cluster: Density Functional Theory Calculations. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 2292-2298.	1.0	5
3990	Bonding Trends in Lewis Acid Adducts of S <sub>4</sub> N <sub>4</sub> - X-ray Structure of TeCl <sub>4</sub> ·S <sub>4</sub> N <sub>4</sub> . <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 2951-2958.	1.0	6
3991	Computation of vertical excitation energies of retinal and analogs: Scope and limitations. <i>Journal of Computational Chemistry</i> , 2006, 27, 116-123.	1.5	25
3992	Electronic structure, chemical bonding, and finite-temperature magnetic properties of full Heusler alloys. <i>Journal of Computational Chemistry</i> , 2006, 27, 90-102.	1.5	23
3993	DFT calculations of <sup>57</sup> Fe Mössbauer isomer shifts and quadrupole splittings for iron complexes in polar dielectric media: Applications to methane monooxygenase and ribonucleotide reductase. <i>Journal of Computational Chemistry</i> , 2006, 27, 1292-1306.	1.5	61
3994	A QM/MM study on the aqueous solvation of the tetrahydroxouranyl [UO <sub>2</sub> (OH) <sub>4</sub> ] <sup>2-</sup> complex ion. <i>Journal of Computational Chemistry</i> , 2006, 27, 1156-1162.	1.5	12
3995	On the accuracy of density functional theory for iron-sulfur clusters. <i>Journal of Computational Chemistry</i> , 2006, 27, 1385-1397.	1.5	107
3996	Assessment of the performance of density-functional methods for calculations on iron porphyrins and related compounds. <i>Journal of Computational Chemistry</i> , 2006, 27, 1577-1592.	1.5	78
3997	Berry Pseudorotation Mechanism for the Interpretation of the <sup>19</sup> F NMR Spectrum in PF <sub>5</sub> by Ab Initio Molecular Dynamics Simulations. <i>ChemPhysChem</i> , 2006, 7, 407-413.	1.0	13
3998	Enantiodiscrimination between an N-Acetyl-L-cysteine SAM and Proline: An In Situ Spectroscopic and Computational Study. <i>ChemPhysChem</i> , 2006, 7, 514-523.	1.0	16
3999	Migration of Carbon into Subsurface Layers of Rh(100): A DFT Study. <i>ChemPhysChem</i> , 2006, 7, 1022-1025.	1.0	10

#	ARTICLE	IF	CITATIONS
4000	Acetylene Decomposition on Rh(100): Theory and Experiment. ChemPhysChem, 2006, 7, 1068-1074.	1.0	6
4001	Atom-Molecule Interactions on Transition Metal Surfaces: A DFT Study of CO and Several Atoms on Rh(100), Pd(100) and Ir(100). ChemPhysChem, 2006, 7, 1075-1080.	1.0	7
4002	Novel Superalkali Superhalogen Compounds (Li <sub>3</sub> ) <sup>+</sup> (SH) <sup>-</sup> (SH=LiF <sub>2</sub> , BeF <sub>3</sub> , and BF <sub>4</sub> ) with Aromaticity: New Electrides and Alkalides. ChemPhysChem, 2006, 7, 1136-1141.	1.0	65
4003	Asymmetry Induction by Cooperative Intermolecular Hydrogen Bonds in Surface-Anchored Layers of Achiral Molecules. ChemPhysChem, 2006, 7, 2197-2204.	1.0	46
4004	Hydrocarbon Bond Dissociation Enthalpies: From Substituted Aromatics to Large Polyaromatics. ChemPhysChem, 2006, 7, 2205-2214.	1.0	45
4005	Theoretical Analysis of the Terahertz Spectrum of the High Explosive PETN. ChemPhysChem, 2006, 7, 2398-2408.	1.0	98
4006	Design of the Sandwich-like Compounds Based on the All-Metal Aromatic Unit Al <sub>3</sub> <sup>+</sup> . ChemPhysChem, 2006, 7, 2478-2482.	1.0	17
4007	Ferrocene-Containing Optically Active Liquid-Crystalline Side-Chain Polysiloxanes with Planar Chirality. Advanced Functional Materials, 2006, 16, 260-267.	7.8	79
4008	Defect Formation Energies in Chalcopyrite-Type AgInSe <sub>2</sub> and the Related Chalcopyrite Compounds by First Principles Calculations. , 2006, , .		4
4009	First-Principles Calculation for the Polarity During ZnO Crystals Grown on the C-Terminated 6H-SiC(0001) Surface. Japanese Journal of Applied Physics, 2006, 45, 4926-4928.	0.8	1
4010	TiNi Monatomic Chains Stabilized by Alloying: a First-Principles Study. Chinese Physics Letters, 2006, 23, 182-185.	1.3	6
4011	Analysis of Time-Dependent Density Functional Theory of Transition Wavelengths of Thioaldehydes and Thioketones. Chinese Physics Letters, 2006, 23, 1738-1741.	1.3	1
4012	Thermodynamic modeling of the sodium alanates and the Na-Al-H system. International Journal of Materials Research, 2006, 97, 1484-1494.	0.1	26
4013	Possible graphitic-boron-nitride-based metal-free molecular magnets from first principles study. Journal of Physics Condensed Matter, 2006, 18, 569-575.	0.7	23
4014	The Properties of Co <sub>2</sub> Cr <sub>1-x</sub> Fe <sub>x</sub> Al Heusler Compounds. Lecture Notes in Physics, 2006, , 113-152.	0.3	6
4015	Electronic Structure and Magnetic Property of Mn-Incorporated $\beta$ -SiC(100). Japanese Journal of Applied Physics, 2006, 45, 5560-5562.	0.8	4
4016	First-Principles Study of the Step Oxidation at Vicinal Si(001) Surfaces. Japanese Journal of Applied Physics, 2006, 45, 2144-2147.	0.8	4
4017	Basal-plane slip systems and polymorphic phase transformation in Ti <sub>2</sub> AlC and Ti <sub>2</sub> AlN: a first-principles study. Journal of Physics Condensed Matter, 2006, 18, 6183-6192.	0.7	29

#	ARTICLE	IF	CITATIONS
4018	Computational study of GaAs $_{1-x}$ N $_x$ and GaN $_{1-y}$ As $_y$ alloys and arsenic impurities in GaN. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 10097-10114.	0.7	14
4019	Adsorption of methanol and methoxy on the $\sqrt{3}\times\sqrt{3}$ -Cr $_2$ O $_3$ (0001) surface. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 10751-10763.	0.7	19
4020	Characterization of the electronic properties of YB $_2$ , ZrB $_2$ , and LuB $_2$ using $^{11}\text{B}$ NMR and first-principles calculations. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 2525-2535.	0.7	42
4021	First-principles studies of chiral step reconstructions of Cu(100) by adsorbed glycine and alanine. <i>Journal of Chemical Physics</i> , 2006, 124, 074703.	1.2	44
4022	Electric dipole polarizabilities and C $_6$ dipole-dipole dispersion coefficients for sodium clusters and C $_6$ . <i>Journal of Chemical Physics</i> , 2006, 125, 124306.	1.2	35
4023	The chemisorption of coronene on Si(001)- $2\times 1$ . <i>Journal of Chemical Physics</i> , 2006, 124, 054701.	1.2	19
4024	Formation and interaction of hydrated alkali metal ions at the graphite-water interface. <i>Journal of Chemical Physics</i> , 2006, 125, 014708.	1.2	32
4025	Vibrational lifetimes of molecular adsorbates on metal surfaces. <i>Journal of Chemical Physics</i> , 2006, 125, 054706.	1.2	89
4026	Coexistence of ferroelectricity and ferromagnetism in tantalum clusters. <i>Journal of Chemical Physics</i> , 2006, 125, 114305.	1.2	25
4027	Intensity enhancement of the vibrational spectrum of oxygen when attached to a platinum nanocluster. <i>Journal of Chemical Physics</i> , 2006, 125, 174302.	1.2	1
4028	Size-dependent alternation of magnetoresistive properties in atomic chains. <i>Journal of Chemical Physics</i> , 2006, 125, 121102.	1.2	11
4029	Calculation of nonadiabatic couplings with restricted open-shell Kohn-Sham density-functional theory. <i>Journal of Chemical Physics</i> , 2006, 125, 224103.	1.2	19
4030	Density functional theory study of water adsorption at reduced and stoichiometric ceria (111) surfaces. <i>Journal of Chemical Physics</i> , 2006, 125, 204704.	1.2	61
4031	O $_2$ -coverage-dependent CO oxidation on reduced TiO $_2$ (110): A first principles study. <i>Journal of Chemical Physics</i> , 2006, 125, 144706.	1.2	34
4032	Nature of reactive O $_2$ and slow CO $_2$ evolution kinetics in CO oxidation by TiO $_2$ supported Au cluster. <i>Journal of Chemical Physics</i> , 2006, 125, 144714.	1.2	8
4033	Calculation of nuclear magnetic resonance shieldings using frozen-density embedding. <i>Journal of Chemical Physics</i> , 2006, 125, 194104.	1.2	69
4034	Thiol and thiolate bond formation of ferrocene-1,1-dithiol to a Ag(111) surface. <i>Journal of Chemical Physics</i> , 2006, 125, 194705.	1.2	7
4035	Role of Heme Iron Coordination and Protein Structure in the Dynamics and Geminate Rebinding of Nitric Oxide to the H93G Myoglobin Mutant. <i>Journal of Biological Chemistry</i> , 2006, 281, 10389-10398.	1.6	28

#	ARTICLE	IF	CITATIONS
4036	Structural characterization of a new layered-ternary Ta <sub>4</sub> AlC <sub>3</sub> ceramic. Journal of Materials Research, 2006, 21, 2587-2592.	1.2	72
4037	A Theoretical Study of the Effect of Eu ion Dopant on the Electronic Excitations of Yttrium Oxide and Yttrium Oxy-Sulphide. Japanese Journal of Applied Physics, 2006, 45, 5782-5785.	0.8	3
4038	Molecular dynamics study of the ternary compound Li <sub>3</sub> AlB <sub>2</sub> O <sub>6</sub> . Chinese Physics B, 2006, 15, 428-431.	1.3	2
4039	Reaction Energy for LiMn[sub 2]O[sub 4] Spinel Dissolution in Acid. Electrochemical and Solid-State Letters, 2006, 9, A265.	2.2	76
4040	Structural, electronic, and magnetic properties of FeSi: hybrid functionals and non-local exchange. Journal of Physics Condensed Matter, 2006, 18, 7437-7447.	0.7	19
4041	Computation of Bond Dissociation Energies for Removal of Nitrogen Dioxide Groups in Certain Aliphatic Nitro Compounds. Chinese Physics Letters, 2006, 23, 819-821.	1.3	4
4042	First-principle Thoery of Phase Stability, Phase Equilibria and Phase Transition of Ordered Compounds. Materials Research Society Symposia Proceedings, 2006, 980, 1.	0.1	0
4043	Adsorption of Methane on the (100) Surface of MgO: Insight into Surface-Adsorbate and Adsorbate-Adsorbate Interactions from First-Principles Calculations. Materials Research Society Symposia Proceedings, 2006, 928, 1.	0.1	1
4044	H Adsorption On Rh (110) Surface. Materials Research Society Symposia Proceedings, 2006, 927, 1.	0.1	0
4045	Ab initio characterization of the electronic and optical properties of a new IR nonlinear optical crystal: K <sub>3</sub> V <sub>5</sub> O <sub>14</sub> . Journal of Physics Condensed Matter, 2006, 18, 5535-5544.	0.7	5
4046	Stability and electronic structure of InN nanotubes from first-principles study. Chinese Physics B, 2006, 15, 798-801.	1.3	6
4047	Deformation Mechanism of Nanocrystalline Al-Fe Alloys by Analysis from Ab-Initio Calculations. Materials Science Forum, 2006, 503-504, 209-214.	0.3	10
4048	Could the relaxed and the O-deficient CrO <sub>2</sub> (100) surface retain half-metallicity?. Applied Physics Letters, 2006, 88, 121903.	1.5	9
4049	Deformation modes and ideal strengths of ternary layered Ti <sub>2</sub> AlC and Ti <sub>2</sub> AlN from first-principles calculations. Physical Review B, 2006, 73, .	1.1	78
4050	Role of Lateral Alkyl Chains in Modulation of Molecular Structures on Metal Surfaces. Physical Review Letters, 2006, 96, 226101.	2.9	51
4051	Bonding nature of metal/oxide incoherent interfaces by first-principles calculations. Physical Review B, 2006, 74, .	1.1	55
4052	First-principles calculations of the adsorption and hydrogenation reactions of CH <sub>x</sub> (x=0,4) species on a Fe(100) surface. Physical Review B, 2006, 73, .	1.1	88
4053	Neutral and negatively charged Al <sub>12</sub> X(X=Si, Ge, Sn, Pb) clusters studied from first principles. Physical Review B, 2006, 74, .	1.1	43



#	ARTICLE	IF	CITATIONS
4054	Magic Structures and Quantum Conductance of [110] Silver Nanowires. <i>Physical Review Letters</i> , 2006, 96, 096104.	2.9	47
4055	Ab initio simulations in liquid caesium at high pressure and temperature. <i>Physical Review B</i> , 2006, 73, .	1.1	28
4056	DFT Study of the Effect of Temperature on ZnO Adsorbed on $\alpha$ -Al <sub>2</sub> O <sub>3</sub> (0001) Surface. <i>Chinese Journal of Chemical Physics</i> , 2006, 19, 137-142.	0.6	3
4057	Model of annealing-induced short-range order effects in (GaIn)(NP) alloys. <i>Physical Review B</i> , 2006, 74, .	1.1	8
4058	Relaxation effects on the magnetism of decorated step edges: Co/Pt(664). <i>Physical Review B</i> , 2006, 73, .	1.1	28
4059	Atomistic deformation modes and intrinsic brittleness of Al <sub>4</sub> SiC <sub>4</sub> : A first-principles investigation. <i>Physical Review B</i> , 2006, 74, .	1.1	57
4060	Possible ground-state structure of Au <sub>26</sub> : A highly symmetric tubelike cage. <i>Journal of Chemical Physics</i> , 2006, 124, 114310.	1.2	67
4061	Metastability of single-bonded cubic-gauche structure of N under ambient pressure. <i>Physical Review B</i> , 2006, 73, .	1.1	30
4062	Ab initio study of biphenyl chemisorption on Si(001): Configurational stability. <i>Physical Review B</i> , 2006, 73, .	1.1	25
4063	Theoretical examination of whether phonon dispersion in Nb <sub>3</sub> Sn is anomalous. <i>Physical Review B</i> , 2006, 74, .	1.1	11
4064	Impact of nitridation on open volumes in HfSiO <sub>x</sub> studied using monoenergetic positron beams. <i>Applied Physics Letters</i> , 2006, 88, 171912.	1.5	10
4065	Two-Dimensional Roughening of Adsorbate Islands in Thermodynamic Equilibrium. <i>Physical Review Letters</i> , 2006, 96, 166102.	2.9	7
4066	Understanding and controlling the weakly interacting interface in perylene/Ag(110). <i>Physical Review B</i> , 2006, 73, .	1.1	29
4067	Local-orbital occupancy formulation of density functional theory: Application to Si, C, and graphene. <i>Physical Review B</i> , 2006, 73, .	1.1	26
4068	Symmetry-mediated H <sub>2</sub> O diffusion on Al{100}. <i>Physical Review B</i> , 2006, 74, .	1.1	11
4069	Bonding Trends and Dimensionality Crossover of Gold Nanoclusters on Metal-Supported MgO Thin Films. <i>Physical Review Letters</i> , 2006, 97, 036106.	2.9	268
4070	Multidimensional Effects on Dissociation of N <sub>2</sub> on Ru(0001). <i>Physical Review Letters</i> , 2006, 96, 096102.	2.9	89
4071	Spontaneous symmetry breaking of the r(100) $\sqrt{5} \times \sqrt{1}$ hex surface induced by hydrogen adsorption. <i>Physical Review B</i> , 2006, 74, .	1.1	13

#	ARTICLE	IF	CITATIONS
4072	Chemical tuning of band alignments for metal gate/high- $\epsilon$ oxide interfaces. <i>Physical Review B</i> , 2006, 73, .	1.1	40
4073	Theoretical study of the $\text{YLiF}_4$ phase transitions under pressure. <i>Physical Review B</i> , 2006, 73, .	1.1	13
4074	Oxygen-Deficient Line Defects in an Ultrathin Aluminum Oxide Film. <i>Physical Review Letters</i> , 2006, 97, 046101.	2.9	123
4075	First-principles investigation of the $\text{WC}/\text{HfO}_2$ interface properties. <i>Journal of Applied Physics</i> , 2006, 99, 084104.	1.1	11
4076	Surface electronic structures of $\text{La}(0001)$ and $\text{Lu}(0001)$ . <i>Physical Review B</i> , 2006, 73, .	1.1	21
4077	Adsorption of water on chlorine-terminated $\text{Si}(111)$ from first principles: Substrate-induced ordering versus intermolecular interactions. <i>Physical Review B</i> , 2006, 73, .	1.1	5
4078	Linear and nonlinear optical properties of $\text{Li}$ under pressure. <i>Physical Review B</i> , 2006, 73, .	1.1	9
4079	Ferromagnetism in $\text{Mg}$ -doped $\text{AlN}$ from ab initio study. <i>Applied Physics Letters</i> , 2006, 89, 142501.	1.5	104
4080	Stabilization mechanism of $\text{Si}_{12}$ cage clusters by encapsulation of a transition-metal atom: A density-functional theory study. <i>Physical Review B</i> , 2006, 74, .	1.1	60
4081	Oxygen-induced step bunching and faceting of $\text{Rh}(553)$ : Experiment and ab initio calculations. <i>Physical Review B</i> , 2006, 74, .	1.1	71
4082	Structural transitions in indium under high pressure: Ab initio electronic structure calculations. <i>Physical Review B</i> , 2006, 74, .	1.1	18
4083	Energetics of $\text{CO}$ on stepped and kinked $\text{Cu}$ surfaces: A comparative theoretical study. <i>Physical Review B</i> , 2006, 74, .	1.1	29
4084	Electronic structure and magnetic coupling in $\text{FeSbO}_4$ : A DFT study using hybrid functionals and GGA+ $U$ methods. <i>Physical Review B</i> , 2006, 73, .	1.1	43
4085	First principles calculations of oxygen vacancy passivation by fluorine in hafnium oxide. <i>Applied Physics Letters</i> , 2006, 89, 152904.	1.5	36
4086	DFT Investigation of $\text{O}_2$ Adsorption on $\text{Si}(001)$ - $(221)$ :H. <i>Chinese Journal of Chemical Physics</i> , 2006, 19, 485-487.	0.6	3
4087	Effects of $\text{Ge}$ content on the diffusion of group-V dopants in $\text{SiGe}$ alloys. <i>Applied Physics Letters</i> , 2006, 88, 173502.	1.5	16
4088	Ab initio studies on the reaction of $\text{O}_2$ with $\text{Ba}_n$ ( $n=2,5$ ) clusters. <i>Journal of Chemical Physics</i> , 2006, 124, 224711.	1.2	6
4089	Extended lattice gas interactions of $\text{Cu}$ on $\text{Cu}(111)$ and $\text{Cu}(001)$ : Ab initio evaluation and implications. <i>Physical Review B</i> , 2006, 73, .	1.1	34

#	ARTICLE	IF	CITATIONS
4090	Nanocables made of a transition metal wire and boron nitride sheath: Density functional calculations. <i>Physical Review B</i> , 2006, 74, .	1.1	24
4091	Surface and interface structures of epitaxial ZrO <sub>2</sub> films on Pt(111): Experiment and density-functional theory calculations. <i>Physical Review B</i> , 2006, 74, .	1.1	24
4092	Theoretical analysis of highly spin-polarized transport in the iron nitride Fe <sub>4</sub> N. <i>Physical Review B</i> , 2006, 73, .	1.1	186
4093	Ordering tendencies in the binary alloys of Rh, Pd, Ir, and Pt: Density functional calculations. <i>Physical Review B</i> , 2006, 74, .	1.1	31
4094	On the structure and chemical bonding of Si <sub>6</sub> and Si <sub>6</sub> in NaSi <sub>6</sub> upon Na <sup>+</sup> coordination. <i>Journal of Chemical Physics</i> , 2006, 124, 124305.	1.2	28
4095	Effects of Al addition on the native defects in hafnia. <i>Applied Physics Letters</i> , 2006, 88, 182903.	1.5	24
4096	Spin-dependent electronic structure of transition-metal atomic chains adsorbed on single-wall carbon nanotubes. <i>Physical Review B</i> , 2006, 74, .	1.1	41
4097	Ga-rich GaAs(001) surface from ab initio calculations: Atomic structure of the (4 $\times$ 6) and (6 $\times$ 6) reconstructions. <i>Physical Review B</i> , 2006, 73, .	1.1	19
4098	Atomic structure and spin magnetism of self-assembled Co nanowires on Pt(332). <i>Physical Review B</i> , 2006, 74, .	1.1	3
4099	Fe <sub>3</sub> O <sub>4</sub> (001) films on Fe(001): Termination and reconstruction of iron-rich surfaces. <i>Physical Review B</i> , 2006, 74, .	1.1	63
4100	First-principles potential energy surfaces and vibrational states of H <sub>2</sub> and D <sub>2</sub> on Rh(111) at 0.25 and 1 monolayer coverages. <i>Journal of Applied Physics</i> , 2006, 99, 113704.	1.1	5
4101	Vibrational spectra of ammonia, benzene, and benzene adsorbed on Si(001) by first principles calculations with periodic boundary conditions. <i>Physical Review B</i> , 2006, 73, .	1.1	46
4102	Effect of coadsorption and Ru alloying on the adsorption of CO on Pt. <i>Physical Review B</i> , 2006, 74, .	1.1	38
4103	Ab initio and tight-binding calculations of noncollinear magnetism in manganese clusters. <i>Physical Review B</i> , 2006, 73, .	1.1	13
4104	Quantum dynamical study of the H <sub>2</sub> and D <sub>2</sub> dissociative adsorption and diffraction from the NiAl(110) alloy surface. <i>Physical Review B</i> , 2006, 73, .	1.1	24
4105	Dihydrogen bonding, p-type conductivity, and origin of change in work function of hydrogenated diamond (001) surfaces. <i>Physical Review B</i> , 2006, 74, .	1.1	10
4106	Non-free-electron momentum- and thickness-dependent evolution of quantum well states in the Cu <sub>2</sub> CoCu(001) system. <i>Physical Review B</i> , 2006, 73, .	1.1	14
4107	First-principles thermoelasticity of bcc iron under pressure. <i>Physical Review B</i> , 2006, 74, .	1.1	55

#	ARTICLE	IF	CITATIONS
4108	Structure, energetics, and vibrational spectra of perylene adsorbed on Si(001): First-principles calculations compared with STM and HREELS. <i>Physical Review B</i> , 2006, 74, .	1.1	12
4109	Calculations of hydrogen coverage on single-walled carbon nanotubes: Dependence on nanotube size, temperature, and pressure. <i>Physical Review B</i> , 2006, 74, .	1.1	28
4110	Comparative study of Ag, Au, Pd, and Pt adsorption on Mo and Ta(112) surfaces. <i>Physical Review B</i> , 2006, 74, .	1.1	10
4111	Fermi level alignment in molecular nanojunctions and its relation to charge transfer. <i>Physical Review B</i> , 2006, 74, .	1.1	84
4112	Influence of local electron interactions on phonon spectrum in iron. <i>Physical Review B</i> , 2006, 74, .	1.1	13
4113	First-principles study of lattice dynamics and diffusion in DO <sub>3</sub> -type Fe <sub>3</sub> Si. <i>Physical Review B</i> , 2006, 73, .	1.1	34
4114	Electron transport in a Pt-CO-Pt nanocontact: Density functional theory calculations. <i>Physical Review B</i> , 2006, 73, .	1.1	28
4115	Stability of conductance oscillations in monatomic sodium wires. <i>Physical Review B</i> , 2006, 74, .	1.1	17
4116	Energy gradients with respect to atomic positions and cell parameters for the Kohn-Sham density-functional theory at the $\Gamma^c$ point. <i>Journal of Chemical Physics</i> , 2006, 124, 224107.	1.2	2
4117	N doping of TiO <sub>2</sub> (110): Photoemission and density-functional studies. <i>Journal of Chemical Physics</i> , 2006, 125, 094706.	1.2	127
4118	The energetics and structure of rutile TiO <sub>2</sub> (110). <i>Journal of Physics Condensed Matter</i> , 2006, 18, 4207-4217.	0.7	69
4119	Kinetic-Anisotropy-Induced Ordering-Orientation Transition in Epitaxial Growth: A Method to Synthesize Ordering-Orientation Superlattices. <i>Physical Review Letters</i> , 2006, 97, 126105.	2.9	5
4120	The chemisorption of dibenzo[a,j]coronene on Si(001)-2 $\times$ 1. <i>Journal of Chemical Physics</i> , 2006, 124, 224708.	1.2	10
4121	Proton Diffusion Mechanism in Amorphous SiO <sub>2</sub> . <i>Physical Review Letters</i> , 2006, 97, 155901.	2.9	62
4122	Chemical Reactivity of Ni-Rh Nanowires. <i>Physical Review Letters</i> , 2006, 97, 126102.	2.9	42
4123	Electrostrictive deformations in small carbon clusters, hydrocarbon molecules, and carbon nanotubes. <i>Physical Review A</i> , 2006, 74, .	1.0	5
4124	High-density limit of the Perdew-Burke-Ernzerhof generalized gradient approximation and related density functionals. <i>Physical Review A</i> , 2006, 74, .	1.0	52
4125	Structural Stabilities and Electronic Structures of Ga Atomic Chains. <i>Chinese Journal of Chemical Physics</i> , 2006, 19, 219-222.	0.6	2

#	ARTICLE	IF	CITATIONS
4126	Selective Analysis of Molecular States by Functionalized Scanning Tunneling Microscopy Tips. <i>Physical Review Letters</i> , 2006, 96, 156102.	2.9	44
4127	Martensitic fcc-to-hcp Transformations in Solid Xenon under Pressure: A First-Principles Study. <i>Physical Review Letters</i> , 2006, 96, 035504.	2.9	33
4128	Ab initio density-functional study of NO on close-packed transition and noble metal surfaces: I. Molecular adsorption. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 13-40.	0.7	85
4129	Comment on "Structural Stability of Complex Hydrides: LiBH <sub>4</sub> Revisited" <i>Physical Review Letters</i> , 2006, 97, 119601; author reply 119602.	2.9	16
4130	Epitaxial Stabilization of Ferromagnetism in the Nanophase of FeGe. <i>Physical Review Letters</i> , 2006, 96, 127201.	2.9	19
4131	Low Photoemission Intensity near E <sub>F</sub> Induced by the Surface Relaxed Structure of CrO <sub>2</sub> (001). <i>Physical Review Letters</i> , 2006, 96, 167206.	2.9	10
4132	Formation kinetics of the Mo(100)-Ag <sub>2</sub> (2 $\times$ 2) surface alloy. <i>Physical Review B</i> , 2006, 74, .	1.1	7
4133	Density functional study of $\alpha$ -CrCl <sub>2</sub> : Structural, electronic, and magnetic properties. <i>Physical Review B</i> , 2006, 74, .	1.1	14
4134	High-order correlation effects on dynamic hyperpolarizabilities and their geometric derivatives: A comparison with density functional results. <i>Journal of Chemical Physics</i> , 2006, 124, 114101.	1.2	46
4135	First-principles calculations of the electronic band structure of In <sub>4</sub> Sn <sub>3</sub> O <sub>12</sub> and In <sub>5</sub> SnSbO <sub>12</sub> . <i>Journal of Applied Physics</i> , 2006, 99, 023706.	1.1	14
4136	First-principles calculations for the structural stabilities of ordered Nb <sub>4</sub> clusters on the Cu(111) surface. <i>Physical Review B</i> , 2006, 73, .	1.1	16
4137	Tuning the surface metal work function by deposition of ultrathin oxide films: Density functional calculations. <i>Physical Review B</i> , 2006, 73, .	1.1	231
4138	Multiple adsorption configurations of NH <sub>3</sub> molecules on the Si(001) surface. <i>Physical Review B</i> , 2006, 73, .	1.1	33
4139	Quantum Monte Carlo study of the Ne atom and the Ne <sup>+</sup> ion. <i>Journal of Chemical Physics</i> , 2006, 124, 224104.	1.2	35
4140	Optical functions of KTaO <sub>3</sub> as determined by spectroscopic ellipsometry and comparison with band structure calculations. <i>Physical Review B</i> , 2006, 74, .	1.1	58
4141	Stability of Ti in NaAlH <sub>4</sub> . <i>Applied Physics Letters</i> , 2006, 88, 161917.	1.5	32
4142	Structural, magnetic, and chemical properties of thin Fe films grown on Rh(100) surfaces investigated with density functional theory. <i>Physical Review B</i> , 2006, 73, .	1.1	16
4143	h-BN monolayer adsorption on the Ni(111) surface: A density functional study. <i>Physical Review B</i> , 2006, 74, .	1.1	61

#	ARTICLE	IF	CITATIONS
4144	Ab initiomolecular dynamics simulations on structural change of liquid eutectic alloyGe <sub>15</sub> Te <sub>85</sub> from573to1073K. Physical Review B, 2006, 74, .	1.1	11
4145	Structural and magnetic stabilities of cubic and orthorhombic phases of CeMnNi <sub>4</sub> . Applied Physics Letters, 2006, 89, 222502.	1.5	11
4146	Atomic structure of a thin silica film on aMo(112)substrate: A combined experimental and theoretical study. Physical Review B, 2006, 73, .	1.1	61
4147	Comparative NMR study of hybridization effect and structural stability inD022-typeNbAl <sub>3</sub> andNbGa <sub>3</sub> . Physical Review B, 2006, 74, .	1.1	31
4148	Vibrational assignments and line shapes in inelastic tunneling spectroscopy: H onCu(100). Physical Review B, 2006, 74, .	1.1	8
4149	Adsorption of phenylglycine on copper: Density functional calculations. Physical Review B, 2006, 74, .	1.1	17
4150	Electronic structure and optical properties of layered perovskitesSr <sub>2</sub> MO <sub>4</sub> (M=Ti, V, Cr, and Mn): Anab initio study. Physical Review B, 2006, 74, .	1.1	32
4151	Influence of electronic correlations on the ground-state properties of cerium dioxide. Journal of Chemical Physics, 2006, 124, 234711.	1.2	30
4152	Structure of Au <sub>8</sub> : Planar or nonplanar?. Journal of Chemical Physics, 2006, 124, 024316.	1.2	84
4153	Electronic state of interstitial Cu in bulk Si: Density functional calculations. Physical Review B, 2006, 73, .	1.1	11
4154	Clean and pyrrole-functionalized Si- and C-terminated SiC surfaces: First-principles calculations of geometry and energetics compared with LEED and XPS. Physical Review B, 2006, 74, .	1.1	16
4155	Orbital-dependent nonlocal correlation energy functional constructed from a Jastrow function: Application to atoms and ions. Physical Review A, 2006, 73, .	1.0	3
4156	Unusual adsorption site of hydrogen on the unreconstructed Ir(100) surface. Physical Review B, 2006, 73, .	1.1	67
4157	Complex adsorbate-substrate interplay of H onIr(100)̂ <sup>~</sup> (5̂-1)-hex: Density functional calculations. Physical Review B, 2006, 74, .	1.1	10
4158	Adsorption of fullerenesC <sub>n</sub> (n=32,36,40,44,48,60)on theGaAs(001)̂ <sup>~</sup> c(4̂-4)reconstructed surface. Physical Review B, 2006, 73, .	1.1	5
4159	Importance of charging in atomic resolution scanning tunneling microscopy: Study of a single phosphorus atom in aSi(001)surface. Physical Review B, 2006, 74, .	1.1	14
4160	First-principles prediction of the mechanical properties and electronic structure of ternary aluminum carbideZr <sub>3</sub> Al <sub>3</sub> C <sub>5</sub> . Physical Review B, 2006, 73, .	1.1	67
4161	Interface reconstruction ofMSi <sub>2</sub> ̂ <sup>•</sup> Si(001)(M=Co,Ni)from first principles. Physical Review B, 2006, 74, .	1.1	10

#	ARTICLE	IF	CITATIONS
4162	From local hybrid functionals to $\epsilon$ -localized local hybrid $\epsilon$ -potentials: Formalism and thermochemical tests. <i>Journal of Chemical Physics</i> , 2006, 124, 204102.	1.2	64
4163	Geometrical and electronic structures of $\text{Au}_m\text{Ag}_n$ ( $2 \leq m+n \leq 8$ ). <i>Journal of Chemical Physics</i> , 2006, 125, 014303.	1.2	55
4164	Crystal growth and elastic properties of orthorhombic $\text{Bi}_2\text{Ga}_4\text{O}_9$ . <i>Journal of Physics Condensed Matter</i> , 2006, 18, 10977-10988.	0.7	27
4165	FIRST PRINCIPLES CALCULATIONS OF ADSORPTION AND DIFFUSION OF Ba ON A RECONSTRUCTED Si(001) SURFACE. <i>Surface Review and Letters</i> , 2006, 13, 365-368.	0.5	2
4166	Ab initio study of molecular adsorption on hydrogenated diamond (001) surfaces. <i>Journal of Physics: Conference Series</i> , 2006, 29, 145-149.	0.3	14
4167	Optimization of ionic conductivity in doped ceria. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 3518-3521.	3.3	464
4168	FIRST-PRINCIPLES STUDY OF THE ELECTRONIC PROPERTIES OF GaAs(114)A ( $2 \times 1$ ) SURFACE. <i>Modern Physics Letters B</i> , 2006, 20, 1275-1285.	1.0	1
4169	Flip-flop Motion of Circular Hydrogen Bond Array in Thiocalix[4]arene. <i>Supramolecular Chemistry</i> , 2006, 18, 371-381.	1.5	14
4170	Modulation of band structure in wurtzite ZnO via site-selective Ga-N codoping. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 6281-6287.	0.7	2
4171	Accurate and efficient method for the treatment of exchange in a plane-wave basis. <i>Journal of Chemical Physics</i> , 2006, 124, 064105.	1.2	87
4172	Electronic, linear, and nonlinear optical properties of III-V indium compound semiconductors. <i>Journal of Chemical Physics</i> , 2006, 125, 034710.	1.2	47
4173	Structural distortion and electronic properties of NiO under high pressure: an ab initio GGA+U study. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 9691-9701.	0.7	8
4174	Ab initio density-functional study of NO adsorption on close-packed transition and noble metal surfaces: II. Dissociative adsorption. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 41-54.	0.7	47
4175	The ferroelectric and cubic phases in $\text{BaTiO}_3$ ferroelectrics are also antiferroelectric. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 14695-14700.	3.3	119
4176	AB INITIO TEMPERATURE-DEPENDENT SIMULATION OF ZnO ADSORBED ON THE $\alpha\text{-Al}_2\text{O}_3$ (0001) SURFACE. <i>Surface Review and Letters</i> , 2006, 13, 27-33.	0.5	2
4177	Vibrational spectra of vitreous $\text{SiO}_2$ and vitreous $\text{GeO}_2$ from first principles. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 415112.	0.7	30
4178	THE ADSORPTION OF Au ON Si(111)- $7 \times 7$ SURFACE: A FIRST-PRINCIPLES STUDY. <i>Surface Review and Letters</i> , 2007, 14, 657-660.	0.5	5
4179	A THEORETICAL INVESTIGATION OF STRUCTURAL, SPECTROSCOPIC AND THERMODYNAMIC PROPERTIES OF CYCLODECANE. <i>Journal of Theoretical and Computational Chemistry</i> , 2007, 06, 281-299.	1.8	4



#	ARTICLE	IF	CITATIONS
4180	A DFT INVESTIGATION OF SULFUR ADSORPTION ON Ir(100). Journal of Theoretical and Computational Chemistry, 2007, 06, 177-185.	1.8	2
4181	FIRST-PRINCIPLES STUDY OF ADSORPTION OF CN ON Cu(111). Journal of Theoretical and Computational Chemistry, 2007, 06, 523-529.	1.8	3
4182	ELECTRONIC STRUCTURES OF S-DOPED ANATASE AND RUTILE TiO <sub>2</sub> . Journal of Theoretical and Computational Chemistry, 2007, 06, 23-32.	1.8	7
4183	First-Principles Investigations of Electrochemical Oxidation of Hydrogen at Solid Oxide Fuel Cell Operating Conditions. Journal of the Electrochemical Society, 2007, 154, B919.	1.3	43
4184	Simulating Molecular Properties of Liquid Crystals. Advances in Chemical Physics, 2007, , 39-113.	0.3	16
4185	<i>Ab initio</i> calculations of structural, elastic and electronic properties of Li <sub>2</sub> O <sub>2</sub> . Philosophical Magazine, 2007, 87, 3373-3383.	0.7	17
4186	Experimental observation of quantum oscillation of surface chemical reactivities. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 9204-9208.	3.3	123
4187	A thermochemically competitive local hybrid functional without gradient corrections. Journal of Chemical Physics, 2007, 126, 011103.	1.2	113
4188	Effects of coverage on the structures, energetics, and electronics of oxygen adsorption on RuO <sub>2</sub> (110). Journal of Chemical Physics, 2007, 127, 064706.	1.2	42
4189	Structural properties of amorphous GeSe <sub>2</sub> . Journal of Physics Condensed Matter, 2007, 19, 415111.	0.7	10
4190	Band structure and optical spectra of ferroelectric triglycine sulphate. Phase Transitions, 2007, 80, 31-37.	0.6	6
4191	DYNAMICS OF DIFFUSION AND ADSORPTION: ZnO/±Al <sub>2</sub> O <sub>3</sub> (0001). Modern Physics Letters B, 2007, 21, 645-654.	1.0	1
4192	ADSORPTION, DIFFUSION AND GROWTH MODE OF ZnO THIN FILM FROM FIRST PRINCIPLES. International Journal of Modern Physics B, 2007, 21, 1891-1901.	1.0	2
4193	Polynitrogen/Nanoaluminum Surface Interactions. , 2007, , .		0
4194	Interatomic bonds and the tensile anisotropy of trialuminides in the elastic limit: a density functional study for Al <sub>3</sub> (Sc,±Ti,±V,±Cr). Philosophical Magazine, 2007, 87, 1769-1794.	0.7	24
4195	Mineralogy of the Earth “ Phase Transitions and Mineralogy of the Lower Mantle. , 2007, , 33-62.		30
4196	Structure, energetics, and bonding of amorphous Au±Si alloys. Journal of Chemical Physics, 2007, 127, 224710.	1.2	27
4197	First-principles study of hydrogen-passivated single-crystalline silicon nanotubes: electronic and optical properties. Nanotechnology, 2007, 18, 505707.	1.3	17

#	ARTICLE	IF	CITATIONS
4198	Isotope quantum effects in the electron momentum density of water. <i>Journal of Chemical Physics</i> , 2007, 126, 154508.	1.2	25
4199	On the structure of the first hydration layer on NaCl(100): Role of hydrogen bonding. <i>Journal of Chemical Physics</i> , 2007, 126, 214707.	1.2	14
4200	Interaction of oxygen with TiN(001): N <sup>15</sup> O exchange and oxidation process. <i>Journal of Chemical Physics</i> , 2007, 126, 244713.	1.2	51
4201	Oxygen adsorption on Mo(112) surface studied by ab initio genetic algorithm and experiment. <i>Journal of Chemical Physics</i> , 2007, 126, 234710.	1.2	37
4202	Kinetic Monte Carlo simulations of the interaction of oxygen with Pt(111). <i>Journal of Chemical Physics</i> , 2007, 127, 014704.	1.2	36
4203	Density functional theory study of CH <sub>x</sub> (x=1-3) adsorption on clean and CO precovered Rh(111) surfaces. <i>Journal of Chemical Physics</i> , 2007, 127, 024705.	1.2	18
4204	Xe <sup>129</sup> chemical shift by the perturbational relativistic method: Xenon fluorides. <i>Journal of Chemical Physics</i> , 2007, 127, 084312.	1.2	33
4205	Time-dependent density functional theory calculation of van der Waals coefficient of sodium clusters. <i>Journal of Chemical Physics</i> , 2007, 127, 134103.	1.2	23
4206	Vibrational lifetimes of cyanide and carbon monoxide on noble and transition metal surfaces. <i>Journal of Chemical Physics</i> , 2007, 127, 154303.	1.2	37
4207	Dissociative chemisorption of H <sub>2</sub> on the Cu(110) surface: A quantum and quasiclassical dynamical study. <i>Journal of Chemical Physics</i> , 2007, 127, 164722.	1.2	36
4208	Biatomic substrates for bulk-molecule interfaces: The PtCo-oxygen interface. <i>Journal of Chemical Physics</i> , 2007, 127, 244706.	1.2	15
4209	Methane dissociation on Ni(111): The effects of lattice motion and relaxation on reactivity. <i>Journal of Chemical Physics</i> , 2007, 127, 224702.	1.2	62
4210	Supersonic molecular beam studies of dissociative adsorption of H <sub>2</sub> on Ru(0001). <i>Journal of Chemical Physics</i> , 2007, 127, 244701.	1.2	47
4211	Magnetic Properties and Electronic Structure of Transition Metal Adsorbed Polar-ZnO Surfaces: Ab initio Calculations. <i>Japanese Journal of Applied Physics</i> , 2007, 46, 6312-6314.	0.8	6
4212	A first-principles study of electronic and magnetic properties of a quasi-one-dimensional organic ferromagnet. <i>Europhysics Letters</i> , 2007, 77, 37006.	0.7	8
4213	Identifying Hydrogen Atoms on Graphite. <i>Journal of the Physical Society of Japan</i> , 2007, 76, 114703.	0.7	11
4214	Chapter 4 Au and Ag (n=1-8) nanocluster catalysts: gas-phase reactivity to deposited structures. <i>Chemical Physics of Solid Surfaces</i> , 2007, , 151-199.	0.3	16
4215	First-principles calculation of electronic structure and magnetic properties of copper adsorbed polar-ZnO surface. <i>Journal of Vacuum Science &amp; Technology B</i> , 2007, 25, 2616.	1.3	1

#	ARTICLE	IF	CITATIONS
4216	Ionization induced relaxation in solvation structure: A comparison between Na(H <sub>2</sub> O) <sub>n</sub> and Na(NH <sub>3</sub> ) <sub>n</sub> . Journal of Chemical Physics, 2007, 126, 084501.	1.2	41
4217	Electronic spectrum of UO <sub>2</sub> <sup>2+</sup> and [UO <sub>2</sub> Cl <sub>4</sub> ] <sup>2-</sup> calculated with time-dependent density functional theory. Journal of Chemical Physics, 2007, 126, 194311.	1.2	70
4218	Exact functional derivative of the nonadditive kinetic-energy bifunctional in the long-distance limit. Journal of Chemical Physics, 2007, 126, 234116.	1.2	68
4219	Density functional theory study of $\beta$ -hydride elimination of ethyl on flat and stepped Cu surfaces. Journal of Chemical Physics, 2007, 127, 144710.	1.2	10
4220	Observable consequences of formation of Au anions from deposition of Au atoms on ultrathin oxide films. Journal of Chemical Physics, 2007, 127, 144713.	1.2	29
4221	Theoretical predictions of nuclear magnetic resonance parameters in a novel organo-xenon species: Chemical shifts and nuclear quadrupole couplings in HXeCCH. Journal of Chemical Physics, 2007, 127, 234314.	1.2	36
4222	Oscillatory exchange coupling in magnetic molecules. Journal of Physics Condensed Matter, 2007, 19, 216205.	0.7	3
4223	Oxygen adsorption on the clean and O-precovered Fe (110) and (100) surfaces. Journal of Physics Condensed Matter, 2007, 19, 096011.	0.7	23
4224	Potential Energy of H <sub>2</sub> Dissociation and Adsorption on Pt(111) Surface: First-Principles Calculation. Japanese Journal of Applied Physics, 2007, 46, 4233-4237.	0.8	36
4225	CO adsorption on a Au/Ni(111) surface alloy: a DFT study. Journal of Physics Condensed Matter, 2007, 19, 246219.	0.7	10
4226	Fermi level alignment in single molecule junctions and its dependence on interface structure. Journal of Physics: Conference Series, 2007, 61, 1097-1101.	0.3	23
4227	Development of Constraint Algorithm for the Number of Electrons in Molecular Orbitals Consisting Mainly 4f Atomic Orbitals of Rare-Earth Elements and Its Introduction to Tight-Binding Quantum Chemical Molecular Dynamics Method. Japanese Journal of Applied Physics, 2007, 46, 2505-2509.	0.8	8
4228	The role of ab initio electronic structure calculations in multiscale modelling of materials. , 2007, , 1-24.		0
4229	An ab initio study of the field-induced position change of a C <sub>60</sub> molecule adsorbed on a gold tip. Nanotechnology, 2007, 18, 165501.	1.3	6
4230	Quantum states of hydrogen atom motion on the Pd(111) surface and in the subsurface. Journal of Physics Condensed Matter, 2007, 19, 365214.	0.7	18
4231	Large-Scale Electronic Structure Calculation on Blue Phosphor BaMgAl <sub>10</sub> O <sub>17</sub> :Eu <sup>2+</sup> Using Tight-Binding Quantum Chemistry Method Implemented for Rare-Earth Elements. Japanese Journal of Applied Physics, 2007, 46, 2534-2541.	0.8	12
4232	Effect of electronic correlation on the Na ordering of Na <sub>x</sub> CoO <sub>2</sub> . Journal of Physics Condensed Matter, 2007, 19, 086203.	0.7	7
4233	Evolution of a symmetry gap and synergetic quantum well states in ultrathin Ag films on Au(111) substrates. Europhysics Letters, 2007, 78, 57003.	0.7	14



#	ARTICLE	IF	CITATIONS
4252	Atomic scale model interfaces between high-khafnium silicates and silicon. Physical Review B, 2007, 75, .	1.1	24
4253	First-principles studies on clean and oxygen-adsorbed Ir(110) surfaces. Physical Review B, 2007, 76, .	1.1	17
4254	Magnetically induced dynamical stability of a Fe monolayer on W(110). Physical Review B, 2007, 76, .	1.1	11
4255	Traits of bulk Pu phases in Pb-Pu superlattice phases from first principles. Physical Review B, 2007, 76, .	1.1	3
4256	Combining multiconfigurational wave functions with correlation density functionals: A size-consistent method based on natural orbitals and occupation numbers. Physical Review A, 2007, 75, .	1.0	37
4257	Ab initio studies of structural, vibrational, and electronic properties of durene crystals and molecules. Physical Review B, 2007, 75, .	1.1	23
4258	Interplay between structural, magnetic, and electronic properties in a $\text{Fe}/\text{O}/\text{Pt}$ thin film. Physical Review B, 2007, 76, .	1.1	129
4259	Formation of electron traps in amorphous silica. Physical Review B, 2007, 76, .	1.1	12
4260	Local zero-bias anomaly in tunneling spectra of a transition-metal oxide thin film. Physical Review B, 2007, 75, .	1.1	20
4261	Response of triluminides to [110] uniaxial loading: An ab initio study for $\text{Al}_3\text{Ti}$ . Physical Review B, 2007, 75, .	1.1	22
4262	Magnetic momentum density, Fermi surface, and directional magnetic Compton profiles in $\text{LaSr}_2\text{Mn}_2\text{O}_7$ and $\text{La}_{1.2}\text{Sr}_{1.8}\text{Mn}_2\text{O}_7$ . Physical Review B, 2007, 75, .	1.1	13
4263	Trimming Si surfaces for molecular electronics. Journal of Applied Physics, 2007, 101, 081719.	1.1	6
4264	Oxygen pressure dependence of $\text{HfO}_2$ stoichiometry: An ab initio investigation. Applied Physics Letters, 2007, 91, 022904.	1.5	9
4265	Stress in silicon interlayers at the $\text{SiO}_2/\text{Ge}$ interface. Applied Physics Letters, 2007, 90, 143511.	1.5	2
4266	Ab-initio Atomic Scale Study of Nearly Frictionless Surfaces. , 2007, , 57-77.		2
4267	Two-dimensional localization of fast electrons in $\text{Cs}/\text{Cu}$ . Physical Review B, 2007, 76, .	1.1	
4268	THE PROBLEM OF THE BAND GAP IN LDA CALCULATIONS. Surface Review and Letters, 2007, 14, 481-487.	0.5	69
4269	Single hydrogen atoms on the Si(001) surface. Physical Review B, 2007, 76, .	1.1	28



#	ARTICLE	IF	CITATIONS
4288	Theoretical study of deep-defect states in bulk PbTe and in thin films. Physical Review B, 2007, 76, .	1.1	57
4289	First-principles investigation of the structural and vibrational properties of vitreous GeSe <sub>2</sub> . Physical Review B, 2007, 75, .	1.1	40
4290	First-principles calculations of the electronic and magnetic properties of $\text{CsAg}_2\text{F}_4$ . Physical Review B, 2007, 76, .	1.1	14
4291	Diffusion of O vacancies near Si:HfO <sub>2</sub> interfaces: An ab initio investigation. Physical Review B, 2007, 76, .	1.1	48
4292	Detection of intrinsic stress in cubic boron nitride films by x-ray absorption near-edge structure: Stress relaxation mechanisms by simultaneous ion implantation during growth. Physical Review B, 2007, 76, .	1.1	11
4293	First-principles calculations of the effects of Cu and Ag additions on the electromigration of Sn-based solder. Journal of Applied Physics, 2007, 102, .	1.1	10
4294	Atomic arrangement and impurity bonding at Al <sub>2</sub> O <sub>3</sub> (001)-Al(771) interface: First-principles calculations. Physical Review B, 2007, 76, .	1.1	2
4295	Convergence of the many-body expansion of interaction potentials: From van der Waals to covalent and metallic systems. Physical Review A, 2007, 76, .	1.0	74
4296	Oxidation of Pd(553): From ultrahigh vacuum to atmospheric pressure. Physical Review B, 2007, 76, .	1.1	70
4297	Nanotemplate with Holes: Ultrathin Alumina on Ni <sub>3</sub> Al(111). Physical Review Letters, 2007, 99, 196104.	2.9	122
4298	Effects of an electric field on a water bilayer on Ag(111). Physical Review B, 2007, 75, .	1.1	28
4299	Water adsorption on O(2 $\bar{1}$ -2)-Ru(0001): STM experiments and first-principles calculations. Physical Review B, 2007, 76, .	1.1	22
4300	Confined states in multiple quantum well structures of $\text{Si}_n\text{Ge}_{1-n}$ nanowire superlattices. Physical Review B, 2007, 76, .	1.1	18
4301	Water adsorption on Pd {100} from first principles. Physical Review B, 2007, 76, .	1.1	37
4302	Energy decomposition analysis of metal silicide nanowires from first principles. Physical Review B, 2007, 75, .	1.1	12
4303	Formation and evolution of a self-organized hierarchy of Ge nanostructures on Si(111)-(7 $\bar{7}$ -7): STM observations and first-principles calculations. Physical Review B, 2007, 75, .	1.1	20
4304	Calculations of superconducting properties in yttrium and calcium under high pressure. Physical Review B, 2007, 75, .	1.1	32
4305	Localization of oxygen donor states in gallium nitride from first-principles calculations. Physical Review B, 2007, 76, .	1.1	25



#	ARTICLE	IF	CITATIONS
4306	Hf defects in $\text{Si}$ and their importance for the $\text{HfO}_2/\text{Si}$ interface: Density-functional calculations. <i>Physical Review B</i> , 2007, 75, .	1.1	4
4307	Including the probe tip in theoretical models of inelastic scanning tunneling spectroscopy: CO on Cu(100). <i>Physical Review B</i> , 2007, 76, .	1.1	27
4308	Relationship between magnetic and structural properties of Ni thin films on GaAs(100) and bulk bcc Ni: First-principles calculations. <i>Physical Review B</i> , 2007, 75, .	1.1	11
4309	Imaging Intrinsic Diffusion of Bridge-Bonded Oxygen Vacancies on $\text{TiO}_2(110)$ . <i>Physical Review Letters</i> , 2007, 99, 126105.	2.9	86
4310	Half-Metallic Silicon Nanowires: First-Principles Calculations. <i>Physical Review Letters</i> , 2007, 99, 256806.	2.9	70
4311	Long-Range Chiral Recognition due to Substrate Locking and Substrate-Adsorbate Charge Transfer. <i>Physical Review Letters</i> , 2007, 99, 196107.	2.9	48
4312	Effect of Carbon Adsorption on the Isomer Stability of $\text{Ir}_4$ Clusters. <i>Physical Review Letters</i> , 2007, 99, 165501.	2.9	16
4313	Influence of Temperature on the Interaction between Pd Clusters and the $\text{TiO}_2(110)$ Surface. <i>Physical Review Letters</i> , 2007, 99, 066102.	2.9	11
4314	Atomic Row Doubling in the STM Images of $\text{Cu}(014)\text{-O}$ Obtained with MnNi Tips. <i>Physical Review Letters</i> , 2007, 98, 206101.	2.9	16
4315	Proton-Induced Fixed Positive Charge at the $\text{Si}/\text{SiO}_2$ Interface. <i>Physical Review Letters</i> , 2007, 99, 126102.	2.9	21
4316	Density functional study of the interaction between small Au clusters, $\text{Au}_n$ ( $n=1-7$ ) and the rutile $\text{TiO}_2$ surface. II. Adsorption on a partially reduced surface. <i>Journal of Chemical Physics</i> , 2007, 127, 244708.	1.2	52
4317	Mixing of Electronic States in Pentacene Adsorption on Copper. <i>Physical Review Letters</i> , 2007, 99, 046802.	2.9	132
4318	<i>Ab initio</i> calculations of the mechanical properties of $\text{SrAl}_2\text{O}_4$ stuffed tridymite. <i>Journal of Applied Physics</i> , 2007, 102, .	1.1	14
4319	Transferable force-constant modeling of vibrational thermodynamic properties in fcc-based $\text{AlTM}$ ( $\text{TM}=\text{Ti}, \text{Zr}, \text{Hf}$ ) alloys. <i>Physical Review B</i> , 2007, 75, .	1.1	44
4320	Conductance model of gold-molecule-silicon and carbon nanotube-molecule-silicon junctions. <i>Physical Review B</i> , 2007, 76, .	1.1	15
4321	Kadowaki-Woods ratio for strongly coupled Fermi liquids. <i>Physical Review B</i> , 2007, 76, .	1.1	1
4322	Calculating carbon nanotube-catalyst adhesion strengths. <i>Physical Review B</i> , 2007, 75, .	1.1	39
4323	Atomic and electronic structure of the cleaved $\text{6H}\text{-SiC}(112\bar{0})$ surface. <i>Physical Review B</i> , 2007, 75, .	1.1	6

#	Systematic study on the pressure dependence of	IF	CITATIONS
4324	$M^2 \frac{dA}{dC}$ phases		

#	ARTICLE	IF	CITATIONS
4342	Structural and electronic properties of Runclusters( $n=2\text{--}14$ ) studied by first-principles calculations. Physical Review B, 2007, 76, .	1.1	50
4343	Surface oxides on Pd(111): STM and density functional calculations. Physical Review B, 2007, 76, .	1.1	69
4344	Cationic and anionic vacancies on the NiO(100) surface: DFT+U and hybrid functional density functional theory calculations. Journal of Chemical Physics, 2007, 127, 174711.	1.2	93
4345	First-Principles Studies on Grain Boundary Energies of [110] Tilt Grain Boundaries in Aluminum. Materials Science Forum, 2007, 561-565, 1837-1840.	0.3	11
4346	First Principles Study of Al(100) Twisted Interfaces. Solid State Phenomena, 2007, 129, 131-136.	0.3	1
4347	Alkali Atoms Intercalating Induced Metal-Semiconductor and Semiconductor-Semiconductor Transitions in Carbon Nanotubes. Solid State Phenomena, 2007, 121-123, 1003-1006.	0.3	0
4348	Theoretical Tensile Deformation of $\Sigma 13$ Pyramidal Twin Grain Boundary in Alumina. Key Engineering Materials, 2007, 352, 21-24.	0.4	0
4349	First-principles study on the electronic structure and optical properties of $\text{Tl}_{2\text{--}3}\text{Cd}_{2\text{--}4}(\text{SO}_4)_3$ and $\text{Rb}_{2\text{--}3}\text{Cd}_2(\text{SO}_4)_3$ . Journal of Materials Research, 2007, 22, 3058-3066.	1.2	31
4350	Layered stacking characteristics of ternary zirconium aluminum carbides. Journal of Materials Research, 2007, 22, 3058-3066.	1.2	31
4351	STUDY OF NANO-STRUCTURED SILICON-PHENYL NANOCLUSTERS TOWARDS SINGLE MOLECULE SENSING. International Journal of High Speed Electronics and Systems, 2007, 17, 327-338.	0.3	3
4352	First Principles Study on the Adsorption of Alkali Metal on C(100) ( $2\text{--}1$ ). Advanced Materials Research, 2007, 26-28, 1341-1344.	0.3	0
4353	Comparative Study of Electronic Properties of Point Defects in Monoclinic Hafnium Dioxide. Materials Research Society Symposia Proceedings, 2007, 996, 1.	0.1	1
4354	Photodissociation of Chromium Oxide Cluster Cations. Journal of Physical Chemistry A, 2007, 111, 8080-8089.	1.1	42
4355	Stacking Fault Energy of Cu-Ga Alloys from First Principles. Materials Science Forum, 2007, 561-565, 1915-1918.	0.3	0
4356	Atomistic Studies of Deformation Mechanism of Nanocrystalline Al-Ti and Al-Fe Alloys from First-Principles. Materials Science Forum, 2007, 561-565, 977-980.	0.3	4
4357	First-Principle Molecular-Dynamics Study of Hydrogen and Aluminium Nanowires in Carbon Nanotubes. Materials Science Forum, 2007, 539-543, 1409-1414.	0.3	5
4358	First Principle Study on Electronic Structure of Nanocrystalline $\text{BaTiO}_3$ Ceramics. Key Engineering Materials, 2007, 336-338, 2510-2512.	0.4	0
4359	First-principles Calculations on the $\text{Zn}_{1-x}\text{Mg}_x\text{O}$ Window Layer Material for CIS Thin Film Solar Cells. Materials Research Society Symposia Proceedings, 2007, 1012, 1.	0.1	2

#	ARTICLE	IF	CITATIONS
4360	Oxygen at high pressures: a theoretical approach to monoatomic phases. Journal of Physics Condensed Matter, 2007, 19, 365211.	0.7	5
4361	Density functional study of the charge on Aun clusters (n=1-7) supported on a partially reduced rutile TiO <sub>2</sub> (110): Are all clusters negatively charged?. Journal of Chemical Physics, 2007, 126, 104701.	1.2	72
4362	First-Principles Calculations on Crystal Structure and Thermodynamic Properties of Ceramics. Key Engineering Materials, 2007, 336-338, 2517-2520.	0.4	0
4363	A First-Principles Analysis for Sulfur Tolerance of CeO <sub>2</sub> in Solid Oxide Fuel Cells. Journal of Physical Chemistry C, 2007, 111, 11117-11122.	1.5	63
4364	Electronic Structure and Defect States of Transition Metal Doped Rutile TiO <sub>2</sub> . Solid State Phenomena, 2007, 124-126, 787-790.	0.3	0
4365	First principles studies on the electronic structures of Li M x Fe 1-x PO 4 ( M = Co, Ni and Rh). Chinese Physics B, 2007, 16, 3042-3045.	1.3	6
4366	Structure, Composition, and Electronic Properties of TiOx/Mo(112) Thin Films. Journal of Physical Chemistry C, 2007, 111, 7437-7445.	1.5	11
4367	Surface states and surface stability in half-metallic systems: the cases of zinc-blende-structure MnSb {111}A, {111}B and {001}. Journal of Physics Condensed Matter, 2007, 19, 315214.	0.7	5
4368	Simulation of Nanoscale Electronic Systems. Advances in Computers, 2007, , 167-249.	1.2	0
4369	A Quest for Efficient Methods of Disintegration of Organophosphorus Compounds: Modeling Adsorption and Decomposition Processes. Challenges and Advances in Computational Chemistry and Physics, 2007, , 565-592.	0.6	1
4370	Anomalous Optical and Electronic Properties of CaTiO <sub>3</sub> Perovskites. Communications in Theoretical Physics, 2007, 48, 563-570.	1.1	3
4371	First-Principles Calculations of Grain Boundary-Surface for Various Grain Boundaries with Different Energies in Aluminum. Materials Science Forum, 2007, 551-552, 331-336.	0.3	3
4372	Reactivity of ideal and defected rutile TiO <sub>2</sub> (110) surface with oxygen. Advances in Applied Ceramics, 2007, 106, 95-100.	0.6	10
4373	Trend in crystal structure of layered ternary T-Al-C carbides (T = Sc, Ti, V, Cr, Zr, Nb, Mo,) Tj ETQq1 1 0,784314 rgBT /Over	1.2	31
4374	Functionalizing AlOOH Surface with Silanol – an Ab-initio Study. Materials Research Society Symposia Proceedings, 2007, 1000, 1.	0.1	0
4375	Understanding the Structural Stability of Compound Mo-S Clusters at Sub-Nanometer Level. Materials Transactions, 2007, 48, 658-661.	0.4	7
4376	Structure and Stability of Small Bimetallic Al-Based Clusters: An ab initio DFT Study. Materials Transactions, 2007, 48, 689-692.	0.4	8
4377	Metal Sandwich Molecules: Planar Metal Atom Arrays between Aromatic Hydrocarbons. Materials Transactions, 2007, 48, 693-699.	0.4	6

#	ARTICLE	IF	CITATIONS
4378	CO Oxidation Process on Pt-M(111) Alloys (M=Ru, Sn): An <i>ab initio</i> Study. <i>Materials Transactions</i> , 2007, 48, 1907-1912.	0.4	1
4380	Native defects and impurities in Zn <sub>3</sub> N <sub>2</sub> : first-principle studies using gradient-correction approximation. <i>Physica Scripta</i> , 2007, T129, 340-344.	1.2	3
4381	Interstitial Oxygen and Dopant Atoms Arrangement in Tin-Doped Indium Oxide. <i>Materials Transactions</i> , 2007, 48, 666-669.	0.4	13
4382	CO oxidation reaction on Pt(111) studied by the dynamic Monte Carlo method including lateral interactions of adsorbates. <i>Journal of Chemical Physics</i> , 2007, 126, 044704.	1.2	44
4383	Chapter 1 Electrical characteristics of bulk-molecule interfaces. <i>Theoretical and Computational Chemistry</i> , 2007, 18, 1-33.	0.2	0
4384	First-Principles Electronic Structure Calculation of LaCo <sub>2</sub> in MgCu <sub>2</sub> Structure. <i>Journal of the Physical Society of Japan</i> , 2007, 76, 084711.	0.7	2
4385	Structural and electronic properties of Al <sub>12</sub> X <sup>+</sup> (X=C, Si, Ge, Sn, and Pb) clusters. <i>Journal of Chemical Physics</i> , 2007, 126, 014703.	1.2	14
4386	Computer simulations for the nano-scale. <i>Acta Physica Slovaca</i> , 2007, 57, 1-176.	1.4	9
4387	Methanol and Methoxide Decomposition on Silver. <i>Journal of Physical Chemistry C</i> , 2007, 111, 9867-9876.	1.5	29
4388	Short-Range Order in Liquid Aluminum Chloride: <i>Ab Initio</i> Molecular Dynamics Simulations and Quantum-Chemical Calculations. <i>Journal of Physical Chemistry B</i> , 2007, 111, 5316-5321.	1.2	11
4389	BFW: A Density Functional for Transition Metal Clusters. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2625-2628.	1.1	8
4390	Recent Advances in Fullerene Deposition on Semiconductor Surfaces. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2007, , 533-563.	0.6	0
4391	Electronic spin transitions in iron-bearing MgSiO <sub>3</sub> perovskite. <i>Earth and Planetary Science Letters</i> , 2007, 253, 282-290.	1.8	93
4392	First-principles study of the tensile and fracture of the Al/TiN interface. <i>Computational Materials Science</i> , 2007, 38, 800-806.	1.4	35
4393	Atomistic study of structural, elastic, electronic and thermal properties of perovskites Ba(Ti,Zr,Nb)O <sub>3</sub> . <i>Computational Materials Science</i> , 2007, 39, 896-902.	1.4	40
4394	Atomistic modeling of an Fe system with a small concentration of C. <i>Computational Materials Science</i> , 2007, 40, 119-129.	1.4	165
4395	<i>Ab initio</i> calculations of mechanical and thermodynamic properties for the B2-based AlRE. <i>Computational Materials Science</i> , 2007, 40, 226-233.	1.4	38
4396	<i>Ab initio</i> simulations of clustering and precipitation in Al-Mg-Si alloys. <i>Computational Materials Science</i> , 2007, 40, 309-318.	1.4	17

#	ARTICLE	IF	CITATIONS
4397	Thermodynamic modelling of the Ba-Ca, Ba-Sr and Ba-Ba systems. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2007, 31, 286-291.	0.7	17
4398	Thermodynamic modelling of the Cu-Pd-H system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2007, 31, 315-329.	0.7	44
4399	Ab initio modeling of Li-B-H boron-chain alloys for hydrogen storage applications. Physical Review B, 2007, 76, .	1.1	13
4400	Control of the Charge State of Metal Atoms on Thin MgO Films. Physical Review Letters, 2007, 98, 096107.	2.9	310
4401	First-principle molecular dynamics study of the structural and electronic properties of liquid and amorphous Ni-Al alloys. Journal of Non-Crystalline Solids, 2007, 353, 2638-2645.	1.5	21
4402	pH Modulates the Quinone Position in the Photosynthetic Reaction Center from Rhodospirillum rubrum sphaeroides in the Neutral and Charge Separated States. Journal of Molecular Biology, 2007, 371, 396-409.	2.0	132
4403	Thermodynamic modeling of the Ba-Ni-Ti system. Journal of Alloys and Compounds, 2007, 430, 188-193.	2.8	9
4404	Two polymorphs of Ba <sub>3</sub> Sn <sub>2</sub> P <sub>4</sub> : Single crystal and electronic structures. Journal of Alloys and Compounds, 2007, 430, 54-59.	2.8	7
4405	First-principle study of the ferroelectricity and optical properties of the BaBi <sub>2</sub> Ta <sub>2</sub> O <sub>9</sub> . Journal of Alloys and Compounds, 2007, 438, 25-29.	2.8	11
4406	First-principles study on the structure and elasticity of LaNi <sub>5</sub> and LaNi <sub>4.25</sub> Al <sub>0.75</sub> . Journal of Alloys and Compounds, 2007, 439, 25-32.	2.8	14
4407	First-principles study of GaP(001) surfaces. Journal of Alloys and Compounds, 2007, 440, 229-235.	2.8	4
4408	First principles screening of destabilized metal hydrides for high capacity H <sub>2</sub> storage using scandium. Journal of Alloys and Compounds, 2007, 446-447, 23-27.	2.8	33
4409	La(TM) <sub>5</sub> hydrides (TM=Fe, Co, Ni): Theoretical perspectives. Journal of Alloys and Compounds, 2007, 446-447, 188-194.	2.8	22
4410	Hydrogen storage properties of Na-Li-Mg-Al-H complex hydrides. Journal of Alloys and Compounds, 2007, 446-447, 228-231.	2.8	38
4411	The importance of vibrations in modelling complex metal hydrides. Journal of Alloys and Compounds, 2007, 446-447, 455-458.	2.8	16
4412	Hydrogen interactions with the PdCu ordered B <sub>2</sub> alloy. Journal of Alloys and Compounds, 2007, 446-447, 583-587.	2.8	55
4413	Point defect dynamics in sodium aluminum hydrides: A combined quasielastic neutron scattering and density functional theory study. Journal of Alloys and Compounds, 2007, 446-447, 469-473.	2.8	33
4414	Moisture-induced embrittlement mechanism for (Ni,Fe)Ti alloys. Intermetallics, 2007, 15, 288-293.	1.8	3

#	ARTICLE	IF	CITATIONS
4415	First-principles investigation of the structural and electronic properties of $\text{Cu}_{6-x}\text{Ni}_x\text{Sn}_5$ ( $x=0, 1, 2$ ) intermetallic compounds. <i>Intermetallics</i> , 2007, 15, 1471-1478.	1.8	103
4416	Structural distortion of $\gamma$ -structured MnO and FeO. <i>Solid State Communications</i> , 2007, 142, 6-9.	0.9	19
4417	Physisorption of nucleobases on graphene: Density-functional calculations. <i>Physical Review B</i> , 2007, 76, .	1.1	296
4418	Band gap calculations with Becke-Johnson exchange potential. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 196208.	0.7	195
4419	Stability analysis of doped materials for reversible hydrogen storage in destabilized metal hydrides. <i>Physical Review B</i> , 2007, 76, .	1.1	26
4420	A density functional theory study of atomic oxygen and nitrogen adsorption over $\gamma$ -alumina (0001). <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5112.	1.3	21
4421	Multiple Charge States of Ag Atoms on Ultrathin NaCl Films. <i>Physical Review Letters</i> , 2007, 98, .	2.9	105
4422	Evidence for a Single Hydrogen Molecule Connected by an Atomic Chain. <i>Physical Review Letters</i> , 2007, 98, 146802.	2.9	78
4423	Infrared Spectrum and Bonding in Uranium Methylidene Dihydride, $\text{CH}_2\text{UH}_2$ . <i>Inorganic Chemistry</i> , 2007, 46, 4917-4925.	1.9	73
4424	General Performance of Density Functionals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10439-10452.	1.1	907
4425	Band-gap variation in Mg- and Cd-doped ZnO nanostructures and molecular clusters. <i>Physical Review B</i> , 2007, 76, .	1.1	94
4426	Critical Assessment of the Performance of Density Functional Methods for Several Atomic and Molecular Properties. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 407-433.	2.3	295
4427	Atomistic mechanism of interfacial reaction and asymmetric growth kinetics in an immiscible Cu-Ru system at equilibrium. <i>Physical Review B</i> , 2007, 75, .	1.1	22
4428	Tuning LDA+U for electron localization and structure at oxygen vacancies in ceria. <i>Journal of Chemical Physics</i> , 2007, 127, 244704.	1.2	313
4429	Structure and Bonding in $\text{SnWO}_4$ , $\text{PbWO}_4$ , and $\text{BiVO}_4$ : Lone Pairs vs Inert Pairs. <i>Inorganic Chemistry</i> , 2007, 46, 3839-3850.	1.9	279
4430	Electron Transfer from a Diamond (100) Surface to an Atmospheric Water Adlayer: A Quantum Mechanical Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 13804-13812.	1.5	30
4431	Adsorption of Pd Atoms and Dimers on the $\text{TiO}_2(110)$ Surface: A First Principles Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 3949-3955.	1.5	51
4432	Theory of Metal Clusters on the MgO Surface: The Role of Point Defects. <i>Nanoscience and Technology</i> , 2007, , 193-243.	1.5	2



#	ARTICLE	IF	CITATIONS
4433	Nucleation of Pd <sub>n</sub> (n=1-5) clusters and wetting of Pd particles on Al <sub>2</sub> O <sub>3</sub> surfaces: A density functional theory study. <i>Physical Review B</i> , 2007, 75, .	1.1	84
4434	First Row Transition Metal Atom Adsorption on Defect-Free MgO(100) Surface. <i>Journal of Physical Chemistry C</i> , 2007, 111, 6781-6788.	1.5	20
4435	Structure and Stability of Small Boron and Boron Oxide Clusters. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6539-6551.	1.1	65
4436	First-principles study of the Pt-CeO <sub>2</sub> (111) interface. <i>Physical Review B</i> , 2007, 76, .	1.1	82
4437	Assessment of the exchange-correlation functionals for the physical description of spin transition phenomena by density functional theory methods: All the same?. <i>Journal of Chemical Physics</i> , 2007, 126, 014105.	1.2	102
4438	Probing chiral interfaces by infrared spectroscopic methods. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 671-685.	1.3	60
4439	Adsorption of H, NH <sub>x</sub> , BH <sub>x</sub> and BBr <sub>x</sub> on a (110) surface of c-BN: A quantum-mechanical DFT study. <i>Diamond and Related Materials</i> , 2007, 16, 131-137.	1.8	8
4440	Size dependence of the structures and energetic and electronic properties of gold clusters. <i>Journal of Chemical Physics</i> , 2007, 126, 084505.	1.2	166
4441	Single P and As dopants in the Si(001) surface. <i>Journal of Chemical Physics</i> , 2007, 127, 184706.	1.2	8
4442	ON THE EVALUATION OF THE RIGOROUS ELECTROSTATIC POTENTIAL/ATOMIC ENERGY RELATIONSHIP. <i>Journal of Theoretical and Computational Chemistry</i> , 2007, 06, 761-788.	1.8	0
4443	Density-Functional and Coupled-Cluster Singles-and-Doubles Calculations of the Nuclear Shielding and Indirect Nuclear Spin-Spin Coupling Constants of o-Benzynes. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 86-94.	2.3	43
4444	Electronic Effects in CO Chemisorption on Pt-Pb Intermetallic Surfaces: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 17357-17369.	1.5	19
4445	Ab initio molecular dynamics simulations of the static, dynamic, and electronic properties of liquid Pb using real-space pseudopotentials. <i>Physical Review B</i> , 2007, 76, .	1.1	34
4446	A computational investigation of stoichiometric and calcium-deficient oxy- and hydroxy-apatites. <i>Faraday Discussions</i> , 2007, 134, 195-214.	1.6	65
4447	Chemical Properties of Small Au Clusters: An Analysis of the Local Site Reactivity. <i>Journal of Physical Chemistry C</i> , 2007, 111, 6668-6677.	1.5	72
4448	Ab initio study of oxygen interstitial diffusion near Si:HfO <sub>2</sub> interfaces. <i>Physical Review B</i> , 2007, 75, .	1.1	19
4449	Ab initio calculations of the electronic and optical properties of germanium selenide. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 186211.	0.7	47
4450	Potassium intercalation in graphite: A van der Waals density-functional study. <i>Physical Review B</i> , 2007, 76, .	1.1	155

#	ARTICLE	IF	CITATIONS
4451	Theoretical investigation of structural, energetic and electronic properties of titanate pyrochlores. Journal of Physics Condensed Matter, 2007, 19, 346203.	0.7	41
4452	Investigation of the Typical Triangular Structure B <sub>3</sub> in Boron Chemistry: An Insight into Bare All-Boron Clusters Used as Ligands or Building Blocks. Journal of Physical Chemistry A, 2007, 111, 9122-9129.	1.1	26
4453	Lattice dynamics of CoO from first principles. Physical Review B, 2007, 75, .	1.1	65
4454	Electronic Excitations of Glycine, Alanine, and Cysteine Conformers from First-Principles Calculations. Journal of Physical Chemistry A, 2007, 111, 4370-4377.	1.1	36
4455	Quantum chemical and vibrational investigation of sodium exchanged $\gamma$ -alumina surfaces. Physical Chemistry Chemical Physics, 2007, 9, 2577-2582.	1.3	26
4456	Ground state structure of sodium ions in $\gamma$ -alumina. $\text{Na} \times \text{Co} \text{O}_2$ A combined Monte Carlo and first-principles approach. Physical Review B, 2007, 76, .	1.1	25
4457	Adsorption structure and scanning tunneling data of a prototype organic-inorganic interface: PTCDA on Ag(111). Physical Review B, 2007, 76, .	1.1	136
4458	Density functional theory study of flat and stepped NaCl(001). Physical Review B, 2007, 76, .	1.1	40
4459	Vibrational Exciton Couplings for the Amide I, II, III, and A Modes of Peptides. Journal of Physical Chemistry B, 2007, 111, 11032-11046.	1.2	85
4460	The mechanism of chemical disordering in Cu <sub>3</sub> Au nanometre-sized systems. Nanotechnology, 2007, 18, 235706.	1.3	19
4461	Clean and metal-doped bundles of boron-carbide nanotubes: A density functional study. Physical Review B, 2007, 76, .	1.1	4
4462	Hydrogen Cycle on CeO <sub>2</sub> (111) Surfaces: Density Functional Theory Calculations. Journal of Physical Chemistry C, 2007, 111, 15337-15341.	1.5	131
4463	Surface functionalization through adsorption of organic molecules. Journal of Physics Condensed Matter, 2007, 19, 305018.	0.7	6
4464	The high-temperature elasticity of MgSiO <sub>3</sub> post-perovskite. Geophysical Monograph Series, 2007, , 99-113.	0.1	14
4465	A Series of New Copper Iodobismuthates: Structural Relationships, Optical Band Gaps Affected by Dimensionality, and Distinct Thermal Stabilities. Inorganic Chemistry, 2007, 46, 8698-8704.	1.9	75
4466	Modeling of CeO <sub>2</sub> , Ce <sub>2</sub> O <sub>3</sub> , and CeO <sub>2</sub> in the LDA+U formalism. Physical Review B, 2007, 75, .	1.1	333
4467	First-principles calculations of structural, electronic, and thermodynamic properties of $\text{Na}_2\text{Be}_4\text{H}$ . Physical Review B, 2007, 76, .	1.1	7
4468	Nontrivial Tuning of the Hydrogen-Binding Energy to Fullerenes with Endohedral Metal Dopants. Journal of Physical Chemistry C, 2007, 111, 13275-13279.	1.5	11

#	ARTICLE	IF	CITATIONS
4469	A Mixed Structural Motif in 34-Atom Pd <sup>2+</sup> Pt Clusters. Journal of Physical Chemistry C, 2007, 111, 2936-2941.	1.5	90
4470	Density functional theory calculation of crystal-field energy levels for $\text{Yb}^{3+}$ ions. Journal of Physical Chemistry C, 2007, 111, 2936-2941.	1.1	7
4471	Applications of Quantum Chemical Methods in Zeolite Science. Studies in Surface Science and Catalysis, 2007, , 701-XXI.	1.5	16
4472	Ab initio simulations of the electrochemical activation of water. Molecular Simulation, 2007, 33, 429-436.	0.9	21
4473	Photophysics and Bonding in Neutral Gold(I) Organometallic Complexes with an Extended Auophilic Supramolecular Structure. Organometallics, 2007, 26, 2550-2560.	1.1	34
4474	First-principles study of ternary fcc solution phases from special quasirandom structures. Physical Review B, 2007, 76, .	1.1	72
4475	Formation of sp <sup>3</sup> Hybridized Bonds and Stability of CaCO <sub>3</sub> at Very High Pressure. Physical Review Letters, 2007, 98, 268501.	2.9	32
4476	Importance of spin-orbit effects on the isomerism profile of Au <sub>3</sub> : An ab initio study. Journal of Chemical Physics, 2007, 127, 164322.	1.2	31
4477	Synthesis, Growth Mechanism, and Work Function at Highly Oriented {001} Surfaces of Bismuth Sulfide Microbelts. Journal of Physical Chemistry C, 2007, 111, 12145-12148.	1.5	34
4478	Au <sub>34</sub> : A Fluxional Core-Shell Cluster. Journal of Physical Chemistry C, 2007, 111, 8228-8232.	1.5	103
4479	Adsorption of small Au clusters on MgO and MgO/Mo: the role of oxygen vacancies and the Mo-support. New Journal of Physics, 2007, 9, 339-339.	1.2	74
4480	Structural transition of Li <sub>2</sub> BeH <sub>4</sub> under high pressure: A first-principles study. Physical Review B, 2007, 75, .	1.1	9
4481	Surface electronic structures of Ba overlayers on W(100), W(110), and W(111). Physical Review B, 2007, 76, .	1.1	12
4482	Ab initio analysis of electron currents through benzene, naphthalene, and anthracene nanojunctions. Nanotechnology, 2007, 18, 485701.	1.3	19
4483	The structural evolution of boron carbide via ab initio calculations. Applied Physics Letters, 2007, 91, .	1.5	61
4484	Potential energy of hydrogen atom motion on Pd(111) surface and in subsurface: A first principles calculation. Journal of Applied Physics, 2007, 101, 123530.	1.1	48
4485	Cross linking of thiolated carbon nanotubes: An ab initio study. Journal of Applied Physics, 2007, 102, 024317.	1.1	14
4486	Dynamical stability of the hardest known oxide and the cubic solar material: TiO <sub>2</sub> . Applied Physics Letters, 2007, 90, 171903.	1.5	42

#	ARTICLE	IF	CITATIONS
4487	Phase diagram and adsorption-desorption kinetics of CO on Ru(0001) from first principles. Journal of Chemical Physics, 2007, 126, 094701.	1.2	38
4488	Solvation and electronic structures of M+Ln, with M+ $\hat{=}$ $\hat{=}$ Mg+ and Ca+, L $\hat{=}$ $\hat{=}$ H <sub>2</sub> O, CH <sub>3</sub> OH, and NH <sub>3</sub> , and n $\hat{=}$ $\hat{=}$ 6. Canadian Journal of Chemistry, 2007, 85, 873-884.	0.6	3
4489	Oxidation of some cage hydrocarbons by dioxiranes. Nature of the transition structure for the reaction of C $\hat{=}$ $\hat{=}$ H bonds with dimethyldioxirane: a comparison of B3PW91 density functional theory with experiment. Organic and Biomolecular Chemistry, 2007, 5, 2302-2310.	1.5	12
4490	Slab model studies of water adsorption and decomposition on clean and X- (X = C, N and O) contaminated Pd(111) surfaces. Physical Chemistry Chemical Physics, 2007, 9, 739-746.	1.3	64
4491	Organolanthanide mediated catalytic cycles: a computational perspective. Dalton Transactions, 2007, , 1743.	1.6	61
4492	Controlling energy and charge transfer in linear chlorophyll dimers. Chemical Communications, 2007, , 4407.	2.2	19
4493	Melting curve of tantalum from first principles. Physical Review B, 2007, 75, .	1.1	99
4494	Effect of Surface Oxygen Vacancy on Pt Cluster Adsorption and Growth on the Defective Anatase TiO <sub>2</sub> (101) Surface. Journal of Physical Chemistry C, 2007, 111, 16397-16404.	1.5	57
4495	NaAlH <sub>4</sub> Clusters with Two Titanium Atoms Added. Journal of Physical Chemistry C, 2007, 111, 8206-8213.	1.5	22
4496	The c(4 $\hat{=}$ 2) Structure of Short- and Intermediate-Chain Length Alkanethiolate Monolayers on Au(111): $\hat{=}$ % A DFT Study. Journal of Physical Chemistry C, 2007, 111, 12149-12151.	1.5	54
4497	Surface Energy Estimation of Catalytically Relevant fcc Transition Metals Using DFT Calculations on Nanorods. Journal of Physical Chemistry C, 2007, 111, 4998-5005.	1.5	36
4498	Role of charged defects and impurities in kinetics of hydrogen storage materials: A first-principles study. Physical Review B, 2007, 76, .	1.1	92
4499	A computational study of H <sub>2</sub> dissociation on silver surfaces: The effect of oxygen in the added row structure of Ag(110). Physical Chemistry Chemical Physics, 2007, 9, 1247-1254.	1.3	43
4500	Electronic Structure and Optical Properties of Semiconducting Orthorhombic BaSi <sub>2</sub> . Chinese Physics Letters, 2007, 24, 2646-2649.	1.3	5
4501	<i>Ab Initio</i> thermodynamic and elastic properties of alkaline-earth metals and their hydrides. Physical Review B, 2007, 76, .	1.1	99
4502	An ytterbium(ii) complex with dimethyl ester of oxydiacetic acid. Dalton Transactions, 2007, , 2779.	1.6	2
4503	Molecular recognition in molecular tweezers systems: quantum-chemical calculation of NMR chemical shifts. Physical Chemistry Chemical Physics, 2007, 9, 4552.	1.3	21
4504	Spectroscopic properties of trichlorofluoromethane CCl <sub>3</sub> F calculated by density functional theory. Physical Chemistry Chemical Physics, 2007, 9, 5027.	1.3	2

#	ARTICLE	IF	CITATIONS
4505	Prediction of a new layered phase of nitrogen from first-principles simulations. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 425226.	0.7	32
4506	Prediction and characterization of a new kind of alkali "superhalogen species with considerable stability: MBeX <sub>3</sub> (M = Li, Na; X = F, Cl, Br). <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5721.	1.3	23
4507	Theoretical and experimental determination of the electronic structure of V <sub>2</sub> O <sub>5</sub> , reduced V <sub>2</sub> O <sub>5</sub> and sodium intercalated NaV <sub>2</sub> O <sub>5</sub> . <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2564-2576.	1.3	67
4508	Optical Properties of the Phosphorescent Trinuclear Copper(I) Complexes of Pyrazolates: Insights from Theory. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4965-4973.	1.1	42
4509	Density Functional Theory and Kinetic Studies of Methanation on Iron Surface. <i>Journal of Physical Chemistry C</i> , 2007, 111, 11012-11025.	1.5	50
4510	Use of Drug Discovery Tools in Rational Organometallic Catalyst Design. <i>Inorganic Chemistry</i> , 2007, 46, 8613-8624.	1.9	20
4511	Geometry Optimization of a Ru(IV) Allyl Dicationic Complex: A DFT Failure?. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 665-670.	2.3	17
4512	Dipole Formation at Interfaces of Alkanethiolate Self-assembled Monolayers and Ag(111). <i>Journal of Physical Chemistry C</i> , 2007, 111, 14448-14456.	1.5	55
4513	First-Principles Investigation of Adsorption and Dissociation of Hydrogen on Mg <sub>2</sub> Si Surfaces. <i>Journal of Physical Chemistry C</i> , 2007, 111, 6910-6916.	1.5	21
4514	Influence of End Group and Surface Structure on the Current-Voltage Characteristics of Alkanethiol Monolayers on Au(111). <i>Journal of Physical Chemistry A</i> , 2007, 111, 12381-12385.	1.1	16
4515	Structure of Mixed Carboxylic Acid Terminated Self-Assembled Monolayers: Experimental and Theoretical Investigation. <i>Journal of Physical Chemistry C</i> , 2007, 111, 4294-4304.	1.5	41
4516	The Effect of Coadsorbed Oxygen on the Adsorption and Diffusion of Potassium on Rh(110): A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 7446-7455.	1.5	12
4517	A Pnictogen of Peculiar Posture. <i>Inorganic Chemistry</i> , 2007, 46, 9146-9154.	1.9	2
4518	Model for the Formation Energies of Alanates and Boranates. <i>Journal of Physical Chemistry C</i> , 2007, 111, 9592-9594.	1.5	9
4519	Adsorption of Copper Clusters in TS-1 Pores: Ti versus Si and Gold versus Copper. <i>Journal of Physical Chemistry C</i> , 2007, 111, 11888-11896.	1.5	7
4520	Structure of Active Sites in Pd-Exchanged Mordenite: A Density Functional Investigation. <i>Journal of Physical Chemistry C</i> , 2007, 111, 6454-6464.	1.5	17
4521	Three Novel Phases in the Sm-Co-Ga System. Syntheses, Crystal and Electronic Structures, and Electrical and Magnetic Properties. <i>Inorganic Chemistry</i> , 2007, 46, 4177-4186.	1.9	16
4522	Testing if the Interstitial Atom, X, of the Nitrogenase Molybdenum-Iron Cofactor Is N or C: ENDOR, ESEEM, and DFT Studies of the $S=3/2$ Resting State in Multiple Environments. <i>Inorganic Chemistry</i> , 2007, 46, 11437-11449.	1.9	89

#	ARTICLE	IF	CITATIONS
4523	On the Chemical Bonding of Gold in Auro-Boron Oxide Clusters $Au_nBO_{-(n-1)}$ . Journal of Physical Chemistry A, 2007, 111, 1648-1658.	1.1	44
4524	On the Copper(II) Ion Coordination by Prion Protein HGGGW Pentapeptide Model. Journal of Physical Chemistry B, 2007, 111, 635-640.	1.2	34
4525	Hydrogen Dissociation Dynamics on Precovered Pd Surfaces: Langmuir is Still Right. Physical Review Letters, 2007, 98, 206107.	2.9	105
4526	Structure of a TiO <sub>x</sub> Zigzag-Like Monolayer on Pt(111). Journal of Physical Chemistry C, 2007, 111, 6095-6102.	1.5	45
4527	Spontaneous Emergence of Cl-Anions from NaCl(100) at Low Relative Humidity. Journal of Physical Chemistry C, 2007, 111, 8000-8004.	1.5	17
4528	Computational Studies of Intramolecular Hydrogen Atom Transfers in the $\dot{I}^2$ -Hydroxyethylperoxy and $\dot{I}^2$ -Hydroxyethoxy Radicals. Journal of Physical Chemistry A, 2007, 111, 5032-5042.	1.1	37
4529	Structural, Electronic, and Optical Properties of Oxygen Defects in Zn <sub>3</sub> N <sub>2</sub> . Journal of Physical Chemistry B, 2007, 111, 3379-3383.	1.2	27
4530	Ab initio study of oxygen adsorption on the Ti(0001) surface. Journal of Physics Condensed Matter, 2007, 19, 226004.	0.7	21
4531	Origin of the photoactivity in boron-doped anatase and rutile $TiO_2$ calculated from first principles. Physical Review B, 2007, 76, .	1.1	107
4532	Theoretical Investigation of the Deposition of Cu, Ag, and Au Atoms on the ZrO <sub>2</sub> (111) Surface. Journal of Physical Chemistry C, 2007, 111, 10448-10454.	1.5	58
4533	Representative Benchmark Suites for Barrier Heights of Diverse Reaction Types and Assessment of Electronic Structure Methods for Thermochemical Kinetics. Journal of Chemical Theory and Computation, 2007, 3, 569-582.	2.3	207
4534	Ligand-Field Dependence of the Excited State Dynamics of Hangman Bisporphyrin Dyad Complexes. Journal of Physical Chemistry B, 2007, 111, 8258-8268.	1.2	16
4535	Theoretical Studies on Novel Main Group Metallocene-like Complexes Involving Planar Hexacoordinate Carbon $\dot{I}^6$ -B <sub>6</sub> C <sub>2</sub> - Ligand. Journal of Physical Chemistry A, 2007, 111, 2930-2934.	1.1	23
4536	Role of Germanium in the Formation of Double Four Rings in Zeolites. Journal of Physical Chemistry C, 2007, 111, 3575-3583.	1.5	47
4537	Adsorption of NO in Fe <sup>2+</sup> -Exchanged Ferrierite. A Density Functional Theory Study. Journal of Physical Chemistry C, 2007, 111, 586-595.	1.5	37
4538	Vanadium Oxides on Aluminum Oxide Supports. 3. Metastable $\dot{I}^{\alpha}$ -Al <sub>2</sub> O <sub>3</sub> (001) Compared to $\dot{I}^{\pm}$ -Al <sub>2</sub> O <sub>3</sub> (0001). Journal of Physical Chemistry C, 2007, 111, 5141-5153.	1.5	27
4539	Infrared Spectroscopic Study of the Adsorption of HCN by $\dot{I}^{\beta}$ -Al <sub>2</sub> O <sub>3</sub> : Competition with Triethylenediamine for Adsorption Sites. Journal of Physical Chemistry C, 2007, 111, 5416-5425.	1.5	24
4540	Ab Initio Analysis of Electron Transport in Oligoglycines. Journal of Physical Chemistry C, 2007, 111, 14552-14559.	1.5	16



#	ARTICLE	IF	CITATIONS
4541	Dielectric relaxation and electronic structure of $\text{CaTiO}_3$ . Physical Review B, 2007, 76, .	1.1	89
4542	Adsorption of Atomic and Molecular Oxygen on the Au(321) Surface: A DFT Study. Journal of Physical Chemistry C, 2007, 111, 17311-17321.	1.5	65
4543	Influence of Single Impurity Atoms on the Structure, Electronic, and Magnetic Properties of Ni <sub>5</sub> Clusters. Journal of Physical Chemistry A, 2007, 111, 2067-2076.	1.1	10
4544	Is the Preadsorbed Sulfur Atom Always Acting as a Poison for the Surface Reaction?. Journal of Physical Chemistry C, 2007, 111, 2223-2228.	1.5	19
4545	First-Principles Calculation of Solution Energy of Alkaline-Earth Metal Elements to BaTiO <sub>3</sub> . Japanese Journal of Applied Physics, 2007, 46, 7136-7140.	0.8	26
4546	Interaction of Carbon Monoxide with Small Gold Clusters Inside TS-1 Pores. Journal of Physical Chemistry C, 2007, 111, 11424-11436.	1.5	13
4547	O-H Bond Dissociation Enthalpies of Oximes: A Theoretical Assessment and Experimental Implications. Journal of Physical Chemistry A, 2007, 111, 13112-13125.	1.1	34
4548	Simple Energy Corrections for Precise Atomization Energies of CHON Molecules. Journal of Physical Chemistry A, 2007, 111, 11160-11165.	1.1	6
4549	Theoretical Study of Aqueous Solvation of $\text{K}^+$ Comparing ab Initio, Polarizable, and Fixed-Charge Models. Journal of Chemical Theory and Computation, 2007, 3, 2068-2082.	2.3	87
4550	An Unexpected Pathway for the Catalytic Oxidation of Methylidyne on Rh{111} as a Route to Syngas. Journal of the American Chemical Society, 2007, 129, 1751-1759.	6.6	56
4551	Adsorption of Atoms on Cu Surfaces: A Density Functional Theory Study. Langmuir, 2007, 23, 4910-4917.	1.6	49
4552	Equilibrium Geometries of Noncovalently Bound Intermolecular Complexes Derived from Subsystem Formulation of Density Functional Theory. Journal of Chemical Theory and Computation, 2007, 3, 735-745.	2.3	45
4553	Deactivation Mechanism of a Au/CeZrO <sub>4</sub> Catalyst During a Low-Temperature Water Gas Shift Reaction. Journal of Physical Chemistry C, 2007, 111, 16927-16933.	1.5	92
4554	Structural distortions in AlF <sub>3</sub> : A test for density-functional methods. Physical Review B, 2007, 75, .	1.1	3
4555	Enantiospecific Adsorption of Alanine on the Chiral Cu{531} Surface. Journal of Physical Chemistry C, 2007, 111, 8331-8336.	1.5	63
4556	First-Principles Investigation of the Structure, Energetics, and Electronic Properties of Ru/HfO <sub>2</sub> Interfaces. Journal of Physical Chemistry C, 2007, 111, 9203-9210.	1.5	11
4557	Density Functional Study of the Adsorption of Atomic Oxygen on the (001) Surface of Early Transition-Metal Carbides. Journal of Physical Chemistry C, 2007, 111, 1307-1314.	1.5	66
4558	On the Sequential Hydrogen Dissociative Chemisorption on Small Platinum Clusters: A Density Functional Theory Study. Journal of Physical Chemistry C, 2007, 111, 12773-12778.	1.5	130



#	ARTICLE	IF	CITATIONS
4559	Predicting Reaction Equilibria for Destabilized Metal Hydride Decomposition Reactions for Reversible Hydrogen Storage. <i>Journal of Physical Chemistry C</i> , 2007, 111, 1584-1591.	1.5	84
4560	Haptotropic Shifts and Fluxionality of Cyclopentadienyl in Mixed-Hapticity Complexes: A DFT Mechanistic Study. <i>Organometallics</i> , 2007, 26, 1777-1781.	1.1	12
4561	Effects of Hydrogen on the Reactivity of O <sub>2</sub> toward Gold Nanoparticles and Surfaces. <i>Journal of Physical Chemistry C</i> , 2007, 111, 19001-19008.	1.5	75
4562	First-principles study of cation and hydrogen arrangements in the Li-Mg-N-H hydrogen storage system. <i>Physical Review B</i> , 2007, 76, .	1.1	23
4563	Precursor $\pi$ -Complex in the Addition of Vinyl Bromide on Si(100). <i>Journal of Physical Chemistry C</i> , 2007, 111, 6365-6371.	1.5	7
4564	Molecular Dynamics Simulations of the Coalescence of Iridium Clusters. <i>Journal of Physical Chemistry C</i> , 2007, 111, 6713-6719.	1.5	14
4565	Bonding in Low-Coordinate Environments: Electronic Structure of Pseudotetrahedral Iron <sup>II</sup> Imido Complexes. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 448-457.	2.3	36
4566	Theoretical Studies of the Formation and Reactivity of C <sub>2</sub> Hydrocarbon Species on the Fe(100) Surface. <i>Journal of Physical Chemistry C</i> , 2007, 111, 13149-13162.	1.5	41
4567	A Systematic Density Functional Study of Molecular Oxygen Adsorption and Dissociation on the (001) Surface of Group IV <sup>IV-VI</sup> Transition Metal Carbides. <i>Journal of Physical Chemistry C</i> , 2007, 111, 16982-16989.	1.5	60
4568	Influence of Anatase Support on Geometrical Structure of Vanadium Oxide at Varying Temperatures and Pressures. Periodic DFT Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 4216-4225.	1.5	18
4569	Equation of state of solid nickel aluminide. <i>Physical Review B</i> , 2007, 76, .	1.1	8
4570	First-Principles Prediction of Equilibrium Potentials for Water Activation by a Series of Metals. <i>Journal of the Electrochemical Society</i> , 2007, 154, F217.	1.3	30
4571	Methane Activation on Pt and Pt <sub>4</sub> : A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1657-1663.	1.2	70
4572	Binding Formation of 12-Hydroxydodecanoic Acid on Si(001)-(2 $\times$ 2). <i>Journal of Physical Chemistry C</i> , 2007, 111, 4375-4378.	1.5	3
4573	Ab initio investigation of ammonia-borane complexes for hydrogen storage. <i>Journal of Chemical Physics</i> , 2007, 126, 184703.	1.2	116
4574	Reactions of Hydroxyl on the Topmost Layer of Ag(111): A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 1333-1341.	1.5	7
4575	Ab initio Study of Structural Stability of Mo <sup>IV</sup> S Clusters and Size Specific Stoichiometries of Magic Clusters. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2778-2782.	1.1	27
4576	Methanol Adsorption and Dissociation on TiO <sub>2</sub> (110) from First Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2007, 111, 10023-10028.	1.5	106

#	ARTICLE	IF	CITATIONS
4577	Theoretical Study of Tungsten $\text{W}^3$ -Silaallyl/ $\text{W}^3$ -Vinylsilyl and Vinyl Silylene Complexes: Interesting Bonding Nature and Relative Stability. <i>Organometallics</i> , 2007, 26, 4413-4423.	1.1	23
4578	Adsorption and Decomposition Pathways of Vinyl Phosphonic and Ethanoic Acids on the Al(111) Surface: A Density Functional Analysis. <i>Journal of Physical Chemistry C</i> , 2007, 111, 7366-7375.	1.5	14
4579	New phases of hydrogen-bonded systems at extreme conditions. <i>Phase Transitions</i> , 2007, 80, 1073-1084.	0.6	9
4580	Adsorption and Dissociation of $\text{H}_2\text{O}$ on a W(111) Surface: A Computational Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 17333-17339.	1.5	29
4581	Simulation of the Electron Transfer between the Tetraheme Subunit and the Special Pair of the Photosynthetic Reaction Center Using a Microstate Description. <i>Journal of Physical Chemistry B</i> , 2007, 111, 2957-2968.	1.2	20
4582	S1 and S2 Excited States of Gas-Phase Schiff-Base Retinal Chromophores: A Time-Dependent Density Functional Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2946-2950.	1.1	34
4583	Dinuclear and Tetranuclear Gold-Nitrogen Complexes. Solvent Influences on Oxidation and Nuclearity of Gold Guanidinate Derivatives. <i>Inorganic Chemistry</i> , 2007, 46, 11165-11172.	1.9	38
4584	Chemisorption of 3-Aminopropyltrimethoxysilane on Si(001)-(2 $\times$ 2). <i>Journal of Physical Chemistry C</i> , 2007, 111, 15020-15025.	1.5	10
4585	Spin Exchange Effects on the Physicochemical Properties of Tetraoxolene-Bridged Bimetallic Complexes. <i>Inorganic Chemistry</i> , 2007, 46, 3257-3274.	1.9	60
4586	Detailed Mechanism for CO Oxidation on AuNi <sub>3</sub> (111) Extended Surface: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 12335-12339.	1.5	15
4587	Pseudopotential hyperfine calculations through perturbative core-level polarization. <i>Physical Review B</i> , 2007, 76, .	1.1	25
4588	First-Principle Study of Sulfur Adsorption on Ir(100) Surface. <i>Materials Science Forum</i> , 2007, 561-565, 2435-2438.	0.3	1
4589	Band-structure anomalies of the chalcopyrite semiconductors $\text{CuGaX}_2$ versus $\text{AgGaX}_2$ (X=S and Se) and their alloys. <i>Physical Review B</i> , 2007, 75, .	1.1	132
4590	Structural studies of $\text{Ni}_2+\text{xMn}_{1-\text{x}}\text{Ga}$ powder x-ray diffraction and total energy calculations. <i>Physical Review B</i> , 2007, 75, .	1.1	90
4591	Electronic structure of biphenyl on Si(100). <i>Physical Review B</i> , 2007, 76, .	1.1	13
4592	Adsorption of gold on TiC(001): Au-C interactions and charge polarization. <i>Journal of Chemical Physics</i> , 2007, 127, 211102.	1.2	66
4593	On the Role of Subsurface Oxygen and Ethylenedioxy in Ethylene Epoxidation on Silver. <i>Journal of Physical Chemistry C</i> , 2007, 111, 7992-7999.	1.5	40
4594	Hydrogen sorption in defective hexagonal BN sheets and BN nanotubes. <i>Physical Review B</i> , 2007, 76, .	1.1	128

#	ARTICLE	IF	CITATIONS
4595	Ultralow-Density Nanocage-Based Metal-Oxide Polymorphs. <i>Physical Review Letters</i> , 2007, 99, 235502.	2.9	119
4596	Density Function Theory Study of Copper Agglomeration on the WN(001) Surface. <i>Journal of Physical Chemistry C</i> , 2007, 111, 9403-9406.	1.5	16
4597	Chemisorption of Sulfur and Sulfur-Based Simple Molecules on Au(111). <i>Journal of Physical Chemistry C</i> , 2007, 111, 12383-12390.	1.5	20
4598	Predicted Oxidation of CO Catalyzed by Au Nanoclusters on a Thin Defect-Free MgO Film Supported on a Mo(100) Surface. <i>Journal of the American Chemical Society</i> , 2007, 129, 2228-2229.	6.6	167
4599	Cyclopropanation of Cyclohexenone by Diazomethane Catalyzed by Palladium Diacetate: Evidence for the Formation of Palladium(0) Nanoparticles. <i>Organometallics</i> , 2007, 26, 3306-3314.	1.1	38
4600	Hydrogen Dynamics in Na <sub>3</sub> AlH <sub>6</sub> : A Combined Density Functional Theory and Quasielastic Neutron Scattering Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 3886-3892.	1.2	38
4601	Electronic Structure of xDNA. <i>Journal of Physical Chemistry B</i> , 2007, 111, 9057-9061.	1.2	31
4602	First-Principles Study of the Four Polymorphs of Crystalline Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine. <i>Journal of Physical Chemistry B</i> , 2007, 111, 12715-12722.	1.2	108
4603	Reaction Mechanisms for C=O Bond Coupling from Pt <sub>4</sub> CH <sub>2</sub> <sup>+</sup> and O <sub>2</sub> : A Relativistic Density Functional Study. <i>Organometallics</i> , 2007, 26, 6076-6081.	1.1	5
4604	Factors Controlling the Interaction of CO <sub>2</sub> with Transition Metal Surfaces. <i>Journal of Physical Chemistry C</i> , 2007, 111, 16934-16940.	1.5	152
4605	Dissociative Adsorption of Water at Vacancy Defects in Graphite. <i>Journal of Physical Chemistry C</i> , 2007, 111, 18258-18263.	1.5	86
4606	First Principle Study of Ethanol Adsorption and Formation of Hydrogen Bond on Rh(111) Surface. <i>Journal of Physical Chemistry C</i> , 2007, 111, 7403-7410.	1.5	50
4607	Electronic Structure Investigation of Surface Adsorbate and Adsorbate-Adsorbate Interactions in Multilayers of CH <sub>4</sub> on MgO(100). <i>Journal of Physical Chemistry C</i> , 2007, 111, 966-976.	1.5	14
4608	Metal-Diboride Nanotubes as High-Capacity Hydrogen Storage Media. <i>Nano Letters</i> , 2007, 7, 663-667.	4.5	115
4609	Hyperelectronic Metal-Carborane Analogues of Cymantrene (MnCp(CO) <sub>3</sub> ) Anions: Electronic and Structural Noninnocence of the Tricarbadeboranyl Ligand. <i>Organometallics</i> , 2007, 26, 4471-4482.	1.1	24
4610	Theoretical Analysis of Intermolecular Covalent H-Bonding and Magnetic Properties of Phenalenyl and spiro-Biphenalenyl Radical H-Dimers. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6304-6315.	1.1	39
4611	Site-Specific Kondo Effect at Ambient Temperatures in Iron-Based Molecules. <i>Physical Review Letters</i> , 2007, 99, 106402.	2.9	242
4612	Theoretical Investigation of the Formation of Hydrogen Peroxide from H <sub>2</sub> and O <sub>2</sub> over Anionic Gold Clusters Au <sub>n</sub> <sup>-</sup> (n = 1-4). <i>Journal of Physical Chemistry C</i> , 2007, 111, 11590-11597.	1.5	24

#	ARTICLE	IF	CITATIONS
4613	Bonding Analyses, Formation Energies, and Vibrational Properties of $M^2$ d <sub>8</sub> Complexes (M = Ag(I), Ni(II), Cu(II), or Zn(II)). Journal of Physical Chemistry A, 2007, 111, 13075-13087.	1.1	31
4614	Kinetic Study of the Reactions of Cl Atoms with CF <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> OH, CF <sub>3</sub> CF <sub>2</sub> CH <sub>2</sub> OH, CHF <sub>2</sub> CF <sub>2</sub> CH <sub>2</sub> OH, and CF <sub>3</sub> CHFCF <sub>2</sub> CH <sub>2</sub> OH. Journal of Physical Chemistry A, 2007, 111, 11608-11617.	1.1	29
4615	Performance on molecules, surfaces, and solids of the Wu-Cohen GGA exchange-correlation energy functional. Physical Review B, 2007, 75, .	1.1	306
4616	Spintronic materials based on main-group elements. Journal of Physics Condensed Matter, 2007, 19, 165203.	0.7	26
4617	Steric effects and chirality in the adsorption of glycine and phenylglycine on Cu(110). Nanotechnology, 2007, 18, 424030.	1.3	24
4618	Effect of boron on the superconducting transition of heavily doped diamond. Diamond and Related Materials, 2007, 16, 353-358.	1.8	11
4619	Electronic Structure of Trigonal-Planar Transition-Metal <sup>II</sup> Imido Complexes: Spin-State Energetics, Spin-Density Profiles, and the Remarkable Performance of the OLYP Functional. Journal of Chemical Theory and Computation, 2007, 3, 689-702.	2.3	110
4620	Surface segregation in CuPt alloys by means of an improved modified embedded atom method. Physical Review B, 2007, 76, .	1.1	15
4621	An Infrared Spectroscopic Study of the Conformational Transition of Elastin-Like Polypeptides. Biophysical Journal, 2007, 93, 2429-2435.	0.2	54
4622	Electronic structure and electrical conductivity of MgO protecting layer in plasma-display panels: A tight-binding quantum chemical study. Journal of the Society for Information Display, 2007, 15, 307.	0.8	2
4623	Magnetic exchange interactions in the paramagnetic state of hcp Gd. Journal of Physics Condensed Matter, 2007, 19, 326218.	0.7	24
4624	Competition between magnetic structures in the Fe rich fcc FeNi alloys. Physical Review B, 2007, 76, .	1.1	119
4625	First-principles LDA+U and GGA+U study of cerium oxides: Dependence on the effective U parameter. Physical Review B, 2007, 75, .	1.1	634
4626	Understanding Ceria Nanoparticles from First-Principles Calculations. Journal of Physical Chemistry C, 2007, 111, 10142-10145.	1.5	99
4627	Statistical Thermodynamics and Model Calculations. , 0, , 525-588.		10
4628	Local hybrid functionals: An assessment for thermochemical kinetics. Journal of Chemical Physics, 2007, 127, 194102.	1.2	87
4629	Basis Set Limit Coupled Cluster Study of H-Bonded Systems and Assessment of More Approximate Methods. Journal of Physical Chemistry A, 2007, 111, 11122-11133.	1.1	87
4630	An Evaluation of Harmonic Vibrational Frequency Scale Factors. Journal of Physical Chemistry A, 2007, 111, 11683-11700.	1.1	2,264

#	ARTICLE	IF	CITATIONS
4631	CO adsorption on Cu-Pd alloy surfaces: ligand versus ensemble effects. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2216-2225.	1.3	79
4632	Ab initio study of Cr interactions with point defects in bcc Fe. <i>Physical Review B</i> , 2007, 75, .	1.1	269
4633	Long-Range Repulsive Interaction between Molecules on a Metal Surface Induced by Charge Transfer. <i>Physical Review Letters</i> , 2007, 99, 176103.	2.9	163
4634	First-principles investigations of the structure and stability of oxygen adsorption and surface oxide formation at Au(111). <i>Physical Review B</i> , 2007, 76, .	1.1	119
4635	A density functional study on water-sulfuric acid-ammonia clusters and implications for atmospheric cluster formation. <i>Journal of Geophysical Research</i> , 2007, 112, .	3.3	111
4636	Oxide-Supported Metal Thin-Film Catalysts: The How and Why. , 2007, , 13-21.		6
4637	Ab Initio Calculation of a Graphene-Ribbon-Based Molecular Switch. <i>Journal of Physical Chemistry C</i> , 2007, 111, 14266-14273.	1.5	27
4638	Novel Precursors for Boron Nanotubes: The Competition of Two-Center and Three-Center Bonding in Boron Sheets. <i>Physical Review Letters</i> , 2007, 99, 115501.	2.9	751
4639	Study of the Nitrogen Concentration Influence on N-Doped TiO <sub>2</sub> Anatase from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2007, 111, 12086-12090.	1.5	220
4640	Properties of the gold oxides Au <sub>2</sub> O <sub>3</sub> and Au <sub>2</sub> O: First-principles investigation. <i>Physical Review B</i> , 2007, 75, .	1.1	101
4641	Ab initio study of K adsorption on graphene and carbon nanotubes: Role of long-range ionic forces. <i>Physical Review B</i> , 2007, 76, .	1.1	104
4642	Description of Carbo-oxocarbons and Assessment of Exchange-Correlation Functionals for the DFT Description of Carbo-mers. <i>Journal of Physical Chemistry A</i> , 2007, 111, 136-149.	1.1	32
4643	Importance of Van Der Waals Interaction for Organic Molecule-Metal Junctions: Adsorption of Thiophene on Cu(110) as a Prototype. <i>Physical Review Letters</i> , 2007, 99, 176401.	2.9	159
4644	First-Principles Calculation of the Structural, Magnetic, and Electronic Properties of the Co <sub>x</sub> Cu <sub>1-x</sub> Solid Solutions Using Special Quasirandom Structures. <i>Journal of the Physical Society of Japan</i> , 2007, 76, 024605.	0.7	12
4645	Van der Waals density functional: Self-consistent potential and the nature of the van der Waals bond. <i>Physical Review B</i> , 2007, 76, .	1.1	1,058
4646	Understanding Photocatalytic Activity of S- and P-Doped TiO <sub>2</sub> under Visible Light from First-Principles. <i>Journal of Physical Chemistry C</i> , 2007, 111, 18985-18994.	1.5	236
4647	DFT-Based Characterization of the Multiple Adsorption Modes of Nitrogen Oxides on Pt(111). <i>Journal of Physical Chemistry C</i> , 2007, 111, 389-397.	1.5	84
4648	Adsorption Behavior of Iron Phthalocyanine on Au(111) Surface at Submonolayer Coverage. <i>Journal of Physical Chemistry C</i> , 2007, 111, 9240-9244.	1.5	140

#	ARTICLE	IF	CITATIONS
4649	Study on the structural relationship between the liquid and amorphous Fe <sub>78</sub> Si <sub>9</sub> B <sub>13</sub> alloys by ab initio molecular dynamics simulation. Applied Physics Letters, 2007, 90, 201909.	1.5	48
4650	Why Urea Eliminates Ammonia Rather than Hydrolyzes in Aqueous Solution. Journal of Physical Chemistry B, 2007, 111, 720-730.	1.2	85
4651	Spin-Forbidden Ligand Binding to the Ferrous <sup>2+</sup> Heme Group: Ab Initio and DFT Studies. Journal of Physical Chemistry B, 2007, 111, 841-852.	1.2	181
4652	A Theoretical Study of the Energetic Stability and Geometry of Hydrogen- and Oxygen-Terminated Diamond (100) Surfaces. Journal of Physical Chemistry C, 2007, 111, 795-801.	1.5	61
4653	Why does the B3LYP hybrid functional fail for metals?. Journal of Chemical Physics, 2007, 127, 024103.	1.2	481
4654	Conservation of dielectric constant upon amorphization in perovskite oxides. Physical Review B, 2007, 76, .	1.1	10
4655	Density functional study of the interaction between small Au clusters, Au <sub>n</sub> (n=1-7) and the rutile TiO <sub>2</sub> surface. I. Adsorption on the stoichiometric surface. Journal of Chemical Physics, 2007, 127, 084704.	1.2	55
4656	Structure and Bonding of the Water <sup>2+</sup> Hydroxyl Mixed Phase on Pt(111). Journal of Physical Chemistry C, 2007, 111, 15003-15012.	1.5	117
4657	Assessment of Density Functional Theory Methods for the Computation of Heats of Formation and Ionization Potentials of Systems Containing Third Row Transition Metals. Journal of Physical Chemistry A, 2007, 111, 6044-6053.	1.1	94
4658	Bonding differences between single iron atoms versus iron chains with carbon nanotubes: First-principles calculations. Physical Review B, 2007, 76, .	1.1	22
4659	Structural Requirements and Reaction Pathways in Dimethyl Ether Combustion Catalyzed by Supported Pt Clusters. Journal of the American Chemical Society, 2007, 129, 13201-13212.	6.6	49
4660	Optimizing performance of half-metals at finite temperature. Journal of Physics Condensed Matter, 2007, 19, 315212.	0.7	20
4661	The Structure and Energy of Oxygen Vacancy Formation in Clean and Doped, Very Thin Films of ZnO. Journal of Physical Chemistry C, 2007, 111, 12715-12722.	1.5	30
4662	Local Atomic Ordering in BaTaO <sub>2.5</sub> Studied by Neutron Pair Distribution Function Analysis and Density Functional Theory. Chemistry of Materials, 2007, 19, 4037-4042.	3.2	96
4663	Ab initio study of the effect of solute atoms on the stacking fault energy in aluminum. Physical Review B, 2007, 75, .	1.1	94
4664	Electronic structure and optical properties of lightweight metal hydrides. Physical Review B, 2007, 75, .	1.1	120
4665	Surface Verwey Transition in Magnetite. Physical Review Letters, 2007, 99, 206402.	2.9	97
4666	Carbocation Branching Observed in a Simulation. Journal of Physical Chemistry A, 2007, 111, 5945-5947.	1.1	14

#	ARTICLE	IF	CITATIONS
4667	Kinetic energy density study of some representative semilocal kinetic energy functionals. <i>Journal of Chemical Physics</i> , 2007, 127, 144109.	1.2	57
4668	Single Phosphorus Atoms in Si(001): Doping-Induced Charge Transfer into Isolated Si Dangling Bonds. <i>Journal of Physical Chemistry C</i> , 2007, 111, 6428-6433.	1.5	5
4669	Proton Hopping in Phosphoric Acid Solvated Nafion Membrane: A Molecular Simulation Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 6357-6363.	1.2	43
4670	Infrared Spectroscopic Study of ClCN Adsorption on Clean and Triethylenediamine-Precovered $\text{Al}_2\text{O}_3$ . <i>Journal of Physical Chemistry C</i> , 2007, 111, 18226-18235.	1.5	12
4671	Origin of the Verwey transition in magnetite: Group theory, electronic structure, and lattice dynamics study. <i>Physical Review B</i> , 2007, 76, .	1.1	93
4672	Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry. <i>Reviews in Computational Chemistry</i> , 2007, , 1-86.	1.5	775
4673	Theoretical Study of Metal-Ligand Interaction in Sm(III), Eu(III), and Tb(III) Complexes of Coumarin-3-Carboxylic Acid in the Gas Phase and Solution. <i>Inorganic Chemistry</i> , 2007, 46, 10926-10936.	1.9	27
4674	A Computational Study of the Adsorption of Small Ag and Au Nanoclusters on Graphite. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12317-12326.	1.1	48
4675	Analysis of Dynamical Properties of Surfaces and Thin Films using Molecular Dynamics. <i>Shinku/Journal of the Vacuum Society of Japan</i> , 2007, 50, 82-88.	0.2	0
4676	Design of Reactive Ion Etching Process Based on ab-initio Calculation-The First Step-. <i>Shinku/Journal of the Vacuum Society of Japan</i> , 2007, 50, 437-439.	0.2	3
4677	Ab-Initio Modeling of Defects in Germanium. , 2007, , 187-210.		1
4678	A DFT Study of Activation of H <sub>2</sub> and D <sub>2</sub> over Zn-MOR. <i>Studies in Surface Science and Catalysis</i> , 2007, 172, 397-400.	1.5	0
4679	Sandwich-like Compounds Based on the All-Metal Aromatic Unit Al <sub>4</sub> and the Main-Group Metals M (M=Li, Na, K, Be, Mg, Ca). <i>Chemistry - A European Journal</i> , 2007, 13, 2546-2555.	1.7	31
4680	Structure of Ag Clusters Grown on Fs-Defect Sites of an MgO(100) Surface. <i>Chemistry - A European Journal</i> , 2007, 13, 6408-6418.	1.7	46
4681	Infrared Spectrum and Structure of Thorimine (HN <sub>3</sub> ThH <sub>2</sub> ). <i>Chemistry - A European Journal</i> , 2007, 13, 5601-5606.	1.7	33
4682	Supramolecular Self-Assembly Initiated by Solid-Solid Wetting. <i>Chemistry - A European Journal</i> , 2007, 13, 7785-7790.	1.7	27
4683	Spintronics: A Challenge for Materials Science and Solid-State Chemistry. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 668-699.	7.2	963
4684	Low-Basicity Oxygen Atoms: A Key in the Search for Propylene Epoxidation Catalysts. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 2055-2058.	7.2	134



#	ARTICLE	IF	CITATIONS
4685	Manipulation and Patterning of the Surface Hydrogen Concentration on Pd(111) by Electric Fields. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 5757-5761.	7.2	16
4686	Catalytic Consequences of Composition in Polyoxometalate Clusters with Keggin Structure. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 7864-7868.	7.2	108
4691	An Interatomic Potential for Studying CuZr Bulk Metallic Glasses. <i>Advanced Engineering Materials</i> , 2007, 9, 505-508.	1.6	26
4692	Comprehensive analysis of chemical bonding in boron clusters. <i>Journal of Computational Chemistry</i> , 2007, 28, 251-268.	1.5	228
4693	The existence of secondary orbital interactions. <i>Journal of Computational Chemistry</i> , 2007, 28, 344-361.	1.5	92
4694	Global minimum structure searches via particle swarm optimization. <i>Journal of Computational Chemistry</i> , 2007, 28, 1177-1186.	1.5	147
4695	DFT studies using supercells and projector-augmented waves for structure, energetics, and dynamics of glycine, alanine, and cysteine. <i>Journal of Computational Chemistry</i> , 2007, 28, 1817-1833.	1.5	45
4696	Merging multiconfigurational wavefunctions and correlation functionals to predict magnetic coupling constants. <i>Journal of Computational Chemistry</i> , 2007, 28, 2559-2568.	1.5	9
4697	A self-contained and portable density functional theory library for use in Ab Initio quantum chemistry programs. <i>Journal of Computational Chemistry</i> , 2007, 28, 2569-2575.	1.5	22
4698	A Theoretical Study of the Nearest Cu-Cu Antiferromagnetic Exchange Coupling Interactions in [LaCu <sub>6</sub> ] and [YCu <sub>6</sub> ]. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 1261-1267.	1.0	3
4699	Conformational Analysis of One-Dimensional Coordination Polymers Based on [Cp <sub>2</sub> Cr <sub>2</sub> (CO) <sub>4</sub> ( $\eta^1$ -P <sub>2</sub> )] by Solid-State Multinuclear NMR Spectroscopy and Density Functional Calculations. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 2775-2782.	1.0	35
4700	Adsorption, Diffusion and Desorption of Chlorine on and from Rutile TiO <sub>2</sub> {110}: A Theoretical Investigation. <i>ChemPhysChem</i> , 2007, 8, 444-451.	1.0	28
4701	Ab Initio Study of Poly(vinyl chloride) Propagation Kinetics: Head-to-Head versus Head-to-Tail Additions. <i>ChemPhysChem</i> , 2007, 8, 541-552.	1.0	26
4702	FTIR and FT-Raman spectra and density functional computations of the vibrational spectra, molecular geometry and atomic charges of the biomolecule: 5-bromouracil. <i>Journal of Raman Spectroscopy</i> , 2007, 38, 1227-1241.	1.2	79
4703	First principles study of structural phase transition of YSb and ScSb compounds. <i>Solid State Communications</i> , 2007, 141, 359-364.	0.9	18
4704	Adsorption and diffusion of OH on Mo modified Pt(111) surface: First-principles theory. <i>Solid State Communications</i> , 2007, 142, 148-153.	0.9	10
4705	First-principles investigation of pressure-induced changes in structural and electronic properties of Y <sub>2</sub> C <sub>3</sub> superconductor. <i>Solid State Communications</i> , 2007, 142, 536-540.	0.9	4
4706	Ab initio study on the structural and elastic properties of MAiSi (M=Ca, Sr, and Ba). <i>Solid State Communications</i> , 2007, 143, 425-428.	0.9	63

#	ARTICLE	IF	CITATIONS
4707	Chemical routes to ultra thin films for copper barriers and liners. <i>Surface and Coatings Technology</i> , 2007, 201, 9256-9259.	2.2	16
4708	TEM and DFT investigation of CVD TiN/Al <sub>2</sub> O <sub>3</sub> multilayer coatings. <i>Surface and Coatings Technology</i> , 2007, 202, 522-531.	2.2	16
4709	Oxygen vacancies in transition metal and rare earth oxides: Current state of understanding and remaining challenges. <i>Surface Science Reports</i> , 2007, 62, 219-270.	3.8	1,102
4710	Density functional theory analysis of reactivity of Pt <sub>x</sub> Pd <sub>y</sub> alloy clusters. <i>Surface Science</i> , 2007, 601, 165-171.	0.8	32
4711	Segregation of Pt at clean surfaces of (Pt, Ni) <sub>3</sub> Al. <i>Surface Science</i> , 2007, 601, 376-380.	0.8	14
4712	Investigation of the dissociative adsorption for cyclopropane on the copper surface by density functional theory and quantum chemical molecular dynamics method. <i>Surface Science</i> , 2007, 601, 679-685.	0.8	3
4713	A comparative study of ethylene oxide and diethylene dioxide adsorption on silicon (001). <i>Surface Science</i> , 2007, 601, 2576-2579.	0.8	4
4714	Kinetic aspect of CO <sub>2</sub> reforming of CH <sub>4</sub> on Ni(111): A density functional theory calculation. <i>Surface Science</i> , 2007, 601, 1271-1284.	0.8	140
4715	Mechanism of two-dimensional chiral growth of 6,13-pentacenequinone thin films on Si(111). <i>Surface Science</i> , 2007, 601, 1311-1318.	0.8	13
4716	Driving force for the WO <sub>3</sub> (001) surface relaxation. <i>Surface Science</i> , 2007, 601, 1481-1488.	0.8	40
4717	The surface oxide: A LEED, DFT and STM study. <i>Surface Science</i> , 2007, 601, 1574-1581.	0.8	96
4718	CO adsorption energies on metals with correction for high coordination adsorption sites – A density functional study. <i>Surface Science</i> , 2007, 601, 1747-1753.	0.8	259
4719	Coverage-dependent magnetization of 3d transition-metal adatoms on Co(001) in the submonolayer regime. <i>Surface Science</i> , 2007, 601, 1763-1767.	0.8	4
4720	The bonding geometry of alkylsilanes on gold: Relation to surface pattern development and STM image contrast. <i>Surface Science</i> , 2007, 601, 1937-1943.	0.8	5
4721	Ab-initio calculations and STM observations on tetrapyrrolyl and Fe(II)-tetrapyrrolyl-porphyrin molecules on Ag(111). <i>Surface Science</i> , 2007, 601, 2409-2414.	0.8	46
4722	Study of Si(001)4Å–2-Ga structure by scanning tunneling microscopy and ab initio calculation. <i>Surface Science</i> , 2007, 601, 2415-2419.	0.8	4
4723	A theoretical study of CH <sub>4</sub> dissociation on Pt(100) surface. <i>Surface Science</i> , 2007, 601, 3697-3701.	0.8	20
4724	An ab initio study of 3-aminopropyltrimethoxysilane molecule on Si(111)-() surface. <i>Surface Science</i> , 2007, 601, 3740-3744.	0.8	10

#	ARTICLE	IF	CITATIONS
4725	Chemisorption of 4-(4-amino-phenylazo) benzoic acid molecule on the Si(001)-(4 $\times$ 2) surface. <i>Surface Science</i> , 2007, 601, 3760-3764.	0.8	4
4726	Doping and STM tip-induced changes to single dangling bonds on Si(001). <i>Surface Science</i> , 2007, 601, 4036-4040.	0.8	10
4727	Interaction of SiH <sub>x</sub> precursors with hydrogen-covered Si surfaces: Impact dynamics and adsorption sites. <i>Surface Science</i> , 2007, 601, 3970-3973.	0.8	5
4728	Spin-flop structure at an antiferromagnetic/ferromagnetic interface: Mn/Fe(100). <i>Surface Science</i> , 2007, 601, 4348-4351.	0.8	5
4729	A nanoscale understanding of the adhesion of polybutylene terephthalate on aluminum. <i>Surface Science</i> , 2007, 601, 5241-5245.	0.8	5
4730	NH <sub>3</sub> on Si(001): Can Gaussian cluster and planewave slab models agree on energetics?. <i>Surface Science</i> , 2007, 601, 3020-3033.	0.8	14
4731	NO dissociation pathways on Rh(100), (110), and (111) surfaces: A comparative density functional theory study. <i>Surface Science</i> , 2007, 601, 3186-3195.	0.8	38
4732	Vibrational entropy-driven dealloying of Mo(100) and W(100) surface alloys. <i>Surface Science</i> , 2007, 601, L95-L101.	0.8	9
4733	When adding an unreactive metal enhances catalytic activity: NO <sub>x</sub> decomposition over silver-rhodium bimetallic surfaces. <i>Surface Science</i> , 2007, 601, L103-L108.	0.8	55
4734	The structure of a stoichiometric TiO <sub>2</sub> nanophase on Pt(1 1 1). <i>Surface Science</i> , 2007, 601, 3488-3496.	0.8	40
4735	First-principles studies of the structure of sulfur on the Pd(111) surface. <i>Surface Science</i> , 2007, 601, 4899-4909.	0.8	12
4736	Ice formation on kaolinite: Lattice match or amphoterism?. <i>Surface Science</i> , 2007, 601, 5378-5381.	0.8	101
4737	On the performance of DFT methods in (hyper)polarizability calculations: N <sub>4</sub> (Td) as a test case. <i>Computational and Theoretical Chemistry</i> , 2007, 804, 41-46.	1.5	15
4738	Structure and aromaticity of and Sb <sub>5</sub> M (M=Li, Na, and K) clusters. <i>Computational and Theoretical Chemistry</i> , 2007, 807, 17-23.	1.5	5
4739	A density-functional study of nickel/aluminum microclusters. <i>Computational and Theoretical Chemistry</i> , 2007, 807, 153-158.	1.5	15
4740	Energetics and bonding in small lithiated carbon clusters. <i>Computational and Theoretical Chemistry</i> , 2007, 807, 163-172.	1.5	8
4741	Spectroscopic properties of aromatic heterocyclic systems: XAl <sub>3</sub> (X=Si, Ge, Sn, Pb) and their anions and cations. <i>Computational and Theoretical Chemistry</i> , 2007, 809, 45-54.	1.5	1
4742	Sandwich complexes of the aromatic ring with the first row transition metal. <i>Computational and Theoretical Chemistry</i> , 2007, 810, 1-6.	1.5	20

#	ARTICLE	IF	CITATIONS
4743	Determination of precise harmonic force constants for alanine polypeptides. Computational and Theoretical Chemistry, 2007, 818, 125-129.	1.5	11
4744	Energetics and bonding in beryllium metallized carbon clusters. Computational and Theoretical Chemistry, 2007, 824, 39-47.	1.5	17
4745	Chemical vapor deposition of amorphous ruthenium-phosphorus alloy films. Thin Solid Films, 2007, 515, 5298-5307.	0.8	40
4746	Photocatalytic decolorization of Remazol Black 5 (RB5) and Procion Red MX-5B Isotherm of adsorption, kinetic of decolorization and mineralization. Applied Catalysis B: Environmental, 2007, 77, 100-109.	10.8	107
4747	Hybridization energies of double strands composed of DNA, RNA, PNA and LNA. Chemical Physics Letters, 2007, 434, 133-138.	1.2	33
4748	A computational study of the molecular structure of 1,3,4,2,2,4-benzodithiadiazine. Chemical Physics Letters, 2007, 434, 200-204.	1.2	6
4749	First-principles calculations of N <sub>2</sub> O adsorption and decomposition on GaN (0001) surface. Chemical Physics Letters, 2007, 438, 213-217.	1.2	10
4750	Local hybrid exchange-correlation functionals based on the dimensionless density gradient. Chemical Physics Letters, 2007, 440, 160-168.	1.2	98
4751	Adsorption of S on Ir(100) surface from first-principles calculations. Chemical Physics Letters, 2007, 441, 53-57.	1.2	8
4752	Nuclear shielding constants from localized local hybrid exchange-correlation potentials. Chemical Physics Letters, 2007, 442, 496-503.	1.2	26
4753	CO adsorbs upside-down on small Pt <sub>n</sub> Au <sub>n</sub> clusters. Chemical Physics Letters, 2007, 443, 304-308.	1.2	10
4754	Growth pattern and bonding trends in Pt (n= 2-13) clusters: Theoretical investigation based on first principle calculations. Chemical Physics Letters, 2007, 446, 374-379.	1.2	77
4755	Experimental equilibrium crystal structures: Molecular dynamics as a probe for atomic probability density functions. Chemical Physics Letters, 2007, 448, 61-64.	1.2	15
4756	Hydrogen pairing on graphene. Carbon, 2007, 45, 218-220.	5.4	60
4757	A TD-DFT investigation of the visible spectra of fluoro-antraquinones. Dyes and Pigments, 2007, 72, 185-191.	2.0	12
4758	Ab initio studies of structural and electronic properties of Li <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> spinel. Electrochemistry Communications, 2007, 9, 1107-1112.	2.3	265
4759	Bulk sensitive photo emission spectroscopy of compounds. Journal of Electron Spectroscopy and Related Phenomena, 2007, 156-158, 97-101.	0.8	15
4760	Determination of the thermal stability and isothermal bulk modulus of the ZrO <sub>2</sub> polymorphs at room temperature by molecular dynamics with a semi-empirical quantum-chemical model. Ceramics International, 2007, 33, 705-709.	2.3	21

#	ARTICLE	IF	CITATIONS
4761	First principles study of the coking resistance and the activity of a boron promoted Ni catalyst. <i>Chemical Engineering Science</i> , 2007, 62, 5039-5041.	1.9	27
4762	COSMO-RS modeling on the extraction of stimulant drugs from urine sample by the double actions of supercritical carbon dioxide and ionic liquid. <i>Chemical Engineering Science</i> , 2007, 62, 3940-3950.	1.9	65
4763	Ab initio study of the change from $\eta^5$ - to $\eta^1$ -coordination in group 12 dimetallocenes $M\eta^2(C_5H_5)_2$ with M, $M = Zn, Cd, Hg$ . <i>Chemical Physics</i> , 2007, 333, 201-207.	0.9	20
4764	Quantum dynamics study of the Langmuir-Hinshelwood H+H recombination mechanism and H <sub>2</sub> formation on a graphene model surface. <i>Chemical Physics</i> , 2007, 338, 1-10.	0.9	20
4765	Chemical bonding in metal sandwich molecules $MnR_2$ with R=pyrene C <sub>16</sub> H <sub>10</sub> and tetracene C <sub>18</sub> H <sub>12</sub> . <i>Chemical Physics</i> , 2007, 337, 55-67.	0.9	12
4766	Interconfigurational energies and ionization potentials: Test of a correlation energy functional. <i>Chemical Physics</i> , 2007, 337, 161-167.	0.9	16
4767	Bonding and magnetism in transition metal sandwich structures with the aromatic hydrocarbon coronene C <sub>24</sub> H <sub>12</sub> outer layers. <i>Chemical Physics</i> , 2007, 342, 223-235.	0.9	15
4768	Site preference of early transition metal elements in C <sub>15</sub> NbCr <sub>2</sub> . <i>Acta Materialia</i> , 2007, 55, 1599-1605.	3.8	47
4769	Site preference of transition-metal elements in B <sub>2</sub> NiAl: A comprehensive study. <i>Acta Materialia</i> , 2007, 55, 4799-4806.	3.8	78
4770	Defects and threshold displacement energies in SrTiO <sub>3</sub> perovskite using atomistic computer simulations. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2007, 254, 211-218.	0.6	69
4771	Theoretical investigations on the functionalization of carbon nanotubes. <i>Inorganica Chimica Acta</i> , 2007, 360, 785-793.	1.2	28
4772	A nickel(II) di- $\eta^4$ -phenolato bridged dinuclear complex: Weak antiferromagnetic interactions in nickel(II) dimers. <i>Inorganica Chimica Acta</i> , 2007, 360, 2245-2254.	1.2	46
4773	The role of water in the initial steps of methanol oxidation on Pt(200). <i>Electrochimica Acta</i> , 2007, 52, 2236-2243.	2.6	37
4774	Enhanced secondary ion emission with a bismuth cluster ion source. <i>International Journal of Mass Spectrometry</i> , 2007, 262, 144-153.	0.7	35
4775	A theoretical investigation of the adsorption surface sites of the activated MgCl <sub>2</sub> . <i>Journal of Molecular Catalysis A</i> , 2007, 270, 164-170.	4.8	35
4776	Density functional theory study of CO adsorption on the (100), (001) and (010) surfaces of Fe <sub>3</sub> C. <i>Journal of Molecular Catalysis A</i> , 2007, 269, 169-178.	4.8	60
4777	1,6-Bis(4-methoxyphenylsulfanyl) perchlorofluoranthene: A molecule with sandwiched $\pi$ - $\pi$ stacking linked by a flexible five-membered ring. <i>Journal of Molecular Structure</i> , 2007, 829, 51-56.	1.8	5
4778	On the ground state $T_g$ - $\mu_g$ ( $T_g=2T_2g, 3T_1g$ ) Jahn-Teller-coupling in hexacyano complexes of 3d-transition metals. <i>Journal of Molecular Structure</i> , 2007, 838, 157-163.	1.8	12

#	ARTICLE	IF	CITATIONS
4779	First-principles calculations of energetics of sigma phase formation and thermodynamic modelling in the Cr-Fe-W system. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2007, 462, 153-158.	2.6	7
4780	A methodology to aid in the design of naval steels: Linking first principles calculations to mesoscale modeling. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2007, 452-453, 558-568.	2.6	14
4781	First-principles study of Sn adsorption on Ni(100), (110) and (111) surfaces. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2007, 460-461, 50-57.	2.6	14
4782	First-principles study of the Ni(111)()R30°-Pb surface. <i>Physica B: Condensed Matter</i> , 2007, 392, 217-220.	1.3	13
4783	Theoretical study of FCC-HCP phase coexistence and phase stability in Al by FP-LAPW method with GGA for exchange and correlation. <i>Physica B: Condensed Matter</i> , 2007, 393, 278-284.	1.3	16
4784	Transition phase and electronic structure of SrS under pressure from first-principles calculations. <i>Physica B: Condensed Matter</i> , 2007, 399, 66-69.	1.3	29
4785	Theoretical and experimental studies on oxygen vacancy in p-type ZnO. <i>Physica B: Condensed Matter</i> , 2007, 401-402, 417-420.	1.3	11
4786	What is the product of ketene hydrogenation on Fe5C2(001): Oxygenates or hydrocarbons?. <i>Journal of Molecular Catalysis A</i> , 2007, 272, 275-287.	4.8	24
4787	Ab initio calculations about intrinsic point defects and He in W. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2007, 255, 23-26.	0.6	197
4788	First-principle calculations of the cohesive energy and the electronic properties of PbTiO3. <i>Physica B: Condensed Matter</i> , 2007, 391, 316-321.	1.3	56
4789	and nitrides bands structure and theoretical determination of bulk modulus. <i>Physica B: Condensed Matter</i> , 2007, 396, 1-7.	1.3	0
4790	Calculation of the thermodynamic properties of B2 AlRE (RE=Sc, Y, La, Ce-Lu). <i>Physica B: Condensed Matter</i> , 2007, 399, 27-32.	1.3	43
4791	Effect of Mg-doping on the structural and electronic properties of LiCoO2: A first-principles investigation. <i>Journal of Power Sources</i> , 2007, 171, 908-912.	4.0	79
4792	The fabrication of Te nanowires with different orientations by vacuum vapor deposition. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2007, 362, 61-65.	0.9	19
4793	Magnetic and optical properties of Fe2VAl and Fe3Al. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2007, 363, 312-316.	0.9	17
4794	Wigner film ground state in a three-dimensional electron gas. <i>Journal of Magnetism and Magnetic Materials</i> , 2007, 310, 1073-1075.	1.0	3
4795	Electronic structure and magnetism of Fe wire in carbon nanotubes. <i>Journal of Magnetism and Magnetic Materials</i> , 2007, 310, 1640-1641.	1.0	1
4796	Rotational spectrum and structure of asymmetric dinitrogen trioxide, N2O3. <i>Journal of Molecular Spectroscopy</i> , 2007, 244, 160-169.	0.4	11

#	ARTICLE	IF	CITATIONS
4797	Heterolytic CH-bond activation in the synthesis of Ni{(2-aryl- $\hat{C}^2$ )pyridine- $\hat{N}$ } <sub>2</sub> and derivatives. Journal of Organometallic Chemistry, 2007, 692, 4774-4783.	0.8	19
4798	Theoretical investigation of the bonding properties of N-heterocyclic carbenes coordinated to electron-rich d8 metal centers. Journal of Organometallic Chemistry, 2007, 692, 5709-5716.	0.8	40
4799	First-principles study of electronic structure and ferromagnetism in Ti-doped ZnO. Journal of Physics and Chemistry of Solids, 2007, 68, 1500-1503.	1.9	26
4800	Electronic structure and optical properties of crystalline strontium azide and barium azide by ab initio pseudopotential plane-wave calculations. Journal of Physics and Chemistry of Solids, 2007, 68, 1762-1769.	1.9	14
4801	Numerical evidence of Luttinger liquid to Fermi liquid transformation in lithium doped trans-polyacetylene chain. Journal of Physics and Chemistry of Solids, 2007, 68, 1856-1862.	1.9	1
4802	Band structure and optical spectra of RbNH <sub>4</sub> SO <sub>4</sub> crystals. Journal of Physics and Chemistry of Solids, 2007, 68, 1892-1896.	1.9	11
4803	Structure- $\hat{C}$ reactivity relationship for bimetallic electrodes: Pt overlayers and PtAu surface alloys on Au(111). Journal of Electroanalytical Chemistry, 2007, 607, 47-53.	1.9	41
4804	Adsorption of formic acid on Pt(111) in the presence of water. Journal of Electroanalytical Chemistry, 2007, 607, 133-139.	1.9	44
4805	Alkane metathesis by a tungsten carbyne complex grafted on gamma alumina: Is there a direct chemical role of the support?. Journal of Catalysis, 2007, 251, 507-513.	3.1	27
4806	Model computations for Cd adsorption on the (001) surface of CdTe. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 3191-3203.	0.8	3
4807	Influence of sequential lithium insertions on the physical properties of spinel manganese oxide. International Journal of Quantum Chemistry, 2007, 107, 225-231.	1.0	3
4808	Electron transport in Nano-Gold-Silicon interfaces. International Journal of Quantum Chemistry, 2007, 107, 440-450.	1.0	34
4809	Cascade configuration of logical gates processing information encoded in molecular potentials. International Journal of Quantum Chemistry, 2007, 107, 754-761.	1.0	14
4810	Theoretical study of structure and vibrational properties of Mg <sub>n</sub> O <sub>n</sub> (n = 3-10) clusters. International Journal of Quantum Chemistry, 2007, 107, 962-967.	1.0	2
4811	Theoretical study on Al <sub>n</sub> O <sub>2</sub> (n = 1-10) clusters and O <sub>2</sub> adsorption on the Al(111) surface. International Journal of Quantum Chemistry, 2007, 107, 1915-1924.	1.0	9
4812	Reaction mechanism of platinum dimer cation with ammonia based on the relativistic density functional study. International Journal of Quantum Chemistry, 2007, 107, 1985-1993.	1.0	6
4813	First principles electronic structure and band gap pressure coefficient for cadmium-oxide. International Journal of Quantum Chemistry, 2007, 107, 2988-2994.	1.0	9
4814	Pressure dependence of superconducting transition temperature of MgB <sub>2</sub> up to 8 GPa. Physica Status Solidi (B): Basic Research, 2007, 244, 1082-1087.	0.7	2



#	ARTICLE	IF	CITATIONS
4815	Effect of substituted IIIB transition metals on electronic properties of indium oxide by first-principles calculations. <i>Physica Status Solidi (B): Basic Research</i> , 2007, 244, 619-628.	0.7	7
4816	Ab initio study of elastic, thermal physical properties and electronic structure of Fe-Ga alloys. <i>Physica Status Solidi (B): Basic Research</i> , 2007, 244, 3583-3592.	0.7	8
4817	Magnetism of linear Fe, Co, and Ni nanowires encapsulated in zigzag (n,0) carbon nanotubes (CNT) with n = 5 to 9: A first-principles study. <i>Physica Status Solidi (B): Basic Research</i> , 2007, 244, 4407-4410.	0.7	8
4818	Initiation of petroleum formation and antioxidant function – a DFT study of sulfur-sulfur bond dissociation enthalpies. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 754-763.	0.9	4
4819	Cooperative mechanisms of fast-ion conduction in gallium-based oxides with tetrahedral moieties. <i>Nature Materials</i> , 2007, 6, 871-875.	13.3	185
4820	Atomic Structures and Electrical Properties of ZnO Grain Boundaries. <i>Journal of the American Ceramic Society</i> , 2007, 90, 337-357.	1.9	96
4821	Dependence of structural properties of ZnO on high pressure. <i>Materials Chemistry and Physics</i> , 2007, 106, 11-15.	2.0	28
4822	Effect of pressure on the structural and elastic properties of ZnS and MgS alloys in the B3 and B1 phases. <i>Materials Letters</i> , 2007, 61, 1978-1981.	1.3	19
4823	First-principles study of the effect of hydrogen on the Ti self-diffusion characteristics in the alpha Ti-H system. <i>Scripta Materialia</i> , 2007, 56, 77-80.	2.6	47
4824	Positive correlation between the magnetic moment of Fe and atomic volume in the binary Fe-(Cu, Ag) system. <i>Journal of Applied Physics</i> , 2007, 101, 074314.	2.6	8
4825	Phase stability of hafnium oxide and zirconium oxide on silicon substrate. <i>Scripta Materialia</i> , 2007, 57, 201-204.	2.6	19
4826	Thermodynamic modelling of the partially ordered solid solution Hf <sub>5-x</sub> NbxGe <sub>4</sub> supported by ab initio calculations. <i>Solid State Sciences</i> , 2007, 9, 159-165.	1.5	8
4827	Mixed-ligand complexes based on asymmetric gadolinium(II)-diketonates: Synthesis, crystal structure, and theoretical modeling. <i>Russian Journal of Inorganic Chemistry</i> , 2007, 52, 1365-1377.	0.3	1
4828	Ab initio calculations of the stability and structural defects of the B2 CuxFe1-xAl phases. <i>Physics of the Solid State</i> , 2007, 49, 1253-1258.	0.2	12
4829	A theoretical investigation on the isomerism and the NMR properties of thiosemicarbazones. <i>Open Chemistry</i> , 2007, 5, 396-419.	1.0	6
4830	Ab initio heat capacity and atomic temperature factors of chalcopyrites. <i>Physical Review B</i> , 2007, 75, .	1.1	17
4831	Thermodynamic functions and pressure-temperature phase diagram of lithium alanates by ab initio calculations. <i>Physical Review B</i> , 2007, 76, .	1.1	34
4832	Creation of paired electron states in the gap of semiconducting carbon nanotubes by correlated hydrogen adsorption. <i>New Journal of Physics</i> , 2007, 9, 275-275.	1.2	33

#	ARTICLE	IF	CITATIONS
4833	Using first principles calculations to identify new destabilized metal hydride reactions for reversible hydrogen storage. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 1438.	1.3	173
4834	Structural investigation and electronic properties of the nickel ferrite NiFe <sub>2</sub> O <sub>4</sub> : a periodic density functional theory approach. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 346219.	0.7	85
4835	Formation of Carbon Species on Ni(111): Structure and Stability. <i>Journal of Physical Chemistry C</i> , 2007, 111, 10894-10903.	1.5	38
4836	Pressure-Driven Phase Transitions in NaBH <sub>4</sub> : Theory and Experiments. <i>Journal of Physical Chemistry B</i> , 2007, 111, 13873-13876.	1.2	37
4837	Thermodynamic guidelines for the prediction of hydrogen storage reactions and their application to destabilized hydride mixtures. <i>Physical Review B</i> , 2007, 76, .	1.1	127
4838	How tight is the Lieb-Oxford bound?. <i>Journal of Chemical Physics</i> , 2007, 127, 054106.	1.2	53
4839	Electronic properties of oxygen-deficient and aluminum-doped rutile $\text{Ti}_{1-x}\text{O}_2$ from first-principles calculations. <i>Physical Review B</i> , 2007, 76, .	1.1	119
4840	Hydrogen storage capacity of boron-nitride and substituted carbon nanotubes. <i>Physical Review B</i> , 2007, 76, .	1.1	86
4841	Simulation of interstitial diffusion in graphite. <i>Physical Review B</i> , 2007, 76, .	1.1	40
4842	Atomic-volume variations of $\text{Pu}$ alloyed with Al, Ga, and Am from first-principles theory. <i>Journal of Computer-Aided Materials Design</i> , 2007, 14, 349-355.	0.7	3
4843	New aspects of the energetics of ordered Ti <sub>2</sub> C and Ti <sub>2</sub> N. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 196226.	0.7	16
4844	DFT study of BaTiO <sub>3</sub> (001) surface with O and O <sub>2</sub> adsorption. <i>European Physical Journal B</i> , 2007, 57, 291-297.	0.6	16
4845	The electronic properties of SiCAlN quaternary compounds. <i>European Physical Journal B</i> , 2007, 59, 29-34.	0.6	6
4846	Structure and magnetism in carbon nanotubes including magnetic wire. <i>European Physical Journal D</i> , 2007, 43, 129-132.	0.6	2
4847	Structure and electronic properties of a heterojunction between a single wall carbon nanotube and a TiC cluster. <i>European Physical Journal D</i> , 2007, 43, 147-150.	0.6	2
4848	Mechanistic Study on Hydrogen Spillover onto Graphitic Carbon Materials. <i>Journal of Physical Chemistry C</i> , 2007, 111, 18995-19000.	1.5	174
4849	Hybrid density functional theory with a specific reaction parameter: hydrogen abstraction reaction of trifluoromethane by the hydroxyl radical. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 383-395.	0.5	11
4850	The role of quantum chemistry in the elucidation of the elementary mechanisms of catalytic processes: from atoms, to surfaces, to enzymes. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 765-779.	0.5	37

#	ARTICLE	IF	CITATIONS
4851	Theory of oxides surfaces, interfaces and supported nano-clusters. Theoretical Chemistry Accounts, 2007, 117, 827-845.	0.5	30
4852	Raman spectroscopic investigation of the antimalarial agent mefloquine. Analytical and Bioanalytical Chemistry, 2007, 387, 1749-1757.	1.9	41
4853	The three-dimensional equilibrium crystal shape of Pb: Recent results of theory and experiment. Applied Physics A: Materials Science and Processing, 2007, 87, 391-397.	1.1	15
4854	Ab initio investigation of the laser induced desorption of iodine from KI(100). Applied Physics A: Materials Science and Processing, 2007, 88, 579-586.	1.1	7
4855	Potential routes to carbon inclusion in apatite minerals: a DFT study. Physics and Chemistry of Minerals, 2007, 34, 495-506.	0.3	16
4856	Can five-membered Te <sub>2</sub> N <sub>2</sub> S rings be considered aromatic?. Structural Chemistry, 2007, 18, 841-847.	1.0	3
4857	A DFT study on benzene adsorption over tungsten sulfides: surface model and adsorption geometries. Topics in Catalysis, 2007, 45, 175-179.	1.3	9
4858	H <sub>2</sub> adsorption and H/D exchange on Au/TS-1 and Au/S-1 catalysts. Topics in Catalysis, 2007, 44, 27-39.	1.3	13
4859	Factors in gold nanocatalysis: oxidation of CO in the non-scalable size regime. Topics in Catalysis, 2007, 44, 145-158.	1.3	190
4860	Continuum and Quantum-Chemical Modeling of Oxygen Reduction on the Cathode in a Solid Oxide Fuel Cell. Topics in Catalysis, 2007, 46, 386-401.	1.3	30
4861	Convergence of density functional iterative procedures with a Newton-Raphson algorithm. Journal of Computational Electronics, 2007, 6, 349-352.	1.3	1
4862	An efficient methodology to study cyclodextrin clusters: application to $\beta$ -CD hydrated monomer, dimer, trimer and tetramer. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2007, 59, 265-277.	1.6	16
4864	Ab initio study on fracture toughness of Ti <sub>0.75</sub> X <sub>0.25</sub> C ceramics. Journal of Materials Science, 2007, 42, 9713-9716.	1.7	13
4865	The Physical and Electronic Structure of M <sub>2</sub> Quadruply Bonded Complexes: A Density Functional Theory Study. Journal of Cluster Science, 2007, 18, 27-49.	1.7	10
4866	Hydrocarbon Molecules Deposited onto Silicon Surfaces: A DFT Study of Adsorption and Conductance. Journal of Cluster Science, 2007, 18, 869-881.	1.7	0
4867	Hybrid exchange correlation functionals and potentials: Concept elaboration. Journal of Structural Chemistry, 2007, 48, S1-S31.	0.3	40
4868	Recent Advances in Understanding CO Oxidation on Gold Nanoparticles Using Density Functional Theory. Catalysis Letters, 2007, 119, 21-28.	1.4	66
4869	Interaction energies in non-covalently bound intermolecular complexes derived using the subsystem formulation of density functional theory. Journal of Molecular Modeling, 2007, 13, 631-642.	0.8	26

#	ARTICLE	IF	CITATIONS
4870	Development of realistic models for Double Metal Cyanide catalyst active sites. <i>Journal of Molecular Modeling</i> , 2007, 13, 751-756.	0.8	42
4871	Optimization of parameters for semiempirical methods V: Modification of NDDO approximations and application to 70 elements. <i>Journal of Molecular Modeling</i> , 2007, 13, 1173-1213.	0.8	3,060
4872	Hybrid density functional theory with a specific reaction parameter: hydrogen abstraction reaction of difluoromethane by the hydroxyl radical. <i>Journal of Molecular Modeling</i> , 2007, 13, 1109-1121.	0.8	4
4873	π-π stacking tackled with density functional theory. <i>Journal of Molecular Modeling</i> , 2007, 13, 1245-1257.	0.8	126
4874	Density functional theory characterisation of 4-hydroxyazobenzene. <i>Journal of Molecular Modeling</i> , 2007, 13, 1227-1235.	0.8	17
4875	The correlation between the electronic structure and elastic properties of nanolaminates. <i>Jom</i> , 2007, 59, 60-64.	0.9	71
4876	The Stability of Al <sub>11</sub> Sm <sub>3</sub> (Al <sub>4</sub> Sm) Phases in the Al-Sm Binary System. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2007, 38, 1145-1151.	1.1	23
4877	Electronic structure of nanograin barium titanate ceramics. <i>Frontiers of Materials Science in China</i> , 2007, 1, 316-318.	0.5	4
4878	A density functional theory study of the adsorption of Hg and HgCl <sub>2</sub> on a CaO(001) surface. <i>Frontiers of Energy and Power Engineering in China</i> , 2007, 1, 101-104.	0.4	1
4879	Iodine ion transport in solid electrolyte LiI(C <sub>3</sub> H <sub>5</sub> NO) <sub>2</sub> : a first-principles identification. <i>Ionics</i> , 2007, 12, 343-347.	1.2	13
4880	Materials simulations using VASP—a quantum perspective to materials science. <i>Computer Physics Communications</i> , 2007, 177, 6-13.	3.0	262
4881	Tuning catalytic properties of bimetallic surfaces: Oxygen adsorption on pseudomorphic Pt/Ru overlayers. <i>Electrochimica Acta</i> , 2007, 52, 2219-2228.	2.6	93
4882	Monolayer adsorption of water on NaCl(100). <i>Applied Surface Science</i> , 2007, 254, 87-91.	3.1	2
4883	The influence of the X atoms and Al 3p occupied states in intermetallics. <i>Physica B: Condensed Matter</i> , 2007, 388, 303-311.	1.3	6
4884	Optical properties of the filled skutterudite LaFe <sub>4</sub> P <sub>12</sub> . <i>Physica B: Condensed Matter</i> , 2007, 390, 147-150.	1.3	5
4885	Electronic structures and shape-memory behavior of Ti <sub>50</sub> Ni <sub>50-x</sub> Cu <sub>x</sub> (x=0, 6.25, 12.5, 18.75 and 25.0at%) by density functional theory. <i>Physica B: Condensed Matter</i> , 2007, 393, 18-23.	1.3	17
4886	Oxygen vacancy formation energy at the Pd/CeO <sub>2</sub> (111) interface. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2007, 369, 132-139.	0.9	70
4887	An ab initio analysis of adsorption and diffusion of silver atoms on alumina surfaces. <i>Surface Science</i> , 2007, 601, 134-145.	0.8	55

#	ARTICLE	IF	CITATIONS
4888	Correlations between magnetic properties and bond formation in Rh/MgO(001). <i>Surface Science</i> , 2007, 601, 1218-1230.	0.8	4
4889	Effect of hydrogenation on P/Si(001)-(1 $\times$ 2). <i>Surface Science</i> , 2007, 601, 1489-1493.	0.8	3
4890	Effect of hydrogenation on B/Si(001)-(1 $\times$ 2). <i>Surface Science</i> , 2007, 601, 3711-3716.	0.8	2
4891	Local reactivity of ultrathin platinum overlayers and surface alloys on a gold surface. <i>Surface Science</i> , 2007, 601, 3702-3706.	0.8	23
4892	Towards hybrid silicon-organic molecular electronics: The stability of acetone on the Si(001) surface. <i>Surface Science</i> , 2007, 601, 5757-5761.	0.8	6
4893	The surface stress of the (110) and (100) surfaces of rutile and the effect of water adsorbents. <i>Surface Science</i> , 2007, 601, 4824-4836.	0.8	36
4894	Density-functional study of the CO adsorption on ferromagnetic Co(0001) and Co(111) surfaces. <i>Surface Science</i> , 2007, 601, 5571-5575.	0.8	39
4895	A first-principles analysis of the chemisorption of hydroxide on copper under electrochemical conditions: A probe of the electronic interactions that control chemisorption at the electrochemical interface. <i>Journal of Electroanalytical Chemistry</i> , 2007, 607, 167-174.	1.9	29
4896	Ab initio structural, electronic and optical properties of orthorhombic. <i>Journal of Solid State Chemistry</i> , 2007, 180, 974-980.	1.4	20
4897	First-principles study of structural and vibrational properties of crystalline silver azide under high pressure. <i>Journal of Solid State Chemistry</i> , 2007, 180, 3521-3528.	1.4	37
4898	Selective oxidation of methanol over supported vanadium oxide catalysts as studied by solid-state NMR spectroscopy. <i>Journal of Molecular Catalysis A</i> , 2007, 270, 257-263.	4.8	12
4899	Atomic diffusion mechanism of Xe in UO <sub>2</sub> . <i>Journal of Nuclear Materials</i> , 2008, 378, 40-44.	1.3	74
4900	Li <sub>1+x</sub> FePO <sub>4</sub> (O <sub>3</sub> ) as anode material for lithium ion batteries: From ab initio studies. <i>Journal of Power Sources</i> , 2008, 175, 891-896.	4.0	17
4901	A DFT study on benzene adsorption over a corner site of tungsten sulfides. <i>Catalysis Today</i> , 2008, 130, 178-182.	2.2	13
4902	Density-functional calculation of the adsorption and reaction of CO and H <sub>2</sub> O molecules over a 4Rh/CeO <sub>2</sub> (111) surface. <i>Chemical Physics</i> , 2008, 348, 161-168.	0.9	22
4903	First-principles study of sulfur adsorption on Mo(110). <i>Chemical Physics</i> , 2008, 353, 109-114.	0.9	13
4904	Study of high-pressure and high-temperature behaviors and $\hat{I}_1$ -to- $\hat{I}_2$ phase transition of forsterite by first-principles and quasi-harmonic Debye model. <i>Computer Physics Communications</i> , 2008, 179, 417-423.	3.0	14
4905	Introducing PROFESS: A new program for orbital-free density functional theory calculations. <i>Computer Physics Communications</i> , 2008, 179, 839-854.	3.0	90

#	ARTICLE	IF	CITATIONS
4906	Experimental and theoretical studies of l-cysteine adsorbed at Ag(111) electrodes. <i>Electrochimica Acta</i> , 2008, 53, 6807-6817.	2.6	32
4907	Ab initio study of interfacial correlations in polymer electrolyte membranes for fuel cells at low hydration. <i>Electrochimica Acta</i> , 2008, 53, 6920-6927.	2.6	19
4908	First-principles study of MgB <sub>2</sub> film on the MgO(111) polar surface. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2008, 372, 1671-1675.	0.9	9
4909	Distribution and magnetization of Co near the rutile TiO <sub>2</sub> (110) surface: A first-principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2008, 372, 2098-2102.	0.9	6
4910	The quantum-chemical calculation of NMR indirect spin-spin coupling constants. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2008, 53, 249-268.	3.9	252
4911	Monolayer bimetallic surfaces: Experimental and theoretical studies of trends in electronic and chemical properties. <i>Surface Science Reports</i> , 2008, 63, 201-254.	3.8	472
4912	DFT characterization of coverage dependent molecular water adsorption modes on $\hat{\Gamma}$ -Al <sub>2</sub> O <sub>3</sub> (0001). <i>Surface Science</i> , 2008, 602, 268-275.	0.8	73
4913	2-Chlorophenol adsorption on Cu(100): First-principles density functional study. <i>Surface Science</i> , 2008, 602, 1554-1562.	0.8	14
4914	DFT characterization of adsorption and diffusion mechanisms of H, As, S, and Se on the zinc orthotitanate(010) surface. <i>Surface Science</i> , 2008, 602, 1877-1882.	0.8	2
4915	Theoretical study of low-index surfaces of trigonal B <sub>2</sub> O <sub>3</sub> . <i>Surface Science</i> , 2008, 602, 2217-2221.	0.8	10
4916	First-principles studies of H <sub>2</sub> S adsorption and dissociation on metal surfaces. <i>Surface Science</i> , 2008, 602, 2758-2768.	0.8	161
4917	Atomic and electronic properties of furan on the Si(001)-(2 $\times$ 2) surface. <i>Surface Science</i> , 2008, 602, 2845-2848.	0.8	5
4918	Step enhanced dehydrogenation of ethanol on Rh. <i>Surface Science</i> , 2008, 602, 3057-3063.	0.8	23
4919	Investigation of submonolayer SiO <sub>x</sub> species formed from oxidation of silane on Pt(111). <i>Surface Science</i> , 2008, 602, 3225-3231.	0.8	7
4920	Surface termination effects on metal atom adsorption on $\hat{\Gamma}$ -alumina. <i>Surface Science</i> , 2008, 602, 3445-3453.	0.8	31
4921	Structural and dynamical properties of Ru(0001) surface. <i>Surface Science</i> , 2008, 602, 3654-3659.	0.8	7
4922	Density functional theory studies of submonolayer oxidized silicon structures on Pd(111) and Pt(111). <i>Surface Science</i> , 2008, 602, 3603-3610.	0.8	4
4923	Pd(110) surface oxide structures investigated by STM and DFT. <i>Surface Science</i> , 2008, 602, 3706-3713.	0.8	14

#	ARTICLE	IF	CITATIONS
4924	A test of empirical correction to site preference: DFT calculations for CO adsorption on Co(0001) surface. <i>Computational and Theoretical Chemistry</i> , 2008, 864, 68-71.	1.5	7
4925	Theoretical study of molecular nitrogen adsorption on Wn clusters. <i>Computational and Theoretical Chemistry</i> , 2008, 867, 17-21.	1.5	19
4926	Hydrogenation of conjugated CC and CO bonds: Quantum chemical preview before metal catalysis. <i>Computational and Theoretical Chemistry</i> , 2008, 870, 61-64.	1.5	4
4927	Water adsorption on fullerene-like carbon nitride overcoats. <i>Thin Solid Films</i> , 2008, 517, 1106-1110.	0.8	40
4928	Gamma-alumina: An Active Support to Obtain Immobilized Electron Poor Zr Complexes. <i>Topics in Catalysis</i> , 2008, 48, 114-119.	1.3	11
4929	Hydrocarbon Selective Oxidation on Vanadium Phosphorus Oxide Catalysts: Insights from Electronic Structure Calculations. <i>Topics in Catalysis</i> , 2008, 50, 116-123.	1.3	7
4930	Selectivity in Methanol Oxidation as Studied on Model Systems Involving Vanadium Oxides. <i>Topics in Catalysis</i> , 2008, 50, 106-115.	1.3	53
4931	Modeling the Adsorption of CO on Small Pt, Fe and Co Clusters for the Fischer-Tropsch Synthesis. <i>Journal of Cluster Science</i> , 2008, 19, 601-614.	1.7	12
4932	Structure and dielectric characteristics of epitaxially strained BaTiO <sub>3</sub> thin films. <i>Journal of Materials Science: Materials in Electronics</i> , 2008, 19, 466-470.	1.1	4
4933	Electronic structures of ZnO(0001)-Zn and (000 $\bar{1}$ )-O polar surfaces. <i>Journal of Materials Science: Materials in Electronics</i> , 2008, 19, 229-233.	1.1	13
4934	Geometry, electronic structure and energy barriers of all possible isomers of Fe <sub>2</sub> C <sub>3</sub> nanoparticle. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 313-318.	0.5	17
4935	The Si-doped planar tetracoordinate carbon (ptC) unit CAl <sub>3</sub> Si $\bar{1}$ could be used as a building block or inorganic ligand during cluster-assembly. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 335-342.	0.5	22
4936	Adsorption of transition metal atoms on the NiO(100) surface and on NiO/Ag(100) thin films. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 575-582.	0.5	15
4937	Trans to cis isomerization of an azobenzene derivative on Cu(100) surface. <i>Applied Physics A: Materials Science and Processing</i> , 2008, 93, 241-246.	1.1	53
4938	Theoretical observation of hexatomic molecules containing pentacoordinate planar carbon. <i>Science in China Series B: Chemistry</i> , 2008, 51, 1030-1035.	0.8	21
4939	Ab initio study of the effects of Ag/Mn doping on the electronic structure of LiFePO <sub>4</sub> . <i>Science Bulletin</i> , 2008, 53, 1763-1767.	4.3	9
4940	Modeling of Thermodynamic Properties and Phase Equilibria for the Al-Sm Binary System. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2008, 39, 502-512.	1.1	23
4941	Practical Surface Treatments and Surface Chemistry of n-Type and p-Type GaN. <i>Journal of Electronic Materials</i> , 2008, 37, 439-447.	1.0	25



#	ARTICLE	IF	CITATIONS
4942	Bonding analysis and stability on alternant B16N16 cage and its dimers. <i>Journal of Molecular Modeling</i> , 2008, 14, 789-795.	0.8	28
4943	Adsorption and reaction of organic molecules on solid surfaces – ab-initio density functional investigations. <i>Monatshefte für Chemie</i> , 2008, 139, 373-387.	0.9	14
4944	Potential energy surfaces for H <sub>2</sub> dissociative adsorption on Pt(111) surface – effects of vacancies. <i>Surface and Interface Analysis</i> , 2008, 40, 1103-1107.	0.8	11
4945	Adsorption and diffusion property of a hydrogen atom on a Pd <sub>3</sub> Ag(111) surface. <i>Surface and Interface Analysis</i> , 2008, 40, 1108-1112.	0.8	17
4946	DFT study on the adsorption of NO on iron tetrakisporphyrin. <i>Surface and Interface Analysis</i> , 2008, 40, 1082-1084.	0.8	9
4947	Understanding the bond-making and bond-breaking of Fe-filled SWNT on Ni(111). <i>Surface and Interface Analysis</i> , 2008, 40, 1098-1102.	0.8	3
4948	Harmonic force field for glycine oligopeptides. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 180-188.	1.0	18
4949	First principle MD study on the structural and electronic properties of liquid and amorphous Ni <sub>81</sub> B <sub>19</sub> and Ni <sub>80</sub> P <sub>20</sub> alloy. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 370-377.	1.0	1
4950	Ab initio reaction path for cisplatin interaction with L-cysteine and L-methionine. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 401-414.	1.0	19
4951	Effects of methods and basis set on ab initio calculations of electronic transport through hydrogenated Pt nanocontacts. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1637-1644.	1.0	6
4952	Effects of substituents on molecular devices. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1546-1554.	1.0	14
4953	Empirical analysis of the Lieb-Oxford bound in ions and molecules. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2428-2432.	1.0	15
4954	On the electronic structures and spectroscopic properties of polyyne and its derivatives. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1565-1571.	1.0	3
4955	Electronic structure and linear optical properties of the double perovskite La <sub>2</sub> NaRuO <sub>6</sub> . <i>Physica Status Solidi (B): Basic Research</i> , 2008, 245, 720-725.	0.7	4
4956	Structure and energetics for an additional H absorbed into superionic phase of CsHSO <sub>4</sub> by a first-principles study. <i>Physica Status Solidi (B): Basic Research</i> , 2008, 245, 657-665.	0.7	3
4957	Structural, electronic and optical properties of spinel MgAl <sub>2</sub> O <sub>4</sub> oxide. <i>Physica Status Solidi (B): Basic Research</i> , 2008, 245, 2800-2807.	0.7	90
4958	Hydroxyl radical reactions with halogenated ethanols in aqueous solution: Kinetics and thermochemistry. <i>International Journal of Chemical Kinetics</i> , 2008, 40, 174-188.	1.0	34
4959	Density Functional Theory Study of <i>trans</i> - $\mu$ -Dioxo Complexes of Iron, Ruthenium, and Osmium with Saturated Amine Ligands, <i>trans</i> -[M(O) <sub>2</sub> (NH <sub>3</sub> ) <sub>2</sub> (NMeH <sub>2</sub> ) <sub>2</sub> ] <sup>2±<math>\pi</math></sup> (M=Fe, Ru, Os), and Detection of [Fe(qpy)(O) <sub>2</sub> ] <sup>n+</sup> (n=1, 2) by High-Resolution ESI Mass Spectrometry. <i>Chemistry – A European Journal</i> , 2008, 14, 5495-5506.		13

#	ARTICLE	IF	CITATIONS
4960	Understanding the Reactivity and Basicity of Zeolites: A Periodic DFT Study of the Disproportionation of $N_2O_4$ on Alkali-Exchanged Zeolite Y. <i>Chemistry - A European Journal</i> , 2008, 14, 5168-5177.	1.7	30
4961	The Elusive Structure of $CrCl_2$ —A Combined Computational and Gas-Phase Electron-Diffraction Study. <i>Chemistry - A European Journal</i> , 2008, 14, 5130-5143.	1.7	20
4962	Models of the ox1 State of Methylcoenzyme M Reductase: Where are the Electrons?. <i>Chemistry - A European Journal</i> , 2008, 14, 9981-9989.	1.7	3
4963	Synthesis and Reactivity of [Penta(4-halogenophenyl)cyclopentadienyl][hydrotris(indazolyl)borato]ruthenium(II) Complexes: Rotation-Induced Fosbury Flop in an Organometallic Molecular Turnstile. <i>Chemistry - A European Journal</i> , 2008, 14, 8147-8156.	1.7	50
4964	Reactions of Uranium Atoms with Ammonia: Infrared Spectra and Quasi-Relativistic Calculations of the $U:NH_3$ , $H_2U:NH_3$ , and $H_2U:NH_3$ Complexes. <i>Chemistry - A European Journal</i> , 2008, 14, 9192-9201.	1.7	40
4965	The Role of Noninnocent Solvent Molecules in Organocatalyzed Asymmetric Michael Addition Reactions. <i>Chemistry - A European Journal</i> , 2008, 14, 10472-10485.	1.7	51
4966	DFT Study of Effects of Potassium Doping on Band Structure of Crystalline Cuprous Azide. <i>Chinese Journal of Chemistry</i> , 2008, 26, 2145-2149.	2.6	15
4967	Unique Reactivity of Confined Metal Atoms on a Silicon Substrate. <i>ChemPhysChem</i> , 2008, 9, 975-979.	1.0	24
4968	Evidence for a Size-Selective Adsorption Mechanism on Oxide Surfaces: Pd and Au atoms on $SiO_2/Mo(112)$ . <i>ChemPhysChem</i> , 2008, 9, 1367-1370.	1.0	31
4969	Ab initio Studies on $Li_4Ti_5O_{12}$ Compounds as Anode Materials for Lithium-Ion Batteries. <i>ChemPhysChem</i> , 2008, 9, 2104-2108.	1.0	110
4970	Hangman Salen Platforms Containing Dibenzofuran Scaffolds. <i>ChemSusChem</i> , 2008, 1, 941-949.	3.6	18
4971	Ab initio study of electronic structure and optical properties of heavy-metal azides: $TlN_3$ , $AgN_3$ , and $CuN_3$ . <i>Journal of Computational Chemistry</i> , 2008, 29, 176-184.	1.5	74
4972	QUILD: QUantum regions interconnected by local descriptions. <i>Journal of Computational Chemistry</i> , 2008, 29, 724-734.	1.5	135
4973	Determination of spin-orbit coupling contributions in the framework of density functional theory. <i>Journal of Computational Chemistry</i> , 2008, 29, 912-920.	1.5	29
4974	Calculation of weakly polar interaction energies in polypeptides using density functional and local Møller-Plesset perturbation theory. <i>Journal of Computational Chemistry</i> , 2008, 29, 1344-1352.	1.5	30
4975	Adsorption of benzene, fluorobenzene and meta-fluorobenzene on $Cu(110)$ : A computational study. <i>Journal of Computational Chemistry</i> , 2008, 29, 1589-1595.	1.5	17
4976	Ab-initio simulations of materials using VASP: Density functional theory and beyond. <i>Journal of Computational Chemistry</i> , 2008, 29, 2044-2078.	1.5	2,717
4977	Density Functional Theory Studies of the Magnetostructural Correlations in the Cyano-Bridged $Mo_2Ni$ and $Mo_2Ni_3$ Systems. <i>European Journal of Inorganic Chemistry</i> , 2008, 2008, 2199-2206.	1.0	4

#	ARTICLE	IF	CITATIONS
4978	Theoretical Study on a Class of Organometallic Complexes Based on All-metal Aromatic Ga <sub>3</sub> Through Sandwiching Stabilization. <i>European Journal of Inorganic Chemistry</i> , 2008, 2008, 2099-2106.	1.0	6
4979	Complexes of Yb <sup>3+</sup> with EDTA and CDTA – Molecular and Electronic Structure. <i>European Journal of Inorganic Chemistry</i> , 2008, 2008, 3075-3082.	1.0	24
4980	Combined Experimental and Density Functional Theory Studies on the Crystal Structures and Magnetic Properties of Mg <sub>1-x</sub> Mn <sub>x</sub> Sb <sub>2</sub> (x = 0.25) and BaMn <sub>2</sub> Sb <sub>2</sub> . <i>European Journal of Inorganic Chemistry</i> , 2008, 2008, 4262-4269.	1.0	33
4981	The role of weakly polar and H-bonding interactions in the stabilization of the conformers of FGG, WGG, and YGG; An aqueous phase computational study. <i>Biopolymers</i> , 2008, 89, 1002-1011.	1.2	6
4982	Stable Deacon Process for HCl Oxidation over RuO <sub>2</sub> . <i>Angewandte Chemie - International Edition</i> , 2008, 47, 2131-2134.	7.2	123
4983	Understanding Palladium Hydrogenation Catalysts: When the Nature of the Reactive Molecule Controls the Nature of the Catalyst Active Phase. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 9274-9278.	7.2	185
4984	Lattice Widening in Niobium-Doped TiO <sub>2</sub> Nanotubes: Efficient Ion Intercalation and Swift Electrochromic Contrast. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 7934-7937.	7.2	101
4985	Hydrothermal Reaction Mechanism and Pathway for the Formation of K <sub>2</sub> Ti <sub>6</sub> O <sub>13</sub> Nanowires. <i>Advanced Functional Materials</i> , 2008, 18, 3018-3025.	7.8	25
4989	Elastic properties of Ti <sub>n+1</sub> AlC <sub>n</sub> and Ti <sub>n+1</sub> AlN <sub>n</sub> MAX phases. <i>Advanced Engineering Materials</i> , 2008, 10, 935-938.	1.6	46
4990	An investigation of secondary ion yield enhancement using Bi <sub>n</sub> <sup>2+</sup> (n=1) Tj ETQq <sub>1.1</sub> 0.784314 rgBT 1.2 17		
4991	Tomonaga-Luttinger liquid feature in sodium-doped quasi-one-dimensional trans-polyacetylene chain. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2008, 40, 2736-2741.	1.3	2
4992	Detecting the lowest-energy structures of. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2008, 372, 6392-6395.	0.9	11
4993	Pressure effects on the structural and electronic properties of ABX <sub>4</sub> scintillating crystals. <i>Progress in Materials Science</i> , 2008, 53, 711-773.	16.0	316
4994	Synthesis and characterization of dinuclear pyrazolato bridged platinum(IV) complexes. <i>Polyhedron</i> , 2008, 27, 914-922.	1.0	14
4995	A europium(II) complex with bis-pyridino-18-crown-6. <i>Polyhedron</i> , 2008, 27, 2688-2692.	1.0	14
4996	An effect of side chain length on the solution structure of poly(9,9-dialkylfluorene)s in toluene. <i>Polymer</i> , 2008, 49, 2033-2038.	1.8	31
4997	First-principles study of the micro-arrangement of hydrogen atoms and electronic properties of LaNi <sub>5</sub> H <sub>x</sub> (x: 0.5-7). <i>Physica B: Condensed Matter</i> , 2008, 403, 2372-2382.	1.3	23
4998	Mott state and quantum critical points in rare-earth oxypnictides (). <i>Physica B: Condensed Matter</i> , 2008, 403, 3653-3657.	1.3	31

#	ARTICLE	IF	CITATIONS
4999	Thermal stabilities of nanoporous metallic electrodes at elevated temperatures. <i>Journal of Power Sources</i> , 2008, 175, 75-81.	4.0	92
5000	Computational studies of CO and CO+: Density functional theory and time-dependent density functional theory. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2008, 109, 2546-2560.	1.1	9
5001	Structure and properties of ordered Li <sub>2</sub> IrO <sub>3</sub> and Li <sub>2</sub> PtO <sub>3</sub> . <i>Journal of Solid State Chemistry</i> , 2008, 181, 1803-1809.	1.4	109
5002	An ab initio study of possible pathways in the thermal decomposition of NaAlH <sub>4</sub> . <i>Journal of Solid State Chemistry</i> , 2008, 181, 3037-3043.	1.4	10
5003	Effective work functions for ionic and electronic emissions from mono- and polycrystalline surfaces. <i>Progress in Surface Science</i> , 2008, 83, 1-165.	3.8	120
5004	Reaction dynamics of H <sub>2</sub> on Si. Ab initio supported model calculations. <i>Progress in Surface Science</i> , 2008, 83, 263-336.	3.8	36
5005	Phase stability of Fe and Mn within density-functional theory plus on-site Coulomb interaction approaches. <i>Journal of Magnetism and Magnetic Materials</i> , 2008, 320, 100-106.	1.0	16
5006	Electronic and magnetic properties of basic nanosystems of early 3d transition metals (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn). <i>Journal of Magnetism and Magnetic Materials</i> , 2008, 320, 107-114.	1.0	14
5007	Magnetic properties, electronic structure, and optical properties of the filled skutterudite BaFe <sub>4</sub> Sb <sub>12</sub> . <i>Journal of Magnetism and Magnetic Materials</i> , 2008, 320, 2591-2595.	1.0	7
5008	Ligand effects on the stability of the insertion products: A DFT study of oxidative addition of NH <sub>3</sub> to iridium(I) complex. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 1547-1551.	0.8	3
5009	First-principle study of electronic properties of Ti <sub>3</sub> Si <sub>1-x</sub> Al <sub>x</sub> C <sub>2</sub> solid solutions. <i>Journal of Physics and Chemistry of Solids</i> , 2008, 69, 1356-1361.	1.9	17
5010	CoO under pressure from first principles. <i>Journal of Physics and Chemistry of Solids</i> , 2008, 69, 1698-1703.	1.9	18
5011	First-principles investigations of iridium low index surfaces. <i>Journal of Physics and Chemistry of Solids</i> , 2008, 69, 2457-2464.	1.9	7
5012	Density functional study of structures and mechanical properties of Y-doped $\hat{\pm}$ -SiAlONs. <i>Journal of the European Ceramic Society</i> , 2008, 28, 995-1002.	2.8	14
5013	The bulk band structure and inner potential of layered In <sub>4</sub> Se <sub>3</sub> . <i>Applied Surface Science</i> , 2008, 254, 4322-4325.	3.1	10
5014	Gas-phase reactivities of charged platinum dimers with ammonia: A combined experimental/theoretical study. <i>Chemical Physics Letters</i> , 2008, 450, 268-273.	1.2	16
5015	A first principle study of terahertz (THz) spectra of acephate. <i>Chemical Physics Letters</i> , 2008, 452, 59-66.	1.2	34
5016	Field-assisted oxidation of rhodium. <i>Chemical Physics Letters</i> , 2008, 452, 133-138.	1.2	26

#	ARTICLE	IF	CITATIONS
5017	Evidence for spontaneous CO <sub>2</sub> activation on cobalt surfaces. <i>Chemical Physics Letters</i> , 2008, 454, 262-268.	1.2	76
5018	Low energy electron impact on gas phase 5-nitouracil. <i>Chemical Physics Letters</i> , 2008, 455, 169-173.	1.2	6
5019	First-principles calculations for geometrical structures and electronic properties of Si-doped TiO <sub>2</sub> . <i>Chemical Physics Letters</i> , 2008, 456, 71-75.	1.2	89
5020	Small Au clusters on a defective MgO(100) surface. <i>Chemical Physics Letters</i> , 2008, 457, 143-147.	1.2	15
5021	Magnetism in germanium-doped boron-nitride nanotubes. <i>Chemical Physics Letters</i> , 2008, 457, 169-173.	1.2	22
5022	Dominant role of the interstitial 4d transition-metal in $TM@Zr$ (TM = Yb, Cd, Zr, O, Au) icosahedral cages. <i>Chemical Physics Letters</i> , 2008, 457, 49-53.	1.2	10
5023	On the move of strongly chemisorbed species on metals: The example of O diffusion on Pd(111) surface. <i>Chemical Physics Letters</i> , 2008, 458, 92-95.	1.2	4
5024	Nano-wire formation by self-assembly of silicon metal cage-like molecules. <i>Chemical Physics Letters</i> , 2008, 458, 170-174.	1.2	28
5025	Local atomic structure and chemical bonding in liquid Te: An ab initio molecular-dynamics simulation. <i>Chemical Physics Letters</i> , 2008, 458, 101-107.	1.2	2
5026	Ab initio simulation of the fundamental vibrational frequencies of selected pyrite-type pnictides. <i>Chemical Physics Letters</i> , 2008, 461, 38-41.	1.2	19
5027	Effect of pressure and temperature on structural stability of potential hydrogen storage compound Li <sub>3</sub> AlH <sub>6</sub> . <i>Chemical Physics Letters</i> , 2008, 460, 442-446.	1.2	8
5028	Theoretical study on the photoabsorption of $M^{n+}Au$ (M = V, Nb and Ta). <i>Chemical Physics Letters</i> , 2008, 462, 358-364.	1.2	16
5029	Towards size-converged properties of model ceria nanoparticles: Monitoring by adsorbed CO using DFT +U approach. <i>Chemical Physics Letters</i> , 2008, 465, 106-109.	1.2	31
5030	Atomic-scale microstructure and elastic properties of quaternary ZrAlSiC ceramics. <i>Acta Materialia</i> , 2008, 56, 2022-2031.	3.8	54
5031	Modeling of phase stability of the fcc phases in the NiIrAl system using the cluster/site approximation method coupling with first-principles calculations. <i>Acta Materialia</i> , 2008, 56, 2576-2584.	3.8	16
5032	Point defect thermodynamics and diffusion in Fe <sub>3</sub> C: A first-principles study. <i>Acta Materialia</i> , 2008, 56, 3236-3244.	3.8	26
5033	Atomic mobilities, diffusivities and simulation of diffusion growth in the CoSi system. <i>Acta Materialia</i> , 2008, 56, 3940-3950.	3.8	69
5034	First-principles study of site occupancy of dilute 3d, 4d and 5d transition metal solutes in L10 TiAl. <i>Acta Materialia</i> , 2008, 56, 6224-6231.	3.8	49

#	ARTICLE	IF	CITATIONS
5035	Optimal promoter edge decoration of CoMoS catalysts: A combined theoretical and experimental study. <i>Catalysis Today</i> , 2008, 130, 149-159.	2.2	184
5036	Mixed sites and promoter segregation: A DFT study of the manifestation of Le Chatelier's principle for the Co(Ni)MoS active phase in reaction conditions. <i>Catalysis Today</i> , 2008, 130, 160-169.	2.2	147
5037	Coupled theoretical and experimental analysis of surface coverage effects in Pt-catalyzed NO and O <sub>2</sub> reaction to NO <sub>2</sub> on Pt(111). <i>Catalysis Today</i> , 2008, 136, 84-92.	2.2	79
5038	Theoretical study of methane adsorption on perfect and defective Ni(111) surfaces. <i>Catalysis Today</i> , 2008, 138, 77-83.	2.2	18
5039	Hydrogen and dihydrogen bonding of transition metal hydrides. <i>Chemical Physics</i> , 2008, 345, 95-102.	0.9	30
5040	Transition metal sandwich molecules with large (C <sub>n</sub> , n ≥ 24) zigzag poly aromatic hydrocarbons. <i>Chemical Physics</i> , 2008, 348, 69-82.	0.9	10
5041	Geometry, bonding and magnetism in planar triangulene graphene molecules with D <sub>3h</sub> symmetry: Zigzag (m=2, n=15). <i>Chemical Physics</i> , 2008, 354, 1-15.	0.9	47
5042	First-principles phase transition and equation of state of titanium. <i>Solid State Communications</i> , 2008, 146, 105-109.	0.9	25
5043	The structure properties of LaNi <sub>3.5</sub> Al <sub>1.5</sub> . <i>Solid State Communications</i> , 2008, 146, 368-371.	0.9	2
5044	Atomic ordering recognized by convergence characteristics of the radial distribution function. <i>Solid State Communications</i> , 2008, 146, 468-471.	0.9	4
5045	Interaction of cholesterol with carbon nanotubes: A density functional theory study. <i>Solid State Communications</i> , 2008, 147, 146-151.	0.9	10
5046	First-principles study of sulfur passivation of GaP(001) surfaces at one-monolayer coverage. <i>Solid State Communications</i> , 2008, 147, 141-145.	0.9	9
5047	Pushing p-type conductivity in ZnO by (Zr, N) codoping: A first-principles study. <i>Solid State Communications</i> , 2008, 147, 194-197.	0.9	32
5048	First-principles calculations on the crystal and electronic structures of LaNi <sub>4.5</sub> Al <sub>0.5</sub> H <sub>6-x</sub> Hex (x = 0, 0.5). <i>Tj ETQq1 1 0.784314 rgBT /Overl</i>	0.9	5
5049	Elastic constants of B <sub>2</sub> -MgRE (RE = Sc, Y, La-Lu) calculated with first-principles. <i>Solid State Communications</i> , 2008, 148, 314-318.	0.9	54
5050	Structural and electronic properties of M <sub>2</sub> InC (M = Ti, Zr, and Hf). <i>Solid State Communications</i> , 2008, 148, 459-463.	0.9	27
5051	First-principles electronic structure of copper phthalocyanine (CuPc). <i>Solid State Communications</i> , 2008, 148, 559-562.	0.9	18
5052	Interfacial fracture toughness of transition metal nitrides. <i>Surface and Coatings Technology</i> , 2008, 203, 598-601.	2.2	69

#	ARTICLE	IF	CITATIONS
5053	Adsorption and dissociation of methanol on the fully oxidized and partially reduced (111) cerium oxide surface: Dependence on the configuration of the cerium 4f electrons. <i>Surface Science</i> , 2008, 602, 162-175.	0.8	61
5054	DFT study of the Au(321) surface reconstruction by consecutive deposition of oxygen atoms. <i>Surface Science</i> , 2008, 602, 424-435.	0.8	22
5055	Au-induced charge redistribution on Si(111)-7 $\times$ 7 surface. <i>Surface Science</i> , 2008, 602, 638-643.	0.8	15
5056	Interaction of carbon dioxide with Cu overlayers on Pt(111). <i>Surface Science</i> , 2008, 602, 702-711.	0.8	44
5057	First principles study of hydrogen atom adsorption and diffusion on Pd <sub>3</sub> Ag(1 1 1) surface and in its subsurface. <i>Surface Science</i> , 2008, 602, 859-863.	0.8	29
5058	Water on the hydroxylated (001) surface of kaolinite: From monomer adsorption to a flat 2D wetting layer. <i>Surface Science</i> , 2008, 602, 960-974.	0.8	155
5059	Sensitivity of short-range trio interactions to lateral relaxation of adatoms: Challenges for detailed lattice-gas modeling. <i>Surface Science</i> , 2008, 602, 1243-1249.	0.8	11
5060	Ammonia adsorption on Cl/Si(001): First-principles calculations. <i>Surface Science</i> , 2008, 602, 1207-1211.	0.8	14
5061	First-principles study of decomposition of NH <sub>3</sub> on Ir(100). <i>Surface Science</i> , 2008, 602, 1288-1294.	0.8	50
5062	Atomic and electronic structures of Ti/Si(111)-. <i>Surface Science</i> , 2008, 602, 1376-1380.	0.8	12
5063	DFT calculations of adenine adsorption on coin metal (110) surfaces. <i>Surface Science</i> , 2008, 602, 2170-2174.	0.8	49
5064	Oxygen adsorption on Zr(0001) surfaces: Density functional calculations and a multiple-layer adsorption model. <i>Surface Science</i> , 2008, 602, 2212-2216.	0.8	23
5065	The structure and reactivity of 2-butanol on Pd(111). <i>Surface Science</i> , 2008, 602, 2264-2270.	0.8	18
5066	Facile dissociation of CO on Fe{211}: Evidence from microcalorimetry and first-principles theory. <i>Surface Science</i> , 2008, 602, 2325-2332.	0.8	42
5067	First principles calculations of methylamine and methanol adsorption on hydroxylated quartz (0001). <i>Surface Science</i> , 2008, 602, 2478-2485.	0.8	25
5068	Lateral electronic confinement in unidimensional noble metal (Au, Pt) nanowires. <i>Surface Science</i> , 2008, 602, L104-L107.	0.8	4
5069	Stressing Pd atoms: Initial oxidation of the Pd(110) surface. <i>Surface Science</i> , 2008, 602, 2440-2447.	0.8	31
5070	The chemistry of chlorine on Ag(1 1 1) over the sub-monolayer range: A density functional theory investigation. <i>Surface Science</i> , 2008, 602, 2639-2642.	0.8	9



#	ARTICLE	IF	CITATIONS
5071	Examining the redox and formate mechanisms for water-gas shift reaction on Au/CeO <sub>2</sub> using density functional theory. <i>Surface Science</i> , 2008, 602, 2828-2834.	0.8	76
5072	Reactivity descriptors for direct methanol fuel cell anode catalysts. <i>Surface Science</i> , 2008, 602, 3424-3431.	0.8	168
5073	DFT study of reconstructed Cu(100) surface with high oxygen coverages. <i>Surface Science</i> , 2008, 602, 3239-3245.	0.8	22
5074	Formation of one-dimensional molybdenum oxide on Mo(112). <i>Surface Science</i> , 2008, 602, 3338-3342.	0.8	23
5075	Analysis of defects on BN nano-structures using high-resolution electron microscopy and density-functional calculations. <i>Ultramicroscopy</i> , 2008, 108, 1484-1489.	0.8	4
5076	First-principles calculations-based model for the reactive ion etching of metal oxide surfaces. <i>Vacuum</i> , 2008, 83, 599-601.	1.6	9
5077	Origin of reverse stability of diphosphouracil tautomers compared to their analogue uracil: DFT and ab initio study. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 54-62.	1.5	9
5078	Structure and aromaticity of $\text{Bi}_5\text{M}$ (M=Li, Na, K) and $\text{Bi}_5\text{M}^+$ (M=Be, Mg, Ca) clusters. <i>Computational and Theoretical Chemistry</i> , 2008, 854, 46-53.	1.5	14
5079	Properties of the multi-electron densities between the Hohenberg-Kohn theorems and variational principle. <i>Computational and Theoretical Chemistry</i> , 2008, 858, 1-11.	1.5	13
5080	CHH-DFT computational molecular characterization of phenanthro [9,10-c]-1,2,5-thiadiazole 1,1-dioxide. <i>Computational and Theoretical Chemistry</i> , 2008, 862, 60-65.	1.5	6
5081	Assessment of density functionals for the investigation of iridium(III) complexes. <i>Computational and Theoretical Chemistry</i> , 2008, 861, 97-102.	1.5	19
5082	A first-principles investigation on the hydrogen bond interaction in DATB. <i>Computational and Theoretical Chemistry</i> , 2008, 864, 89-92.	1.5	7
5083	Atomic geometry and electronic structure of defects in Zn <sub>3</sub> N <sub>2</sub> . <i>Thin Solid Films</i> , 2008, 516, 1297-1301.	0.8	34
5084	Theoretical study of structural, optical and electrical properties of zirconium-doped zinc oxide. <i>Applied Surface Science</i> , 2008, 254, 6983-6986.	3.1	23
5085	Optical properties of cadmium telluride in zinc-blende and wurzite structure. <i>Physica B: Condensed Matter</i> , 2008, 403, 1907-1915.	1.3	50
5086	Ab initio investigation of half-metal state in zinc-blende MnSn and MnC. <i>Physica B: Condensed Matter</i> , 2008, 403, 2473-2476.	1.3	9
5087	Ab initio study of formation, migration and binding properties of helium-vacancy clusters in aluminum. <i>Physica B: Condensed Matter</i> , 2008, 403, 2719-2724.	1.3	32
5088	Adsorption of Al on the Si(001) surface. <i>Physica B: Condensed Matter</i> , 2008, 403, 2979-2986.	1.3	9

#	ARTICLE	IF	CITATIONS
5089	Electronic band structure of calcium selenide under pressure. <i>Physica B: Condensed Matter</i> , 2008, 403, 3022-3026.	1.3	8
5090	Electronic structure and magnetic state of. <i>Physica B: Condensed Matter</i> , 2008, 403, 4232-4235.	1.3	11
5091	The electronic structures and properties of transition metal-doped silicon nanoclusters: A density functional investigation. <i>Chemical Physics</i> , 2008, 353, 170-176.	0.9	31
5092	Computer simulation study of defect formation and migration energy in calcium fluoride. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2008, 266, 2698-2701.	0.6	8
5093	The electronic structure of Ti(BH <sub>4</sub> ) <sub>3</sub> : Photoelectron spectra and calculation of vertical ionization energies. <i>Inorganica Chimica Acta</i> , 2008, 361, 462-466.	1.2	7
5094	Structural model studies for the high-valent intermediate Q of methane monooxygenase from broken-symmetry density functional calculations. <i>Inorganica Chimica Acta</i> , 2008, 361, 973-986.	1.2	61
5095	Reaction of carbon monoxide with tri-tert-butylgallium: The first example of CO insertion into a gallium-carbon bond. <i>Inorganica Chimica Acta</i> , 2008, 361, 3332-3337.	1.2	16
5096	Atomistic simulation of water adsorption and cation siting in polyoxoniobate materials. <i>Microporous and Mesoporous Materials</i> , 2008, 116, 532-539.	2.2	3
5097	Density Functional Theory studies of dehydrogenated and zwitterionic glycine and alanine on Pd and Cu surfaces. <i>Journal of Molecular Catalysis A</i> , 2008, 281, 44-48.	4.8	21
5098	Density functional theory study of H <sub>2</sub> adsorption on the (100), (001) and (010) surfaces of Fe <sub>3</sub> C. <i>Journal of Molecular Catalysis A</i> , 2008, 292, 14-20.	4.8	20
5099	First-principles study of the electronic structure and mechanical properties of CaMg <sub>2</sub> Laves phase. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2008, 489, 444-450.	2.6	37
5100	New generation of Ni-based superalloys designed on the basis of first-principles calculations. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2008, 497, 18-24.	2.6	38
5101	Ab initio calculations of magnetic structure and lattice dynamics of Fe/Pt multilayers. <i>European Physical Journal B</i> , 2008, 61, 173-179.	0.6	3
5102	Effect of S adsorption on magnetic Co(0001) surface: a DFT study. <i>European Physical Journal B</i> , 2008, 61, 319-324.	0.6	3
5103	Interaction of Au nanowires with impurities. <i>European Physical Journal B</i> , 2008, 61, 441-444.	0.6	8
5104	Interfacial properties of Ce <sub>0.75</sub> Zr <sub>0.25</sub> O <sub>2</sub> supported noble metals (Pd, Pt) from first principles. <i>European Physical Journal B</i> , 2008, 63, 455-460.	0.6	4
5105	Ground-state energy of a classical artificial molecule. <i>European Physical Journal B</i> , 2008, 64, 81-86.	0.6	0
5106	Electronic structure, ferroelectricity and optical properties of CaBi <sub>2</sub> Ta <sub>2</sub> O <sub>9</sub> . <i>European Physical Journal B</i> , 2008, 66, 483-487.	0.6	41

#	ARTICLE	IF	CITATIONS
5107	Simulating CH <sub>4</sub> physisorption on ionic crystals. European Physical Journal D, 2008, 46, 69-76.	0.6	2
5108	Superlattice structures of graphene-based armchair nanoribbons. Physical Review B, 2008, 78, .	1.1	148
5109	Orbital-dependent density functionals: Theory and applications. Reviews of Modern Physics, 2008, 80, 3-60.	16.4	1,069
5110	Short and intermediate range order in amorphous $\text{GeSe}_2$ . Physical Review B, 2008, 77, .	1.1	55
5111	Evidence for graphene growth by C cluster attachment. New Journal of Physics, 2008, 10, 093026.	1.2	262
5112	The electronic structure of surface chains in the layered semiconductor In <sub>4</sub> Se <sub>3</sub> (100). Applied Physics Letters, 2008, 92, 122107.	1.5	30
5113	A first-principles study of molecular oxygen dissociation at an electrode surface: a comparison of potential variation and coadsorption effects. Physical Chemistry Chemical Physics, 2008, 10, 3613.	1.3	76
5114	Functionalization of carbon-based nanostructures with light transition-metal atoms for hydrogen storage. Physical Review B, 2008, 77, .	1.1	315
5115	Influence of Density Functionals and Basis Sets on One-Bond Carbon <sup>13</sup> C NMR Spin <sup>1</sup> Spin Coupling Constants. Journal of Chemical Theory and Computation, 2008, 4, 448-456.	2.3	40
5116	Energy level structure of 4f5d states and the Stokes shift in LaPO <sub>4</sub> :Pr <sup>3+</sup> : A theoretical study. Physical Review B, 2008, 78, .	1.1	20
5117	Work function changes induced by deposition of ultrathin dielectric films on metals: A theoretical analysis. Physical Review B, 2008, 78, .	1.1	180
5118	First-principles calculations of carbon nanotubes adsorbed on diamond (100) surfaces. Journal of Physics Condensed Matter, 2008, 20, 225016.	0.7	7
5119	Interplay between magnetism and structure in atomic-size Pd contacts: <i>Ab initio</i> studies. Physical Review B, 2008, 77, .	1.1	16
5120	Titanium and native defects in LiBH <sub>4</sub> and NaAlH <sub>4</sub> . Journal of Physics Condensed Matter, 2008, 20, 465210.	0.7	25
5121	Searching for the optimum structures of alloy nanoclusters. Physical Chemistry Chemical Physics, 2008, 10, 640-649.	1.3	185
5122	High-Capacity Room-Temperature Hydrogen Storage in Carbon Nanotubes via Defect-Modulated Titanium Doping. Journal of Physical Chemistry C, 2008, 112, 17456-17464.	1.5	71
5123	Configurational thermodynamics of alloys from first principles: effective cluster interactions. Reports on Progress in Physics, 2008, 71, 046501.	8.1	264
5124	Molybdenum at High Pressure and Temperature: Melting from Another Solid Phase. Physical Review Letters, 2008, 100, 135701.	2.9	127

#	ARTICLE	IF	CITATIONS
5125	Application of First Principles Methods in the Study of Fuel Cell Air-Cathode Electrocatalysis. , 2008, , 289-329.		3
5126	Hydrogen Adsorption on Lithium-Functionalized Calixarenes: A Computational Study. Journal of Physical Chemistry C, 2008, 112, 19676-19679.	1.5	27
5127	Chromium Aromatic Hydrocarbon Sandwich Molecules and the Eighteen-Electron Rule. Journal of Physical Chemistry A, 2008, 112, 2034-2042.	1.1	12
5128	First-principles study of physisorption of nucleic acid bases on small-diameter carbon nanotubes. Nanotechnology, 2008, 19, 125701.	1.3	160
5129	A first-principles studies on TlX (X=P, As). Open Physics, 2008, 6, .	0.8	13
5130	Effect of chromium on the electronic structure and magnetic properties of cementite. Physics of Metals and Metallography, 2008, 105, 568-573.	0.3	12
5131	A DFT study of hydrogen chemisorption on V (100) surfaces. Russian Journal of Physical Chemistry A, 2008, 82, 2354-2361.	0.1	11
5132	Theoretical analysis of the alloying system and design of new nickel-base superalloys. Doklady Physics, 2008, 53, 438-441.	0.2	11
5133	Ground-state properties of boron-doped diamond. Journal of Experimental and Theoretical Physics, 2008, 106, 781-787.	0.2	7
5134	Effect of oxygen on structure and electronic properties of silicon nanoclusters Si <sub>n</sub> (n = 5, 6, 10, 18). Semiconductors, 2008, 42, 800-804.	0.2	6
5135	Thermochemical and Mechanical Stabilities of the Oxide Scale of ZrB <sub>2</sub> +SiC and Oxygen Transport Mechanisms. Journal of the American Ceramic Society, 2008, 91, 1475-1480.	1.9	83
5136	First-Principles Calculations and Thermodynamic Modeling of the Al <sub>2</sub> O <sub>3</sub> -Nd <sub>2</sub> O <sub>3</sub> System. Journal of the American Ceramic Society, 2008, 91, 3355-3361.	1.9	12
5137	A chemically driven insulatorâ€“metal transition in non-stoichiometric and amorphous gallium oxide. Nature Materials, 2008, 7, 391-398.	13.3	166
5138	Dipole-directed assembly of lines of 1,5-dichloropentane on silicon substrates by displacement of surface charge. Nature Nanotechnology, 2008, 3, 222-228.	15.6	57
5139	A DFT study of the origin of the HDS/HydO selectivity on Co(Ni)MoS active phases. Journal of Catalysis, 2008, 260, 276-287.	3.1	66
5140	Towards an understanding of promoter action in heterogeneously catalyzed ethene epoxidation: Why chlorine is the best halogen. Journal of Catalysis, 2008, 260, 380-383.	3.1	44
5141	A first-principles investigation of the phase stability of Ti <sub>2</sub> AlC with Al vacancies. Scripta Materialia, 2008, 58, 227-230.	2.6	132
5142	Formation of nonequilibrium phases and associated structural transitions in the Rhâ€“Ta system induced by ion beam mixing. Scripta Materialia, 2008, 59, 3-6.	2.6	10

#	ARTICLE	IF	CITATIONS
5143	Ab initio study of electronic and thermodynamic properties of NdNi <sub>4</sub> Mg and NdNi <sub>4</sub> MgH <sub>4</sub> . <i>Scripta Materialia</i> , 2008, 59, 147-150.	2.6	5
5144	Ab initio modeling of the formation and migration of monovacancies in Ti <sub>2</sub> AlC. <i>Scripta Materialia</i> , 2008, 59, 854-857.	2.6	58
5145	The lower-valence coexisting ferrimagnetic Cr <sub>2</sub> VX (X=Ga, Si, Ge, Sb) Heusler compounds: A first-principles study. <i>Scripta Materialia</i> , 2008, 59, 1107-1110.	2.6	21
5146	Identification of the B33 martensite phase in Cu <sup>ε</sup> Zr using first-principles and X-ray diffraction. <i>Scripta Materialia</i> , 2008, 59, 1143-1146.	2.6	37
5147	Ideal mechanical strengths of Ir and Ir <sub>3</sub> Zr. <i>Scripta Materialia</i> , 2008, 59, 1197-1199.	2.6	17
5148	A first-principles study on the structural stability of Al <sub>2</sub> Ca Al <sub>4</sub> Ca and Mg <sub>2</sub> Ca phases. <i>Materials Letters</i> , 2008, 62, 206-210.	1.3	50
5149	Synthesis, crystal and electronic structure of Li <sub>13</sub> Ag <sub>5</sub> Si <sub>6</sub> , a potential anode for Li-ion batteries. <i>Solid State Sciences</i> , 2008, 10, 5-11.	1.5	21
5150	Two novel Zintl compounds Na <sub>12</sub> Ge <sub>8</sub> Sn and Na <sub>15</sub> Ge <sub>8</sub> SnP: Single crystal and electronic structures. <i>Solid State Sciences</i> , 2008, 10, 525-532.	1.5	1
5151	Carburization of the Fe <sub>3</sub> O <sub>4</sub> (111) Surface. <i>Journal of Physical Chemistry C</i> , 2008, 112, 6372-6379.	1.5	17
5152	Chapter 10 Electron Transfer and Nonadiabaticity. <i>Handbook of Surface Science</i> , 2008, , 429-524.	0.3	6
5153	Pseudopolymorphism in Nickel(II) Complexes with 6-Methylpicolinate. <i>Synthesis, Structural, Spectroscopic, Thermal, and Density Functional Theory Studies. Crystal Growth and Design</i> , 2008, 8, 3465-3473.	1.4	23
5154	E <sub>2</sub> and S <sub>N</sub> <sup>2</sup> Reactions of X <sup>+</sup> + CH <sub>3</sub> CH <sub>2</sub> X (X = F, Cl); an <i>ab Initio</i> and DFT Benchmark Study. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 929-940.	2.3	86
5155	Influence of vacancy defect density on electrical properties of armchair single wall carbon nanotube. <i>Diamond and Related Materials</i> , 2008, 17, 563-566.	1.8	12
5156	Size-Dependence of Adsorption Properties of Metal Nanoparticles: A Density Functional Study on Palladium Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2008, 112, 20269-20275.	1.5	86
5157	[Re(̇-5-C <sub>5</sub> H <sub>5</sub> )(CO) <sub>3</sub> ]+Family of 17-Electron Compounds: Monomer/Dimer Equilibria and Other Reactions. <i>Journal of the American Chemical Society</i> , 2008, 130, 2692-2703.	6.6	69
5158	Highly Accurate First-Principles Benchmark Data Sets for the Parametrization and Validation of Density Functional and Other Approximate Methods. Derivation of a Robust, Generally Applicable, Double-Hybrid Functional for Thermochemistry and Thermochemical Kinetics. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12868-12886.	1.1	680
5159	O <sub>2</sub> evolution on a clean partially reduced rutile TiO <sub>2</sub> (110) surface and on the same surface precovered with Au <sub>1</sub> and Au <sub>2</sub> : The importance of spin conservation. <i>Journal of Chemical Physics</i> , 2008, 129, 074705.	1.2	113
5160	Bridging the temperature and pressure gaps: close-packed transition metal surfaces in an oxygen environment. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 184021.	0.7	27

#	ARTICLE	IF	CITATIONS
5161	Theoretical Modeling of Zeolite Nanoparticle Surface Acidity for Heavy Oil Upgrading. Journal of Physical Chemistry C, 2008, 112, 6794-6810.	1.5	55
5162	Identification of the Matrix Shift: A Fingerprint for Neutral Neon Complex?. Journal of Physical Chemistry A, 2008, 112, 1018-1023.	1.1	13
5163	First-Principles Studies of the Structural and Electronic Properties of the (Ga <sub>1-x</sub> Zn <sub>x</sub> ) <sub>2</sub> (N <sub>1-x</sub> O <sub>x</sub> ) Solid Solution Photocatalyst. Journal of Physical Chemistry C, 2008, 112, 3439-3446.	1.5	11
5164	Plane-Wave DFT Investigations of the Adsorption, Diffusion, and Activation of CO on Kinked Fe(710) and Fe(310) Surfaces. Journal of Physical Chemistry C, 2008, 112, 10472-10489.	1.5	48
5165	Enhanced adsorption energy of Au <sub>1</sub> and O <sub>2</sub> on the stoichiometric TiO <sub>2</sub> (110) surface by coadsorption with other molecules. Journal of Chemical Physics, 2008, 128, 044714.	1.2	54
5166	Atomic Scale Insights on Chlorinated $\gamma$ -Alumina Surfaces. Journal of the American Chemical Society, 2008, 130, 11030-11039.	6.6	61
5167	Zero-Point Fluctuations in Naphthalene and Their Effect on Charge Transport Parameters. Journal of Physical Chemistry A, 2008, 112, 9113-9117.	1.1	14
5168	First-principles studies of water adsorption on graphene: The role of the substrate. Applied Physics Letters, 2008, 93, .	1.5	294
5169	Electrical response of molecular chains in density functional theory: Ultranonlocal response from a semilocal functional. Physical Review B, 2008, 77, .	1.1	58
5170	Bulk and surface analysis of H <sub>2</sub> Agg Fe carbide (Fe <sub>5</sub> C <sub>2</sub> ): a density functional theory study. Journal of Physics Condensed Matter, 2008, 20, 064238.	0.7	38
5171	First-principles investigation of intrinsic defects and (N, O) impurity atom stimulated Al vacancy in Ti <sub>2</sub> AlC. Applied Physics Letters, 2008, 93, .	1.5	38
5172	No Cage, No Tube: Relative Stabilities of Nanostructures. Journal of Physical Chemistry C, 2008, 112, 13200-13203.	1.5	11
5173	Stone-Wales Defects in Single-Walled Boron Nitride Nanotubes: Formation Energies, Electronic Structures, and Reactivity. Journal of Physical Chemistry C, 2008, 112, 1365-1370.	1.5	105
5174	Crystal packing of TCNQ anion $\dot{\text{C}}\text{N}^{\ominus}$ radicals governed by intermolecular covalent $\text{C}\text{--}\text{N}$ bonding: DFT calculations and statistical analysis of crystal structures. Physical Chemistry Chemical Physics, 2008, 10, 2625.	1.3	61
5175	<i>Ab initio</i> calculations of free-energy reaction barriers. Journal of Physics Condensed Matter, 2008, 20, 064211.	0.7	54
5176	<i>Ab initio</i> study of substitutional impurity atoms in 4H-SiC. Journal of Applied Physics, 2008, 104, .	1.1	15
5177	Hybrid exchange-correlation functional for accurate prediction of the electronic and structural properties of ferroelectric oxides. Physical Review B, 2008, 77, .	1.1	315
5178	First-Principles Study on Water and Oxygen Adsorption on Surfaces of Indium Oxide and Indium Tin Oxide Nanoparticles. Journal of Physical Chemistry C, 2008, 112, 14015-14020.	1.5	36

#	ARTICLE	IF	CITATIONS
5179	Computational Study of Brønsted Acidity of Faujasite. Effect of the Al Content on the Infrared OH Stretching Frequencies. <i>Journal of Physical Chemistry C</i> , 2008, 112, 19293-19301.	1.5	30
5180	Synergetic Effects of the Cu/Pt{110} Surface Alloy: Enhanced Reactivity of Water and Carbon Monoxide. <i>Journal of Physical Chemistry C</i> , 2008, 112, 6422-6429.	1.5	20
5181	Density functional studies of model cerium oxide nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 5730.	1.3	125
5182	Atomic and Electronic Structure of Cerium Oxide Stepped Model Surfaces. <i>Journal of Physical Chemistry C</i> , 2008, 112, 17643-17651.	1.5	40
5183	Phase transition and elastic constants of zirconium from first-principles calculations. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 235230.	0.7	35
5184	Predictive Molecular Thermodynamic Models for Liquid Solvents, Solid Salts, Polymers, and Ionic Liquids. <i>Chemical Reviews</i> , 2008, 108, 1419-1455.	23.0	137
5185	Stability of MgO(111) Polar Surface: Effect of the Environment. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3327-3333.	1.5	26
5186	Ab Initio Study of Temperature and Pressure Dependence of Energy and Phonon-Induced Dephasing of Electronic Excitations in CdSe and PbSe Quantum Dots. <i>Journal of Physical Chemistry C</i> , 2008, 112, 7800-7808.	1.5	89
5187	Platinum-group and noble metals under oxidizing conditions. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 184023.	0.7	52
5188	Trends in adsorption of noble gases He, Ne, Ar, Kr, and Xe on Pd <sub>111</sub> . All-electron d. <i>Physical Review B</i> , 2008, 77, .	1.1	59
5189	Theory and simulation in heterogeneous gold catalysis. <i>Chemical Society Reviews</i> , 2008, 37, 2046.	18.7	136
5190	Electric Field Control of Structure, Dimensionality, and Reactivity of Gold Nanoclusters on Metal-Supported MgO Films. <i>Physical Review Letters</i> , 2008, 100, 056102.	2.9	58
5191	DFT Calculation of <sup>1</sup> J( <sup>119</sup> Sn, <sup>13</sup> C) and <sup>2</sup> J( <sup>119</sup> Sn, <sup>1</sup> H) Coupling Constants in Di- and Trimethyltin(IV) Compounds. <i>Inorganic Chemistry</i> , 2008, 47, 4796-4807.	1.9	46
5192	Oxoperoxo Vanadium(V) Complexes of L-Lactic Acid: Density Functional Theory Study of Structure and NMR Chemical Shifts. <i>Inorganic Chemistry</i> , 2008, 47, 7317-7326.	1.9	28
5193	A Periodic DFT Study of N <sub>2</sub> O <sub>4</sub> Disproportionation on Alkali-Exchanged Zeolites X. <i>Journal of Physical Chemistry C</i> , 2008, 112, 5510-5519.	1.5	37
5194	Dynamics of Hydrogen Spillover on Carbon-Based Materials. <i>Journal of Physical Chemistry C</i> , 2008, 112, 17465-17470.	1.5	62
5195	Ab initio study of evolution of mechanical and transport properties of clean and contaminated Au nanowires along the deformation path. <i>Physical Review B</i> , 2008, 77, .	1.1	44
5196	F and F <sup>+</sup> Centers on MgO/Ag(100) or MgO/Mo(100) Ultrathin Films: Are They Stable?. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3857-3865.	1.5	31



#	ARTICLE	IF	CITATIONS
5197	Methane Activation and Oxygen Vacancy Formation over CeO <sub>2</sub> and Zr, Pd Substituted CeO <sub>2</sub> Surfaces. Journal of Physical Chemistry C, 2008, 112, 14955-14964.	1.5	180
5198	Migration of Ag in low-temperature Ag <sub>2</sub> S from first principles. Journal of Chemical Physics, 2008, 128, 014704.	1.2	26
5199	Stable Geometric and Electronic Structures of Gold-Coated Nanoparticles M@Au <sub>12</sub> (M =) Tj ETQq0 0 0 rgBT /Overlock 10 T Journal of Physical Chemistry C, 2008, 112, 12646-12652.	1.5	23
5200	Transition-Metal-Substituted Indium Thiospinels as Novel Intermediate-Band Materials: Prediction and Understanding of Their Electronic Properties. Physical Review Letters, 2008, 101, 046403.	2.9	129
5201	Combined Ligand Field and Density Functional Theory Analysis of the Magnetic Anisotropy in Oligonuclear Complexes Based on Fe <sup>III</sup> and Mn <sup>II</sup> Exchange-Coupled Pairs. Inorganic Chemistry, 2008, 47, 2449-2463.	1.9	78
5202	Correlation of Global Electrophilicity with the Activation Energy in Single-Step Concerted Reactions. Journal of Physical Chemistry A, 2008, 112, 97-105.	1.1	13
5203	Methanol and Water Dissociation on TiO <sub>2</sub> (110): The Role of Surface Oxygen. Journal of Physical Chemistry C, 2008, 112, 17737-17740.	1.5	92
5204	Adsorption of diatomic molecules on iron tape-porphyrin: A comparative study. Physical Review B, 2008, 77, .	1.1	26
5205	Origin of hardness in WB <sub>4</sub> and its implications for ReB <sub>4</sub> , TaB <sub>4</sub> , MoB <sub>4</sub> , TcB <sub>4</sub> , and OsB <sub>4</sub> . Applied Physics Letters, 2008, 93, .	1.5	154
5206	Stability and magnetism of hydrogen dimers on graphene. Physical Review B, 2008, 78, .	1.1	103
5207	Determination of elastic constants of Na <sub>0.5</sub> Bi <sub>0.5</sub> TiO <sub>3</sub> from <i>ab initio</i> calculations. Phase Transitions, 2008, 81, 1117-1124.	0.6	21
5208	All-Electron Scalar Relativistic Basis Sets for Third-Row Transition Metal Atoms. Journal of Chemical Theory and Computation, 2008, 4, 908-919.	2.3	1,061
5209	On the Mechanisms of Hydrogen Spillover in MoO <sub>3</sub> . Journal of Physical Chemistry C, 2008, 112, 1755-1758.	1.5	98
5210	Electronic and magnetic properties of transition-metal atom adsorbed graphene and graphene nanoribbons. Physical Review B, 2008, 77, .		452
5211	Compression curves of transition metals in the Mbar range: Experiments and projector augmented-wave calculations. Physical Review B, 2008, 78, .	1.1	383
5212	Evaluation of first-principles techniques for obtaining materials parameters of ground- and excited-state properties from first-principles calculations. Physical Review B, 2008, 77, .	1.1	86
5213	Compression curves of transition metals in the Mbar range: Experiments and projector augmented-wave calculations. Physical Review B, 2008, 78, .	1.1	93
5214	OH Formation from O and H Atoms Physisorbed on a Graphitic Surface through the Langmuir-Hinshelwood Mechanism: A Quasi-Classical Approach. Journal of Physical Chemistry A, 2008, 112, 11921-11930.	1.1	38

#	ARTICLE	IF	CITATIONS
5215	Adsorption of NO on Cu-SAPO-34 and Co-SAPO-34: A Periodic DFT Study. Journal of Physical Chemistry C, 2008, 112, 2632-2639.	1.5	17
5216	Developing paradigms of chemical bonding: adaptive natural density partitioning. Physical Chemistry Chemical Physics, 2008, 10, 5207.	1.3	1,206
5217	The Effect of Water on the CO Oxidation on Ag(111) and Au(111) Surfaces: A First-Principle Study. Journal of Physical Chemistry C, 2008, 112, 17303-17310.	1.5	160
5218	Hydroxyl Chain Formation on the Cu(110) Surface: Watching Water Dissociation. Journal of Physical Chemistry C, 2008, 112, 17672-17677.	1.5	52
5219	Wetting of mixed OH•H <sub>2</sub> O layers on Pt(111). Journal of Chemical Physics, 2008, 128, 074701.	1.2	37
5220	Effect of dopants on grain boundary decohesion of Ni: A first-principles study. Applied Physics Letters, 2008, 93, .	1.5	48
5221	The structure of mixed H <sub>2</sub> O•OH monolayer films on Ru(0001). Journal of Chemical Physics, 2008, 129, 154109.	1.2	50
5222	Short-range and long-range contributions to the size effect in metal-ferroelectric-metal heterostructures. Physical Review B, 2008, 77, .	1.1	108
5223	Modeling doped and defective oxides in catalysis with density functional theory methods: Room for improvements. Journal of Chemical Physics, 2008, 128, 182505.	1.2	221
5224	Chain metallicity and competition between paramagnetism and antiferromagnetism in underdoped YBaCu <sub>3</sub> . A first principles de. Physical Review B, 2008, 78, .	1.1	13
5225	Computational Techniques at the Organic•Inorganic Interface in Biomineralization. Chemical Reviews, 2008, 108, 4823-4854.	23.0	113
5226	Mechanism of the Water Gas Shift Reaction on Pt: First Principles, Experiments, and Microkinetic Modeling. Journal of Physical Chemistry C, 2008, 112, 4608-4617.	1.5	452
5227	N Doping of Rutile TiO <sub>2</sub> (110) Surface. A Theoretical DFT Study. Journal of Physical Chemistry C, 2008, 112, 2624-2631.	1.5	107
5228	Comparison of the Adsorption of Ni, Pd, and Pt on the (0001) Surface of •Alumina. Journal of Physical Chemistry C, 2008, 112, 18948-18954.	1.5	32
5229	Combined experimental and theoretical investigation of optical, structural, and electronic properties of Ca <sub>3</sub> N <sub>2</sub> H <sub>3</sub> . Journal of Physical Chemistry C, 2008, 112, 18948-18954.	1.1	128
5230	Infrared Spectroscopy of Discrete Uranyl Anion Complexes. Journal of Physical Chemistry A, 2008, 112, 508-521.	1.1	53
5231	TD-DFT investigation of the electronic spectra of (DOEO) <sub>4</sub> HgBr <sub>4</sub> •TCE salt. Molecular Physics, 2008, 106, 33-42.	0.8	5
5232	Hydrogen adsorption, dissociation and diffusion on the •U(001) surface. Journal of Physics Condensed Matter, 2008, 20, 445001.	0.7	13

#	ARTICLE	IF	CITATIONS
5233	A density functional theory-based study of the electronic structures and properties of cage like metal doped silicon clusters. Journal of Applied Physics, 2008, 104, .	1.1	39
5234	Origin of Selectivity Switch in Fischer-Tropsch Synthesis over Ru and Rh from First-Principles Statistical Mechanics Studies. Journal of the American Chemical Society, 2008, 130, 7929-7937.	6.6	64
5235	First-principles solution to the problem of Mo lattice stability. Physical Review B, 2008, 77, .	1.1	58
5236	High-Resolution Raman Spectroscopy Study of Phonon Modes in LiBH <sub>4</sub> and LiBD <sub>4</sub> . Journal of Physical Chemistry A, 2008, 112, 9716-9722.	1.1	43
5237	DFT study of the adsorption of microsolvated glycine on a hydrophilic amorphous silica surface. Physical Chemistry Chemical Physics, 2008, 10, 6360.	1.3	84
5238	Interactions in Large, Polyaromatic Hydrocarbon Dimers: Application of Density Functional Theory with Dispersion Corrections. Journal of Physical Chemistry A, 2008, 112, 10968-10976.	1.1	136
5239	Electronic Band Structure of Tetracene-TCNQ and Perylene-TCNQ Compounds. Journal of Physical Chemistry A, 2008, 112, 2497-2502.	1.1	46
5240	Exploring the Limit of Accuracy of the Global Hybrid Meta Density Functional for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2008, 4, 1849-1868.	2.3	956
5241	First-principles calculations of the electronic structure and pressure-induced magnetic transition in siderite $\text{FeCO}_3$ . Physical Review B, 2008, 78, .	1.1	42
5242	Changes in single-walled carbon nanotube chirality during growth and regrowth. Journal of Chemical Physics, 2008, 128, 124708.	1.2	12
5243	Electronic structure of bulk- and Na-intercalated $\text{TiS}_2$ from a GGA+U calculation with the Hubbard terms obtained <i>ab initio</i> . Physical Review B, 2008, 78, .	1.1	24
5244	On the prediction of the crystal and electronic structure of mixed-valence materials by periodic density functional calculations: The case of Prussian Blue. Journal of Chemical Physics, 2008, 128, 044713.	1.2	35
5245	Electronic structures of SiC nanoribbons. Journal of Chemical Physics, 2008, 129, 174114.	1.2	222
5246	Structural motifs, mixing, and segregation effects in 38-atom binary clusters. Journal of Chemical Physics, 2008, 128, 134517.	1.2	147
5247	The structure of LiMg(AlD <sub>4</sub> ) <sub>3</sub> . Journal of Alloys and Compounds, 2008, 455, 249-254.	2.8	35
5248	Lattice stability of intermediate phases of the Sr-Si system. Journal of Alloys and Compounds, 2008, 457, 29-35.	2.8	16
5249	On the formation of LaFe <sub>5</sub> Hn. Journal of Alloys and Compounds, 2008, 461, 26-33.	2.8	15
5250	First principles calculation of elastic and lattice constants of orthorhombic Cu <sub>3</sub> Sn crystal. Journal of Alloys and Compounds, 2008, 466, 517-520.	2.8	36

#	ARTICLE	IF	CITATIONS
5251	Phase equilibria, thermodynamics and solidification microstructures of Mg–Sn–Ca alloys, Part 1: Experimental investigation and thermodynamic modeling of the ternary Mg–Sn–Ca system. <i>Intermetallics</i> , 2008, 16, 299-315.	1.8	86
5252	Elastic properties of the post-perovskite phase of Fe <sub>2</sub> O <sub>3</sub> and implications for ultra-low velocity zones. <i>Physics of the Earth and Planetary Interiors</i> , 2008, 170, 260-266.	0.7	15
5253	MoS <sub>2</sub> Nanoribbons: High Stability and Unusual Electronic and Magnetic Properties. <i>Journal of the American Chemical Society</i> , 2008, 130, 16739-16744.	6.6	876
5254	A First-Principle Study of Chain Propagation Steps in the Fischer–Tropsch Synthesis on Fe(100). <i>Journal of Physical Chemistry C</i> , 2008, 112, 13681-13691.	1.5	17
5255	First-principles calculations of the crystal structure, electronic structure, and thermodynamic stability of $\text{Be}$ . <i>Physical Review B</i> , 2008, 77, .	1.1	31
5256	A Density Functional Study of $\hat{\pm}\text{-Mg}(\text{BH}_4)_2$ . <i>Chemistry of Materials</i> , 2008, 20, 4952-4956.	3.2	76
5257	Structure of Ca(BD <sub>4</sub> ) <sub>2</sub> $\hat{2}$ -Phase from Combined Neutron and Synchrotron X-ray Powder Diffraction Data and Density Functional Calculations. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8042-8048.	1.2	91
5258	Revealing Intuitively Assessable Chemical Bonding Patterns in Organic Aromatic Molecules via Adaptive Natural Density Partitioning. <i>Journal of Organic Chemistry</i> , 2008, 73, 9251-9258.	1.7	242
5259	Predicting Enthalpies of Molecular Substances: Application to $\text{LiBH}_4$ . <i>Physical Review Letters</i> , 2008, 100, 040602.	2.9	40
5260	Ni-induced destabilization dynamics of crystalline zinc borohydride. <i>Applied Physics Letters</i> , 2008, 92, 134101.	1.5	8
5261	Probing Silver Nanoparticles During Catalytic H <sub>2</sub> Evolution. <i>Journal of the American Chemical Society</i> , 2008, 130, 7067-7076.	6.6	49
5262	Advances in Correlated Electronic Structure Methods for Solids, Surfaces, and Nanostructures. <i>Annual Review of Physical Chemistry</i> , 2008, 59, 261-290.	4.8	210
5263	Adsorption and Dissociation of the HCl and Cl <sub>2</sub> Molecules on W(111) Surface: A Computational Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 12342-12348.	1.5	10
5264	Adsorption and Dissociation of CO <sub>x</sub> ( <i>x</i> = 1, 2) on W(111) Surface: A Computational Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3341-3348.	1.5	21
5265	Simulating charge transport in tris(8-hydroxyquinoline) aluminium (Alq <sub>3</sub> ). <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 1852.	1.3	169
5266	Density Functional Characterization of the Band Edges, the Band Gap States, and the Preferred Doping Sites of Halogen-Doped TiO <sub>2</sub> . <i>Chemistry of Materials</i> , 2008, 20, 6528-6534.	3.2	165
5267	Large-Scale Screening of Metal Hydride Mixtures for High-Capacity Hydrogen Storage from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2008, 112, 5258-5262.	1.5	97
5268	Experiment and first principles calculation of hydrogen-induced reduction of Young's modulus of BaTiO <sub>3</sub> single crystal. <i>Journal Physics D: Applied Physics</i> , 2008, 41, 092004.	1.3	1

#	ARTICLE	IF	CITATIONS
5269	Analysis of semi-empirical interatomic potentials appropriate for simulation of crystalline and liquid Al and Cu. Philosophical Magazine, 2008, 88, 1723-1750.	0.7	374
5270	Structural, electronic, and magnetic properties of $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"> \langle \text{mml:mrow}> \langle \text{mml:mn}> 3 \langle \text{mml:mn}> \langle \text{mml:mi}> d \langle \text{mml:mi}> \langle \text{mml:mrow}> \langle \text{mml:math}> \text{transition metal monatomic chains: First-principles calculations. Physical Review B, 2008, 77, .$	1.1	63
5271	Temperature-dependent diffusion coefficients from <i>ab initio</i> computations: Hydrogen, deuterium, and tritium in nickel. Physical Review B, 2008, 77, .	1.1	186
5272	Enthalpy of mixing for ternary fcc solid solutions from special quasirandom structures. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2008, 32, 74-81.	0.7	22
5273	Combined <i>ab initio</i> /CALPHAD modeling of fcc-based phase-equilibria in the Ir-Nb system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2008, 32, 353-360.	0.7	9
5274	First-principles based calculation of binary and multicomponent phase diagrams for titanium carbonitride. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2008, 32, 543-565.	0.7	31
5275	Thermodynamic description of the Mg-Eu binary system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2008, 32, 462-465.	0.7	8
5276	Thermodynamic modeling of the Na-Al-Ti-H system and Ti dissolution in sodium alanates. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2008, 32, 624-636.	0.7	16
5277	<i>Ab initio</i> study of the composition dependence of the pressure-induced spin crossover in perovskite (Mg <sub>1-x</sub> Fe <sub>x</sub> )SiO <sub>3</sub> . Earth and Planetary Science Letters, 2008, 265, 535-545.	1.8	70
5278	Surface complexation of U(VI) on goethite ( $\alpha$ -FeOOH). Geochimica Et Cosmochimica Acta, 2008, 72, 298-310.	1.6	186
5279	First-principles study of structural and elastic properties of MgSe under hydrostatic pressure. Computational Materials Science, 2008, 41, 538-541.	1.4	15
5280	Initial stage of Ag deposition on regular MgO(001) surface: A DFT study. Computational Materials Science, 2008, 42, 43-49.	1.4	15
5281	First-principles study of heavily B-doped silicon. Computational Materials Science, 2008, 42, 161-167.	1.4	8
5282	Structural and bonding properties of stannate pyrochlores: A density functional theory investigation. Computational Materials Science, 2008, 42, 653-658.	1.4	44
5283	Stability and magnetic properties of Mn-substituted ScN semiconductor from first principles. Computational Materials Science, 2008, 43, 392-398.	1.4	15
5284	Structural and electronic properties of cubic HfO <sub>2</sub> surfaces. Computational Materials Science, 2008, 44, 46-52.	1.4	61
5285	Effect of impurities on grain boundary cohesion in bcc iron. Computational Materials Science, 2008, 43, 736-743.	1.4	62
5286	Zirconium and hafnium oxide interface with silicon: Computational study of stress and strain effects. Computational Materials Science, 2008, 43, 930-937.	1.4	11

#	ARTICLE	IF	CITATIONS
5287	The effect of excess titanium and crystal symmetry on electronic properties of $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$ compounds. Computational Materials Science, 2008, 43, 909-916.	1.4	20
5288	Formation and stability of di-transition-metal carbides $\text{Ti}_x\text{Zr}_{1-x}\text{C}$ , $\text{Ti}_x\text{Hf}_{1-x}\text{C}$ and $\text{Hf}_x\text{Zr}_{1-x}\text{C}$ . Computational Materials Science, 2008, 44, 347-350.	1.4	18
5289	Ab initio calculation of the total energy and elastic properties of Laves phase $\text{C}_{15}\text{Al}_2\text{RE}$ (RE=Sc, Y, La). <i>Journal of Applied Physics</i> , 2008, 104, 043505.	1.4	43
5290	Electronic structure, elasticity and hardness of diborides of zirconium and hafnium: First principles calculations. Computational Materials Science, 2008, 44, 411-421.	1.4	134
5291	Ab initio equation of state for the body-centered-cubic phase of iron at high pressure and temperature. Physical Review B, 2008, 78, .	1.1	34
5292	Pressure effect on the structural and elastic properties of ternary compounds $\text{M}_2\text{AlC}$ (M = Ti, V, Cr). <i>Journal of Applied Physics</i> , 2008, 104, 043505.	0.3	14
5293	Stable $\text{M}_2\text{AlC}(0001)$ surfaces (M = Ti, V and Cr) by first-principles investigation. Journal of Physics Condensed Matter, 2008, 20, 225006.	0.7	25
5294	First-principles study of interphase $\text{Ni}_3\text{Sn}$ in $\text{Sn}\epsilon$ -Ni alloy for anode of lithium ion battery. Chinese Physics B, 2008, 17, 3422-3427.	0.7	20
5295	Diffusion of Interstitial Mn in the Dilute Magnetic Semiconductor (Ga,Mn)As: The Effect of a Charge State. Physical Review Letters, 2008, 101, 177204.	2.9	15
5296	Recent density functional studies of hydrodesulfurization catalysts: insight into structure and mechanism. Journal of Physics Condensed Matter, 2008, 20, 064236.	0.7	25
5297	Novel High Pressure Phases of $\text{Hf}_2\text{-AlH}_3$ : A Density-Functional Study. Chemistry of Materials, 2008, 20, 5997-6002.	3.2	31
5298	Generation of vacancy-interstitial pairs as a possible origin of resistivity switching and ferroelectric properties in $\text{CdTiO}_3$ . <i>Physical Review B</i> , 2008, 77, .	1.1	25
5299	Intercalation processes and diffusion paths of lithium ions in spinel-type structured $\text{LiTi}_2\text{O}_6$ . <i>Physical Review B</i> , 2008, 77, .	1.1	25
5300	Theory: Periodic Electronic Structure Calculations. <i>Journal of Applied Physics</i> , 2008, 104, 043505.		1
5301	On the Mechanism of Low-Temperature Water Gas Shift Reaction on Copper. Journal of the American Chemical Society, 2008, 130, 1402-1414.	6.6	839
5302	Modelling of bitumen fragment adsorption on $\text{Cu}^+$ and $\text{Ag}^+$ exchanged zeolite nanoparticles. Molecular Simulation, 2008, 34, 943-951.	0.9	15
5303	Electronic structure of $\text{ZnO:GaN}$ compounds: Asymmetric bandgap engineering. Physical Review B, 2008, 78, .	1.1	93
5304	Theoretical Study of the Thermodynamic and Kinetic Aspects of Terminated (111) Diamond Surfaces. Journal of Physical Chemistry C, 2008, 112, 3018-3026.	1.5	47



#	ARTICLE	IF	CITATIONS
5305	Water Clusters Confined in Nonpolar Cavities by Ab Initio Calculations. <i>Journal of Physical Chemistry C</i> , 2008, 112, 11779-11785.	1.5	28
5306	Density functional theory for hydrogen storage materials: successes and opportunities. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 064229.	0.7	52
5307	In-silico investigations in heterogeneous catalysisâ€”combustion and synthesis of small alkanes. <i>Chemical Society Reviews</i> , 2008, 37, 2274.	18.7	52
5308	Charge-induced formation of linear Au clusters on thin MgO films: Scanning tunneling microscopy and density-functional theory study. <i>Physical Review B</i> , 2008, 78, .	1.1	64
5309	First-principles approach to monitoring the band gap and magnetic state of a graphene nanoribbon via its vacancies. <i>Physical Review B</i> , 2008, 78, .	1.1	120
5310	Mapping the dâ€”d Excited-State Manifolds of Transition Metal Î²-Diiminatoâ€”Imido Complexes. Comparison of Density Functional Theory and CASPT2 Energetics. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12792-12798.	1.1	19
5311	Dissociative dynamics of spin-triplet and spin-singlet O2 on Ag(100). <i>Journal of Chemical Physics</i> , 2008, 129, 224702.	1.2	39
5312	Low Dimensional Nanomaterials for Spintronics. , 2008, , 247-271.		0
5313	Phase stability of cation-doped LiMnO<sub>2</sub> within the GGA+U approximation. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2008, 16, 055008.	0.8	9
5314	Kinetics-driven anisotropic growth of pentacene thin films. <i>Physical Review B</i> , 2008, 77, .	1.1	42
5315	Spin and band-gap engineering in doped graphene nanoribbons. <i>Physical Review B</i> , 2008, 78, .	1.1	128
5316	Characterization of the Fe Site in Ironâ€”Sulfur Cluster-Free Hydrogenase (Hmd) and of a Model Compound via Nuclear Resonance Vibrational Spectroscopy (NRVS). <i>Inorganic Chemistry</i> , 2008, 47, 3969-3977.	1.9	97
5317	Stable nanoporous alkali halide polymorphs: a first principles bottom-up study. <i>Journal of Materials Chemistry</i> , 2008, 18, 5871.	6.7	30
5318	A study of bimetallic Cuâ€”Ag, Auâ€”Ag and Pdâ€”Ag clusters adsorbed on a double-vacancy-defected MgO(100) terrace. <i>Faraday Discussions</i> , 2008, 138, 37-47.	1.6	27
5319	Dependence of charge transfer reorganization energy on carrier localisation in organic molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 121-127.	1.3	43
5320	Lattice match in density functional calculations: ice Ih vs. Î²-Agl. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 4688.	1.3	55
5321	Cluster-assembled compounds comprising an all-metal subunit Li3Al4â€”. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2020.	1.3	6
5322	Metal adsorption on oxide polar ultrathin films. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 1876.	1.3	24





#	ARTICLE	IF	CITATIONS
5341	On the possibility of ferromagnetism in carbon-doped anatase TiO <sub>2</sub> . Applied Physics Letters, 2008, 93, 132507.	1.5	125
5342	Theoretical Investigation of the Uranyl Ion Sorption on the Rutile TiO <sub>2</sub> (110) Face. Inorganic Chemistry, 2008, 47, 10991-10997.	1.9	35
5343	Theoretical and Experimental Vibrational Characterizations of Amine-Coated Silver Nanoparticles. Journal of Physical Chemistry C, 2008, 112, 13851-13855.	1.5	7
5344	Physisorption and Chemisorption of Hydrocarbons in H-FAU Using QM-Pot(MP2//B3LYP) Calculations. Journal of Physical Chemistry C, 2008, 112, 11796-11812.	1.5	55
5345	Hydrogen Storage in Ti-Decorated BC <sub>4</sub> N Nanotube. Journal of Physical Chemistry C, 2008, 112, 17487-17491.	1.5	37
5346	First-principles study of interaction of molecular hydrogen with Li-doped carbon nanotube peapod structures. Physical Review B, 2008, 77, .	1.1	36
5347	Carbon-13 NMR Relaxation Study of 1,8-Bis(dimethylamino)naphthalene in Isotropic Solution. Journal of Physical Chemistry A, 2008, 112, 4711-4714.	1.1	4
5348	Thermodynamics of Environment-Dependent Oxygen Chemisorption on Pt(111). Journal of Physical Chemistry C, 2008, 112, 9559-9572.	1.5	173
5349	Adsorption and Decomposition of CO on Stepped Fe(310) Surfaces. Journal of Physical Chemistry C, 2008, 112, 3692-3700.	1.5	17
5350	First-Principles Calculation of <sup>13</sup> C NMR Chemical Shifts of Infinite Single-Walled Carbon Nanotubes: New Data for Large-Diameter and Four-Helical Nanotubes. Journal of Physical Chemistry C, 2008, 112, 16417-16421.	1.5	18
5351	Reaction Mechanism of the Oxidation of HCl over RuO <sub>2</sub> (110). Journal of Physical Chemistry C, 2008, 112, 9966-9969.	1.5	68
5352	Structural, Electronic, and Magnetic Properties of Fe <sub>3</sub> C <sub>2</sub> Cluster. Journal of Physical Chemistry A, 2008, 112, 4556-4561.	1.1	11
5353	Near optical isotropy in noncubic SrI <sub>2</sub> : Density functional calculations. Applied Physics Letters, 2008, 92, 201908.	1.5	31
5354	Bonding in Low-Coordinate Environments: Electronic Structure of Distorted Square-Planar Iron-Imido Complexes With Pincer-Type Ligands. Journal of Chemical Theory and Computation, 2008, 4, 1576-1584.	2.3	3
5355	Binding Strength of Sodium Ions in Cellulose for Different Water Contents. Journal of Physical Chemistry B, 2008, 112, 8985-8989.	1.2	27
5356	Lithium Calcium Imide [Li <sub>2</sub> Ca(NH) <sub>2</sub> ] for Hydrogen Storage: Structural and Thermodynamic Properties. Journal of Physical Chemistry B, 2008, 112, 11381-11384.	1.2	21
5357	Density Functional and Basis Set Dependence of Hydrated Ln(III) Properties. Journal of Chemical Theory and Computation, 2008, 4, 708-718.	2.3	53
5358	Gold Nanostructures on TiO <sub>x</sub> /Mo(112) Thin Films. Journal of Physical Chemistry C, 2008, 112, 191-200.	1.5	15

#	ARTICLE	IF	CITATIONS
5359	Origin of the OH Vibrational Blue Shift in the LiOH Crystal. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13487-13494.	1.1	9
5360	Insight into the Reduction of Pyruvic Acid to Lactic Acid over Cu{110}: The Crucial Role of Intramolecular Tunneling in Direct Hydrogenation. <i>Journal of the American Chemical Society</i> , 2008, 130, 14483-14492.	6.6	12
5361	Effect of particle size and surface structure on adsorption of O and OH on platinum nanoparticles: A first-principles study. <i>Physical Review B</i> , 2008, 77, .	1.1	173
5362	Intrinsic Metal Size Effect on Adsorption of Organic Molecules on Platinum. <i>Journal of Physical Chemistry C</i> , 2008, 112, 6822-6831.	1.5	17
5363	Stacking and Solvent Effects on the Electronic and Optical Properties of Gold and Mercury Acetylide Aggregations: A Theoretical Study. <i>Organometallics</i> , 2008, 27, 4636-4648.	1.1	16
5364	Orbital Interpretation of Kinetic Energy Density and a Direct Space Comparison of Chemical Bonding in Tetrahedral Network Solids. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7705-7716.	1.1	4
5365	A Density Functional Study on Transition-Metal-Coated Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2008, 112, 9128-9132.	1.5	15
5366	Adsorption of Water on O(2 Å <sup>-2</sup> )/Ru(0001): Thermal Stability and Inhibition of Dissociation. <i>Journal of Physical Chemistry C</i> , 2008, 112, 14052-14057.	1.5	12
5367	Allene as the Parent Substrate in Zinc-Mediated Biomimetic Hydration Reactions of Cumulenes. <i>Journal of Organic Chemistry</i> , 2008, 73, 8265-8278.	1.7	7
5368	<i>Ab initio</i> prediction of stable boron sheets and boron nanotubes: Structure, stability, and electronic properties. <i>Physical Review B</i> , 2008, 77, .	1.1	315
5369	Oxygen-mediated electron transport through hybrid silicon-organic interfaces. <i>Nanotechnology</i> , 2008, 19, 285201.	1.3	7
5370	The structural properties of wurtzite and rocksalt Mg <sub>x</sub> Zn <sub>1-x</sub> O. <i>Semiconductor Science and Technology</i> , 2008, 23, 025008.	1.0	30
5371	Combined Density Functional Theory and Interatomic Potential Study of the Bulk and Surface Structures and Properties of the Iron Sulfide Mackinawite (FeS). <i>Journal of Physical Chemistry C</i> , 2008, 112, 10960-10967.	1.5	70
5372	On the Thermodynamic Stability of (S <sub>3</sub> )R <sub>3</sub> O Methanethiolate Lattice on Reconstructed Au(111) Surface Models. <i>Journal of Physical Chemistry C</i> , 2008, 112, 19121-19124.	1.5	20
5373	Ab Initio Molecular Dynamics Simulation on the Aggregation of a Cu Monolayer on a WN(001) Surface. <i>Journal of Physical Chemistry C</i> , 2008, 112, 9798-9802.	1.5	13
5374	Thermodynamic Properties of Trialkali (Li, Na, K) Hexa-alanates: A Combined DFT and Experimental Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 18598-18607.	1.5	15
5375	Vibrational Spectra of ±-Amino Acids in the Zwitterionic State in Aqueous Solution and the Solid State: DFT Calculations and the Influence of Hydrogen Bonding. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10333-10347.	1.1	63
5376	Effect of Ag Adatoms on High-Coverage Alkanethiolate Adsorption on Au(111). <i>Journal of Physical Chemistry C</i> , 2008, 112, 4557-4563.	1.5	8

#	ARTICLE	IF	CITATIONS
5377	Chemical Behavior and in Vitro Activity of Mixed Phosphine Gold(I) Compounds on Melanoma Cell Lines. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 1584-1591.	2.9	22
5378	Toward Calculations of the $^{129}\text{Xe}$ Chemical Shift in $\text{Xe}@C_{60}$ at Experimental Conditions: Relativity, Correlation, and Dynamics. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2658-2668.	1.1	60
5379	Axial Coordination of NHC Ligands on Dirhodium(II) Complexes: Generation of a New Family of Catalysts. <i>Journal of Organic Chemistry</i> , 2008, 73, 4076-4086.	1.7	94
5380	Insertion of Internal Alkynes and Ethene into Permethylated Singly Tucked-in Titanocene. <i>Organometallics</i> , 2008, 27, 5532-5547.	1.1	42
5381	Density Functional Theory Calculations of the Lowest Energy Quintet and Triplet States of Model Hemes: Role of Functional, Basis Set, and Zero-Point Energy Corrections. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3700-3711.	1.1	25
5382	Ab initio study of Co and Ni under uniaxial and biaxial loading and in epitaxial overlayers. <i>Physical Review B</i> , 2008, 78, .	1.1	26
5383	Chemisorption of hydrogen molecules on carbon nanotubes: charging effect from first-principles calculations. <i>Nanotechnology</i> , 2008, 19, 075707.	1.3	15
5384	DFT Study of the CO Oxidation on the Au(321) Surface. <i>Journal of Physical Chemistry C</i> , 2008, 112, 17291-17302.	1.5	65
5385	Counting Electrons Transferred through a Thin Alumina Film into Au Chains. <i>Physical Review Letters</i> , 2008, 100, 096802.	2.9	101
5386	Electronic Correlations Decimate the Ferroelectric Polarization of Multiferroic $\text{HoMn}_2\text{O}_5$ . <i>Physical Review Letters</i> , 2008, 100, 227602.	2.9	71
5387	Study of Lattice Constant and Bulk Modulus in Zincblende InGaN Using Local Density Approximation and Generalized Gradient Approximation. <i>Japanese Journal of Applied Physics</i> , 2008, 47, 3350-3353.	0.8	12
5388	Adsorption Configurations and Reactions of Boric Acid on a $\text{TiO}_2$ Anatase (101) Surface. <i>Journal of Physical Chemistry C</i> , 2008, 112, 8276-8287.	1.5	44
5389	Crystal and Molecular Structure of Piceatannol; Scavenging Features of Resveratrol and Piceatannol on Hydroxyl and Peroxyl Radicals and Docking with Transthyretin. <i>Journal of Agricultural and Food Chemistry</i> , 2008, 56, 10557-10566.	2.4	68
5390	Effect of Coadsorbed Dopants on Diamond Initial Growth Processes: $\text{CH}_3$ Adsorption. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5429-5435.	1.1	19
5391	Competitive Chemisorption of Bifunctional Carboxylic Acids on H:Si(100): A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 10167-10175.	1.5	4
5392	Polyfunctional Methodology for Improved DFT Thermochemical Predictions. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10624-10634.	1.1	1
5393	Oxygen-Centered Hexatantalum Tetradecaimido Cluster Complexes. <i>Inorganic Chemistry</i> , 2008, 47, 1053-1066.	1.9	20
5394	A first principles theoretical study of vibrational spectral diffusion and hydrogen bond dynamics in aqueous ionic solutions: D2O in hydration shells of $\text{Cl}^-$ ions. <i>Journal of Chemical Physics</i> , 2008, 129, 194512.	1.2	102

#	ARTICLE	IF	CITATIONS
5395	First-Principles Study of Experimental and Hypothetical Mg(BH <sub>4</sub> ) <sub>2</sub> Crystal Structures. <i>Journal of Physical Chemistry C</i> , 2008, 112, 4391-4395.	1.5	61
5396	Synthesis, Resolution, and VCD Analysis of an Enantiopure Diazaoxatricornan Derivative. <i>Journal of the American Chemical Society</i> , 2008, 130, 6507-6514.	6.6	39
5397	The Mechanism of Propane Oxidation over Iron Antimony Oxide. <i>Journal of Physical Chemistry C</i> , 2008, 112, 9783-9797.	1.5	4
5398	Redox Behavior of the Model Catalyst Pd/CeO <sub>2</sub> /Pt(111). <i>Journal of Physical Chemistry C</i> , 2008, 112, 10918-10922.	1.5	62
5399	Energetics, Structure, and Electron Detachment Spectra of Calcium and Zinc Neutral and Anion Clusters: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11052-11060.	1.1	7
5400	Synthesis and Characterization of Metallomacrocyclic Palladium(II) Complexes with New Hybrid Pyrazole Ligands. Diffusion NMR Studies and Theoretical Calculations. <i>Inorganic Chemistry</i> , 2008, 47, 11084-11094.	1.9	27
5401	A first-principles investigation of the effect of Pt cluster size on CO and NO oxidation intermediates and energetics. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 6009.	1.3	45
5402	Formation of CH <sub>x</sub> Species from CO Dissociation on Double-Stepped Co(0001): Exploring Fischer-Tropsch Mechanism. <i>Journal of Physical Chemistry C</i> , 2008, 112, 14108-14116.	1.5	71
5403	Structure of Isolated Molybdenum(VI) Oxide Species on $\gamma$ -Alumina: A Periodic Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 14456-14463.	1.5	41
5404	Benzene and Its Dissociation Products on Ir{100}. <i>Journal of Physical Chemistry C</i> , 2008, 112, 14417-14427.	1.5	4
5405	New Data on the Structure of Uranium Monocarbide. <i>Chemistry of Materials</i> , 2008, 20, 3199-3204.	3.2	25
5406	Adsorption of Au and Pd Atoms on Thin SiO <sub>2</sub> Films: the Role of Atomic Structure. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3405-3409.	1.5	29
5407	Comparative Theoretical Study of CO Adsorption and Desorption Kinetics on (111) Surfaces of Transition Metals. <i>Journal of Physical Chemistry C</i> , 2008, 112, 14377-14384.	1.5	28
5408	Structural Model Studies for the Peroxo Intermediate P and the Reaction Pathway from P to Q of Methane Monooxygenase Using Broken-Symmetry Density Functional Calculations. <i>Inorganic Chemistry</i> , 2008, 47, 2975-2986.	1.9	58
5409	Adsorption of NO on Pd-Exchanged Mordenite: Ab Initio DFT Modeling. <i>Journal of Physical Chemistry C</i> , 2008, 112, 12349-12362.	1.5	13
5410	Atomic Layer Deposition of Hafnium Oxide from Hafnium Chloride and Water. <i>Journal of the American Chemical Society</i> , 2008, 130, 11996-12006.	6.6	45
5411	Adsorption and Dissociation of CO as Well as CH <sub>x</sub> Coupling and Hydrogenation on the Clean and Oxygen Pre-covered Co(0001) Surfaces. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3840-3848.	1.5	36
5412	Experimental and Theoretical Investigations of the Thermodynamic Stability of BaC <sub>60</sub> and K <sub>x</sub> C <sub>60</sub> Compound Clusters. <i>ACS Nano</i> , 2008, 2, 1000-1014.	7.3	11

#	ARTICLE	IF	CITATIONS
5413	Oxidation of Ir(111): From O <sub>2</sub> Trilayer to Bulk Oxide Formation. <i>Journal of Physical Chemistry C</i> , 2008, 112, 11946-11953.	1.5	77
5414	Examining the Performance of DFT Methods in Uranium Chemistry: Does Core Size Matter for a Pseudopotential?. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7632-7642.	1.1	44
5415	Design of Mold Materials with Excellent Releasability for IC Encapsulation using Epoxy Compounds. , 2008, , .		0
5416	First Principles Study of the Stability and the Formation Kinetics of Subsurface and Bulk Carbon on a Ni Catalyst. <i>Journal of Physical Chemistry C</i> , 2008, 112, 9679-9685.	1.5	37
5417	Canonical Variational Transition-State Theory Study of the CF <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub> + OH Reaction. <i>Journal of Physical Chemistry B</i> , 2008, 112, 328-335.	1.2	16
5418	Carbene Proton Attachment Energies: Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5269-5277.	1.1	7
5419	Toward a Chemical Mechanism of Proton Pumping by the B-Type Cytochrome <i>c</i> Oxidases: Application of Density Functional Theory to Cytochrome <i>bc<sub>3</sub></i> of <i>Thermus thermophilus</i> . <i>Journal of the American Chemical Society</i> , 2008, 130, 15002-15021.	6.6	63
5420	A Theoretical Investigation of the Selective Oxidation of Methanol to Formaldehyde on Isolated Vanadate Species Supported on Titania. <i>Journal of Physical Chemistry C</i> , 2008, 112, 13204-13214.	1.5	70
5421	Dependence of A-Si:H density of states on hydrogen content: Modeling and experiment.. Conference Record of the IEEE Photovoltaic Specialists Conference, 2008, , .	0.0	1
5422	Cyclic Boron Clusters Enclosing Planar Hypercoordinate Cobalt, Iron, and Nickel. <i>Inorganic Chemistry</i> , 2008, 47, 10906-10910.	1.9	74
5423	Hexanuclear Cobalt Carbonyl Carbide Clusters: The Interplay between Octahedral and Trigonal Prismatic Structures. <i>Inorganic Chemistry</i> , 2008, 47, 9314-9320.	1.9	5
5424	Effect of S on Pt(111) and Pt <sub>3</sub> Ni(111) Surfaces: A First Principles Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 1544-1551.	1.5	24
5425	Ligand-Bound <i>S</i> = <sup>1</sup> / <sub>2</sub> FeMo-Cofactor of Nitrogenase: Hyperfine Interaction Analysis and Implication for the Central Ligand X Identity. <i>Inorganic Chemistry</i> , 2008, 47, 6162-6172.	1.9	57
5426	Structures, Interactions, and Ferromagnetism of Fe-Carbon Nanotube Systems. <i>Journal of Physical Chemistry C</i> , 2008, 112, 8400-8407.	1.5	15
5427	Oxidation of platinum surfaces and reaction with carbon monoxide. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 184022.	0.7	13
5428	Mechanistic Aspects of the Reaction of Th <sup>+</sup> and Th <sup>2+</sup> with Water in the Gas Phase. <i>Inorganic Chemistry</i> , 2008, 47, 2083-2088.	1.9	35
5429	Au <sup>+</sup> N Synergy and N-Doping of Metal Oxide-Based Photocatalysts. <i>Journal of the American Chemical Society</i> , 2008, 130, 12056-12063.	6.6	115
5430	Interaction of Metallic Nanoparticles with a Biologically Active Molecule, Dopamine. <i>Journal of Physical Chemistry B</i> , 2008, 112, 15256-15259.	1.2	22

#	ARTICLE	IF	CITATIONS
5431	Intermediates in the Formation of Graphitic Carbon on a Flat FCC-Co(111) Surface. Journal of Physical Chemistry C, 2008, 112, 12899-12904.	1.5	48
5432	Photodissociation of Yttrium and Lanthanum Oxide Cluster Cations. Journal of Physical Chemistry A, 2008, 112, 5354-5362.	1.1	49
5433	First-Principles Study on the Effects of Zr Dopant on the CO Adsorption on Ceria. Journal of Physical Chemistry C, 2008, 112, 15341-15347.	1.5	27
5434	Density Functional Theory Study of the TiH <sub>2</sub> Interaction with a NaAlH <sub>4</sub> Cluster. Journal of Physical Chemistry C, 2008, 112, 15759-15764.	1.5	21
5435	Chiral Recognition on Catalytic Surfaces: Theoretical Insight in a Biomimetic Heterogeneous Catalytic System. Journal of Physical Chemistry C, 2008, 112, 10200-10208.	1.5	33
5436	Small-Angle Rotation in Individual Colloidal CdSe Quantum Rods. ACS Nano, 2008, 2, 1179-1188.	7.3	19
5437	Dynamic Interplay between Diffusion and Reaction: Nitrogen Recombination on Rh{211} in Car Exhaust Catalysis. Journal of the American Chemical Society, 2008, 130, 2213-2220.	6.6	24
5438	DFT for the energy minimum among eight collinear and noncollinear magnetic structures of GdB <sub>4</sub> . Physical Review B, 2008, 78, .	1.1	12
5439	Hydrogen storage capacities of nanoporous carbon calculated by density functional and MÅller-Plesset methods. Physical Review B, 2008, 78, .	1.1	49
5440	Electronic properties and stabilities of bulk and low-index surfaces of SnO in comparison with SnO <sub>2</sub> : A first-principles density functional approach with an empirical correction of van der Waals interactions. Physical Review B, 2008, 77, .	1.1	115
5441	Cubic metallic phase of aluminum hydride showing improved hydrogen desorption. Applied Physics Letters, 2008, 92, .	1.5	18
5442	Assessing the Perdew-Burke-Ernzerhof exchange-correlation density functional revised for metallic bulk and surface systems. Physical Review B, 2008, 77, .	1.1	163
5443	Reducing the Metal Work Function beyond Pauli Pushback: A Computational Investigation of Tetrathiafulvalene and Viologen on Coinage Metal Surfaces. Journal of Physical Chemistry C, 2008, 112, 20357-20365.	1.5	43
5444	Weak $\pi$ -2-Olefin Bonding in Palladium and Platinum Allyl Cationic Complexes Containing Chiral Monodentate Ligands with $\pm$ -Phenyl Methyl Amine Side Chains. Organometallics, 2008, 27, 2949-2958.	1.1	14
5445	Synergy between Crystal Strain and Surface Energy in Morphological Evolution of Five-Fold-Twinned Silver Crystals. Journal of the American Chemical Society, 2008, 130, 15581-15588.	6.6	84
5446	Two-Dimensional Pentacene:3,4,9,10-Perylenetetracarboxylic Dianhydride Supramolecular Chiral Networks on Ag(111). Journal of the American Chemical Society, 2008, 130, 12285-12289.	6.6	61
5447	Discriminating Reasons for Selectivity Enhancement of CO in Alkyne Hydrogenation on Palladium. Journal of Physical Chemistry C, 2008, 112, 9346-9350.	1.5	38
5448	Long-Range Proton Transport for the Water Reaction on Si(001): Study of Hydrogen-Bonded Systems with a Model Liquid $\sim$ solid Interface. Journal of Physical Chemistry C, 2008, 112, 12879-12886.	1.5	14



#	ARTICLE	IF	CITATIONS
5449	Stability and magnetic properties of $T^2$ xmlns:mml="http://www.w3.org/1998/Math/MathML"		

#	ARTICLE	IF	CITATIONS
5467	A DNA Sensor for Sequencing and Mismatches Based on Electron Transport Through Watson-Crick and Non-Watson-Crick Base Pairs. <i>IEEE Sensors Journal</i> , 2008, 8, 803-814.	2.4	22
5468	2D calculation of anharmonic OH vibrations in a layered hydroxide crystal. <i>Journal of Chemical Physics</i> , 2008, 129, 064502.	1.2	4
5469	An alternative model for electron correlation in Pu. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 422202.	0.7	17
5470	A mechanistic study of hydrogen spillover in MoO <sub>3</sub> and carbon-based graphitic materials. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 064223.	0.7	12
5471	Rational design of new materials for spintronics: Co <sub>2</sub> FeZ (<math>Z=Al, Ga, Si, Ge</math>). <i>Science and Technology of Advanced Materials</i> , 2008, 9, 014102.	2.8	148
5472	Design of water gas shift catalysts for hydrogen production in fuel processors. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 064237.	0.7	13
5473	First-Principles Investigation of the Fundamental Corrosion Properties of a Model Cu <sub>38</sub> Nanoparticle and the (111), (113) Surfaces. <i>Journal of the Electrochemical Society</i> , 2008, 155, C407.	1.3	68
5474	Electronic and structural investigations of gold clusters doped with copper: Au <sup>1</sup> Cu <sup>n</sup> (n=13-19). <i>Journal of Chemical Physics</i> , 2008, 128, 184314.	1.2	33
5475	Ferrocene-1,1-dithiol as molecular wire between Ag electrodes: The role of surface defects. <i>Journal of Chemical Physics</i> , 2008, 128, 064704.	1.2	11
5476	First-principles local density approximation (LDA) +U and generalized gradient approximation (GGA) +U studies of plutonium oxides. <i>Chinese Physics B</i> , 2008, 17, 1364-1370.	0.7	26
5477	First-Principle Calculations for Transition Phase and Elastic Properties of SrS. <i>Communications in Theoretical Physics</i> , 2008, 49, 1611-1614.	1.1	18
5478	Theoretical characterization of titanyl phthalocyanine as a p-type organic semiconductor: Short intermolecular H-H interactions yield large electronic couplings and hole transport bandwidths. <i>Journal of Chemical Physics</i> , 2008, 128, 034701.	1.2	92
5479	First-principles study of the mechanical properties of NiAl microalloyed by M (Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd). <i>Journal Physics D: Applied Physics</i> , 2008, 41, 181901.	1.3	19
5480	Origin of unexpected magnetism in Cu-doped TiO <sub>2</sub> . <i>Europhysics Letters</i> , 2008, 81, 17004.	0.7	10
5481	Free Energies for Acid Attack Reactions of Lithium Cobaltate. <i>Journal of the Electrochemical Society</i> , 2008, 155, A711.	1.3	16
5482	THEORETICAL STUDY OF GLYCINE CONFORMERS. <i>Journal of Theoretical and Computational Chemistry</i> , 2008, 07, 889-909.	1.8	23
5483	First-principles calculations of the thermodynamic and elastic properties of the L1 <sub>2</sub> -based Al <sub>3</sub> RE (RE = Sc, Y, La-Lu). <i>International Journal of Materials Research</i> , 2008, 99, 582-588.	0.1	35
5484	Morphology and Composition of Selected High-k Materials and Their Relevance to Dielectric Properties of Thin Films. <i>Journal of the Electrochemical Society</i> , 2008, 155, G97.	1.3	9

#	ARTICLE	IF	CITATIONS
5485	Density functional studies on Lewis acidity of alkaline earth metal exchanged faujasite zeolite. <i>Molecular Simulation</i> , 2008, 34, 1121-1128.	0.9	3
5486	Coarse-grained model for growth of $\gamma$ - and $\kappa$ -Al <sub>2</sub> O <sub>3</sub> on TiC and TiN(111): thin alumina films from density-functional calculations. <i>Journal of Physics: Conference Series</i> , 2008, 100, 082010.	0.3	2
5487	Combining density functional theory and cluster expansion methods to predict H <sub>2</sub> permeance through Pd-based binary alloy membranes. <i>Journal of Chemical Physics</i> , 2008, 128, 144701.	1.2	71
5488	Adhesive metal transfer at the Al(111)/ $\gamma$ -Fe <sub>2</sub> O <sub>3</sub> (001) interface: a study with <i>ab initio</i> molecular dynamics. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2008, 16, 085001.	0.8	6
5489	Reliability of range-separated hybrid functionals for describing magnetic coupling in molecular systems. <i>Journal of Chemical Physics</i> , 2008, 129, 184110.	1.2	74
5490	New filled P-based skutterudites promising materials for thermoelectricity?. <i>New Journal of Physics</i> , 2008, 10, 053004.	1.2	8
5491	Theoretical Evidences for Enhanced Superconducting Transition Temperature of CaSi <sub>2</sub> in a High-Pressure AlB <sub>2</sub> Phase. <i>Journal of the Physical Society of Japan</i> , 2008, 77, 104712.	0.7	5
5492	Mechanisms for O <sub>2</sub> dissociation over the BaO (100) surface. <i>Journal of Chemical Physics</i> , 2008, 128, 034702.	1.2	10
5493	Nanomicrointerface to read molecular potentials into current-voltage based electronics. <i>Journal of Chemical Physics</i> , 2008, 128, 114711.	1.2	8
5494	The role of exchange-correlation functionals in the potential energy surface and dynamics of N <sub>2</sub> dissociation on W surfaces. <i>Journal of Chemical Physics</i> , 2008, 128, 154704.	1.2	48
5495	Thermodynamics and kinetics of oxygen-induced segregation of 3d metals in Pt <sub>3</sub> Pt(111) and Pt <sub>3</sub> Pt(100) bimetallic structures. <i>Journal of Chemical Physics</i> , 2008, 128, 164703.	1.2	85
5496	$\gamma$ -point lattice free energy estimates from O(1) force calculations. <i>Journal of Chemical Physics</i> , 2008, 128, 184708.	1.2	1
5497	What can we learn from the adiabatic connection formalism about local hybrid functionals?. <i>Journal of Chemical Physics</i> , 2008, 128, 214107.	1.2	44
5498	Ca (AlH <sub>4</sub> ) <sub>2</sub> , CaAlH <sub>5</sub> , and CaH <sub>2</sub> +6LiBH <sub>4</sub> : Calculated dehydrogenation enthalpy, including zero point energy, and the structure of the phonon spectra. <i>Journal of Chemical Physics</i> , 2008, 128, 234505.	1.2	9
5499	Electronic effects induced by single hydrogen atoms on the Ge(001) surface. <i>Journal of Chemical Physics</i> , 2008, 128, 244707.	1.2	6
5500	Stability of suspended gold and silver alloy monatomic chains. <i>Journal of Chemical Physics</i> , 2008, 128, 244703.	1.2	15
5501	On the role of the nonlocal Hartree-Fock exchange in <i>ab initio</i> quantum transport: H <sub>2</sub> in Pt nanocontacts revisited. <i>Journal of Chemical Physics</i> , 2008, 129, 034702.	1.2	5
5502	Self-consistent generalized Kohn-Sham local hybrid functionals of screened exchange: Combining local and range-separated hybridization. <i>Journal of Chemical Physics</i> , 2008, 129, 124110.	1.2	68

#	ARTICLE	IF	CITATIONS
5503	Energetics, structure, and charge distribution of reduced and oxidized n-pyrrole oligomers: A density functional approach. <i>Journal of Chemical Physics</i> , 2008, 129, 164903.	1.2	27
5504	Nonuniform temperature dependence of the reactivity of disordered VO <sub>x</sub> /Al <sub>2</sub> O <sub>3</sub> (001) surfaces: A density functional theory based Monte Carlo study. <i>Journal of Chemical Physics</i> , 2008, 129, 224710.	1.2	5
5505	Predictions of melting, crystallization, and local atomic arrangements of aluminum clusters using a reactive force field. <i>Journal of Chemical Physics</i> , 2008, 129, 244506.	1.2	47
5506	Comparative study of anchoring groups for molecular electronics: structure and conductance of Au-S-Au and Au-NH <sub>2</sub> -Au junctions. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 374101.	0.7	34
5507	Crystallographic phase stabilities and electronic structures in AgNbO <sub>3</sub> by first-principles calculation. <i>Molecular Simulation</i> , 2008, 34, 1105-1114.	0.9	20
5508	Electronic origin of anomalously high shear modulus and intrinsic brittleness of fcc Ir. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 085221.	0.7	17
5509	Chemisorption of Hydrogen Molecule on Axially Strained (8, 0) Carbon Nanotube. <i>Journal of Physical Chemistry C</i> , 2008, 112, 18516-18520.	1.5	5
5510	Ab Initio Alloying of Mg for Hydrogen Storage. <i>Materials Research Society Symposia Proceedings</i> , 2008, 1098, 1.	0.1	1
5511	Prediction of incommensurate crystal structure in Ca at high pressure. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 20627-20630.	3.3	45
5512	Ab initio calculation of the growth of Te nanorods and Bi <sub>2</sub> Te <sub>3</sub> nanoplatelets. <i>Chinese Physics B</i> , 2008, 17, 286-289.	0.7	5
5513	Optical Properties of Filled Skutterudite ThFe <sub>4</sub> P <sub>12</sub> . <i>Communications in Theoretical Physics</i> , 2008, 49, 1049-1051.	1.1	3
5514	First-principles local density approximation (generalized gradient approximation) +U study of catalytic CeO <sub>m</sub> clusters: U value differs from bulk. <i>Journal of Chemical Physics</i> , 2008, 128, 164718.	1.2	21
5515	Electronic structure of the weakly coupled edge-sharing MnO <sub>4</sub> <sup>spin-rac</sup> chain compound LiMnVO <sub>4</sub> : an ab initio study. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 395204.	0.7	5
5516	Structural and mechanical properties of Mg <sub>17</sub> Al <sub>12</sub> and Mg <sub>24</sub> Y <sub>5</sub> from first-principles calculations. <i>Journal Physics D: Applied Physics</i> , 2008, 41, 195408.	1.3	65
5517	Definition of current density in the presence of a non-local potential. <i>Nanotechnology</i> , 2008, 19, 155401.	1.3	23
5518	Adsorption Behavior of CH <sub>2</sub> and CH <sub>3</sub> on Metal Clusters Cu <sub>n</sub> (n = 16). <i>Chinese Journal of Chemical Physics</i> , 2008, 21, 445-450.	0.6	3
5519	Theoretical study of the localization of excess electrons at the surface of ice. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 225003.	0.7	7
5520	Comparison of c(2 × 2)N/Fe(001) and Fe <sub>4</sub> N(002) surfaces: a density-functional theory study. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 075212.	0.7	5

#	ARTICLE	IF	CITATIONS
5521	Zinc cysteine active sites of metalloproteins: A density functional theory and x-ray absorption fine structure study. <i>Journal of Chemical Physics</i> , 2008, 128, 115104.	1.2	10
5522	Density functional study of double ionization energies. <i>Journal of Chemical Physics</i> , 2008, 128, 084112.	1.2	11
5523	Electric-field-gradient tensor and charge densities in LaB6: B11 nuclear-magnetic-resonance single-crystal investigations and first-principles calculations. <i>Journal of Applied Physics</i> , 2008, 103, 083534.	1.1	13
5524	Tuning the work function of ultrathin oxide films on metals by adsorption of alkali atoms. <i>Journal of Chemical Physics</i> , 2008, 128, 164707.	1.2	44
5525	Adsorption processes of hydrogen molecules on SiC(001), Si(001) and C(001) surfaces. <i>New Journal of Physics</i> , 2008, 10, 125028.	1.2	7
5526	Elastic Constants of Co/Pt Superlattice Studied by Acoustic Measurements and <i>Ab initio</i> Calculations. <i>Japanese Journal of Applied Physics</i> , 2008, 47, 3847-3850.	0.8	15
5527	Reliable lateral and vertical manipulations of a single Cu adatom on a Cu(111) surface with multi-atom apex tip: semiempirical and first-principles simulations. <i>Nanotechnology</i> , 2008, 19, 335710.	1.3	12
5528	Optical properties of the intermetallic compound Fe <sub>2</sub> TiSn. <i>Journal Physics D: Applied Physics</i> , 2008, 41, 095404.	1.3	10
5529	Electronic Properties of Nitrogen-Doped Carbon Nanotubes with Strain: <i>Ab initio</i> Method Approach. <i>Japanese Journal of Applied Physics</i> , 2008, 47, 5062-5065.	0.8	4
5530	Predicting the hydrogen pressure to achieve ultralow friction at diamond and diamondlike carbon surfaces from first principles. <i>Applied Physics Letters</i> , 2008, 92, .	1.5	29
5531	Formation and properties of metal-terminated oxygen atomic chains. <i>New Journal of Physics</i> , 2008, 10, 033005.	1.2	39
5532	First-principles calculations of elastic constants of DO <sub>3</sub> -Mg <sub>3</sub> RE (RE = Sc, Y, La). <i>Tj ETQq1</i> 1.0.784314 rgBT / DO	1.2	13
5533	Unique electronic band structures of hydrogen-terminated 112-angle silicon nanowires. <i>Nanotechnology</i> , 2008, 19, 035708.	1.3	10
5534	Structural, electronic and magnetic properties of the surfaces of tetragonal and cubic HfO <sub>2</sub> . <i>New Journal of Physics</i> , 2008, 10, 063031.	1.2	34
5535	Al-induced reduction of the oxygen diffusion in HfO <sub>2</sub> : an <i>ab initio</i> study. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 135206.	0.7	7
5536	Coupling of <i>ab initio</i> density functional theory and molecular dynamics for the multiscale modeling of carbon nanotubes. <i>Nanotechnology</i> , 2008, 19, 055702.	1.3	8
5537	Linear response results for phonons and electron-phonon coupling in hexagonal close packed Sc-spin fluctuations, and implications for superconductivity. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 045209.	0.7	7
5538	Morphology transformation of patterned, uniform and faceted GaN microcrystals. <i>Journal Physics D: Applied Physics</i> , 2008, 41, 015406.	1.3	6

#	ARTICLE	IF	CITATIONS
5539	Antiferromagnetism and segregation in cuboctahedral FePt nanoparticles. Journal Physics D: Applied Physics, 2008, 41, 134015.	1.3	19
5540	Density functional theory calculations of the surface structure of the inverse spinel zinc orthotitanate. Journal of Physics Condensed Matter, 2008, 20, 095001.	0.7	3
5541	Bond strength and interface energy between Pd membranes and TiAl supports. Applied Physics Letters, 2008, 93, .	1.5	24
5542	Charge carrier induced lattice strain and stress effects on As activation in Si. Applied Physics Letters, 2008, 93, .	1.5	10
5543	Structural effect of junction interface on magnetic properties in a Co/MgO/Co system: First-principles calculations. Journal of Applied Physics, 2008, 103, .	1.1	8
5544	Phase transition and thermodynamic properties of SrS via first-principles calculations. Chinese Physics B, 2008, 17, 1355-1359.	0.7	31
5545	Time-dependent density-functional-theory calculation of the van der Waals coefficient $C_6$ of alkali-metal atoms Li, Na, K; alkali-metal dimers $Li_2$ , $Na_2$ , $K_2$ . Physical Review B, 2008, 77, .	1.0	11
5546	Ferromagnetic states in $FeRu$ studied by <i>ab initio</i> calculation and ion-beam mixing. Physical Review B, 2008, 77, .	1.1	14
5547	Ionicity in disordered GeSe <sub>2</sub> : A comparison of first-principles and atomistic potential models. Journal of Chemical Physics, 2008, 128, 244505.	1.2	14
5548	Nature of boron solution and diffusion in $\alpha$ -iron. Physical Review B, 2008, 77, .	1.1	44
5549	Electronic and vibrational properties of $AlH_3$ . Physical Review B, 2008, 77, .	1.1	25
5550	First-principles study of the mode-1 fracture of $FeTi$ interfaces. Physical Review B, 2008, 78, .	1.1	3
5551	High-pressure phases of calcium and their finite-temperature phase boundaries. Physical Review B, 2008, 78, .	1.1	41
5552	Calculation of local excitations in large systems by embedding wave-function theory in density-functional theory. Physical Chemistry Chemical Physics, 2008, 10, 5353.	1.3	145
5553	The adsorption of CO on charged and neutral Au and Au <sub>2</sub> : A comparison between wave-function based and density functional theory. Journal of Chemical Physics, 2008, 128, 124302.	1.2	27
5554	Atomic structure, electronic structure, and defect energetics in $CaO$ boundaries of $CaO$ . Physical Review B, 2008, 78, .	1.1	9
5555	Structure and Local-Equilibrium Thermodynamics of the $(2\sqrt{2}\times 2)$ Reconstruction of Rutile TiO <sub>2</sub> (100). Physical Review Letters, 2008, 100, 086102.	2.9	25
5556	Topology of the Spin-Polarized Charge Density in bcc and fcc Iron. Physical Review Letters, 2008, 100, 017208.	2.9	32

#	ARTICLE	IF	CITATIONS
5557	Adsorption of small hydrocarbon molecules on Si surfaces: Ethylene on Si(001). Physical Review B, 2008, 77, .	1.1	30
5558	First-principles characterization of Ni diffusion kinetics in $\text{NiAl}$ . Physical Review B, 2008, 78, .	1.1	32
5559	Band Offsets at the $\text{Si/SiO}_2$ interface from Many-Body Perturbation Theory. Physical Review Letters, 2008, 100, 186401.	1.1	154
5560	Pinning of graphene to Ir(111) by flat Ir dots. Physical Review B, 2008, 77, .	1.1	126
5561	Highly destabilized Mg-Ti-Ni-H system investigated by density functional theory and hydrogenography. Physical Review B, 2008, 77, .	1.1	39
5562	Nonadiabatic effects in the dissociation of oxygen molecules at the Al(111) surface. Physical Review B, 2008, 77, .	1.1	112
5563	Ge vacancies at $\text{Ge/Si}$ interfaces: Stress-enhanced pairing distortion. Physical Review B, 2008, 77, .	1.1	2
5564	Emergence and Visualization of an Interface State during Contact Formation with a Single Molecule. Physical Review Letters, 2008, 101, 096801.	2.9	3
5565	Describing bond-breaking processes by reactive potentials: Importance of an environment-dependent interaction range. Physical Review B, 2008, 78, .	1.1	149
5566	Structural, electronic, and energetic properties of $\text{SiC}[111]\text{-ZrB}_2[0001]$ heterojunctions: A first-principles density functional theory study. Physical Review B, 2008, 77, .	1.1	11
5567	Spatial modulation of molecular adsorption energies due to indirect interaction. Physical Review B, 2008, 78, .	1.1	23
5568	First-principles Investigation of the Structural and Electronic Properties of Cu Based Intermetallics. , 2008, , .		0
5569	Resolving the Optical Spectrum of Water: Coordination and Electrostatic Effects. Physical Review Letters, 2008, 100, 207403.	2.9	62
5570	Unoccupied states of individual silver clusters and chains on Ag(111). Physical Review B, 2008, 77, .	1.1	35
5571	Magnetism and chemical ordering in icosahedral Al-Pd-Mn quasicrystal. Physical Review B, 2008, 78, .	1.1	7
5572	Atomic Scale Design and Control of Cation Distribution in Hexagonal Ferrites. Physical Review Letters, 2008, 101, 067201.	2.9	31
5573	Thermal-Hydrogen Promoted Selective Desorption and Enhanced Mobility of Adsorbed Radicals in Silicon Film Growth. Physical Review Letters, 2008, 100, 046105.	2.9	16
5574	Density functional calculations of the electronic structure and optical properties of the ternary carbides $\text{Al}_4\text{C}_3$ . Physical Review B, 2008, 78, .	1.1	24



#	ARTICLE	IF	CITATIONS
5575	Atomic structure and energetics of thec-GaN(001) surface. Physical Review B, 2008, 78, .	1.1	2
5576	Wavevector-dependent quantum-size effect in electron decay length at Pb thin film surfaces. Applied Physics Letters, 2008, 93, 093105.	1.5	18
5577	Adsorption of oxygen atoms on the Mg3Nd(001) surface. Journal of Applied Physics, 2008, 104, 033516.	1.1	0
5578	Electronic surface error in the Si interstitial formation energy. Physical Review B, 2008, 77, .	1.1	30
5579	The anisotropic band structure of layered In4Se3(001). Journal of Applied Physics, 2008, 104, .	1.1	37
5580	First-principles study of energetic and electronic properties of A2Ti2O7 (A=Sm, Gd, Er) pyrochlore. Journal of Applied Physics, 2008, 104, .	1.1	24
5581	A study of Hf vacancies at Si:HfO2 heterojunctions. Applied Physics Letters, 2008, 92, 152911.	1.5	4
5582	Biaxial stress-dependent optical band gap, crystalline, and electronic structure in wurtzite ZnO: Experimental and <i>ab initio</i> study. Journal of Applied Physics, 2008, 104, .	1.1	57
5583	Effect of adsorbed hydrogen on the stability of titanium atoms on aluminum surfaces. Physical Review B, 2008, 77, .	1.1	14
5584	Atomic scale study of the degradation mechanism of boron contaminated hafnium oxide. Applied Physics Letters, 2008, 92, 052907.	1.5	1
5585	Phonons and crystal structures of the $\sqrt{2}$ -pyrochlore superconductorsKOs2O6andRbOs2O6from micro-Raman spectroscopy. Physical Review B, 2008, 77, .	1.1	26
5586	Effects of Y doping on the structural stability and defect properties of cubic HfO2. Journal of Applied Physics, 2008, 104, .	1.1	31
5587	Theoretical study of the surface reactivity of alkaline earth oxides: Local density of states evaluation of the local softness. Journal of Chemical Physics, 2008, 128, 034708.	1.2	31
5588	Modeling the sorption dynamics of NaH using a reactive force field. Journal of Chemical Physics, 2008, 128, 164714.	1.2	29
5589	First-principles calculation of defect formation energies and electronic properties in stannate pyrochlores. Journal of Applied Physics, 2008, 104, .	1.1	23
5590	Reliability study of La2O3 capped HfSiON high-permittivity n-type metal-oxide-semiconductor field-effect transistor devices with tantalum-rich electrodes. Journal of Applied Physics, 2008, 104, 044512.	1.1	11
5591	Hydrogen diffusion in MgH2 and NaMgH3 via concerted motions of charged defects. Applied Physics Letters, 2008, 93, .	1.5	62
5592	The effect of La addition on optical transmittance spectra of hydrogenated Mg $\epsilon$ -La thin films. Journal of Applied Physics, 2008, 104, 016110.	1.1	7

#	ARTICLE	IF	CITATIONS
5593	Nonvolatile memories of Ge nanodots self-assembled by depositing ultrasmall amount Ge on SiO <sub>2</sub> at room temperature. Applied Physics Letters, 2008, 92, 093124.	1.5	11
5594	Increase in oxide hole trap density associated with nitrogen incorporation at the SiO <sub>2</sub> /SiC interface. Journal of Applied Physics, 2008, 103, .	1.1	69
5595	Effect of chlorine residue on electrical performance of atomic layer deposited hafnium silicate. Journal of Applied Physics, 2008, 103, 114102.	1.1	10
5596	Basic nanosystems of early 4d and 5d transition metals: Electronic properties and the effect of spin-orbit interaction. Journal of Applied Physics, 2008, 104, 014302.	1.1	9
5597	Lithiated assemblies of metal chalcogenide nanowires. Applied Physics Letters, 2008, 92, .	1.5	10
5598	Dielectric constant boost in amorphous sesquioxides. Applied Physics Letters, 2008, 92, .	1.5	16
5599	Amorphous HfO <sub>2</sub> and Hf <sub>1-x</sub> Si <sub>x</sub> O <sub>y</sub> via a melt-and-quench scheme using ab initio molecular dynamics. Physical Review B, 2008, 77, .	1.1	46
5600	First-principles theory of nanoscale pattern formation in ultrathin alloy films: A comparative study of Fe-Ag on Ru(0001) and Mo(110) substrates. Physical Review B, 2008, 77, .	1.1	13
5601	Dissociative adsorption of $O_2$ molecules on O-precovered Fe(110) and Fe(100): Density-functional calculations. Physical Review B, 2008, 77, .	1.1	34
5602	Electronic properties of bilayered manganite $Ca_{1-x}Mn_{2.5-x}O_6$ . Physical Review B, 2008, 77, .	1.1	1
5603	Dissociative adsorption of $O_2$ on Pt and Au surfaces: Potential energy surfaces and electronic states. Physical Review B, 2008, 77, .	1.1	23
5604	Defect evolution in oxide nanophases: The case of a zigzag-like $TiO_x$ phase on Pt(111). Physical Review B, 2008, 77, .	1.1	43
5605	Surface Modification of Ni-YSZ Using Niobium Oxide for Sulfur-Tolerant Anodes in Solid Oxide Fuel Cells. Journal of the Electrochemical Society, 2008, 155, B449.	1.3	45
5606	Lock and key behaviours of an aromatic carboxylic acid molecule with differing conformations on an Au (111) surface. Molecular Physics, 2008, 106, 2371-2380.	0.8	1
5607	Evidence for Itineracy in the Anticipated Kondo Insulator FeSi: A Quantitative Determination of the Band Renormalization. Physical Review Letters, 2008, 101, 046406.	2.9	53
5608	Dynamical stability of the cubic metallic phase of $AlH_3$ at ambient pressure: Density functional calculations. Physical Review B, 2008, 78, .	1.1	26
5609	Pt-induced nanowires on Ge(001): <i>ab initio</i> study. Physical Review B, 2008, 78, .	1.1	22
5610	Oxygen defect accumulation at Si:HfO <sub>2</sub> interfaces. Applied Physics Letters, 2008, 92, .	1.5	40

#	ARTICLE	IF	CITATIONS
5611	Calculation of dopant segregation ratios at semiconductor interfaces. Physical Review B, 2008, 78, .	1.1	8
5612	Dynamical properties and temperature induced molecular disordering of $\text{LiBH}_4$ . Physical Review B, 2008, 78, .	1.1	69
5613	Hybrid exchange-correlation functionals applied to hyperfine interactions at lanthanide and actinide impurities in Fe. Physical Review B, 2008, 77, .	1.1	21
5614	Electronic structure of Cu <sub>3</sub> N films studied by soft x-ray spectroscopy. Journal of Physics Condensed Matter, 2008, 20, 235212.	0.7	12
5615	Density functional theory study of mercury adsorption on metal surfaces. Physical Review B, 2008, 77, .	1.1	65
5616	Density functional theory study of mercury adsorption on strained pseudomorphic monolayers of Cu and Pd on Ru(0001). Physical Review B, 2008, 77, .	1.1	4
5617	Density functional theory prediction of a hysteretic phase transition in InPu crystals. Physical Review B, 2008, 77, .	1.1	1
5618	First-principles study of transition metal impurities in Si. Physical Review B, 2008, 77, .	1.1	78
5619	Ground-State Properties of Crystalline Ice from Periodic Hartree-Fock Calculations and a Coupled-Cluster-Based Many-Body Decomposition of the Correlation Energy. Physical Review Letters, 2008, 101, 183005.	2.9	80
5620	Second-nearest-neighbor modified embedded-atom potential for binary Ta-W alloys based on first-principles calculations. Physical Review B, 2008, 77, .	1.1	8
5621	Ab initio investigation of interfacial layer formation in the Mo-Si boundary for extreme ultraviolet lithography. Journal of Applied Physics, 2008, 103, 124310.	1.1	0
5622	Bond strength and electronic structures of coherent Ir-Ir <sub>3</sub> Zr interfaces. Applied Physics Letters, 2008, 92, .	1.5	13
5623	Spin Tunneling in Junctions with Disordered Ferromagnets. Physical Review Letters, 2008, 100, 057205.	2.9	31
5624	Ground-state structure of coherent lattice-mismatched zinc-blende A <sub>1-x</sub> B <sub>x</sub> semiconductor alloys (x=0.25 and 0.75). Physical Review B, 2008, 77, .	1.1	10
5625	Structural, electronic, and magnetic properties of 13-, 55-, and 147-atom clusters of Fe, Co, and Ni: A spin-polarized density functional study. Physical Review B, 2008, 78, .	1.1	70
5626	Constructing an Array of Anchored Single-Molecule Rotors on Gold Surfaces. Physical Review Letters, 2008, 101, 197209.	2.9	127
5627	Work function anisotropy and surface stability of half-metallic CrO <sub>2</sub> . Physical Review B, 2008, 77, .	1.1	18
5628	High pressure structural phase transitions in Sr from <i>ab initio</i> calculations. Physical Review B, 2008, 77, .	1.1	13

#	ARTICLE	IF	CITATIONS
5629	Band alignment in molecular devices: Influence of anchoring group and metal work function. Physical Review B, 2008, 77, .	1.1	33
5630	Spin confinement in the superlattices of graphene ribbons. Applied Physics Letters, 2008, 92, .	1.5	79
5631	<i>Ab initio</i> electronic structure and correlations in pristine and potassium-doped molecular crystals of copper phthalocyanine. Physical Review B, 2008, 77, .	1.1	50
5632	Carbon impurity dissolution and migration in bcc Fe-Cr: First-principles calculations. Physical Review B, 2008, 78, .	1.1	35
5633	Microscopic origin of the different colors displayed by MgAl <sub>2</sub> O <sub>4</sub> :Cr <sup>3+</sup> and emerald. Physical Review B, 2008, 78, .	1.1	18
5634	Temperature dependence of the optical response: Application to bulk GaAs using first-principles molecular dynamics simulations. Physical Review B, 2008, 77, .	1.1	23
5635	Intermolecular Overlap Geometry Gives Two Classes of Fulleride Superconductor: Electronic Structure of 38 Å C <sub>60</sub> Tc. Physical Review B, 2008, 77, .	2.9	22
5636	First-principles molecular dynamics of the initial oxidation of Si{001} by ozone. Physical Review B, 2008, 78, .	1.1	8
5637	Electronic structure of a potential optical crystal YBa <sub>3</sub> B <sub>9</sub> O <sub>18</sub> : Experiment and theory. Applied Physics Letters, 2008, 92, 171903.	1.5	7
5638	Electronic states and adhesion properties at metal/MgO incoherent interfaces: First-principles calculations. Physical Review B, 2008, 77, .	1.1	31
5639	Identification of a stable phase for the high-capacity hydrogen-storage material Zn <sub>18</sub> using density functional theory and lattice dynamics. Physical Review B, 2008, 77, .	1.1	18
5640	First-principles theory of the energetics of He defects in bcc transition metals. Physical Review B, 2008, 78, .	1.1	130
5641	Understanding magnetic interactions in the series of bcc transition metal alloys. Physical Review B, 2008, 78, .		

#	ARTICLE	IF	CITATIONS
5647	Quasiatomic orbitals for <i>ab initio</i> tight-binding analysis. Physical Review B, 2008, 78, .	1.1	90
5648	Functionalization of silicon nanowires with transition metal atoms. Physical Review B, 2008, 78, .	1.1	26
5649	Photoemission and quantum chemical study of $\text{SrTiO}_3$ and their interaction with $\text{CO}$ . Physical Review B, 2008, 78, .	1.1	54
5650	Controlling the Kondo Effect in $\text{CoCu}_n$ Clusters Atom by Atom. Physical Review Letters, 2008, 101, 266803.	2.9	77
5651	High-pressure structural behavior of large-void CoSn-type intermetallics: Experiments and first-principles calculations. Physical Review B, 2008, 77, .	1.1	15
5652	Segregation of Cr impurities at bcc iron surfaces: First-principles calculations. Physical Review B, 2008, 78, .	1.1	44
5653	Nearly metastable rhombohedral phases of bcc metals. Physical Review B, 2008, 77, .	1.1	4
5654	Role of Hydrogen in Giant Spin Polarization Observed on Magnetic Nanostructures. Physical Review Letters, 2008, 100, 026806.	2.9	24
5655	Shape and surface structure of gold nanoparticles under oxidizing conditions. Physical Review B, 2008, 77, .	1.1	49
5656	Extrinsic Nature of Point Defects on the Si(001) Surface: Dissociated Water Molecules. Physical Review Letters, 2008, 100, 036107.	2.9	53
5657	Charging of Metal Adatoms on Ultrathin Oxide Films: Au and Pd on $\text{Cu}(111)$ and $\text{FeO}$ . Physical Review B, 2008, 77, .	1.1	8
5658	Structure of $\text{FeO}$ on $\text{Pt}$ and $\text{Tj}$ . Physical Review B, 2008, 78, .	2.9	109
5659	Deuterium occupation of tetrahedral sites in palladium. Physical Review B, 2008, 78, .	1.1	34
5660	Atomic structure and magnetic moments in cluster-assembled nanocomposite Fe/Cu films. Physical Review B, 2008, 78, .	1.1	18
5661	Water adsorption on clean Ni(111) and $\text{Ni}_2\text{O}_3$ calculated from first principles. Physical Review B, 2008, 78, .	1.1	16
5662	Exceptional surface stability in late transition metal alloys driven by lattice strain. Physical Review B, 2008, 77, .	1.1	6
5663	Electronic structure and properties of Li-insertion materials: $\text{Li}_2\text{O}$ and $\text{Li}_3\text{O}$ . Physical Review B, 2008, 77, .	1.1	31
5664	Structure of gold atoms on stoichiometric and defective ceria surfaces. Journal of Chemical Physics, 2008, 129, 194708.	1.2	103

#	ARTICLE	IF	CITATIONS
5665	Disorder and surface effects on work function of Ni-Pt metal gates. Physical Review B, 2008, 78, .	1.1	41

Electronic properties of

5666

$\text{Sc}_{5M_4\text{Si}_{10}}$

#	ARTICLE	IF	CITATIONS
5683	Magnetic Properties of Mn Doped Armchair Graphene Nanoribbon. Materials Transactions, 2008, 49, 2445-2447. Bonding and Magnetism in High Symmetry Nano-Sized Graphene Molecules: Linear Acenes	0.4	10
5684	C <sub>4m+2</sub> H <sub>2m+4</sub> (m=2,⋯,25); Zigzag Hexangulenes C <sub>6m</sub> <sup>**</sup> /H <sub>6m</sub> (m=2,⋯,10); Crenelated Hexangulenes C <sub>6(3m+1)</sub> <sup>**</sup> /H <sub>6(2m+1)</sub> (m=2,⋯,6); Zigzag Triangulenes	0.4	23
5685	Structural, Electronic and Optical Properties of the Al <sub>2</sub> O <sub>3</sub> ; Doped SiO <sub>2</sub> ; First Principles Calculations. Materials Transactions, 2008, 49, 2474-2479.	0.4	7
5686	Structural, energetic, and electronic properties of hydrogenated titanium clusters. Journal of Chemical Physics, 2008, 128, 194714.	1.2	22
5687	Atomistic and electronic structure of bimetallic cobalt/rhenium clusters from density functional theory calculations. Journal of Chemical Physics, 2008, 128, 084712.	1.2	10
5688	Free energy calculation of the reaction path of the N <sub>2</sub> O decomposition over Fe(II)-ferrierite. Studies in Surface Science and Catalysis, 2008, , 689-694.	1.5	1
5689	Parameterized local hybrid functionals from density-matrix similarity metrics. Journal of Chemical Physics, 2008, 128, 084111.	1.2	42
5690	Charge transfer and adhesion in Rh/MgO(001). Journal of Physics: Conference Series, 2008, 100, 082027.	0.3	3
5691	Quantum-Chemical Calculations of the Equilibrium Constants of a Fission Product Mixture in a Steam-Hydrogen Carrier Gas in Severe Accident Conditions. Nuclear Technology, 2008, 163, 245-251.	0.7	0
5692	Investigations of dopants introduction in hafnia: Electronic properties, diffusion, and their role on the gate leakage current. Journal of Applied Physics, 2008, 104, 033709.	1.1	4
5693	Origin of enhanced superconducting transition temperature through structural transformation in CaSi <sub>2</sub> . Journal of Physics: Conference Series, 2008, 121, 052010.	0.3	4
5694	Catalyzed Routes to Molecular Hydrogen Formation and Hydrogen Addition Reactions on Neutral Polycyclic Aromatic Hydrocarbons under Interstellar Conditions. Astrophysical Journal, 2008, 679, 531-536.	1.6	122
5695	Thermal properties of guest-free Si <sub>136</sub> and Ge <sub>136</sub> clathrates: A first-principles study. Journal of Applied Physics, 2008, 104, 033535.	1.1	16
5696	Local reactivity of O <sub>2</sub> with Pt <sub>3</sub> on Co <sub>3</sub> Pt and related backgrounds. Journal of Chemical Physics, 2008, 128, 204701.	1.2	7
5697	Density Functionals of Chemical Bonding. International Journal of Molecular Sciences, 2008, 9, 1050-1095.	1.8	49
5698	Magnetism at surfaces and defects in icosahedral Al-Pd-Mn quasicrystals. Physical Review B, 2009, 80, .	1.1	8
5699	First-principles elastic properties of $\frac{1}{2}\text{Pu}$ . Physical Review B, 2009, 79, .	1.1	31
5700	Modifying the electronic structure of semiconducting single-walled carbon nanotubes by Ar <sup>+</sup> ion irradiation. Physical Review B, 2009, 79, .	1.1	42



#	ARTICLE	IF	CITATIONS
5701	Structure and stability of Au rods on $\text{TiO}_2$ by first-principles calculations. Physical Review B, 2009, 80, .	1.1	16

5702	Surface geometry of Cu <sub>531</sub> . Physical Review B, 2009, 79, .	1.1	16
------	--	-----	----

5703	Structural and electronic properties of		
------	---	--	--

#	ARTICLE	IF	CITATIONS
5719	Two-dimensional metal-organic coordination networks of Mn-7,7,8,8-tetracyanoquinodimethane assembled on Cu(100): Structural, electronic, and magnetic properties. Physical Review B, 2009, 80, .	1.1	41
5720	Properties of helium defects in bcc and fcc metals investigated with density functional theory. Physical Review B, 2009, 80, .	1.1	134
5721	Origin of the anomalous Slater-Pauling curve in cobalt-manganese alloy clusters. Physical Review B, 2009, 80, .	1.1	7
5722	Dye adsorbates BrPDI, BrGly, and BrAsp on anataseTiO2(001)for dye-sensitized solar cell applications. Physical Review B, 2009, 80, .	1.1	25
5723	First-principles study of the optical properties of $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \text{display="inline"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{Mg} \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \times \langle \text{mml:mi} \rangle \langle \text{mml:msub} \rangle$ Physical Review B, 2009, 79, .	1.1	20
5724	Adsorption of metal adatoms on FeO(111) and MgO(111) monolayers: Effects of charge state of adsorbate on rumpling of supported oxide film. Physical Review B, 2009, 80, .	1.1	49
5725	Description of magnetic interactions in strongly correlated solids via range-separated hybrid functionals. Physical Review B, 2009, 79, .	1.1	44
5726	Inelastic scattering in metal- $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \text{display="inline"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mtext} \rangle \text{H} \langle \text{mml:mtext} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \text{display="inline"} \rangle$ junctions. Physical Review B, 2009, 79, .	1.1	41
5727	Density functional theory study of the iron-based porphyrin haem(b) on the Si(111):H surface. Physical Review B, 2009, 79, .	1.1	18
5728	Comparative study of CO adsorption on flat, stepped, and kinked Au surfaces using density functional theory. Physical Review B, 2009, 79, .	1.1	50
5729	Indium on Cu(100) from first principles: Energetics, complex formation, and diffusion of adsorbates and vacancies on terraces and at steps. Physical Review B, 2009, 79, .	1.1	2
5730	Structural and electronic properties of Ge-Si, Sn-Si, and Pb-Si dimers on Si(001) from density-functional calculations. Physical Review B, 2009, 79, . Adsorption of atomic and molecular oxygen on 3C-SiC(111) and $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \text{display="inline"} \rangle$	1.1	1
5731			

#	ARTICLE	IF	CITATIONS
5737	Azobenzene at coinage metal surfaces: Role of dispersive van der Waals interactions. Physical Review B, 2009, 80, .	1.1	462
5738	Shear deformation, ideal strength, and stacking fault formation of fcc metals: A density-functional study of Al and Cu. Physical Review B, 2009, 79, .	1.1	135
5739	Ab initio study of pressure-induced metal-insulator transition in cubic FeGe. Physical Review B, 2009, 80, .	1.1	19
5740	Formation and migration of charged native point defects in $\text{MgH}$ . First-principles calculations. Physical Review B, 2009, 80, .	1.1	48
5741	Ab initio atomistic thermodynamics study on the selective oxidation mechanism of the surfaces of intermetallic compounds. Physical Review B, 2009, 80, .	1.1	29
5742	Assessment through first-principles calculations of an intermediate-band photovoltaic material based on Ti-implanted silicon: Interstitial versus substitutional origin. Physical Review B, 2009, 79, .	1.1	81
5743	FIRST PRINCIPLES CALCULATIONS OF ELASTIC CONSTANTS FOR DEFECTED $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ . Integrated Ferroelectrics, 2009, 108, 21-36.	0.3	10
5744	Mechanism of alkane dehydrogenation catalyzed by acidic zeolites: Ab initio transition path sampling. Journal of Chemical Physics, 2009, 131, 214508.	1.2	55
5745	Exploring $\text{Ce}^{3+}/\text{Ce}^{4+}$ cation ordering in reduced ceria nanoparticles using interionic-potential and density-functional calculations. Journal of Chemical Physics, 2009, 131, 064701.	1.2	50
5746	Lack of surface oxide layers and facile bulk oxide formation on Pd(110). Physical Review B, 2009, 80, .	1.1	41
5747	Ab initio simulations of thermodynamic and chemical properties of detonation product mixtures. Journal of Chemical Physics, 2009, 131, 084107.	1.2	17
5748	Energetics and electronic structure of aluminum point defects in $\text{HfO}_2$ : A first-principles study. Journal of Applied Physics, 2009, 106, 014104.	1.1	21
5749	Theoretical investigation of A-element atom diffusion in $\text{Ti}_2\text{AC}$ (A=Sn, Ga, Cd, In, and Pb). Applied Physics Letters, 2009, 94, .	1.5	52
5750	Polarization Vortices in Germanium Telluride Nanoplatelets: A Theoretical Study. Physical Review Letters, 2009, 103, 247601.	2.9	16
5751	Ab initio molecular dynamics study of the hydrogen-deuterium exchange in bulk lithiumborohydride ( $\text{LiBH}_4$ ). Applied Physics Letters, 2009, 94, 141903.	1.5	13
5752	Density functional estimations of Heisenberg exchange constants in oligonuclear magnetic compounds: Assessment of density functional theory versus ab initio. Journal of Chemical Physics, 2009, 131, 224316.	1.2	15
5753	Diffusion of hydrogen vacancy in $\text{Na}_3\text{AlH}_6$ . Applied Physics Letters, 2009, 95, 111910.	1.5	10
5754	Density functional calculations on atomic and electronic structures of amorphous $\text{HfO}_2/\text{Si}(001)$ interface. Applied Physics Letters, 2009, 95, .	1.5	13

#	ARTICLE	IF	CITATIONS
5755	Effect of high pressure on polymorphic phase transition and electronic structure of XAs (X=Al, Ga). <i>Tj ETQq0 0 0 rgBT/Overlock 10 Tf 50</i>	0.6	11
5756	First-principles study of ionic oxygen mobility of Sr-containing LaAlO <sub>3</sub> perovskite. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 305502.	0.7	2
5757	Ohmic contacts on silicon carbide: The first monolayer and its electronic effect. <i>Physical Review B</i> , 2009, 80, .	1.1	63
5758	Long-range order instead of phase separation in large lattice-mismatch isovalent AX <sup>n</sup> BX systems. <i>Physical Review B</i> , 2009, 80, .	1.1	5
5759	Nitrogen fixation at passivated Fe nanoclusters supported by an oxide surface: Identification of viable reaction routes using density functional calculations. <i>Physical Review B</i> , 2009, 80, .	1.1	2
5760	Dynamic decomposition of aliphatic molecules on Al(111) from <i>ab initio</i> molecular dynamics. <i>Physical Review B</i> , 2009, 79, .	1.1	9
5761	Fundamental interaction process between pure edge dislocation and energetically stable grain boundary. <i>Physical Review B</i> , 2009, 79, .	1.1	33
5762	Correlations in coverage-dependent atomic adsorption energies on Pd(111). <i>Physical Review B</i> , 2009, 79, .	1.1	87
5763	Insight into the performance of GGA functionals for solid-state calculations. <i>Physical Review B</i> , 2009, 80, .	1.1	72
5764	Dielectric and vibrational properties of bixbyite sesquioxides. <i>Physical Review B</i> , 2009, 80, .	1.1	8
5765	First-principles calculations of clean Au(110) surfaces and chemisorption of atomic oxygen. <i>Physical Review B</i> , 2009, 79, .	1.1	31
5766	Diffusion pathways of phosphorus atoms on silicon (001). <i>Physical Review B</i> , 2009, 79, .	1.1	19
5767	Sublayer Si atoms as reactive centers in the chemisorption on Si(100): Adsorption of $C_2$ . <i>Physical Review B</i> , 2009, 79, .	1.1	21
5768	Group-III A versus III B delafossites: Electronic structure study. <i>Physical Review B</i> , 2009, 80, .	1.1	69
5769	Atomic structure of the Ag/Ge(111)-(3 $\sqrt{3}$ ×3) surface: From scanning tunneling microscopy observation to theoretical study. <i>Journal of Chemical Physics</i> , 2009, 131, 224705.	1.2	12
5770	Stability of the ternary perovskites Sc <sub>3</sub> . <i>Physical Review B</i> , 2009, 79, .		

#	ARTICLE	IF	CITATIONS
5773	Ab initiothermodynamic study of the structure and chemical bonding of $\text{Al}_x\text{Ni}_{1-x}\text{Al}_2\text{O}_3$ interface. Physical Review B, 2009, 80, .	1.1	10
5774	Evidence for the formation of a Mott state in potassium-intercalated pentacene. Physical Review B, 2009, 79, .	1.1	38
5775	Stability and work function of $\text{TiC}$ surfaces: Density functional theory calculations. Physical Review B, 2009, 80, .	1.1	19
5776	Impact of the crystal structure of $\text{HfO}_2$ on the transport properties of model $\text{HfO}_2/\text{Si}/\text{HfO}_2$ silicon-on-insulator field-effect transistors: A combined DFT-scattering theory approach. Physical Review B, 2009, 79, .	1.1	5
5777	Quantum Monte Carlo studies of covalent and metallic clusters: Accuracy of density functional approximations. Physical Review B, 2009, 79, .	1.1	36
5778	Stress effects on impurity solubility in crystalline materials: A general model and density-functional calculations for dopants in silicon. Physical Review B, 2009, 79, .	1.1	26
5779	Charge and spin states of metal atoms adsorbed on ultrathin $\text{MgO}/\text{Fe}(001)$ films. Physical Review B, 2009, 79, .	1.1	20
5780	Impact of Surface Chemistry on Grain Boundary Induced Intrinsic Stress Evolution during Polycrystalline Thin Film Growth. Physical Review Letters, 2009, 102, 056101.	2.9	13
5781	Local structure of the $\text{Ag}(100)$ surface reacting with molecular iodine: Experimental and theoretical study. Physical Review B, 2009, 80, .	1.1	22
5782	Predicted High-Temperature Superconducting State in the Hydrogen-Dense Transition-Metal Hydride $\text{YH}_3$ at 40ÅK and 17.7ÅGPa. Physical Review Letters, 2009, 103, 077002.	2.9	79
5783	Nonempirical hyper-generalized-gradient functionals constructed from the Lieb-Oxford bound. Physical Review A, 2009, 79, .	1.0	33
5784	Electronic structure of amorphous indium oxide transparent conductors. Physical Review B, 2009, 80, .	1.1	49
5785	Determination of the Structural Parameters of an Incommensurate Phase from First Principles: The Case of Sc-II. Physical Review Letters, 2009, 102, 085701.	2.9	15
5786	Modifying the Adsorption Characteristic of Inert Silica Films by Inserting Anchoring Sites. Physical Review Letters, 2009, 102, 016102.	2.9	21
5787	Energetics of Al doping and intrinsic defects in monoclinic and cubic zirconia: First-principles calculations. Physical Review B, 2009, 80, .	1.1	26
5788	Hybrid-functional calculations with plane-wave basis sets: Effect of singularity correction on total energies, energy eigenvalues, and defect energy levels. Physical Review B, 2009, 80, .	1.1	112
5789	First-principles model study of the phase stabilities of dilute Fe-Cu alloys: Role of vibrational free energy. Physical Review B, 2009, 80, .	1.1	23
5790	Self-assembly of methanethiol on the reconstructed $\text{Au}(111)$ surface. Physical Review B, 2009, 80, .	1.1	36

#	ARTICLE	IF	CITATIONS
5791	Electron energy loss spectroscopy of the L <sub>2,3</sub> edge of phosphorus skutterudites and electronic structure calculations. <i>Physical Review B</i> , 2009, 80, .	1.1	9
5792	Fermi-surface pockets in YBaCuO. Comparison of <i>ab initio</i> techniques. <i>Physical Review B</i> , 2009, 79, .	1.1	11
5793	Electron-phonon coupling in compressed TaS <sub>2</sub> . Stability and superconductivity from first principles. <i>Physical Review B</i> , 2009, 79, .	1.1	46
5794	First-principles study of Au nanostructures on rutile TiO <sub>2</sub> . <i>Physical Review B</i> , 2009, 79, .	1.1	32
5795	<i>Ab initio</i> study on the surface chemistry and nanotribological properties of passivated diamond surfaces. <i>Physical Review B</i> , 2009, 79, .	1.1	91
5796	<i>Ab initio</i> molecular dynamics study of the hydrogen diffusion in sodium and lithium hydrides. <i>Journal of Applied Physics</i> , 2009, 106, .	1.1	11
5797	Individual charge-trapping dislocations in an ionic insulator. <i>Applied Physics Letters</i> , 2009, 95, .	1.5	7
5798	Theoretical studies of the interactions of ethylene and formaldehyde with gold clusters. <i>Journal of Chemical Physics</i> , 2009, 131, 034710.	1.2	20
5799	Magnetic properties of some metastable Co-Ru alloys studied by ion beam mixing and <i>ab initio</i> calculation. <i>Applied Physics Letters</i> , 2009, 94, 131903.	1.5	6
5800	<i>Ab initio</i> study of lithium and sodium iron fluorophosphate cathodes for rechargeable batteries. <i>Applied Physics Letters</i> , 2009, 94, 151904.	1.5	29
5801	Correlation between local structure of melts and glass forming ability for Fe <sub>78</sub> M <sub>9</sub> B <sub>13</sub> (M=Nb, Si, and Ti). <i>Physical Review B</i> , 2009, 79, .	1.1	21
5802	Site Preference and Alloying Effect of Excess Ni in Mn-Ga Shape Memory Alloys. <i>Chinese Physics Letters</i> , 2009, 26, 047101.	1.3	7
5803	Symmetry-breaking-induced enhancement of visible light absorption in delafossite alloys. <i>Applied Physics Letters</i> , 2009, 94, 251907.	1.5	20
5804	Elimination of phase separation in metalorganic chemical vapor deposition-grown GaInP epilayers by compositionally step-graded Ga <sub>1-x</sub> In <sub>x</sub> P multilayers. <i>Journal of Applied Physics</i> , 2009, 106, 063517.	1.1	2
5805	Relatively low temperature synthesis of hexagonal tungsten carbide films by N doping and its effect on the preferred orientation, phase transition, and mechanical properties. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2009, 27, 167-173.	0.9	19
5806	The origin of p-type conduction in (P, N) codoped ZnO. <i>Journal of Applied Physics</i> , 2009, 106, 043707.	1.1	36
5807	Dynamics of the Negative Thermal Expansion in Tellurium Based Liquid Alloys. <i>Physical Review Letters</i> , 2009, 103, 245901.	2.9	19
5808	Analytic form of the correlation energy of the uniform electron gas. <i>Physical Review A</i> , 2009, 79, .	1.0	7

#	ARTICLE	IF	CITATIONS
5809	Chemisorption of water and carbon dioxide on nanostructured BaTiO <sub>3</sub> /SrTiO <sub>3</sub> (001) surfaces. Journal of Applied Physics, 2009, 106, .	1.1	69
5810	Atomic Structure of the Epitaxial BaO/SiO <sub>2</sub> on TiO <sub>2</sub> (001) Surfaces. Journal of Applied Physics, 2009, 106, 123514.	2.9	45
5811	Atomic hydrogen adsorption and incipient hydrogenation of the Mg(0001) surface: A density-functional theory study. Journal of Chemical Physics, 2009, 131, 034706.	1.2	17
5812	Structural Prediction and Phase Transformation Mechanisms in Calcium at High Pressure. Physical Review Letters, 2009, 103, 055503.	2.9	65
5813	Enhance diamond coating adhesion by oriented interlayer microcracking. Journal of Applied Physics, 2009, 106, 123514.	1.1	2
5814	Benchmarking DFT surface energies with quantum Monte Carlo. Molecular Simulation, 2009, 35, 609-612.	0.9	11
5815	First-Principles Analysis of the Initial Electroreduction Steps of Oxygen over Pt(111). Journal of the Electrochemical Society, 2009, 156, B126.	1.3	207
5816	Ab Initio Study on Structural and Magnetic Properties of Ni-Pd and Ni-Pt Linear and Zigzag Nanowires. Communications in Theoretical Physics, 2009, 52, 123-127.	1.1	4
5817	Molecular adsorption and metal-support interaction for transition-metal clusters in zeolites: NO adsorption on Pd <sub>n</sub> (n=1-6) clusters in mordenite. Journal of Chemical Physics, 2009, 130, 104503.	1.2	26
5818	Relationship between layered crystal structure and mechanical properties of Al <sub>2</sub> O <sub>3</sub> /AlN (M = Al, Ga, In). Journal of Applied Physics, 2009, 106, 123514.	1.2	12
5819	Element Lines: Bonding in the Ternary Gold Polyphosphides, Au <sub>2</sub> MP <sub>2</sub> with M = Pb, Tl, or Hg. Journal of the American Chemical Society, 2009, 131, 2199-2207.	6.6	22
5820	Surface stability and electronic structure of hydrogen- and fluorine-terminated diamond surfaces: A first-principles investigation. Journal of Materials Research, 2009, 24, 2461-2470.	1.2	38
5821	The effects of alloying elements Al and In on Ni-Mn-Ga shape memory alloys, from first principles. Journal of Physics Condensed Matter, 2009, 21, 045506.	0.7	11
5822	First principle study on the elastic and thermodynamic properties of TiB <sub>2</sub> crystal under high temperature. Chinese Physics B, 2009, 18, 1248-1252.	0.7	17
5823	The Lattice Stabilities and Electronic Structure of Ba <sub>1-x</sub> Sr <sub>x</sub> TiO <sub>3</sub> Solid Solutions by First-Principles Calculations. Ferroelectrics, 2009, 388, 172-179.	0.3	6
5824	Ab initio studies on n-type and p-type Li <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> . Chinese Physics B, 2009, 18, 2492-2497.	0.7	8
5825	Kinetic Monte Carlo Simulations of Solid Oxide Fuel Cell. Journal of the Electrochemical Society, 2009, 156, B1406.	1.3	15
5826	Methane dissociation on Ni(111) and Pt(111): Energetic and dynamical studies. Journal of Chemical Physics, 2009, 130, 054701.	1.2	124



#	ARTICLE	IF	CITATIONS
5827	Low-temperature $\hat{\pm}$ -alumina thin film growth:ab initiostudies of Al adatom surface migration. Journal Physics D: Applied Physics, 2009, 42, 125302.	1.3	11
5828	Atomic and electronic structure of the YBa <sub>2</sub> Cu <sub>3</sub> O <sub>7</sub> /SrTiO <sub>3</sub> interface from first principles. Journal of Applied Physics, 2009, 106, 093714.	1.1	13
5829	Effect of the exchange-correlation potential and of surface relaxation on the description of the H <sub>2</sub> O dissociation on Cu(111). Journal of Chemical Physics, 2009, 130, 224702.	1.2	84
5830	General trend for adsorbate-induced segregation of subsurface metal atoms in bimetallic surfaces. Journal of Chemical Physics, 2009, 130, 174709.	1.2	108
5831	FIRST-PRINCIPLES STUDY OF THE MIGRATION OF HELIUM IN TUNGSTEN. International Journal of Modern Physics B, 2009, 23, 2077-2082.	1.0	12
5832	SPIN-POLARIZED DENSITY FUNCTIONAL STUDY ON HETEROFULLERENE AND METALLOFULLERENE CLUSTERS. International Journal of Modern Physics B, 2009, 23, 5119-5130.	1.0	9
5833	A comprehensive survey of M <sub>2</sub> AX phase elastic properties. Journal of Physics Condensed Matter, 2009, 21, 305403.	0.7	138
5834	Real-Time Evaluation of Aluminum Borohydride Trimethylamine for Aluminum Chemical Vapor Deposition. Journal of the Electrochemical Society, 2009, 156, H333.	1.3	5
5835	First-principles study of phase equilibria in Cu–Pt–Rh disordered alloys. Journal of Physics Condensed Matter, 2009, 21, 415401.	0.7	6
5836	Long-range empirical potential model: extension to hexagonal close-packed metals. Journal of Physics Condensed Matter, 2009, 21, 385402.	0.7	23
5837	Do all wurtzite nanotubes prefer faceted ones?. Journal of Chemical Physics, 2009, 130, 204706.	1.2	40
5838	First-principles study of structural and corrected band properties of wurtzite Zn <sub>1-x</sub> Cd <sub>x</sub> O and Zn <sub>1-x</sub> Mg <sub>x</sub> O systems. Chinese Physics B, 2009, 18, 2992-2997.	0.7	16
5839	Hydrogen diffusion in bulk and nanoclusters of MgH <sub>2</sub> and the role of catalysts on the basis of <i>ab initio</i> molecular dynamics. Applied Physics Letters, 2009, 94, .	1.5	15
5840	Post-CCSD(T) <i>ab Initio</i> Thermochemistry of Halogen Oxides and Related Hydrides XOX, XOOX, HOX, XO <sub>n</sub> , and HXO <sub>n</sub> (X = F, Cl), and Evaluation of DFT Methods for These Systems. Journal of Physical Chemistry A, 2009, 113, 4802-4816.	1.1	77
5841	A first-principles density functional study of chlorophenol adsorption on Cu <sub>2</sub> O(110):CuO. Journal of Chemical Physics, 2009, 130, 184505.	1.2	30
5842	A quantum chemistry study of Diels–Alder dimerizations in benzene and anthracene. Journal of Chemical Physics, 2009, 131, 024313.	1.2	16
5843	Direct Approach to Atomistic <i>Ab Initio</i> Studies of Precipitate Growth in Alloys. Materials Research Society Symposia Proceedings, 2009, 1229, 20901.	0.1	0
5844	Electronic structure and phase stability of In-free photovoltaic semiconductors, Cu <sub>2</sub> ZnSnSe <sub>4</sub> and Cu <sub>2</sub> ZnSnS <sub>4</sub> by first-principles calculation. Materials Research Society Symposia Proceedings, 2009, 1165, 1.	0.1	43

#	ARTICLE	IF	CITATIONS
5845	Amorphous Semiconductors Studied by First-principles Simulations: Structure and Electronic Properties. Materials Research Society Symposia Proceedings, 2009, 1153, 1.	0.1	1
5846	Improvement of the Pt/Graphene Interface Adhesion by Metallic Adatoms for Fuel Cell Applications. Materials Research Society Symposia Proceedings, 2009, 1213, 70201.	0.1	2
5847	Studies of LaSn <sub>3</sub> as a Negative Electrode for Lithium-Ion Batteries. Journal of the Electrochemical Society, 2009, 156, A536.	1.3	17
5848	Rapid synthesis of bulk Ti <sub>2</sub> AlC by self-propagating high temperature combustion synthesis with a pseudo-hot isostatic pressing process. Journal of Materials Research, 2009, 24, 2528-2535.	1.2	76
5849	Integrated Experimental, Atomistic, and Microstructurally Based Finite Element Investigation of the Dynamic Compressive Behavior of 2139 Aluminum. Journal of Applied Mechanics, Transactions ASME, 2009, 76, .	1.1	21
5850	Review of Hierarchical Multiscale Modeling to Describe the Mechanical Behavior of Amorphous Polymers. Journal of Engineering Materials and Technology, Transactions of the ASME, 2009, 131, .	0.8	65
5851	Characterization of Vacancy Defect Interaction on the Electric Properties of Zigzag Single-Walled Carbon Nanotubes. Journal of the Physical Society of Japan, 2009, 78, 094715.	0.7	0
5852	Structural and electronic properties of identical-sized Zn nanoclusters grown on Si(111)-(7Å-7) surfaces. Journal of Chemical Physics, 2009, 130, 024701.	1.2	10
5853	Excited state calculations using phaseless auxiliary-field quantum Monte Carlo: Potential energy curves of low-lying C2 singlet states. Journal of Chemical Physics, 2009, 130, 094107.	1.2	62
5854	Influence of a dielectric layer on photon emission induced by a scanning tunneling microscope. Journal of Chemical Physics, 2009, 130, 084706.	1.2	22
5855	Influence of CO in the structural and electrical properties of Pt nanocontacts: Comparison with H <sub>2</sub> molecule addition. Journal of Chemical Physics, 2009, 131, 014702.	1.2	2
5856	Comprehensive study of sodium, copper, and silver clusters over a wide range of sizes 2%N%75. Journal of Chemical Physics, 2009, 131, 174510.	1.2	87
5857	On the structure and dynamics of secondary n-alkyl cations. Journal of Chemical Physics, 2009, 131, 104314.	1.2	14
5858	Mechanisms for chemical transformations of (R,R)-tartaric acid on Cu(110): A first principles study. Journal of Chemical Physics, 2009, 131, 144703.	1.2	6
5859	Model Hamiltonian for the interaction of NO with the Au(111) surface. Journal of Chemical Physics, 2009, 130, 174716.	1.2	64
5860	Glutamic acid adsorbed on Ag(110): direct and indirect molecular interactions. Journal of Physics Condensed Matter, 2009, 21, 185001.	0.7	10
5861	Substantial stabilization of ferromagnetism in ZnO:Mn induced by N codoping. Journal of Physics Condensed Matter, 2009, 21, 185503.	0.7	12
5862	Electron-phonon coupling and spin fluctuations in 3d and 4d transition metals: implications for superconductivity and its pressure dependence. Journal of Physics Condensed Matter, 2009, 21, 025602.	0.7	14

#	ARTICLE	IF	CITATIONS
5863	Surface segregation of Si and its effect on oxygen adsorption on a $\hat{1}^3$ -TiAl(111) surface from first principles. Journal of Physics Condensed Matter, 2009, 21, 225005.	0.7	33
5864	Weak molecular chemisorption of N <sub>2</sub> /Pt(111). Journal of Physics Condensed Matter, 2009, 21, 264009.	0.7	5
5865	Ozonolysis of diamond. Journal of Physics Condensed Matter, 2009, 21, 264010.	0.7	2
5866	CoAl(001) surface structures: a kinetic Monte Carlo simulation. Journal of Physics Condensed Matter, 2009, 21, 445005.	0.7	2
5867	Adsorption states of the self-assembly of NH <sub>3</sub> molecules on the Si(001) surface. Journal of Physics Condensed Matter, 2009, 21, 064237.	0.7	7
5868	Study of pure and doped hydrogenated germanium cages: a density functional investigation. Nanotechnology, 2009, 20, 275202.	1.3	20
5869	Nucleation of gold atoms on vanadyl-terminated V <sub>2</sub> O <sub>3</sub> (0001). New Journal of Physics, 2009, 11, 093007.	1.2	16
5870	<i>Ab initio</i> calculations of structural and magnetic properties of Fe(O <sub>1</sub> ) <sub>1</sub> /MgO(O <sub>1</sub> ) <sub>1</sub> /Fe(O <sub>1</sub> ) <sub>1</sub> magnetic tunnel junction with interfacial Mg vacancy. Journal Physics D: Applied Physics, 2009, 42, 015003.	1.3	2
5871	Magnetic properties of Fe <sub>(1-x)</sub> Co <sub>x</sub> nanowires inside a (6,6) carbon nanotube. Journal Physics D: Applied Physics, 2009, 42, 105008.	1.3	11
5872	First principles calculation of the effects of solute atom on electromigration resistance of Al interconnects. Journal Physics D: Applied Physics, 2009, 42, 125501.	1.3	5
5873	Adsorption of benzene, phenol, propane and carbonic acid molecules on oxidized Al(111) and $\hat{1}^{\pm}$ -Al <sub>2</sub> O <sub>3</sub> (0001) surfaces: a first-principles study. Journal of Physics Condensed Matter, 2009, 21, 225001.	0.7	13
5874	Dissipative effects in the dynamics of N <sub>2</sub> on tungsten surfaces. Journal of Physics Condensed Matter, 2009, 21, 264007.	0.7	30
5875	The complex structure of liquid Cu <sub>6</sub> Sn <sub>5</sub> alloy. Journal of Physics Condensed Matter, 2009, 21, 155106.	0.7	5
5876	Nanorod Calculations on Body-Centered Cubic Iron: A Method for Estimation of Size-Dependent Surface Energies of Metal Nanocrystals. Journal of Physical Chemistry C, 2009, 113, 644-649.	1.5	5
5877	Density Functional Study on Relative Energies, Structures, and Bonding of Low-lying Electronic States of Lutetium Dimer. Chinese Journal of Chemical Physics, 2009, 22, 371-379.	0.6	1
5878	Role of hydrogen adsorption on the carbon terminated $\hat{1}^2$ -SiC(100)-c(2 Å × 2) surface structure: a theoretical approach. Journal of Physics Condensed Matter, 2009, 21, 055004.	0.7	2
5879	Effect of iron additions on intergranular cohesion in chromium. Journal of Physics Condensed Matter, 2009, 21, 485002.	0.7	12
5880	Comparison of the Density of States Obtained from the X-ray Photoelectron Spectra with the Electronic Structure Calculations for $\hat{1}^{\pm}$ -BiB <sub>3</sub> O <sub>6</sub> . Japanese Journal of Applied Physics, 2009, 48, 011601.	0.8	9

#	ARTICLE	IF	CITATIONS
5881	Electronic Structures of 4H-SiC with Group I and VII Elements: First-Principles Study of Possible p-Type Doping. Japanese Journal of Applied Physics, 2009, 48, 041301.	0.8	6
5882	Pressure-induced structural phase transitions on Na <sub>0.5</sub> CoO <sub>2</sub> : a first principles study. Journal of Physics Condensed Matter, 2009, 21, 155401.	0.7	0
5883	Evolution of unoccupied resonance during the synthesis of a silver dimer on Ag(111). New Journal of Physics, 2009, 11, 063020.	1.2	24
5884	Characterization of platinum nitride from first-principles calculations. Journal of Physics Condensed Matter, 2009, 21, 485403.	0.7	10
5885	Structural evolution due to Zn and Te adsorption on As-exposed Si(211): density functional calculation. Journal of Physics Condensed Matter, 2009, 21, 375502.	0.7	0
5886	First-Principles Analysis of the Activity of Transition and Noble Metals in the Direct Utilization of Hydrocarbon Fuels at Solid Oxide Fuel Cell Operating Conditions. Journal of the Electrochemical Society, 2009, 156, B1457.	1.3	43
5887	Periodic trends governing the interactions between impurity atoms [H $\hat{e}$ Ar] and $\hat{I}\pm$ -U. Philosophical Magazine, 2009, 89, 465-487.	0.7	8
5888	Review of Stress Effects on Dopant Solubility in Silicon and Silicon-Germanium Layers. Solid State Phenomena, 0, 156-158, 173-180.	0.3	1
5889	Spin-Flip Reaction of Re + CH <sub>4</sub> A Relativistic Density Functional Theory Investigation. Journal of Physical Chemistry A, 2009, 113, 8471-8477.	1.1	5
5890	Step decoration of chiral metal surfaces. Journal of Chemical Physics, 2009, 130, 124710.	1.2	27
5891	Fast three dimensional migration of He clusters in bcc Fe and Fe $\hat{e}$ Cr alloys. Journal of Applied Physics, 2009, 105, .	1.1	79
5892	Shape prediction of two-dimensional adatom islands on crystal surfaces during homoepitaxial growth. Applied Physics Letters, 2009, 94, 183107.	1.5	13
5893	Electronic and magnetic properties of graphene absorbed with S atom: A first-principles study. Journal of Applied Physics, 2009, 105, .	1.1	32
5894	Enhanced magnetic moments of Fe clusters supported on MgO/Fe(001) ultrathin films. Journal of Chemical Physics, 2009, 130, 184711.	1.2	7
5895	A first principles study on the full-Heusler compound Cr <sub>2</sub> MnAl. Applied Physics Letters, 2009, 94, .	1.5	68
5896	First-principles study of structure and quantum transport properties of C <sub>20</sub> fullerene. Journal of Chemical Physics, 2009, 131, 024311.	1.2	56
5897	Network of hydrogen bonds in Pro-Ala-Pro and Pro-Phe-Pro diamides: A first principles study of Ala $\hat{t}$ Phe point mutation in proline environment. Journal of Chemical Physics, 2009, 131, 035105.	1.2	3
5898	Methane combustion on Pd-based model catalysts: Structure sensitive or insensitive?. Journal of Chemical Physics, 2009, 131, 144704.	1.2	36

#	ARTICLE	IF	CITATIONS
5899	Diffusion and clustering of Au adatoms on H-terminated Si(111)-(1 $\times$ 1): A first principles study. Journal of Chemical Physics, 2009, 131, 144702.	1.2	3
5900	Ab initio-derived correlations for defect-dopant interactions in electronic materials. Applied Physics Letters, 2009, 95, 172104.	1.5	0
5901	N codoping induced ferromagnetism in ZnO:Co (101 $\hat{A}$ ) thin films. Journal of Applied Physics, 2009, 106, .	1.1	11
5902	Rescaled potentials for transition metal solutes in $\hat{A}$ -iron. Philosophical Magazine, 2009, 89, 3393-3411.	0.7	8
5903	Computational Study of 3,4-Diphenyl-1,2,5-Thiadiazole 1-Oxide for Organic Photovoltaics. International Journal of Photoenergy, 2009, 2009, 1-8.	1.4	12
5904	Periodic Density Functional Theory Investigation of the Uranyl Ion Sorption on Three Mineral Surfaces: A Comparative Study. International Journal of Molecular Sciences, 2009, 10, 2633-2661.	1.8	32
5905	Predicting New Materials for Hydrogen Storage Application. Materials, 2009, 2, 2296-2318.	1.3	9
5906	Lattice dynamics of Fe-doped CoO from first principles. Journal of Physics Condensed Matter, 2009, 21, 125601.	0.7	13
5907	Hydroxyl vacancies in single-walled aluminosilicate and aluminogermanate nanotubes. Journal of Physics Condensed Matter, 2009, 21, 195301.	0.7	20
5908	Oxygen Reduction on Pt(111) Cathode of Fuel Cells. Journal of the Physical Society of Japan, 2009, 78, 114601.	0.7	7
5909	Phase stabilities and mechanical properties of two new carbon crystals. Europhysics Letters, 2009, 87, 56003.	0.7	33
5910	Effect of Substitutional or Chemisorbed Nitrogen on the Diamond (100) Growth Process. Materials Research Society Symposia Proceedings, 2009, 1203, 1.	0.1	0
5911	Adsorption Mechanism of Hydrogen on Boron-Doped Fullerenes. Chinese Physics Letters, 2009, 26, 086804.	1.3	4
5912	Assessing nanoparticle size effects on metal hydride thermodynamics using the Wulff construction. Nanotechnology, 2009, 20, 204001.	1.3	127
5913	Structural Stabilities of Ordered Arrays of Nb 4 Clusters on NaCl(100) Surface. Chinese Physics Letters, 2009, 26, 016802.	1.3	2
5914	Activation of Ethane C-H and C-C Bonds by Gas Phase Th+ and U+: A Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 14699-14705.	1.1	24
5915	Chemical bonding and mechanical properties of $M_2A_2C$ ( $M = Ti, V, Cr$ ). Tj ETQq0 0 0 rgBT /Overlock 10 2009, 24, 556-564.	1.2	30
5916	Tailoring the reactivity of bimetallic overlayer and surface alloy systems. Journal of Physics Condensed Matter, 2009, 21, 084205.	0.7	48

#	ARTICLE	IF	CITATIONS
5917	First Principles Calculations of Complex Intermediate Band Materials for Photovoltaic Devices. Materials Research Society Symposia Proceedings, 2009, 1211, 1.	0.1	0
5918	Excited state properties of liquid water. Journal of Physics Condensed Matter, 2009, 21, 033101.	0.7	24
5919	First-principles study of oxygen incorporation and migration mechanisms in Ti <sub>2</sub> AlC. Journal of Materials Research, 2009, 24, 3190-3196.	1.2	25
5920	Effects of O and N impurities on the nanostructural evolution during growth of Cr/Sc multilayers. Journal of Materials Research, 2009, 24, 79-95.	1.2	10
5921	First-Principles Study of Lithium Absorption in Boron- or Silicon-Doped Single-Walled Carbon Nanotubes. Advanced Materials Research, 2009, 79-82, 613-616.	0.3	1
5922	Ground-state phase diagram of Na <sub>x</sub> CoO <sub>2</sub> : correlation of Na ordering with CoO <sub>2</sub> stacking sequences. Journal of Physics Condensed Matter, 2009, 21, 035401.	0.7	15
5923	First-principles study of the diffusion of Ga via interstitial-mediated mechanisms in ZnO. Scripta Materialia, 2009, 61, 324-326.	2.6	5
5924	Elastic properties and electronic structures of CdCNi <sub>3</sub> : A comparative study with MgCNi <sub>3</sub> . Solid State Sciences, 2009, 11, 251-258.	1.5	36
5925	First-principles investigation on extraction of lithium ion from monoclinic LiMnO <sub>2</sub> . Solid State Sciences, 2009, 11, 271-274.	1.5	9
5926	Partial ordering in the section Hf <sub>5</sub> Ge <sub>4</sub> –Zr <sub>5</sub> Ge <sub>4</sub> : Crystallographic investigation and modeling based on ab initio calculations. Solid State Sciences, 2009, 11, 395-401.	1.5	11
5927	Structural and electronic properties of lithium ion battery anode material LiMN (M=Ni, Co, Cu). Solid State Sciences, 2009, 11, 1898-1902.	1.5	3
5928	Structural, elastic and electronic properties of $\eta_2$ phase precipitate in Mg–Gd alloy system investigated via first-principles calculation. Solid State Sciences, 2009, 11, 2156-2161.	1.5	37
5929	The effect of Co-promotion on MoS <sub>2</sub> catalysts for hydrodesulfurization of thiophene: A density functional study. Journal of Catalysis, 2009, 268, 201-208.	3.1	136
5930	Pyrolysis Mechanisms of Quinoline and Isoquinoline with Density Functional Theory. Chinese Journal of Chemical Engineering, 2009, 17, 805-813.	1.7	18
5931	$\eta_2$ -Diketones at Water/Supercritical CO <sub>2</sub> Interface: A Molecular Dynamics Simulation. Chinese Journal of Chemical Engineering, 2009, 17, 990-998.	1.7	4
5932	Highly Ordered, Millimeter-Scale, Continuous, Single-Crystalline Graphene Monolayer Formed on Ru (0001). Advanced Materials, 2009, 21, 2777-2780.	11.1	389
5933	Interface Atomic-Scale Structure and its Impact on Quantum Electron Transport. Advanced Materials, 2009, 21, 4966-4969.	11.1	23
5935	Effect of Doped Transition Metal on Reversible Hydrogen Release/Uptake from NaAlH <sub>4</sub> . Chemistry - A European Journal, 2009, 15, 1685-1695.	1.7	36



#	ARTICLE	IF	CITATIONS
5936	How to Build Molecules with Large Magnetic Anisotropy. <i>Chemistry - A European Journal</i> , 2009, 15, 4078-4087.	1.7	163
5937	The Effect of Platinum on Diffusion Kinetics in $\text{NiAl}$ : Implications for Thermal Barrier Coating Lifetimes. <i>ChemPhysChem</i> , 2009, 10, 226-235.	1.0	12
5938	Reversible Structural Modulation of Fe-Pt Bimetallic Surfaces and Its Effect on Reactivity. <i>ChemPhysChem</i> , 2009, 10, 1013-1016.	1.0	68
5939	Investigation of $(1R,2S)$ -Ephedrine by Cryogenic Terahertz Spectroscopy and Solid-State Density Functional Theory. <i>ChemPhysChem</i> , 2009, 10, 2434-2444.	1.0	42
5940	Magnetic Anisotropy in a Family of Experimentally Synthesized and Theoretically Modeled $\text{M}_6\text{M}_8(\text{CN}_{24})$ Systems. <i>ChemPhysChem</i> , 2009, 10, 2496-2502.	1.0	1
5941	A New Class of Boron Nanotube. <i>ChemPhysChem</i> , 2009, 10, 3119-3121.	1.0	19
5942	An Excursion from Normal to Inverted $\text{C}\ddot{\text{C}}$ Bonds Shows a Clear Demarcation between Covalent and Charge-Shift $\text{C}\ddot{\text{C}}$ Bonds. <i>ChemPhysChem</i> , 2009, 10, 2658-2669.	1.0	46
5943	Performance of density functional models to reproduce observed $^{13}\text{C}$ chemical shifts of proteins in solution. <i>Journal of Computational Chemistry</i> , 2009, 30, 884-892.	1.5	27
5944	Chemical bonding in view of electron charge density and kinetic energy density descriptors. <i>Journal of Computational Chemistry</i> , 2009, 30, 1093-1102.	1.5	62
5945	A combined semiempirical-DFT study of oligomers within the finite-chain approximation, evolution from oligomers to polymers. <i>Journal of Computational Chemistry</i> , 2009, 30, 1220-1228.	1.5	11
5946	A combinatorial study of full Heusler alloys by first-principles computational methods. <i>Journal of Computational Chemistry</i> , 2009, 30, 1290-1299.	1.5	101
5947	Interesting properties of Thomas-Fermi kinetic and Parr electron-repulsion DFT energy functional generated compact one-electron density approximation for ground-state electronic energy of molecular systems. <i>Journal of Computational Chemistry</i> , 2009, 30, 1445-1453.	1.5	6
5948	Interaction of NO molecules with Pd clusters: <i>Ab initio</i> density-functional study. <i>Journal of Computational Chemistry</i> , 2009, 30, 1910-1922.	1.5	20
5949	First-principles calculations of the stability and electronic properties of the $\text{PbTiO}_3$ (110) polar surface. <i>Journal of Computational Chemistry</i> , 2009, 30, 1785-1798.	1.5	18
5950	A new hybrid DFT approach to electronic excitation and first hyperpolarizabilities of transition metal complexes. <i>Journal of Computational Chemistry</i> , 2009, 30, 2056-2063.	1.5	27
5951	Performance of plane-wave-based LDA and GGA approaches to describe magnetic coupling in molecular systems. <i>Journal of Computational Chemistry</i> , 2009, 30, 2316-2326.	1.5	35
5952	First-principles study of molecular hydrogen dissociation on doped $\text{Al}_{12}\text{X}$ (X = B, Al, C, Si). <i>Journal of Computational Chemistry</i> , 2009, 30, 1785-1798.	1.5	18
5953	Trends of the bonding effect on the performance of DFT methods in electric properties calculations: A pattern recognition and metric space approach on some $\text{XY}_2$ (X = O, S and Y = H, O, F, S). <i>Journal of Computational Chemistry</i> , 2009, 30, 1785-1798.	1.5	18



#	ARTICLE	IF	CITATIONS
5954	DFT/TDâ€DFT investigation on Ir(III) complexes with <i>N</i> -heterocyclic carbene ligands: Geometries, electronic structures, absorption, and phosphorescence properties. <i>Journal of Computational Chemistry</i> , 2010, 31, 628-638.	1.5	25
5955	Assessment of quantumâ€chemical methods for electronic properties and geometry of signaling biomolecules. <i>Journal of Computational Chemistry</i> , 2010, 31, 1063-1079.	1.5	4
5956	Direct visual evidence for the chemical mechanism of surfaceâ€enhanced resonance Raman scattering via charge transfer. <i>Journal of Raman Spectroscopy</i> , 2009, 40, 137-143.	1.2	79
5957	Direct visual evidence for the chemical mechanism of surfaceâ€enhanced resonance Raman scattering via charge transfer: (II) Bindingâ€site and quantumâ€size effects. <i>Journal of Raman Spectroscopy</i> , 2009, 40, 1172-1177.	1.2	28
5958	Selective Propene Epoxidation on Immobilized Au <sub>6</sub> Clusters: The Effect of Hydrogen and Water on Activity and Selectivity. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 1467-1471.	7.2	246
5959	Theoretical study of the hydroxylation of phenolates by the Cu <sub>2</sub> O <sub>2</sub> (N,Nâ€dimethylethylenediamine) <sub>2</sub> <sup>2+</sup> complex. <i>Journal of Biological Inorganic Chemistry</i> , 2009, 14, 229-242.	1.1	17
5960	First principles calculations on the influence of water-filled cavities on the electronic structure of Prussian Blue. <i>Journal of Molecular Modeling</i> , 2009, 15, 567-572.	0.8	18
5961	Density functional studies of closed-shell attractions of S(AuPH <sub>3</sub> ) <sub>2</sub> and HS(AuPH <sub>3</sub> ) <sub>2</sub> + and their dimers. <i>Journal of Molecular Modeling</i> , 2009, 15, 461-468.	0.8	4
5962	Structural stability and magnetic properties of Co-doped or adsorbed polar-ZnO surface. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2009, 373, 391-395.	0.9	12
5963	Ferromagnetism in carbon-doped ZnO films from first-principle study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2009, 373, 3091-3096.	0.9	27
5964	Molecular modelling by DFT of 1,2-diaminoethane adsorbed on the Zn-terminated and O-terminated, anhydrous and hydroxylated ZnO (0001) surface. <i>Superlattices and Microstructures</i> , 2009, 46, 19-24.	1.4	20
5965	Electronic and optical properties of acetylene and ethylene on Si(001). <i>Superlattices and Microstructures</i> , 2009, 46, 240-245.	1.4	3
5966	Water adsorption on hydrogenated Si(111) surfaces. <i>Surface Science</i> , 2009, 603, 60-64.	0.8	25
5967	Scanning tunneling microscopy and ab initio studies of precursor states of Ga-induced cluster on Si(001) surface. <i>Surface Science</i> , 2009, 603, 183-189.	0.8	2
5968	Reactions of vinyl groups on a model chromia surface: Vinyl chloride on stoichiometric $\gamma$ -Cr <sub>2</sub> O <sub>3</sub> . <i>Surface Science</i> , 2009, 603, 265-272.	0.8	3
5969	Density functional and dynamics study of the dissociative adsorption of hydrogen on Mg (0001) surface. <i>Surface Science</i> , 2009, 603, 304-310.	0.8	29
5970	SiO adsorption on a p(2 $\sqrt{3}$ â€2) reconstructed Si(100) surface. <i>Surface Science</i> , 2009, 603, 901-906.	0.8	4
5971	STM study of Si(113) 3 $\sqrt{3}$ â€2-Ga surface. <i>Surface Science</i> , 2009, 603, 1197-1202.	0.8	4

#	ARTICLE	IF	CITATIONS
5972	CO interaction with Au atoms adsorbed on terrace, edge and corner sites of the MgO(100) surface. Electronic structure and vibrational analysis from DFT. <i>Surface Science</i> , 2009, 603, 1262-1269.	0.8	15
5973	Effect of hydrogenation on the electronic structure of the P/Si(0 0 1)-(1 Å <sup>-2</sup> ) surface. <i>Surface Science</i> , 2009, 603, 2271-2275.	0.8	1
5974	Adsorption of methanol and methoxy on NiAl(110) and Ni3Al(111): A DFT study. <i>Surface Science</i> , 2009, 603, 2378-2386.	0.8	17
5975	Electrostatic field effect on molecular structures at metal surfaces. <i>Surface Science</i> , 2009, 603, 2815-2819.	0.8	13
5976	CO2 dissociation on Ni(211). <i>Surface Science</i> , 2009, 603, 2991-2998.	0.8	47
5977	Tailoring periodic nanostructures of vicinal copper surfaces: Formation and evolution of oxygen-induced faceting on Cu(332). <i>Surface Science</i> , 2009, 603, 3081-3087.	0.8	6
5978	DFT study on H2O activation by stepped and planar Rh surfaces. <i>Surface Science</i> , 2009, 603, 3275-3281.	0.8	31
5979	Structure and reducibility of titania-supported monomeric and dimeric molybdenum oxide entities studied by DFT calculations. <i>Computational and Theoretical Chemistry</i> , 2009, 903, 73-82.	1.5	17
5980	Broken symmetry approach and density functional theory investigation on hetero-spin system consisting of copper(II) and aminoxyl radicals: Comparison and reliability of different basis sets approaches. <i>Computational and Theoretical Chemistry</i> , 2009, 896, 54-62.	1.5	5
5981	Out-of-plane $\pi$ -aromaticity and enhanced $\sigma$ -aromaticity in superatom compounds $Li_3+Na_4^{2+}M_3^+$ (M=Li, Na) $T_j$ $E_{Tj} = 1.0784314$ eV $B_{1g}$	1.5	4
5982	Density functional theory study of hydrogenation mechanism in Fe-doped Mg(0001) surface. <i>Applied Surface Science</i> , 2009, 255, 6338-6344.	3.1	17
5983	Stress induced preferred orientation and phase transition for ternary WCxNy thin films. <i>Applied Surface Science</i> , 2009, 255, 8164-8170.	3.1	7
5984	The effect of defects on the hydrogenation in Mg (0001) surface. <i>Applied Surface Science</i> , 2009, 256, 46-51.	3.1	30
5985	Adsorption of Li on Cu(110): Density-functional calculations. <i>Chemical Physics</i> , 2009, 355, 135-140.	0.9	7
5986	Geometry and bonding in the ground and lowest triplet state of D6h symmetric crenellated edged C6[3m(m <sup>2</sup> +1)+1]H6(2m <sup>2</sup> +1) (m=2, 3, 6) graphene hydrocarbon molecules. <i>Chemical Physics</i> , 2009, 358, 85-95.	0.9	15
5987	First-principles theory for helium and xenon diffusion in uranium dioxide. <i>Journal of Nuclear Materials</i> , 2009, 385, 364-367.	1.3	45
5988	Molecular structure and DFT study of hydrothermally synthesized niobium oxide fluoride. <i>Journal of Molecular Structure</i> , 2009, 928, 171-175.	1.8	5
5989	A web-deployed interface for performing ab initio molecular dynamics, optimization, and electronic structure in Fireball. <i>Computer Physics Communications</i> , 2009, 180, 418-426.	3.0	3

#	ARTICLE	IF	CITATIONS
5990	DFT study of furan adsorption over stable molybdenum sulfide catalyst under HDO conditions. <i>Comptes Rendus Chimie</i> , 2009, 12, 754-761.	0.2	56
5991	Cathode catalysts for fuel cell development: A theoretical study based on band structure calculations for tungsten nitride and cobalt tungsten nitrides. <i>Electrochimica Acta</i> , 2009, 54, 6732-6739.	2.6	21
5992	Bond covalency and electronic structure of CaB <sub>2</sub> O <sub>4</sub> (III) crystal. <i>Structural Chemistry</i> , 2009, 20, 221-226.	1.0	5
5993	Hydrogen binding property of Co- and Ni-based organometallic compounds. <i>Structural Chemistry</i> , 2009, 20, 1107-1113.	1.0	26
5994	Electronic states in ordered and disordered quantum networks: with applications to graphene and to boron nanotubes. <i>Journal of Mathematical Chemistry</i> , 2009, 46, 532-549.	0.7	3
5995	The nature of the electronic states and photoelectron spectra of oxyanion crystals. <i>Journal of Structural Chemistry</i> , 2009, 50, 1021-1028.	0.3	11
5996	3d Transition metal decorated B-C-N composite nanostructures for efficient hydrogen storage: A first-principles study. <i>Bulletin of Materials Science</i> , 2009, 32, 353-360.	0.8	3
5997	Boron rings containing planar octacoordinate iron and cobalt. <i>Science in China Series B: Chemistry</i> , 2009, 52, 288-294.	0.8	12
5998	Structures and aromaticity of the planar Al <sub>2</sub> P <sub>2</sub> N <sup>n-</sup> (n=1-4) clusters. <i>Science in China Series B: Chemistry</i> , 2009, 52, 2237-2242.	0.8	2
5999	Structural stability and magnetism of metastable Ni-Pt intermetallic compounds studied by ab initio calculation. <i>Science in China Series D: Earth Sciences</i> , 2009, 52, 2681-2687.	0.9	7
6000	Electronic structure, chemical bond and thermal stability of hydrogen absorber Li <sub>2</sub> MgN <sub>2</sub> H <sub>2</sub> . <i>Science Bulletin</i> , 2009, 54, 497-503.	4.3	2
6001	Dead lithium phase investigation of Sn-Zn alloy as anode materials for lithium ion battery. <i>Science Bulletin</i> , 2009, 54, 1003-1008.	4.3	14
6002	First-principles investigation on initial stage of 2H-SiC(001) surface oxidation. <i>Science Bulletin</i> , 2009, 54, 1487-1494.	4.3	17
6003	Equilibrium geometric structure and electronic properties of Cl and H <sub>2</sub> O co-adsorption on Fe (100) surface. <i>Science Bulletin</i> , 2009, 54, 1295-1301.	4.3	5
6004	Elastic Properties, Thermal Expansion Coefficients, and Electronic Structures of Mg and Mg-Based Alloys. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2009, 40, 2751-2760.	1.1	37
6005	Thermodynamic Assessment of the Au-Co-Sn Ternary System. <i>Journal of Electronic Materials</i> , 2009, 38, 2158-2169.	1.0	17
6006	First-Principle Calculation Assisted Thermodynamic Assessment of the Pt-Pb System. <i>Journal of Phase Equilibria and Diffusion</i> , 2009, 30, 318-322.	0.5	7
6007	First-Principles Study of the Band Gap Structure of Oxygen-Passivated Silicon Nanonets. <i>Nanoscale Research Letters</i> , 2009, 4, 409-413.	3.1	10

#	ARTICLE	IF	CITATIONS
6008	Density functional theory and tight binding-based dynamical studies of carbon metal systems of relevance to carbon nanotube growth. <i>Nano Research</i> , 2009, 2, 774-782.	5.8	7
6009	Magnetic properties of vanadium-doped silicon carbide nanowires. <i>Metals and Materials International</i> , 2009, 15, 107-111.	1.8	28
6010	Computational study of the ground state properties of iodine and polyiodide ions. <i>Theoretical Chemistry Accounts</i> , 2009, 122, 119-125.	0.5	32
6011	Some questions on the exchange contribution to the effective potential of the Kohn-Sham theory. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 197-205.	0.5	1
6012	A variational density matrix approach with nonlocal effective potential. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 183-187.	0.5	1
6013	Influence of the exchange-correlation potential on the description of the molecular mechanism of oxygen dissociation by Au nanoparticles. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 119-126.	0.5	47
6014	Structural and electronic properties of small platinum metallorganic complexes. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 317-325.	0.5	7
6015	Density functional study on rare gas-noble metal closed-shell interaction in XeMX (M=Au, Ag, Cu; X=F, Cl, Br, I). <i>Theoretical Chemistry Accounts</i> , 2009, 123, 119-126.	0.5	11
6016	DFT studies of pressure effects on structural and vibrational properties of crystalline octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 179-186.	0.5	54
6017	Spontaneous Phosphorus-Halogen Bond Cleavage in <i>N</i> -Heterocyclic Halogenophosphanes Revisited: The Case of P-Br and P-I Bonds. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2009, 635, 245-252.	0.6	27
6018	Syntheses, Structures, and Theoretical Studies of New Mercury Iodobismuthates: (Et <sub>4</sub> N) <sub>4</sub> (Bi <sub>4</sub> Hg <sub>2</sub> I <sub>20</sub> ) and (i-Bu <sub>4</sub> N) <sub>2</sub> (Bi <sub>2</sub> HgI <sub>10</sub> ). <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2009, 635, 1645-1649.	0.6	33
6019	Structures and energetics of H <sub>2</sub> O adsorption on the Fe <sub>3</sub> O <sub>4</sub> (111) surface. <i>Journal of Fuel Chemistry and Technology</i> , 2009, 37, 506-512.	0.9	19
6020	Effects of Alloying Elements Ti, Cr, Al, and Hf on $\hat{1}^2$ -Nb <sub>5</sub> Si <sub>3</sub> from First-principles Calculations. <i>Chinese Journal of Aeronautics</i> , 2009, 22, 206-210.	2.8	18
6021	On the band gap location and core spectra of orthorhombic IV-VI compounds SnS and SnSe. <i>Physica Status Solidi (B): Basic Research</i> , 2009, 246, 183-191.	0.7	64
6022	Hypothetically superhard boron carbide structures with a B <sub>11</sub> C icosahedron and three-atom chain. <i>Physica Status Solidi (B): Basic Research</i> , 2009, 246, 62-70.	0.7	31
6023	Optical properties of pure and transition metal-doped indium oxide. <i>Physica Status Solidi (B): Basic Research</i> , 2009, 246, 1072-1081.	0.7	42
6024	Dispersion interactions in density-functional theory. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 1127-1135.	0.9	322
6025	Conclusive evidence on the insensitivity of additive rules to the combinational details of exchange and correlation functional in hybrid DFT methods. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 160-170.	1.0	2

#	ARTICLE	IF	CITATIONS
6026	Density functional study of aurophilic interaction in Cl(AuPH <sub>3</sub> ) and in its dimerization. International Journal of Quantum Chemistry, 2009, 109, 526-533.	1.0	6
6027	Development of eclipsed and staggered forms in some hydrogen bonded complexes. International Journal of Quantum Chemistry, 2009, 109, 629-638.	1.0	1
6028	Structure and stability of high-spin Au <sub>n</sub> (n = 2-8) clusters. International Journal of Quantum Chemistry, 2009, 109, 861-869.	1.0	2
6029	Time-dependent density functional theory calculation of van der Waals coefficient of potassium clusters. International Journal of Quantum Chemistry, 2009, 109, 1376-1384.	1.0	5
6030	Periodic DFT investigation on the structure and properties of TNAD crystal. International Journal of Quantum Chemistry, 2009, 109, 1598-1608.	1.0	1
6031	Linearized orbital-free embedding potential in self-consistent calculations. International Journal of Quantum Chemistry, 2009, 109, 1886-1897.	1.0	14
6032	Ab initio studies of vacancy-defected fullerenes and single-walled carbon nanotubes. International Journal of Quantum Chemistry, 2009, 109, 3441-3456.	1.0	19
6033	A promiscuous dicopper(II) system promoting the hydrolysis of bis(2,4-dinitrophenyl)phosphate: Gaining mechanistic insight by means of structural and spectroscopic DFT studies. International Journal of Quantum Chemistry, 2010, 110, 1432-1442.	1.0	4
6034	Theoretical zero-temperature isotherm and structural phase stability of thorium dioxide. International Journal of Quantum Chemistry, 2009, 109, 3564-3569.	1.0	12
6035	Density functional study of roles of porphyrin ring in electronic structures of heme. International Journal of Quantum Chemistry, 2009, 109, 3583-3591.	1.0	22
6036	Kinetics of the thermal decomposition of 1,2-dioxaspiro[2,5]octane. Kinetics and Catalysis, 2009, 50, 180-185.	0.3	2
6037	Vibrational predissociation spectra of the , n=3-10, 12 clusters: Even-odd alternation in the core ion. International Journal of Mass Spectrometry, 2009, 283, 94-99.	0.7	11
6038	Isopropanol adsorption on Î³-Al <sub>2</sub> O <sub>3</sub> surfaces: A computational study. Journal of Molecular Catalysis A, 2009, 304, 58-64.	4.8	51
6039	Relationship between molecular structure and Raman spectra of quinolines. Journal of Molecular Structure, 2009, 924-926, 301-308.	1.8	42
6040	Structural analysis of 5-fluorouracil and thymine solid solutions. Journal of Molecular Structure, 2009, 932, 16-30.	1.8	35
6041	Vacancies and E-centers in silicon as multi-symmetry defects. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2009, 159-160, 107-111.	1.7	14
6042	Ab initio study of Kr in hcp Ti: Diffusion, formation and stability of small Kr-vacancy clusters. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 2991-2994.	0.6	6
6043	Study on the ground state of NiO: The LSDA (GGA)+U method. Physica B: Condensed Matter, 2009, 404, 89-94.	1.3	48

#	ARTICLE	IF	CITATIONS
6044	Structural growth sequences and electronic properties of gold clusters: Highly symmetric tubelike cages. <i>Physica B: Condensed Matter</i> , 2009, 404, 1705-1708.	1.3	6
6045	Layered growth model and epitaxial growth structures for SiCAlN alloys. <i>Physica B: Condensed Matter</i> , 2009, 404, 1840-1846.	1.3	0
6046	Investigation of the electronic structure of Me/Al <sub>2</sub> O <sub>3</sub> (0001) interfaces. <i>Physica B: Condensed Matter</i> , 2009, 404, 2065-2071.	1.3	27
6047	Energetics and electronic properties of Mg <sub>7</sub> TMH <sub>16</sub> (TM=Sc, Ti, V, Y, Zr, Nb): An ab initio study. <i>Physica B: Condensed Matter</i> , 2009, 404, 2234-2240.	1.3	42
6048	The adsorption of In on the surface of (001) CdTe. <i>Physica B: Condensed Matter</i> , 2009, 404, 3530-3533.	1.3	2
6049	Study of O <sub>2</sub> and OH adsorption energies on Pd-Cu alloys surface with a quantum chemistry approach. <i>Electrochimica Acta</i> , 2009, 54, 1769-1776.	2.6	57
6050	An evaluation of exchange-correlation functionals for the calculations of the ionization energies for atoms and molecules. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2009, 171, 18-23.	0.8	21
6051	Stereochemistry of the reaction products of the oxidative addition reaction of methyl iodide to [Rh((C <sub>4</sub> H <sub>3</sub> S)COCHCOR)(CO)(PPh <sub>3</sub> )]: A NMR and computational study. R=CF <sub>3</sub> , C <sub>6</sub> H <sub>5</sub> , C <sub>4</sub> H <sub>3</sub> S. <i>Inorganica Chimica Acta</i> , 2009, 362, 519-530.	1.2	42
6052	Isomer distribution and structure of (2,2'-biphenyldiolato)bis(β <sup>2</sup> -diketonato)titanium(IV) complexes: A single crystal X-ray, solution NMR and computational study. <i>Inorganica Chimica Acta</i> , 2009, 362, 3088-3096.	1.2	19
6053	Theoretical investigation on structure and properties of 2,4,5-trinitroimidazole and its three derivatives. <i>Computational and Theoretical Chemistry</i> , 2009, 895, 44-51.	1.5	31
6054	A theoretical study of neutral and anionic Au <sub>5</sub> Al clusters. <i>Computational and Theoretical Chemistry</i> , 2009, 895, 92-95.	1.5	12
6055	Density functional theory study of structural, vibrational, and thermodynamic properties of crystalline 2,4-dinitrophenol, 2,4-dinitroresorcinol, and 4,6-dinitroresorcinol. <i>Computational and Theoretical Chemistry</i> , 2009, 895, 131-137.	1.5	12
6056	Dissociative adsorption of methane on Ni(111) surface with and without adatom: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2009, 903, 83-88.	1.5	20
6057	DFT and TDDFT study of carbon trioxide. <i>Computational and Theoretical Chemistry</i> , 2009, 897, 32-35.	1.5	7
6058	Interaction of NCO with small silver clusters: A density functional study. <i>Computational and Theoretical Chemistry</i> , 2009, 897, 100-105.	1.5	13
6059	First-principles study of crystalline mono-amino-2,4,6-trinitrobenzene, 1,3-diamino-2,4,6-trinitrobenzene, and 1,3,5-triamino-2,4,6-trinitrobenzene. <i>Computational and Theoretical Chemistry</i> , 2009, 900, 84-89.	1.5	33
6060	Coordination and binding of ions in Ca <sup>2+</sup> - and Ba <sup>2+</sup> -containing methanol dehydrogenase and interactions with methanol. <i>Computational and Theoretical Chemistry</i> , 2009, 901, 72-80.	1.5	11
6061	DFT periodic study of adsorption of glycine on the (0001) surface of zinc terminated ZnO. <i>Computational and Theoretical Chemistry</i> , 2009, 903, 49-58.	1.5	35

#	ARTICLE	IF	CITATIONS
6062	Theoretical study of transition metal cation exchanged zeolites: Interaction with NO. Computational and Theoretical Chemistry, 2009, 912, 88-94.	1.5	18
6063	Uncharged analogues of the phenalenyl cation: Hartree-Fock, Møller-Plesset, and density functional computational investigations of the isomers of boraphenalene. Computational and Theoretical Chemistry, 2009, 904, 49-56.	1.5	12
6064	Density functional theory study on the pyrolysis mechanism of thiophene in coal. Computational and Theoretical Chemistry, 2009, 905, 8-12.	1.5	31
6065	Geometry and thermodynamic stabilities of rhodanine tautomers and rotamers: Quantum chemical study. Computational and Theoretical Chemistry, 2009, 907, 66-73.	1.5	15
6066	Approximate time-dependent density functional theory. Computational and Theoretical Chemistry, 2009, 914, 38-49.	1.5	75
6067	Sandwich complexes of the Sb <sub>4</sub> aromatic ring with some transition metals. Computational and Theoretical Chemistry, 2009, 908, 73-78.	1.5	14
6068	First-principles study of identical clusters on the Si(001) surface. Computational and Theoretical Chemistry, 2009, 910, 69-73.	1.5	1
6069	Theoretical study of the structure of neutral, radical and anionic monoperoxo carbonic acid. Computational and Theoretical Chemistry, 2009, 913, 131-138.	1.5	5
6070	A computational study and fragment analysis of the back-bonding in Titanocenyl Complexes containing a five-member L <sub>2</sub> -cyclic ligand, L <sub>2</sub> =O, S, or Se. Computational and Theoretical Chemistry, 2009, 915, 51-57.	1.5	5
6071	First principles study of microscopic structures and layer-anion interactions in layered double hydroxides intercalated various univalent anions. Computational and Theoretical Chemistry, 2009, 915, 122-131.	1.5	19
6072	Structures and electronic properties of thin-films of polycyclic aromatic hydrocarbons. Thin Solid Films, 2009, 517, 3005-3010.	0.8	6
6073	Theoretical and spectroscopic investigations on the structure and bonding in B-C-N thin films. Thin Solid Films, 2009, 518, 1459-1464.	0.8	18
6074	A DFT study of methylamine polyaddition to C <sub>80</sub> fullerene. Superlattices and Microstructures, 2009, 46, 302-305.	1.4	6
6075	Electronic and optical properties of single-layered silicon sheets. Solid State Communications, 2009, 149, 153-155.	0.9	36
6076	First-principles study of diffusion of zinc vacancies and interstitials in ZnO. Solid State Communications, 2009, 149, 199-204.	0.9	48
6077	Ab initio studies on the structural and magnetic properties of RhH. Solid State Communications, 2009, 149, 322-324.	0.9	10
6078	Synthesis, crystal and electronic structures of La <sub>3</sub> Cr <sub>2</sub> N <sub>6</sub> . Solid State Communications, 2009, 149, 273-276.	0.9	8
6079	Ab initio calculations for properties of MAX phases Ti <sub>2</sub> InC, Zr <sub>2</sub> InC, and Hf <sub>2</sub> InC. Solid State Communications, 2009, 149, 564-566.	0.9	49



#	ARTICLE	IF	CITATIONS
6080	Ab initio study of the electronic and atomic structure of the wolframite-type ZnWO <sub>4</sub> . Solid State Communications, 2009, 149, 425-428.	0.9	54
6081	First-principles calculations on the mechanical properties of niobium nitrides. Solid State Communications, 2009, 149, 725-728.	0.9	22
6082	First-principles study of magnetism driven by intrinsic defects in MgO. Solid State Communications, 2009, 149, 855-858.	0.9	80
6083	Ab initio study on the ground states, phase stability, and mechanical properties of the Au-Pt system. Solid State Communications, 2009, 149, 952-956.	0.9	11
6084	Structural, elastic and electronic properties of ACTi <sub>3</sub> (A=Al, In and Tl) antiperovskite. Solid State Communications, 2009, 149, 919-922.	0.9	9
6085	Structural and electronic properties of Zn on a CdTe(001) surface. Solid State Communications, 2009, 149, 982-985.	0.9	9
6086	First-principles study of crystal structures of under pressure. Solid State Communications, 2009, 149, 1342-1346.	0.9	1
6087	The geometric structure influence on the ferromagnetism in Carbon-doped anatase : First-principles study. Solid State Communications, 2009, 149, 1717-1721.	0.9	15
6088	A first-principles study on the structural, elastic and electronic properties of AlCSc <sub>3</sub> and AlNSc <sub>3</sub> . Solid State Communications, 2009, 149, 1840-1842.	0.9	8
6089	Cage-like structure and charge hollow in the immiscible Cu-Ta system. Solid State Communications, 2009, 149, 1974-1977.	0.9	1
6090	First-principles study of structural, elastic, electronic and optical properties of SrMO <sub>3</sub> (M=Ti and Sn). Solid State Communications, 2009, 149, 2244-2249.	0.9	21
6091	An ab initio study of the electronic structure and elastic properties of the newly discovered ternary carbide. Solid State Communications, 2009, 149, 2156-2159.	0.9	30
6092	First-principles study of pressure effects on and. Solid State Communications, 2009, 149, 2125-2129.	0.9	12
6093	Water adsorption on phosphorous-carbide thin films. Surface and Coatings Technology, 2009, 204, 1035-1039.	2.2	15
6094	Composition-constitution-morphology relationship of Al <sub>2</sub> O <sub>3</sub> thin films deposited by plasma assisted chemical vapor deposition. Surface and Coatings Technology, 2009, 204, 215-221.	2.2	21
6095	X-ray spectroscopic techniques are powerful tools for electronic structure investigations of transition metal oxides. Surface Science, 2009, 603, 1613-1621.	0.8	4
6096	Interaction of alkali metals with the Fe <sub>3</sub> O <sub>4</sub> (111) Surface. Surface Science, 2009, 603, 78-83.	0.8	25
6097	Optical anisotropy of the In/Si(111)(4Å-1)/(8Å-2) nanowire array. Surface Science, 2009, 603, 247-250.	0.8	9

#	ARTICLE	IF	CITATIONS
6098	Correlating STM contrast and atomic-scale structure by chemical modification: Vacancy dislocation loops on FeO/Pt(111). <i>Surface Science</i> , 2009, 603, L15-L18.	0.8	53
6099	Effectiveness of in situ NH <sub>3</sub> annealing treatments for the removal of oxygen from GaN surfaces. <i>Surface Science</i> , 2009, 603, 387-399.	0.8	29
6100	Adsorbate influence on the coercive field of ultrathin Co/Cu{110}. <i>Surface Science</i> , 2009, 603, L45-L48.	0.8	7
6101	Realization of an atomic sieve: Silica on Mo(112). <i>Surface Science</i> , 2009, 603, 1145-1149.	0.8	25
6102	Atomic and electronic structures of thin NaCl films grown on a Ge(001) surface. <i>Surface Science</i> , 2009, 603, 2102-2107.	0.8	8
6103	Ab-initio calculations of interactions between Cu adatoms on Cu(110): Sensitivity of strong multi-site interactions to adatom relaxations. <i>Surface Science</i> , 2009, 603, 2387-2392.	0.8	12
6104	Adsorption of methanol on Ni <sub>3</sub> Al(111) and NiAl(110): A high resolution PES study. <i>Surface Science</i> , 2009, 603, 2370-2377.	0.8	12
6105	Structural and electronic properties of the Ti/W(111) adsorption system. <i>Surface Science</i> , 2009, 603, 2507-2519.	0.8	8
6106	Reactivity of surface OH in CH <sub>4</sub> reforming reactions on Ni(111): A density functional theory calculation. <i>Surface Science</i> , 2009, 603, 2600-2606.	0.8	41
6107	Ammonia on Ni(111) surface studied by first principles: Bonding, multilayers structure and comparison with experimental IR and XPS data. <i>Surface Science</i> , 2009, 603, 3025-3034.	0.8	26
6108	Nanoclusters of TiO <sub>2</sub> wetted with gold. <i>Surface Science</i> , 2009, 603, 3131-3135.	0.8	8
6109	Energetics of oxygen embedment into unreconstructed and reconstructed Cu(1 0 0) surfaces: Density functional theory calculations. <i>Surface Science</i> , 2009, 603, 3404-3409.	0.8	26
6110	Theoretical investigations on the high light yield of the LuI <sub>3</sub> :Ce scintillator. <i>Journal of Luminescence</i> , 2009, 129, 1555-1559.	1.5	16
6111	Structure and energetics of hydrogen adsorption on Fe <sub>3</sub> O <sub>4</sub> (111). <i>Journal of Molecular Catalysis A</i> , 2009, 302, 129-136.	4.8	57
6112	On the effectiveness of partial oxidation of propylene by gold: A density functional theory study. <i>Journal of Molecular Catalysis A</i> , 2009, 306, 6-10.	4.8	31
6113	CO hydrogenation reaction on sulfided molybdenum catalysts. <i>Journal of Molecular Catalysis A</i> , 2009, 312, 7-17.	4.8	53
6114	First-principles calculations of elastic and thermo-physical properties of Al, Mg and rare earth lanthanide elements. <i>Physica B: Condensed Matter</i> , 2009, 404, 2299-2304.	1.3	11
6115	Density functional theory study of Ir atom deposited on $\hat{\Gamma}^3$ -Al <sub>2</sub> O <sub>3</sub> (001) surface. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2009, 373, 277-281.	0.9	21

#	ARTICLE	IF	CITATIONS
6116	Hydrogen adsorption on N-decorated single wall carbon nanotubes. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 2588-2591.	0.9	17
6117	New template for metal decoration and hydrogen adsorption on graphene-like C <sub>3</sub> N <sub>4</sub> . Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 2778-2781.	0.9	47
6118	First-principles study of lattice dynamics of LiFePO <sub>4</sub> . Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 4096-4100.	0.9	48
6119	Atomic structure and phase transformations in Pu alloys. Progress in Materials Science, 2009, 54, 909-943.	16.0	43
6120	Theoretical studies on magnetic interactions between Cu(II) ions in salen nucleobases. Polyhedron, 2009, 28, 1945-1949.	1.0	12
6121	Syntheses, crystal structure and theoretical modelling of tetrahedral mono- $\eta^2$ -diketonato titanocenyl complexes. Polyhedron, 2009, 28, 966-974.	1.0	7
6122	A DFT study of the 67Zn, 14N and 2H electric field gradient tensors in Zinc(II)-4-Melm complexes and extrapolation to superoxide dismutase. Journal of Molecular Graphics and Modelling, 2009, 27, 620-627.	1.3	3
6123	Structural, electronic and magnetic properties of Cr-doped (ZnTe) <sub>12</sub> clusters. Journal of Magnetism and Magnetic Materials, 2009, 321, 235-240.	1.0	21
6124	Stabilization of ferromagnetism in Mn doped ZnO with C co-doping. Journal of Magnetism and Magnetic Materials, 2009, 321, 273-276.	1.0	18
6125	Electronic and magnetic behavior of ultrathin Ti nanowires. Journal of Magnetism and Magnetic Materials, 2009, 321, 1856-1862.	1.0	8
6126	Magnetism in strained pseudomorphic ultrathin films of fcc 3d-transition metals (Cr, Mn, Fe, Co and Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.0	9
6127	Electronic and magnetic properties of Pd-Ni multilayers: Study using density functional theory. Journal of Magnetism and Magnetic Materials, 2009, 321, 3478-3482.	1.0	9
6128	First-principles modeling of He-clusters in UO <sub>2</sub> . Journal of Nuclear Materials, 2009, 385, 72-74.	1.3	16
6129	Ab initio study of interstitial migration in Fe-Cr alloys. Journal of Nuclear Materials, 2009, 386-388, 86-89.	1.3	55
6130	A density functional theory assessment of the clustering behaviour of He and H in tungsten. Journal of Nuclear Materials, 2009, 386-388, 109-111.	1.3	136
6131	Theory of He trapping, diffusion, and clustering in UO <sub>2</sub> . Journal of Nuclear Materials, 2009, 385, 510-516.	1.3	40
6132	Radiation damage effects in the uranium-bearing $\gamma$ -phase oxide Y <sub>6</sub> U <sub>10</sub> O <sub>12</sub> . Journal of Nuclear Materials, 2009, 389, 497-499.	1.3	7
6133	Helium atoms in chromium-rich Fe-Cr alloys - Ab initio results. Journal of Nuclear Materials, 2009, 395, 45-49.	1.3	5

#	ARTICLE	IF	CITATIONS
6134	Influence of the ligand donor atoms on the in vitro stability of rhenium(I) and technetium (I)-99m complexes with pyrazole-containing chelators: Experimental and DFT studies. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 950-958.	0.8	19
6135	Density functional theory study of the mechanism for Ni(NHC) <sub>2</sub> catalyzed dehydrogenation of ammonia-borane for chemical hydrogen storage. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 2831-2838.	0.8	35
6136	Influence of elastic properties on superplasticity in doped yttria-stabilized zirconia. <i>Journal of Physics and Chemistry of Solids</i> , 2009, 70, 15-19.	1.9	12
6137	Ab-initio pseudopotential study of electronic structure and chemisorption of oxygen on aluminium surface. <i>Journal of Physics and Chemistry of Solids</i> , 2009, 70, 298-302.	1.9	9
6138	Ab initio simulations on the atomic and electronic structure of single-walled BN nanotubes and nanoarches. <i>Journal of Physics and Chemistry of Solids</i> , 2009, 70, 796-803.	1.9	27
6139	Simulation of elasto optical properties of K <sub>2</sub> SO <sub>4</sub> crystals. <i>Journal of Physics and Chemistry of Solids</i> , 2009, 70, 1109-1112.	1.9	15
6140	Crystal, electronic structures and photoluminescence properties of rare-earth doped LiSi <sub>2</sub> N <sub>3</sub> . <i>Journal of Solid State Chemistry</i> , 2009, 182, 301-311.	1.4	60
6141	The crystal structure of Hf <sub>1.5</sub> Nb <sub>1.5</sub> As and structure-composition relations in the section Hf <sub>3</sub> As-Nb <sub>3</sub> As. <i>Journal of Solid State Chemistry</i> , 2009, 182, 896-904.	1.4	6
6142	The electronic structures of vanadate salts: Cation substitution as a tool for band gap manipulation. <i>Journal of Solid State Chemistry</i> , 2009, 182, 1964-1971.	1.4	141
6143	Theoretical study of different speciation of mercury adsorption on CaO (0 0 1) surface. <i>Proceedings of the Combustion Institute</i> , 2009, 32, 2693-2699.	2.4	55
6144	The interaction between adsorbed OH and O <sub>2</sub> on TiO <sub>2</sub> surfaces. <i>Progress in Surface Science</i> , 2009, 84, 155-176.	3.8	126
6145	Investigation of the interactions between ginsenosides and amino acids by mass spectrometry and theoretical chemistry. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009, 74, 478-483.	2.0	9
6146	Dehydrogenation of ethanol on an O <sub>2</sub> -4Rh/CeO <sub>2</sub> (111) surface: A computational study. <i>Chemical Physics</i> , 2009, 359, 141-150.	0.9	9
6147	New insights on the reaction mechanisms for CO oxidation on Au catalysts. <i>Chemical Physics Letters</i> , 2009, 468, 201-204.	1.2	18
6148	Preparation, characterization and visible-light-driven photocatalytic activity of Fe-doped titania nanorods and first-principles study for electronic structures. <i>Applied Catalysis B: Environmental</i> , 2009, 90, 595-602.	10.8	700
6149	An incremental coupled-cluster approach to metallic lithium. <i>Chemical Physics Letters</i> , 2009, 469, 90-93.	1.2	24
6150	DFT study of molybdena-silica system - A selection of density functionals based on their performance in thermochemistry of molybdenum compounds. <i>Chemical Physics Letters</i> , 2009, 469, 140-144.	1.2	30
6151	The transition from metal-metal bonding to metal-solvent interactions during a dissolution event as assessed from electronic structure. <i>Chemical Physics Letters</i> , 2009, 469, 99-103.	1.2	32

#	ARTICLE	IF	CITATIONS
6152	Long-range interactions between polar molecules and metallic surfaces: A comparison of classical and density functional theory based models. <i>Chemical Physics Letters</i> , 2009, 471, 239-243.	1.2	33
6153	Electronic structure, molecular properties and electronic currents of the luminescent [Au <sub>3</sub> (CH <sub>3</sub> NCOCH <sub>3</sub> ) <sub>3</sub> ] cluster. <i>Chemical Physics Letters</i> , 2009, 474, 290-293.	1.2	22
6154	Pyridine as axial ligand on the [Mo <sub>6</sub> Cl <sub>8</sub> ] <sup>4+</sup> core switches off luminescence. <i>Chemical Physics Letters</i> , 2009, 475, 232-234.	1.2	21
6155	Investigation of crystalline 2-pyridone using terahertz spectroscopy and solid-state density functional theory. <i>Chemical Physics Letters</i> , 2009, 478, 166-171.	1.2	7
6156	Structural, electronic, and magnetic properties of a series of aluminum clusters doped with various transition metals. <i>Chemical Physics Letters</i> , 2009, 480, 258-264.	1.2	62
6157	Density functional studies of the magnetic properties in nitrogen doped TiO <sub>2</sub> . <i>Chemical Physics Letters</i> , 2009, 481, 99-102.	1.2	58
6158	Dangling bond energetics in carbon nitride and phosphorus carbide thin films with fullerene-like and amorphous structure. <i>Chemical Physics Letters</i> , 2009, 482, 110-113.	1.2	41
6159	Adsorption and electronic structure of single C <sub>60</sub> F <sub>18</sub> molecule on Si(111)-7 $\times$ 7 surface. <i>Chemical Physics Letters</i> , 2009, 482, 307-311.	1.2	20
6160	Impedance spectroscopy, electronic structure and X-ray photoelectron spectroscopy studies of Pb(Fe <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub> . <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2009, 169, 80-85.	0.8	24
6161	Kinetics and thermodynamics of carbon segregation and graphene growth on Ru(0001). <i>Carbon</i> , 2009, 47, 1806-1813.	5.4	104
6162	Electric field induced reversible switch in hydrogen storage based on single-layer and bilayer graphenes. <i>Carbon</i> , 2009, 47, 3452-3460.	5.4	93
6163	Experimental investigation and thermodynamic modeling of the Ni-Al-Ru ternary system. <i>Acta Materialia</i> , 2009, 57, 202-212.	3.8	18
6164	Defect energetics and Xe diffusion in UO <sub>2</sub> and ThO <sub>2</sub> . <i>Acta Materialia</i> , 2009, 57, 1655-1659.	3.8	60
6165	Ab-initio calculations of the hydrogen-uranium system: Surface phenomena, absorption, transport and trapping. <i>Acta Materialia</i> , 2009, 57, 4707-4715.	3.8	43
6166	Density functional theory study on water-gas-shift reaction over molybdenum disulfide. <i>Applied Catalysis A: General</i> , 2009, 365, 62-70.	2.2	47
6167	First-principles study of manganese adsorption on Si(100) surface. <i>Applied Surface Science</i> , 2009, 255, 6624-6628.	3.1	10
6168	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 395502.	0.7	18,183
6169	Evidence of the Ge nonreactivity during the initial stage of SiGe oxidation. <i>Applied Physics Letters</i> , 2009, 94, 041912.	1.5	10

#	ARTICLE	IF	CITATIONS
6170	Adsorption and dissociation of $O_2$ on Be(0001): First-principles prediction of an energy barrier on the adiabatic potential energy surface. Physical Review B, 2009, 79, .	1.1	16
6171	Combined Experimental and Theoretical Investigation of Nanosized Effects of Pt Catalyst on Their Underlying Methanol Electro-Oxidation Activity. Journal of Physical Chemistry C, 2009, 113, 9197-9205.	1.5	16
6172	Interatomic potentials for the Be-C-H system. Journal of Physics Condensed Matter, 2009, 21, 445002.	0.7	56
6173	Adsorption of O on Mo(110) surface from first-principles calculation. European Physical Journal B, 2009, 67, 27-34.	0.6	13
6174	Organic superconductors revisited. European Physical Journal B, 2009, 69, 167-171.	0.6	1
6175	Chemisorption of CO and H on Pd, Pt and Au nanoclusters: a DFT approach. European Physical Journal D, 2009, 52, 131-134.	0.6	37
6176	Bonding properties and structures of titanium clusters on (10,0) single wall carbon nano capsule. European Physical Journal D, 2009, 52, 87-90.	0.6	3
6177	Density functional study of the electronic structure and properties of lithium intercalated graphite. European Physical Journal D, 2009, 54, 643-655.	0.6	12
6178	Diels-Alder Reaction between Cyclopentadiene and $C_{60}$ : An Analysis of the Performance of the ONIOM Method for the Study of Chemical Reactivity in Fullerenes and Nanotubes. Journal of Physical Chemistry A, 2009, 113, 9721-9726.	1.1	63
6179	Electronic structure and stability of quaternary chalcogenide semiconductors derived from cation cross-substitution of II-VI and III-VI. Physical Review B, 2009, 79, .	1.1	413
6180	First-Principles Characterization of Bi-based Photocatalysts: $Bi_{12}TiO_{20}$ , $Bi_2Ti_2O_7$ , and $Bi_4Ti_3O_{12}$ . Journal of Physical Chemistry C, 2009, 113, 5658-5663.	1.5	209
6181	Adsorption dynamics of $H_2$ on Pd(100) from first principles. Physical Chemistry Chemical Physics, 2009, 11, 5814.	1.3	26
6182	On the Relative Preference of Enamine/Iminium Pathways in an Organocatalytic Michael Addition Reaction. Chemistry - an Asian Journal, 2009, 4, 714-724.	1.7	27
6183	One-Dimensional Polymers Based on Silver(I) Cations and Organometallic <i>cyclo</i> - $P_3$ Ligand Complexes. Chemistry - an Asian Journal, 2009, 4, 1578-1587.	1.7	26
6184	Theory of tunneling across hydrogen-bonded base pairs for DNA recognition and sequencing. Physical Review E, 2009, 79, 051911.	0.8	15
6185	Factors influencing graphene growth on metal surfaces. New Journal of Physics, 2009, 11, 063046.	1.2	241
6186	Ferromagnetism in the potential cathode material $LiNaFePO_4$ . Europhysics Letters, 2009, 87, 18001.	0.7	4
6187	Kinetic and Thermodynamic Stability of the Group 13 Trihydrides. Inorganic Chemistry, 2009, 48, 7953-7961.	1.9	20

#	ARTICLE	IF	CITATIONS
6188	First-principles study of $\text{Al}_2\text{O}_3$ surface. Physical Review B, 2009, 79, .	1.1	61
6189	First-principles study of hydrogenated amorphous silicon. Physical Review B, 2009, 79, .	1.1	61
6190	Evidence of kinetic-energy-driven antiferromagnetism in double perovskites: A first-principles study of La-doped $\text{Sr}_2\text{FeMoO}_7$ . Physical Review B, 2009, 80, .	1.1	47
6191	Effect of Porphyrin Ligands on the Regioselective Dehydrogenation versus Epoxidation of Olefins by Oxoiron(IV) Mimics of Cytochrome P450. Journal of Physical Chemistry A, 2009, 113, 11713-11722.	1.1	78
6192	Atomic structure of the two intermediate phase glasses $\text{SiSe}_4$ and $\text{GeSe}_4$ . Physical Review B, 2009, 79, .	1.1	61
6193	Accurate Reaction Enthalpies and Sources of Error in DFT Thermochemistry for Aldol, Mannich, and $\alpha$ -Aminoxylation Reactions. Journal of Physical Chemistry A, 2009, 113, 10376-10384.	1.1	124
6194	Experimental and theoretical screening of nanoscale oxide reactivity with $\text{LiBH}_4$ . Nanotechnology, 2009, 20, 204024.	1.3	15
6195	A theoretical design of half-metallic compounds by a long range of doping Mn for Heusler-type $\text{Cr}_3\text{Al}$ . Journal of Applied Physics, 2009, 105, .	1.1	27
6196	Empirical and ab initio computation of the thermochemical parameters of amino acids: I. Monoamino carbonic acids and monoamino dicarbonic acids and their amides. Russian Journal of General Chemistry, 2009, 79, 453-457.	0.3	2
6197	Bromine adsorption on Ge(001) surface: comparative study for coverages of 0.25, 0.5, 0.75 and 1 monolayer. Open Physics, 2009, 7, .	0.8	3
6198	Comparative DFT study on the $\alpha$ -glycosidic bond in reactive species of galactosyl diphosphates. Chemical Papers, 2009, 63, .	1.0	25
6199	Ab initio study of Hg-Hg and E112-E112 van der Waals interactions. Physics of Atomic Nuclei, 2009, 72, 396-400.	0.1	11
6200	Electronic structure, magnetic properties, and stability of the binary and ternary carbides $(\text{Fe,Cr})_3\text{C}$ and $(\text{Fe,Cr})_7\text{C}_3$ . Physics of the Solid State, 2009, 51, 2084-2089.	0.2	40
6201	Electronic States in Zinc Magnesium Oxide Alloy Semiconductors: Hard X-ray Photoemission Spectroscopy and Density Functional Theory Calculations. Chemistry of Materials, 2009, 21, 144-150.	3.2	15
6202	Synthesis and Fundamental Properties of Stable $\text{Ph}_3\text{SnSiH}_3$ and $\text{Ph}_3\text{SnGeH}_3$ Hydrides: Model Compounds for the Design of $\text{Si}^{\sim}\text{Ge}^{\sim}\text{Sn}$ Photonic Alloys. Inorganic Chemistry, 2009, 48, 6314-6320.	1.9	10
6203	Structural and Electronic Properties of a $\text{W}_3\text{O}_9$ Cluster Supported on the $\text{TiO}_2$ (110) Surface. Journal of Physical Chemistry C, 2009, 113, 17509-17517.	1.5	34
6204	Electronic Zero-Point Oscillations in the Strong-Interaction Limit of Density Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 743-753.	2.3	79
6205	Enantiospecific Adsorption of Amino Acids on Hydroxylated Quartz (0001). Langmuir, 2009, 25, 10737-10745.	1.6	29



#	ARTICLE	IF	CITATIONS
6206	Density Functional Studies of the Adsorption and Dissociation of NO <sub>x</sub> ( $x = 1$ ). <i>Journal of Physical Chemistry B</i> , 2009, 113, 10540-10547.	1.5	10
6207	Equation of state of hexagonal closed packed iron under Earth's core conditions from quantum Monte Carlo calculations. <i>Physical Review B</i> , 2009, 79, .	1.1	28
6208	Structural Versatility of the $\mu$ -SmGa <sub>3</sub> Phase: X-Ray, Electron Diffraction, and DFT Studies. <i>Inorganic Chemistry</i> , 2009, 48, 2399-2406.	1.9	5
6209	Coupled-Perturbed Scheme for the Calculation of Electronic g-Tensors with Local Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2985-2995.	2.3	15
6210	Hydrogen Absorption and Diffusion in Bulk $\pm$ -MoO <sub>3</sub> . <i>Journal of Physical Chemistry C</i> , 2009, 113, 11399-11407.	1.5	126
6211	Broken-Symmetry DFT Spin Densities of Iron Nitrosyls, Including Roussin's Red and Black Salts: Striking Differences between Pure and Hybrid Functionals. <i>Journal of Physical Chemistry B</i> , 2009, 113, 10540-10547.	1.2	44
6212	First Principle Study on the Adsorption of Styrene on Si(100)2 Å <sup>-1</sup> . <i>Journal of Physical Chemistry C</i> , 2009, 113, 5263-5273.	1.5	11
6213	Enhancement of Adsorption Inside Single-Walled Carbon Nanotubes: Li Doping Effect on n-Heptane van der Waals Bonding. <i>Journal of Physical Chemistry C</i> , 2009, 113, 4829-4838.	1.5	13
6214	Thermodynamics of hydrogen vacancies in $\text{MgH}$ first-principles calculations and grand-canonical statistical mechanics. <i>Physical Review B</i> , 2009, 80, .	1.1	23
6215	Work Function Measurements of Thin Oxide Films on Metals—MgO on Ag(001). <i>Journal of Physical Chemistry C</i> , 2009, 113, 11301-11305.	1.5	102
6216	Unexpected Trimerization of Pyrazine in the Coordination Sphere of Low-Valent Titanocene Fragments. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2044-2049.	2.3	12
6217	Dehydrogenation of Ethanol on a 2Ru/ZrO <sub>2</sub> (111) Surface: Density Functional Computations. <i>Journal of Physical Chemistry C</i> , 2009, 113, 6132-6139.	1.5	9
6218	Vanadium Oxides Supported on a Thin Silica Film Grown on Mo(112): Insights from Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2009, 113, 8336-8342.	1.5	17
6219	Theoretical Study on the X-ray Absorption at the Sulfur K-Edge in Gold Nanoparticles Protected by Thiolates. <i>Journal of Physical Chemistry C</i> , 2009, 113, 14844-14851.	1.5	6
6220	Evaluation of Density Functionals and Basis Sets for Carbohydrates. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 679-692.	2.3	183
6221	How to Stabilize $\mu$ -3-Silapropargyl/Alkynylsilyl Complex of [Cp <sub>2</sub> M] <sup>+</sup> ( $L = \text{CO}$ , PMe <sub>3</sub> , or PF <sub>3</sub> and M =) <i>Journal of Physical Chemistry B</i> , 2009, 113, 2152-2157.	1.1	9
6222	Density Functional Theory Study of the Reaction Mechanism for Competitive Carbon-Hydrogen and Carbon-Halogen Bond Activations Catalyzed by Transition Metal Complexes. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2152-2157.	1.1	9
6223	Role of Dihydrogen Bonds for the Stabilization of Self-Assembled Molecular Nanostructures. <i>Journal of Physical Chemistry C</i> , 2009, 113, 12653-12657.	1.5	12

#	ARTICLE	IF	CITATIONS
6224	A Dominant Dissociation Mode of cis-Dichloroethylene on Si(100)2 Å <sup>-1</sup> : Adjacent Si Dimer Double Dechlorination. <i>Journal of Physical Chemistry C</i> , 2009, 113, 21797-21804.	1.5	3
6225	THE CO-ADSORPTION OF BENZENE AND CO ON Co(0001). <i>Surface Review and Letters</i> , 2009, 16, 749-755.	0.5	5
6226	First-principles investigation of pentagonal and hexagonal core-shell silicon nanowires with various core compositions. <i>Physical Review B</i> , 2009, 80, .	1.1	22
6227	CO Disproportionation on a Nanosized Iron Cluster. <i>Journal of Physical Chemistry C</i> , 2009, 113, 12939-12942.	1.5	15
6228	Dynamics of Open-Shell Species at Metal Surfaces. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16311-16320.	1.5	18
6229	Is There a Nanosize for the Activity of TiO <sub>2</sub> Compounds?. <i>Journal of Physical Chemistry C</i> , 2009, 113, 12186-12194.	1.5	37
6230	Density Functional Theory Studies of Structural Deformation in Bis(alkynyl)diruthenium(III): Stronger Ru <sup>2+</sup> Ru Bonding by Any Means Necessary. <i>Inorganic Chemistry</i> , 2009, 48, 5608-5610.	1.9	16
6231	Van der Waals Interactions in Density-Functional Theory: Rare-Gas Diatomics. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 719-727.	2.3	145
6232	First-Principles Study of Electronic, Absorption, and Thermodynamic Properties of Crystalline Styphnic Acid and Its Metal Salts. <i>Journal of Physical Chemistry B</i> , 2009, 113, 10315-10321.	1.2	30
6233	Self-Consistent Polarization Density Functional Theory: Application to Argon. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2075-2085.	1.1	19
6234	Surface energies of stoichiometric FePt and CoPt alloys and their implications for nanoparticle morphologies. <i>Physical Review B</i> , 2009, 80, .	1.1	121
6235	Neighboring Amide Participation in Thioether Oxidation: Relevance to Biological Oxidation. <i>Journal of the American Chemical Society</i> , 2009, 131, 13791-13805.	6.6	47
6236	First-Principles Study of Electronic Transport Properties of Dodecahedrane C <sub>20</sub> H <sub>20</sub> and Its Endohedral Complex Li@C <sub>20</sub> H <sub>20</sub> . <i>Journal of Physical Chemistry C</i> , 2009, 113, 15756-15760.	1.5	27
6237	Evaluation of Electronic Coupling in Transition-Metal Systems Using DFT: Application to the Hexa-Aquo Ferric <sup>3+</sup> /Ferrous Redox Couple. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 307-323.	2.3	41
6238	Performance of Ab Initio and Density Functional Methods for Conformational Equilibria of C <sub>n</sub> H <sub>2n+2</sub> Alkane Isomers (n = 4-8). <i>Journal of Physical Chemistry A</i> , 2009, 113, 11974-11983.	1.1	156
6239	Theoretical Investigation of Formamide Adsorption on Ag(111) Surfaces. <i>Journal of Physical Chemistry C</i> , 2009, 113, 10541-10547.	1.5	31
6240	Hg Binding on Pd Binary Alloys and Overlays. <i>Journal of Physical Chemistry C</i> , 2009, 113, 7813-7820.	1.5	49
6241	MoS <sub>2</sub> Nanowires: A Promising Anode Material for Lithium-Ion Batteries. A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 18436-18440.	1.5	14

#	ARTICLE	IF	CITATIONS
6242	Aminoxyl Radicals on the Silicon (001) Surface. <i>Journal of Physical Chemistry C</i> , 2009, 113, 1020-1027.	1.5	2
6243	Concerning the Reaction Pathway of the Metathesis Reaction involving WW and CN Triple Bonds: A Theoretical Study. <i>Inorganic Chemistry</i> , 2009, 48, 10358-10363.	1.9	4
6244	Density Functional Theory Calculations of the Interaction of Hydrazine with Low-Index Copper Surfaces. <i>Journal of Physical Chemistry C</i> , 2009, 113, 15714-15722.	1.5	40
6245	Ca Deposition on TiO <sub>2</sub> (110) Surfaces: Insights from Quantum Calculations. <i>Journal of Physical Chemistry C</i> , 2009, 113, 3740-3745.	1.5	7
6246	First Principles Study of the Effect of Carbon and Boron on the Activity of a Ni Catalyst. <i>Journal of Physical Chemistry C</i> , 2009, 113, 4099-4106.	1.5	39
6247	Norbornadiene-Based Molecules for Functionalizing The Si(001) Surface. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16094-16103.	1.5	4
6248	IR Spectroscopic Measurement of Diffusion Kinetics of Chemisorbed Pyridine through Nanocrystalline MgO Particles. The Involvement of Surface Defect Sites in Slow Diffusion. <i>Journal of Physical Chemistry C</i> , 2009, 113, 2219-2227.	1.5	19
6249	Elastic constants of NaBH <sub>4</sub> and LiBH <sub>4</sub> : Instability of $\hat{\Gamma}^2$ -LiBH <sub>4</sub> . <i>Europhysics Letters</i> , 2009, 88, 36005.	0.7	3
6250	Study of the size-dependent properties of Sc <sub>n</sub> Al (n= 1–14) clusters by density-functional theory. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 046004.	0.7	3
6251	Effects of Lattice Expansion on the Reactivity of a One-Dimensional Oxide. <i>Journal of the American Chemical Society</i> , 2009, 131, 3253-3259.	6.6	12
6252	Jahn–Teller-like origin of the tetragonal distortion in disordered Fe–Pd magnetic shape memory alloys. <i>Applied Physics Letters</i> , 2009, 94, 072508.	1.5	44
6253	Methane C–H Bond Activation by Gas-Phase Th <sup>+</sup> and U <sup>+</sup> : Reaction Mechanisms and Bonding Analysis. <i>Organometallics</i> , 2009, 28, 3716-3726.	1.1	47
6254	Cooperative Phase Transformation in Self-Assembled Metal-on-Oxide Arrays. <i>Journal of Physical Chemistry C</i> , 2009, 113, 1143-1146.	1.5	13
6255	Theoretical Study on the Reaction Mechanism for the Formation of 2-Methylpyridine Cobalt(I) Complex from Cobaltacyclopentadiene and Acetonitrile. <i>Organometallics</i> , 2009, 28, 3636-3649.	1.1	46
6256	Adsorption and Diffusion of Light Gases in ZIF-68 and ZIF-70: A Simulation Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16906-16914.	1.5	126
6257	Density Functional Studies of Ethanol Dehydrogenation on a 2Rh/ $\hat{\Gamma}^3$ -Al <sub>2</sub> O <sub>3</sub> (110) Surface. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16181-16187.	1.5	18
6258	Ti-Decorated BC <sub>4</sub> N Sheet: A planar Nanostructure for High-Capacity Hydrogen Storage. <i>Journal of Physical Chemistry C</i> , 2009, 113, 15783-15787.	1.5	31
6259	Proposed Long-Range Empirical Potential To Study the Metallic Glasses in the Ni–Nb–Ta System. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7282-7290.	1.2	17



#	ARTICLE	IF	CITATIONS
6278	Structure, Bonding, and Relative Stability of the Ground and Low-Lying Electronic States of CuO <sub>2</sub> . The Role of Exact Exchange. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1308-1317.	1.1	19
6279	Toward a Wave-Function-Based Treatment of Metals: Extrapolation from Finite Clusters. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11483-11486.	1.1	7
6280	Impact of Reduction on the Properties of Metal Bisdithiolenes: Multinuclear Solid-State NMR and Structural Studies on Pt(tfd) <sub>2</sub> and Its Reduced Forms. <i>Journal of Physical Chemistry B</i> , 2009, 113, 3298-3313.	1.2	14
6281	Borohydride Oxidation over Au(111): A First-Principles Mechanistic Study Relevant to Direct Borohydride Fuel Cells. <i>Journal of the Electrochemical Society</i> , 2009, 156, B86.	1.3	70
6282	X-ray Photoemission Study of the Charge State of Au Nanoparticles on Thin MgO/Fe(001) Films. <i>Journal of Physical Chemistry C</i> , 2009, 113, 19957-19965.	1.5	27
6283	A potential surface for the interaction between water and coronene as a model for a hydrophobic surface. <i>Molecular Physics</i> , 2009, 107, 1197-1207.	0.8	14
6284	Cryogenic Terahertz Spectrum of (+)-Methamphetamine Hydrochloride and Assignment Using Solid-State Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5119-5127.	1.1	59
6285	Direct Spectroscopic Observation of the Role of Humidity in Surface Diffusion through an Ionic Adsorbent Powder. The Behavior of Adsorbed Pyridine on Nanocrystalline MgO. <i>Journal of Physical Chemistry C</i> , 2009, 113, 2228-2234.	1.5	19
6286	Density Functional Theory Calculations of Solid Nitromethane under Hydrostatic and Uniaxial Compressions with Empirical van der Waals Correction. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3610-3614.	1.1	38
6287	Crystal and Molecular Structure of Manganese(II) Lapacholate, a Novel Polymeric Species Undergoing Temperature-Reversible Metal to Ligand Electron Transfer. <i>Inorganic Chemistry</i> , 2009, 48, 3529-3534.	1.9	14
6288	Influence of Dopants Ti and Ni on Dehydrogenation Properties of NaAlH <sub>4</sub> : Electronic Structure Mechanisms. <i>Journal of Physical Chemistry C</i> , 2009, 113, 10215-10221.	1.5	17
6289	Oxygen vacancy formation on clean and hydroxylated low-index $V_2O_5$ surfaces: A density functional investigation. <i>Physical Review B</i> , 2009, 79, 115411.	1.1	39
6290	Intermediates and Spectators in O <sub>2</sub> Dissociation at the RuO <sub>2</sub> (110) Surface. <i>Journal of Physical Chemistry C</i> , 2009, 113, 15266-15273.	1.5	54
6291	Origin of the High Thermoelectric Performance in Si Nanowires: A First-Principle Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 14001-14005.	1.5	25
6292	A Density Functional Study of Initial Steps in the Oxidation of Early Transition Metal Nitrides, MN (M = Ti, V, Cr, Mn, Fe, Co, Ni). <i>Journal of Physical Chemistry C</i> , 2009, 113, 10215-10221.	1.5	12
6293	Chainlike Au <sup>+</sup> O Structures on Au(110)-(1 $\times$ 1) Surfaces Calculated from First Principles. <i>Journal of Physical Chemistry C</i> , 2009, 113, 5690-5699.	1.5	16
6294	First-Principles Investigation of Surface and Subsurface H Adsorption on Ir(111). <i>Journal of Physical Chemistry C</i> , 2009, 113, 21361-21367.	1.5	42
6295	Platinum Group Metal Adsorption on Clean and Hydroxylated Corundum Surfaces. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16747-16756.	1.5	25

#	ARTICLE	IF	CITATIONS
6296	Examination of Phencyclidine Hydrochloride via Cryogenic Terahertz Spectroscopy, Solid-State Density Functional Theory, and X-ray Diffraction. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13013-13022.	1.1	27
6297	Characteristic Spin <sup>1</sup> Orbit Induced <sup>1</sup> H(CH <sub>2</sub> ) Chemical Shifts upon Deprotonation of Group 9 Polyamine Aqua and Alcohol Complexes. <i>Journal of the American Chemical Society</i> , 2009, 131, 11909-11918.	6.6	25
6298	Degradation of interface integrity between a high-k dielectric thin film and a gate electrode due to excess oxygen in the film. , 2009, , .		1
6299	A Theoretical Study of H <sub>2</sub> Reacting on Ti/Al(100) Surfaces. <i>Journal of Physical Chemistry C</i> , 2009, 113, 11027-11034.	1.5	17
6300	H/Br Exchange in BBr <sub>3</sub> by HSiR <sub>3</sub> (R = H, CH <sub>3</sub> ), Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 587 Td (C<sup>3</sup> Barrier. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12035-12043.	1.1	12
6301	Adsorption and diffusion of Au atoms on the (001) surface of Ti, Zr, Hf, V, Nb, Ta, and Mo carbides. <i>Journal of Chemical Physics</i> , 2009, 130, 244706.	1.2	17
6302	Phonon-Induced Dephasing of Excitons in Semiconductor Quantum Dots: Multiple Exciton Generation, Fission, and Luminescence. <i>ACS Nano</i> , 2009, 3, 2487-2494.	7.3	115
6303	Light-Activated Molecular Conductivity in the Photoreactions of Vitamin D <sub>3</sub> . <i>Journal of Physical Chemistry A</i> , 2009, 113, 6740-6744.	1.1	11
6304	Structure and Decomposition Pathways of Vinyl Acetate on Clean and Oxygen-Covered Pd(100). <i>Journal of Physical Chemistry C</i> , 2009, 113, 971-978.	1.5	16
6305	The Unusual Solid-State Structure of Mercury Oxide: Relativistic Density Functional Calculations for the Group 12 Oxides ZnO, CdO, and HgO. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12427-12432.	1.1	24
6306	Performance of Kinetic Energy Functionals for Interaction Energies in a Subsystem Formulation of Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 3161-3174.	2.3	109
6307	ELASTIC AND ELECTRONIC PROPERTIES OF<font>Hf</font><sub>2</sub><font>SnC</font>AND<font>Hf</font><sub>2</sub><font>SnN</font>. <i>International Journal of Modern Physics B</i> , 2009, 23, 5155-5161.	1.0	2
6308	Surface Phase Diagram and Oxygen Coupling Kinetics on Flat and Stepped Pt Surfaces under Electrochemical Potentials. <i>Journal of Physical Chemistry C</i> , 2009, 113, 9765-9772.	1.5	62
6309	Water adsorption on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</mml:mi><mml:msub><mml:mrow><mml:mtext>-Al</mml:mtext></mml:mrow></mml:msub></mml:math> Physical Review B, 2009, 80, .	1.1	7
6310	Self-Assembly of Diacid Molecules: A Theoretical Approach of Molecular Interactions. <i>Journal of Physical Chemistry C</i> , 2009, 113, 17566-17571.	1.5	7
6311	DFT Study of Planar Boron Sheets: A New Template for Hydrogen Storage. <i>Journal of Physical Chemistry C</i> , 2009, 113, 18962-18967.	1.5	130
6312	Defect-induced magnetic order in pure ZnO films. <i>Physical Review B</i> , 2009, 80, .	1.1	274
6313	Structure of Reduced Ultrathin TiO<sub>x</sub> Polar Films on Pt(111). <i>Journal of Physical Chemistry C</i> , 2009, 113, 5721-5729.	1.5	64



#	ARTICLE	IF	CITATIONS
6314	Potential-Driven Adiabatic Connection in Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 822-826.	2.3	2
6315	Ground-state properties of simple elements from GW calculations. <i>Physical Review B</i> , 2009, 80, .	1.1	61
6316	Manganese Borohydride As a Hydrogen-Storage Candidate: First-Principles Crystal Structure and Thermodynamic Properties. <i>Journal of Physical Chemistry C</i> , 2009, 113, 13416-13424.	1.5	19
6317	Structure-Reactivity Relationship for Catalytic Activity of Gallium Oxide and Sulfide Clusters in Zeolite. <i>Journal of Physical Chemistry C</i> , 2009, 113, 4246-4249.	1.5	32
6318	Pronounced Cluster-Size Effects: Gas-Phase Reactivity of Bare Vanadium Cluster Cations $V_n^+$ ( $n = 1\text{--}7$ ) Toward Methanol. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5625-5632.	1.1	24
6319	Activity and Reactivity of $Fe^{2+}$ Cations in the Zeolite. Ab Initio Free-Energy MD Calculation of the $N_2O$ Dissociation over Iron-Exchanged Ferrierite. <i>Journal of Physical Chemistry C</i> , 2009, 113, 18807-18816.	1.5	9
6320	Chemically Accurate Simulation of a Prototypical Surface Reaction: $H_2$ Dissociation on Cu(111). <i>Science</i> , 2009, 326, 832-834.	6.0	315
6321	Application of Hybrid Functionals to the Modeling of NO Adsorption on $Cu^+SAPO-34$ and $Co^+SAPO-34$ : A Periodic DFT Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 5274-5291.	1.5	22
6322	$SiC/Ti_3SiC_2$ interface: Atomic structure, energetics, and bonding. <i>Physical Review B</i> , 2009, 79, .	1.1	53
6323	Phase transitions in various kinds of clusters. <i>Physics-Uspexhi</i> , 2009, 52, 137-164.	0.8	60
6324	Density Functional Theory Study of the Adsorption and Reaction of $H_2S$ on $TiO_2$ Rutile (110) and Anatase (101) Surfaces. <i>Journal of Physical Chemistry C</i> , 2009, 113, 20411-20420.	1.5	61
6325	Periodic density functional theory study of spin crossover in the cesium iron hexacyanochromate prussian blue analog. <i>Journal of Chemical Physics</i> , 2009, 130, 014702.	1.2	13
6326	Tailoring the Interaction Strength between Gold Particles and Silica Thin Films via Work Function Control. <i>Physical Review Letters</i> , 2009, 103, 056801.	2.9	37
6327	Phase stability and physical properties of $Ta_5Co_7$ from first-principles calculations. <i>Physical Review B</i> , 2009, 80, .	1.1	77
6328	Adsorption of hydrogen on boron-doped graphene: A first-principles prediction. <i>Journal of Applied Physics</i> , 2009, 105, .	1.1	96
6329	Adsorption of Late Transition Metal Atoms on $MgO/Mo(100)$ and $MgO/Ag(100)$ Ultrathin Films: A Comparative DFT Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16694-16701.	1.5	37
6330	An Enhanced Hydrogen Adsorption Enthalpy for Fluoride Intercalated Graphite Compounds. <i>Journal of the American Chemical Society</i> , 2009, 131, 17732-17733.	6.6	50
6331	Aggregation in thin-film silver: Induced by chlorine and inhibited by alloying with two dopants. <i>Corrosion Science</i> , 2009, 51, 2557-2564.	3.0	11



#	ARTICLE	IF	CITATIONS
6332	Electronic, electrical and thermodynamic properties of Ca <sub>5</sub> Si <sub>3</sub> by first principles calculations and low temperature experimental techniques. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009, 33, 260-264.	0.7	6
6333	First-principles calculation of L10 -disorder phase equilibria for Fe-Ni system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009, 33, 244-249.	0.7	26
6334	Thermodynamic investigation of the galvanizing systems, I: Refinement of the thermodynamic description for the Fe-Zn system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009, 33, 433-440.	0.7	44
6335	Thermodynamic modeling of the Sn-V binary system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009, 33, 539-544.	0.7	12
6336	Solution-based thermodynamic modeling of the Ni-Ta and Ni-Mo-Ta systems using first-principle calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009, 33, 631-641.	0.7	32
6337	A thermodynamic description of the Ge-Sr system acquired via a hybrid approach of CALPHAD and first-principles calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009, 33, 719-722.	0.7	7
6338	First-principles study of binary special quasirandom structures for the Al-Cu, Al-Si, Cu-Si, and Mg-Si systems. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009, 33, 769-773.	0.7	17
6339	He incorporation and diffusion pathways in pure and defective zircon ZrSiO <sub>4</sub> : A density functional theory study. <i>Chemical Geology</i> , 2009, 258, 182-196.	1.4	51
6340	First-principles study on the structural, elastic, and electronic properties of <sup>6</sup> LiAlO <sub>2</sub> . <i>Computational Materials Science</i> , 2009, 46, 221-224.	1.4	26
6341	Interfacial interactions in clay-based nylon 6 nanocomposites: A density functional theory study. <i>Computational Materials Science</i> , 2009, 46, 942-949.	1.4	6
6342	First-principles calculations of mechanical and thermodynamic properties of the Laves C15-Mg <sub>2</sub> RE (RE=La, Ce, Pr, Nd, Pm, Sm, Gd). <i>Computational Materials Science</i> , 2009, 47, 297-301.	1.4	23
6343	First-principles study of Ni/Ni <sub>3</sub> Al interface strengthening by alloying elements. <i>Computational Materials Science</i> , 2009, 47, 320-325.	1.4	43
6344	First principles study of structural phase stability of wide-gap semiconductors MgTe, MgS and MgSe. <i>Computational Materials Science</i> , 2009, 47, 593-598.	1.4	71
6345	Ab initio predictions of potassium partitioning between Fe and Al-bearing MgSiO <sub>3</sub> perovskite and post-perovskite. <i>Physics of the Earth and Planetary Interiors</i> , 2009, 174, 247-253.	0.7	7
6346	Ab initio molecular dynamics study of elasticity of akimotoite MgSiO <sub>3</sub> at mantle conditions. <i>Physics of the Earth and Planetary Interiors</i> , 2009, 173, 115-120.	0.7	14
6347	Oxide nitrides: From oxides to solids with mobile nitrogen ions. <i>Progress in Solid State Chemistry</i> , 2009, 37, 81-131.	3.9	66
6348	Thermodynamics, structure and kinetics in the system Ga-O-N. <i>Progress in Solid State Chemistry</i> , 2009, 37, 132-152.	3.9	33
6349	Structural and dynamical properties of Fe <sub>78</sub> Si <sub>9</sub> B <sub>13</sub> alloy during rapid quenching by first principles molecular dynamic simulation. <i>Journal of Non-Crystalline Solids</i> , 2009, 355, 2333-2338.	1.5	24

#	ARTICLE	IF	CITATIONS
6350	First-principles study of indium adsorption on GaP(001)(2 $\times$ 1) surface. Journal of Alloys and Compounds, 2009, 467, 557-561.	2.8	10
6351	Ti cations in sodium alanate. Journal of Alloys and Compounds, 2009, 471, L29-L31.	2.8	8
6352	X-ray photoelectron spectroscopy and full potential studies of the electronic density of state of ternary oxyborate Na <sub>3</sub> La <sub>9</sub> O <sub>3</sub> (BO <sub>3</sub> ) <sub>8</sub> . Journal of Alloys and Compounds, 2009, 472, 30-34.	2.8	5
6353	Jahn-Teller distortion and electronic structure of LiMn <sub>2</sub> O <sub>4</sub> . Journal of Alloys and Compounds, 2009, 474, 370-374.	2.8	169
6354	First-principles studies on surface electronic structure and stability of LiFePO <sub>4</sub> . Journal of Alloys and Compounds, 2009, 476, 462-465.	2.8	48
6355	Electronic and magnetic properties of Al adsorption on $\hat{\Gamma}$ -uranium (001) surface: Ab initio calculations. Journal of Alloys and Compounds, 2009, 476, 675-682.	2.8	15
6356	A first-principles study of the La-H system. Journal of Alloys and Compounds, 2009, 480, 111-113.	2.8	10
6357	On the enthalpy of formation of aluminum diboride, AlB <sub>2</sub> . Journal of Alloys and Compounds, 2009, 477, L11-L12.	2.8	15
6358	Theoretical investigation of zincblende AlSb and GaSb compounds. Journal of Alloys and Compounds, 2009, 478, 653-656.	2.8	14
6359	Copper passivation by metal doping. Journal of Alloys and Compounds, 2009, 482, 33-42.	2.8	13
6360	First-principles investigations of F and Cl impurities in NaAlH <sub>4</sub> . Journal of Alloys and Compounds, 2009, 484, 347-351.	2.8	6
6361	Crystal, electronic structures, optical and magnetic properties of Tb <sub>4</sub> Al <sub>2</sub> O <sub>9</sub> . Journal of Alloys and Compounds, 2009, 484, 943-948.	2.8	14
6362	Microstructure and electronic characteristics of the 6H-type ABACAB LPSO structure in Mg <sub>97</sub> Zn <sub>1</sub> Y <sub>2</sub> alloy. Journal of Alloys and Compounds, 2009, 485, 672-676.	2.8	24
6363	Effects of bias voltage and annealing on the structure and mechanical properties of WC <sub>0.75</sub> N <sub>0.25</sub> thin films. Journal of Alloys and Compounds, 2009, 486, 357-364.	2.8	20
6364	Stereoregularity, Regioselectivity, and Dormancy in Polymerizations Catalyzed by <i>i</i> -C <sub>1</sub> -Symmetric Fluorenyl-Based Metallocenes. A Theoretical Study Based on Density Functional Theory. Organometallics, 2009, 28, 2609-2618.	1.1	22
6365	Lithium incorporation into a silica thin film: Scanning tunneling microscopy and density functional theory. Physical Review B, 2009, 80, .	1.1	21
6366	Is Cerocene Really a Ce(III) Compound? All-Electron Spin-Orbit Coupled CASPT2 Calculations on M( $\hat{\Gamma}$ -C <sub>8</sub> H <sub>8</sub> ) <sub>2</sub> (M = Th, Pa, Ce). Journal of Physical Chemistry A, 2009, 113, 2896-2905.	1.1	72
6367	Direct to indirect band gap transition in ultrathin ZnO nanowires under uniaxial compression. Applied Physics Letters, 2009, 94, .	1.5	52

#	ARTICLE	IF	CITATIONS
6368	Structure of the Orthorhombic $\hat{I}^3$ -Phase and Phase Transitions of $\text{Ca}(\text{BD}_4)_2$ . <i>Journal of Physical Chemistry C</i> , 2009, 113, 17223-17230.	1.5	37
6369	First-principles study of two- and one-dimensional honeycomb structures of boron nitride. <i>Physical Review B</i> , 2009, 79, .	1.1	580
6370	Magnetic anisotropy from density functional calculations. Comparison of different approaches: $\text{Mn}_2\text{O}_7$ acetate as a test case. <i>Journal of Chemical Physics</i> , 2009, 130, 194109.	1.2	68
6371	Switchable Molecular Conductivity. <i>Journal of the American Chemical Society</i> , 2009, 131, 10447-10451.	6.6	23
6372	Modeling Ethanol Decomposition on Transition Metals: A Combined Application of Scaling and Brønsted-Evans-Polanyi Relations. <i>Journal of the American Chemical Society</i> , 2009, 131, 5809-5815.	6.6	275
6373	Magnetic states of zigzag graphene nanoribbons from first principles. <i>Applied Physics Letters</i> , 2009, 94, .	1.5	41
6374	Density functional characterization of the electronic structure and optical properties of Cr-doped $\text{SrTiO}_3$ . <i>Journal Physics D: Applied Physics</i> , 2009, 42, 055401.	1.3	61
6375	Translational energy and state resolved observations of D and D <sub>2</sub> thermally desorbing from D clusters chemisorbed on graphite. <i>Journal of Chemical Physics</i> , 2009, 131, 244707.	1.2	6
6376	Impurities on graphene: Midgap states and migration barriers. <i>Physical Review B</i> , 2009, 80, .	1.1	217
6377	Diffusion of adatoms and small clusters on magnesium oxide surfaces. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 264001.	0.7	22
6378	DFT Analysis of the Reaction Paths of Formaldehyde Decomposition on Silver. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8125-8131.	1.1	28
6380	Catalyzed $\hat{I}^2$ scission of a carbenium ion III. Scission observed in ab initio molecular dynamics simulations. <i>Canadian Journal of Chemistry</i> , 2009, 87, 1512-1520.	0.6	4
6381	Interaction of graphene with FCC-Co(111). <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 803-807.	1.3	53
6382	Density Functional Studies of Methanol Decomposition on Subnanometer Pd Clusters. <i>Journal of Physical Chemistry C</i> , 2009, 113, 21789-21796.	1.5	33
6383	A systematic search for minimum structures of small gold clusters $\text{Au}_n$ ( $n=2-20$ ) and their electronic properties. <i>Journal of Chemical Physics</i> , 2009, 131, 064306.	1.2	259
6384	Theoretical Studies of Palladium-Gold Nanoclusters: Pd-Au Clusters with up to 50 Atoms. <i>Journal of Physical Chemistry C</i> , 2009, 113, 9141-9152.	1.5	152
6385	Theoretical study of $\text{Cu}_{38-n}\text{Au}_n$ clusters using a combined empirical potential-density functional approach. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 10340.	1.3	41
6386	Theory of Scanning Tunneling Microscopy and Applications in Catalysis. , 0, , 97-118.		1

#	ARTICLE	IF	CITATIONS
6387	Ab initio Study on the Structural Stability and Magnetism of Metastable A3B Phases in Ni <sub>1-x</sub> Au <sub>x</sub> (Cu, Zn). <i>Journal of Applied Physics</i> , 2009, 105, 093507.	0.7	10
6388	First-principles calculations of the structural stability and magnetism of metastable A <sub>3</sub> B phases in Ni <sub>1-x</sub> Au <sub>x</sub> (Cu, Zn). <i>Physical Review B</i> , 2009, 80, 080401.	1.1	124
6389	A Methanol-Tolerant Carbon-Supported Pt <sub>1-x</sub> Au <sub>x</sub> Alloy Cathode Catalyst for Direct Methanol Fuel Cells and Its Evaluation by DFT. <i>Journal of Physical Chemistry C</i> , 2009, 113, 7461-7468.	1.5	140
6390	First-principles study of diffusion of oxygen vacancies and interstitials in ZnO. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 195403.	0.7	29
6391	Linear-scaling self-consistent implementation of the van der Waals density functional. <i>Physical Review B</i> , 2009, 79, .	1.1	151
6392	Development of interatomic potentials appropriate for simulation of solid-liquid interface properties in Al-Mg alloys. <i>Philosophical Magazine</i> , 2009, 89, 3269-3285.	0.7	120
6393	First-principles study of typical precipitates in creep resistant magnesium alloys. <i>Journal Physics D: Applied Physics</i> , 2009, 42, 125403.	1.3	25
6394	Hydrogen multicenter bonds and reversible hydrogen storage. <i>Journal of Chemical Physics</i> , 2009, 130, 114301.	1.2	23
6395	Carbon Doping of the TiO <sub>2</sub> (110) Rutile Surface. A Theoretical Study Based on DFT. <i>Chemistry of Materials</i> , 2009, 21, 1431-1438.	3.2	39
6396	Redox properties of gold-substituted zirconia surfaces. <i>Journal of Materials Chemistry</i> , 2009, 19, 710-717.	6.7	12
6397	First-Principles Analysis of NO <sub>x</sub> Adsorption on Anhydrous γ-Al <sub>2</sub> O <sub>3</sub> Surfaces. <i>Journal of Physical Chemistry C</i> , 2009, 113, 7779-7789.	1.5	28
6398	Correlation-induced anomalies and extreme sensitivity in fcc Pu. <i>Philosophical Magazine</i> , 2009, 89, 1813-1822.	0.7	12
6399	Flash and Continuous Photolysis Studies of the Thionitrosyl Complex Cr(CH <sub>3</sub> CN) <sub>5</sub> (NS) <sub>2</sub> <sup>+</sup> and the Nitric Oxide Analogs: Reactions of Nitrogen Monosulfide in Solution. <i>Inorganic Chemistry</i> , 2009, 48, 231-238.	1.9	15
6400	A theoretical study of the effects of the charge state and size of gold clusters on the adsorption and dissociation of H <sub>2</sub> . <i>Journal of Chemical Physics</i> , 2009, 130, 034701.	1.2	38
6401	Temperature of the inner-core boundary of the Earth: Melting of iron at high pressure from first-principles coexistence simulations. <i>Physical Review B</i> , 2009, 79, .	1.1	136
6402	Interface and transport properties of Fe/V/MgO/Fe and Fe/V/Fe/MgO/Fe magnetic tunneling junctions. <i>Physical Review B</i> , 2009, 79, .	1.1	20
6403	Metal- and Hydrogen-Bonding Competition during Water Adsorption on Pd(111) and Ru(0001). <i>Journal of the American Chemical Society</i> , 2009, 131, 18425-18434.	6.6	99
6404	Accurate Hartree-Fock energy of extended systems using large Gaussian basis sets. <i>Physical Review B</i> , 2009, 80, .	1.1	47

#	ARTICLE	IF	CITATIONS
6405	Crystal and electronic band structure of Cu <sub>2</sub> ZnSnX <sub>4</sub> (X=S and Se) photovoltaic absorbers: First-principles insights. Applied Physics Letters, 2009, 94, .	1.5	585
6406	Electronic structures of $\hat{\Gamma}^2$ -Si <sub>3</sub> N <sub>4</sub> (0001)/Si(111) interfaces: Perfect bonding and dangling bond effects. Journal of Applied Physics, 2009, 105, .	1.1	23
6407	Density Functional Theory Study of the Adsorption of Au Atom on Cerium Oxide: Effect of Low-Coordinated Surface Sites. Journal of Physical Chemistry C, 2009, 113, 4948-4954.	1.5	54
6408	Multiferroicity in Rare-Earth Nickelates $R<sub>2</sub>NiO<sub>3</sub>$ . Physical Review Letters, 2009, 103, 156401.	2.9	103
6409	X-ray Emission Spectroscopy To Study Ligand Valence Orbitals in Mn Coordination Complexes. Journal of the American Chemical Society, 2009, 131, 13161-13167.	6.6	135
6410	High-pressure phase transitions of ScPO <sub>4</sub> and YPO <sub>4</sub> . Physical Review B, 2009, 80, .	1.1	51
6411	Effect of magnetic state on the $\hat{\Gamma}^3$ Bain transformation path in iron: First-principles calculations of the Bain transformation path. Physical Review B, 2009, 79, .	1.1	1
6412	Calculation of the lattice constant of solids with semilocal functionals. Physical Review B, 2009, 79, .	1.1	709
6413	Theoretical and Spectroscopic Investigations of the Bonding and Reactivity of (RO) <sub>3</sub> Mn Molecules, where M = Cr, Mo, and W. Inorganic Chemistry, 2009, 48, 828-837.	1.9	8
6414	CO Adsorption on One-, Two-, and Three-Dimensional Au Clusters Supported on MgO/Ag(001) Ultrathin Films. Journal of Physical Chemistry C, 2009, 113, 10256-10263.	1.5	29
6415	Synthesis of Trimethylplatinum(IV) Complexes with <i>N,N</i> - and <i>N,O</i> -Heterocyclic Carbene Ligands and Their Reductive C <sup>α</sup> -C Elimination Reactions. Journal of the American Chemical Society, 2009, 131, 8861-8874.	6.6	41
6416	<i>ab initio</i> thermodynamic evaluation of Pd atom interaction with CeO <sub>2</sub> surfaces. Journal of Chemical Physics, 2009, 131, 084701.	1.2	51
6417	Mechanism of carbon nanotubes unzipping into graphene ribbons. Journal of Chemical Physics, 2009, 131, 031105.	1.2	107
6418	Adsorption and Reactivity of CO <sub>2</sub> on Defective Graphene Sheets. Journal of Physical Chemistry A, 2009, 113, 493-498.	1.1	110
6419	Role of exchange in density-functional theory for weakly interacting systems: Quantum Monte Carlo analysis of electron density and interaction energy. Physical Review A, 2009, 80, .	1.0	21
6420	Assessment of the $\epsilon$ -6-31+G** + LANL2DZ Mixed Basis Set Coupled with Density Functional Theory Methods and the Effective Core Potential: Prediction of Heats of Formation and Ionization Potentials for First-Row-Transition-Metal Complexes. Journal of Physical Chemistry A, 2009, 113, 9843-9851.	1.1	313
6421	Electronic and magnetic structure of Fe <sub>3</sub> GGA+U. Physical Review B, 2009, 79, .	1.1	61
6422	Influence of Pb(II) Ions on the EPR Properties of the Semiquinone Radicals of Humic Acids and Model Compounds: High Field EPR and Relativistic DFT Studies. Journal of Physical Chemistry A, 2009, 113, 14115-14122.	1.1	30

#	ARTICLE	IF	CITATIONS
6423	Molecular Dynamics Simulations of Au Penetration through Alkanethiol Monolayers on the Au(111) Surface. <i>Journal of Physical Chemistry C</i> , 2009, 113, 6360-6366.	1.5	7
6424	Structure Sensitivity of Methanol Electrooxidation on Transition Metals. <i>Journal of the American Chemical Society</i> , 2009, 131, 14381-14389.	6.6	203
6425	Temperature evolution of structure and bonding of formic acid and formate on fully oxidized and highly reduced CeO <sub>2</sub> (111). <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 11171.	1.3	61
6426	Parametrization of a reactive many-body potential for MoS <sub>2</sub> systems. <i>Physical Review B</i> , 2009, 79, .	1.1	241
6427	Molecular dynamics simulation of the effect of pH on the adsorption of rhodamine laser dyes on TiO <sub>2</sub> hydroxylated surfaces. <i>Molecular Simulation</i> , 2009, 35, 1140-1151.	0.9	15
6428	Interactions between hydrogen impurities and vacancies in Mg and Al: A comparative analysis based on density functional theory. <i>Physical Review B</i> , 2009, 80, .	1.1	109
6429	Electronic Structure Engineering via On-Plane Chemical Functionalization: A Comparison Study on Two-Dimensional Polysilane and Graphane. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16741-16746.	1.5	133
6430	First principles studies of silicon as a negative electrode material for lithium-ion batteries. <i>Canadian Journal of Physics</i> , 2009, 87, 625-632.	0.4	53
6431	Surface Concavity~Convexity Sensitive Oxidation Dynamics of Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2009, 113, 3569-3573.	1.5	4
6432	Oxygen Adsorption on Î <sup>2</sup> -Cristobalite Polymorph: Ab Initio Modeling and Semiclassical Time-Dependent Dynamics. <i>Journal of Physical Chemistry A</i> , 2009, 113, 15366-15375.	1.1	21
6433	Magnetism in graphene due to single-atom defects: dependence on the concentration and packing geometry of defects. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 196002.	0.7	96
6434	First-principles study of elastic and phonon properties of the heavy fermion compound CeMg. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 246001.	0.7	24
6435	Density Functional Characterization of the Electronic Structure and Optical Properties of N-Doped, La-Doped, and N/La-Codoped SrTiO <sub>3</sub> . <i>Journal of Physical Chemistry C</i> , 2009, 113, 15046-15050.	1.5	88
6436	Multiple adsorption of NO on cobalt-exchanged chabazite, mordenite, and ferrierite zeolites: A periodic density functional theory study. <i>Journal of Chemical Physics</i> , 2009, 131, 054101.	1.2	8
6437	Promotion of CO Oxidation on Bimetallic Au~Ag(110) Surfaces: A Combined Microscopic and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 13151-13159.	1.5	28
6438	Wall thickness of single-walled carbon nanotubes and its Young's modulus. <i>Physica Scripta</i> , 2009, 79, 025702.	1.2	27
6439	<i>Ab Initio</i> Molecular Dynamics Study of Hot Atom Dynamics after Dissociative Adsorption of $H_2$ on Pd(100). <i>Physical Review Letters</i> , 2009, 103, 246101.	2.9	52
6440	Chemical engineering of prehydrogenated C and BN-sheets by Li: Application in hydrogen storage. <i>Journal of Applied Physics</i> , 2009, 106, .	1.1	40



#	ARTICLE	IF	CITATIONS
6441	Tailoring Bicomponent Supramolecular Nanoporous Networks: Phase Segregation, Polymorphism, and Glasses at the Solid-Liquid Interface. <i>Journal of the American Chemical Society</i> , 2009, 131, 13062-13071.	6.6	134
6442	First-Principles Study of Water Chains Encapsulated in Single-Walled Carbon Nanotube. <i>Journal of Physical Chemistry C</i> , 2009, 113, 5368-5375.	1.5	45
6443	Ab initio examination of ductility features of fcc metals. <i>Physical Review B</i> , 2009, 79, .	1.1	91
6444	Density functional theory based first-principle calculation of Nb-doped anatase TiO <sub>2</sub> and its interactions with oxygen vacancies and interstitial oxygen. <i>Journal of Chemical Physics</i> , 2009, 131, 034702.	1.2	86
6445	Stable calcium adsorbates on carbon nanostructures: Applications for high-capacity hydrogen storage. <i>Physical Review B</i> , 2009, 79, .	1.1	74
6446	Electronic structure models of oxygen adsorption at the solvated, electrified Pt(111) interface. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 10108.	1.3	35
6447	Composition, structure, and stability of the rutile TiO <sub>2</sub> nanotubes. Oxygen depletion, hydroxylation, hydrogen migration, and water adsorption. <i>Physical Review B</i> , 2009, 79, .	1.1	26
6448	Ab initio calculations for the elastic properties of magnesium under pressure. <i>Physical Review B</i> , 2009, 80, .	1.1	19
6449	Ab initio DFT+U study of He atom incorporation into UO <sub>2</sub> crystals. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 7241.	1.3	72
6450	Prediction of half-metallic conductivity in Prussian Blue derivatives. <i>Journal of Materials Chemistry</i> , 2009, 19, 2032.	6.7	41
6451	Geometric and electronic characteristics of active sites on TiO <sub>2</sub> -supported Au nano-catalysts: insights from first principles. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 11006.	1.3	56
6452	Nitrogen-Treated Graphite and Oxygen Electroreduction on Pyridinic Edge Sites. <i>Journal of Physical Chemistry C</i> , 2009, 113, 6730-6734.	1.5	199
6453	Impact of Stoichiometry on the Hydrogen Storage Properties of LiNH <sub>2</sub> ·LiBH <sub>4</sub> ·MgH <sub>2</sub> Ternary Composites. <i>Journal of Physical Chemistry C</i> , 2009, 113, 2004-2013.	1.5	20
6454	Connections between the energy functional and interaction potentials for materials simulations. <i>Physical Review B</i> , 2009, 80, .	1.1	12
6455	First-principles study of defects and phase transition in UO <sub>2</sub> . <i>Journal of Physics Condensed Matter</i> , 2009, 21, 435401.	0.7	71
6456	From bare Ge nanowire to Ge/Si core/shell nanowires: A first-principles study. <i>Physical Review B</i> , 2009, 80, .	1.1	39
6457	The delicate electronic and magnetic structure of the LaFePnO system (Pn = pnictogen). <i>New Journal of Physics</i> , 2009, 11, 025004.	1.2	47
6458	Unravelling the Nature of Gold Surface Sites by Combining IR Spectroscopy and DFT Calculations. Implications in Catalysis. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16772-16784.	1.5	136



#	ARTICLE	IF	CITATIONS
6459	Density Functional Theory Study for the Stability and Ionic Conductivity of Li <sub>2</sub> O Surfaces. Journal of Physical Chemistry C, 2009, 113, 672-676.	1.5	50
6460	Density Functional Theory Comparison of Water Dissociation Steps on Cu, Au, Ni, Pd, and Pt. Journal of Physical Chemistry C, 2009, 113, 7269-7276.	1.5	257
6461	Adsorption Isotherm and Orientation of Alcohols on Hydrophilic SiO <sub>2</sub> under Ambient Conditions. Journal of Physical Chemistry C, 2009, 113, 10632-10641.	1.5	49
6462	Order and disorder in the wetting layer on Ru(0001). Faraday Discussions, 2009, 141, 231-249.	1.6	39
6463	Energetics and Vibrational Analysis of Methyl Salicylate Isomers. Journal of Physical Chemistry A, 2009, 113, 10385-10390.	1.1	23
6464	Active Sites for H <sub>2</sub> Adsorption and Activation in Au/TiO <sub>2</sub> and the Role of the Support. Journal of Physical Chemistry A, 2009, 113, 3750-3757.	1.1	142
6465	Role of Coverage and Surface Oxidation Degree in the Adsorption of Acetone on TiO <sub>2</sub> (110). A Density Functional Study. Journal of Physical Chemistry C, 2009, 113, 19973-19980.	1.5	24
6466	New Metallic Carbon Crystal. Physical Review Letters, 2009, 102, 055703.	2.9	119
6467	Interaction of CO with OH on Au(111): HCOO, CO <sub>3</sub> , and HOCO as Key Intermediates in the Water-Gas Shift Reaction. Journal of Physical Chemistry C, 2009, 113, 19536-19544.	1.5	93
6468	Three Lanthanum MOF Polymorphs: Insights into Kinetically and Thermodynamically Controlled Phases. Inorganic Chemistry, 2009, 48, 4707-4713.	1.9	56
6469	Theoretical study of PTCDA adsorbed on the coinage metal surfaces, Ag(111), Au(111) and Cu(111). New Journal of Physics, 2009, 11, 053010.	1.2	182
6470	Screened hybrid density functionals for solid-state chemistry and physics. Physical Chemistry Chemical Physics, 2009, 11, 443-454.	1.3	384
6471	Adsorption and diffusion of SCH <sub>3</sub> radicals and Au(SCH <sub>3</sub> ) <sub>2</sub> complexes on the unreconstructed Au(111) surface in the submonolayer coverage regime. Physical Review B, 2009, 79, .	1.1	18
6472	Density functional theory simulations of complex hydride and carbon-based hydrogen storage materials. Chemical Society Reviews, 2009, 38, 211-225.	18.7	107
6473	Superhard diamondlike $\langle \text{BC} \rangle_5$ $\langle \text{BC} \rangle_4$ $\langle \text{BC} \rangle_3$ $\langle \text{BC} \rangle_2$ $\langle \text{BC} \rangle_1$ $\langle \text{BC} \rangle_0$ . A first-principles investigation. Physical Review B, 2009, 80, .	1.1	24
6474	A DFT comparative study of carbon adsorption and diffusion on the surface and subsurface of Ni and Ni <sub>3</sub> Pd alloy. Physical Chemistry Chemical Physics, 2009, 11, 11546.	1.3	35
6475	<i>Ab initio</i> thermodynamics of lithium oxides: from bulk phases to nanoparticles. Nanotechnology, 2009, 20, 445703.	1.3	73
6476	Parametrization of a reactive force field for aluminum hydride. Journal of Chemical Physics, 2009, 131, 044501.	1.2	35

#	ARTICLE	IF	CITATIONS
6477	Electronic Structure and Reactivity of Boron Nitride Nanoribbons with Stone-Wales Defects. Journal of Chemical Theory and Computation, 2009, 5, 3088-3095.	2.3	127
6478	Subsurface Incorporation of Oxygen into Palladium(111): A Theoretical Study of Energetics and Kinetics. Journal of Physical Chemistry C, 2009, 113, 15326-15336.	1.5	12
6479	A density functional for sparse matter. Journal of Physics Condensed Matter, 2009, 21, 084203.	0.7	363
6480	First-principles study of zinc oxide honeycomb structures. Physical Review B, 2009, 80, .	1.1	298
6481	Structural, magnetic, and energetic properties of Na <sub>2</sub> FePO <sub>4</sub> F, Li <sub>2</sub> FePO <sub>4</sub> F, NaFePO <sub>4</sub> F, and LiFePO <sub>4</sub> F from <i>ab initio</i> calculations. Journal of Applied Physics, 2009, 106, .	1.1	26
6482	First principles study of the photo-oxidation of water on tungsten trioxide (WO <sub>3</sub> ). Journal of Chemical Physics, 2009, 130, 114701.	1.2	105
6483	Structural Properties of Tetra- <i>tert</i> -butyl Zinc(II) Phthalocyanine Isomers on a Au(111) Surface. Journal of Physical Chemistry C, 2009, 113, 11223-11227.	1.5	18
6484	Ferromagnetic Compounds for High Efficiency Photovoltaic Conversion: The Case of AlP:Cr. Physical Review Letters, 2009, 102, 227204.	2.9	48
6485	Fluorine substituent effects on dihydrogen bonding of transition metal hydrides. Physical Chemistry Chemical Physics, 2009, 11, 7231.	1.3	10
6486	Importance of Kinetics in Surface Alloying: A Comparison of the Diffusion Pathways of Pd and Ag Atoms on Cu(111). Journal of Physical Chemistry C, 2009, 113, 12863-12869.	1.5	46
6487	A benchmark theoretical study of the electronic ground state and of the singlet-triplet split of benzene and linear acenes. Journal of Chemical Physics, 2009, 131, 224321.	1.2	187
6488	Benchmark Thermochemistry of the C <sub>n</sub> H <sub>2n+2</sub> Alkane Isomers ( $n = 2\text{--}8$ ) and Performance of DFT and Composite <i>Ab Initio</i> Methods for Dispersion-Driven Isomeric Equilibria. Journal of Physical Chemistry A, 2009, 113, 8434-8447.	1.1	128
6489	Advances in atomistic simulations of mineral surfaces. Journal of Materials Chemistry, 2009, 19, 7807.	6.7	32
6490	Density functional study of aurophilic interaction in [X(AuPH <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub> (X = F, Cl, Br, I). Physical Chemistry Chemical Physics, 2009, 11, 5796.	1.3	12
6491	Ligand effect on the NMR, vibrational and structural properties of tetra- and hexanuclear ruthenium hydrido clusters: a theoretical investigation. Dalton Transactions, 2009, , 2142.	1.6	20
6492	Electronic charge transfer between ceria surfaces and gold adatoms: a GGA+U investigation. Physical Chemistry Chemical Physics, 2009, 11, 5246.	1.3	83
6493	Experimental and theoretical studies of complexes of [PbmAg] <sup>m+</sup> (m = 1–4). Physical Chemistry Chemical Physics, 2009, 11, 1043.	1.3	7
6494	±-Cr <sub>2</sub> under Pressure: Prediction of a Metallic Phase Transition. Journal of Physical Chemistry A, 2009, 113, 12022-12027.	1.1	1

#	ARTICLE	IF	CITATIONS
6495	Growth and Desorption Kinetics of Ultrathin Zn Layers on Pd(111). <i>Journal of Physical Chemistry C</i> , 2009, 113, 9788-9796.	1.5	36
6496	DFT Investigation of Intermediate Steps in the Hydrolysis of $\text{Al}_2\text{O}_3(0001)$ . <i>Journal of Physical Chemistry C</i> , 2009, 113, 2149-2158.	1.5	81
6497	Frontier Orbital Description of the Si(100) Surface: A Route to Symmetry-Allowed and Concerted [2 + 2] Cycloadditions. <i>Journal of the American Chemical Society</i> , 2009, 131, 6768-6774.	6.6	10
6498	First-Principles Study of Carbon Monoxide Oxidation on Ag(111) in Presence of Subsurface Oxygen and Stepped Ag(221). <i>Journal of Physical Chemistry C</i> , 2009, 113, 8266-8272.	1.5	27
6499	Step Effects on the Dissociation of NO on Close-Packed Rhodium Surfaces. <i>Journal of Physical Chemistry C</i> , 2009, 113, 20623-20631.	1.5	36
6500	Atomization energies of the carbon clusters $\text{C}_n$ ( $n = 2\text{--}10$ ) revisited by means of W4 theory as well as density functional, GGA, and CBS methods. <i>Molecular Physics</i> , 2009, 107, 977-990.	0.8	41
6501	DFT calculations of comparative energetics and ENDOR/Mössbauer properties for two protonation states of the iron dimer cluster of ribonucleotide reductase intermediate X. <i>Dalton Transactions</i> , 2009, , 6045.	1.6	27
6502	Electronic structure and optical properties of Nb-doped $\text{Sr}_2\text{TiO}_4$ by density function theory calculation. <i>Chinese Physics B</i> , 2009, 18, 2945-2952.	0.7	12
6503	A new phase in the decomposition of $\text{Mg}(\text{BH}_4)_2$ : first-principles simulated annealing. <i>Journal of Materials Chemistry</i> , 2009, 19, 7081.	6.7	27
6504	Mechanism of molecular hydrogen dissociation on gold chains and clusters as model prototypes of nanostructures. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 10122.	1.3	25
6505	DFT 2H quadrupolar coupling constants of ruthenium complexes: a good probe of the coordination of hydrides in conjunction with experiments. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5657.	1.3	24
6506	The 559-to-600 nm shift observed in red fluorescent protein eqFP611 is attributed to cis $\rightarrow$ trans isomerization of the chromophore in an anionic protein pocket. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 6042.	1.3	3
6507	The giant magnetic anisotropy energy of $\text{Fe}^{2+}$ ions in $\text{SrCl}_2$ . <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 7545.	1.3	12
6508	Density functional theory study of the oxoperoxo vanadium(V) complexes of glycolic acid. Structural correlations with NMR chemical shifts. <i>Dalton Transactions</i> , 2009, , 9735.	1.6	28
6509	Auto-oligomerization and hydration of pyrrole revealed by x-ray absorption spectroscopy. <i>Journal of Chemical Physics</i> , 2009, 131, 114509.	1.2	20
6510	Further investigations of linear trirhodium complexes: experimental and theoretical studies of $[\text{Rh}_3(\text{dpa})_4\text{Cl}_2]$ and $[\text{Rh}_3(\text{dpa})_4\text{Cl}_2](\text{BF}_4)$ [dpa = bis(2-pyridyl)amido anion]. <i>Dalton Transactions</i> , 2009, , 2623.	1.6	16
6511	Ensemble vs. electronic effects on the reactivity of two-dimensional Pd alloys: a comparison of CO and $\text{CH}_3\text{OH}$ adsorption on Zn/Pd(111) and Cu/Pd(111). <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 10457.	1.3	20
6512	A computational study of electronic structure, thermodynamics and kinetics of hydrogen desorption from Al- and Si-doped $\text{La}$ , $\text{La}^{3-}$ , and $\text{La}^{2-}\text{MgH}_2$ . <i>Journal of Materials Chemistry</i> , 2009, 19, 4348.	6.7	32

#	ARTICLE	IF	CITATIONS
6513	Electronic properties of pentacoordinated heme complexes in cytochrome P450 enzymes: search for an Fe(i) oxidation state. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 10219.	1.3	28
6514	Multinuclear gallium-oxide cations in high-silica zeolites. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 2893.	1.3	50
6515	Chemical and electromagnetic mechanisms of tip-enhanced Raman scattering. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 9412.	1.3	61
6516	Au nanoparticles on a templating TiO <sub>x</sub> /Pt(111) ultrathin polar film: a photoemission and photoelectron diffraction study. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 2177.	1.3	17
6517	Theoretical study of hydrogen dissociative adsorption on strained pseudomorphic monolayers of Cu and Pd deposited onto a Ru(0001) substrate. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 7303.	1.3	27
6518	Unrestricted study of the Eley-Rideal formation of H <sub>2</sub> on graphene using a new multidimensional graphene-H potential: role of the substrate. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 2715.	1.3	36
6519	Anharmonic OH vibrations in Mg(OH) <sub>2</sub> (brucite): Two-dimensional calculations and crystal-induced blueshift. <i>Journal of Chemical Physics</i> , 2009, 131, 244517.	1.2	17
6520	Atomistic Modeling of Voiding Mechanisms at Oxide/Alloy Interfaces. <i>Journal of Physical Chemistry C</i> , 2009, 113, 9978-9981.	1.5	17
6522	Theory of doping properties of Ag acceptors in ZnO. <i>Physical Review B</i> , 2009, 80, .	1.1	84
6523	Experimental and Computational Characterization. <i>Engineering Materials and Processes</i> , 2009, , 39-61.	0.2	0
6524	Changing the physical and chemical properties of titanium oxynitrides $\text{TiN}_x\text{O}_y$ by changing the composition. <i>Physical Review B</i> , 2009, 80, .	1.1	48
6525	The study of the electronic structures and properties of pure and transition metal-doped silicon nanoclusters: a density functional theory approach. <i>Molecular Simulation</i> , 2009, 35, 381-394.	0.9	14
6526	First-principles study of the interaction and charge transfer between graphene and metals. <i>Physical Review B</i> , 2009, 79, .	1.1	1,064
6527	Electronic and elastic properties of CaF <sub>2</sub> under high pressure from <i>ab initio</i> calculations. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 415501.	0.7	23
6528	Vacancy-assisted diffusion mechanism of group-III elements in ZnO: An <i>ab initio</i> study. <i>Journal of Applied Physics</i> , 2009, 105, 073504.	1.1	18
6529	Density functional theory study on hydrogenation mechanism in catalyst-activated Mg(0001) surface. <i>Transactions of Nonferrous Metals Society of China</i> , 2009, 19, 383-388.	1.7	14
6530	Naphthalene-containing polyimides: Synthesis, characterization and photovoltaic properties of novel donor-acceptor dyes used in solar cell. <i>Transactions of Nonferrous Metals Society of China</i> , 2009, 19, s587-s593.	1.7	8
6531	Abrupt Rotation of the Rashba Spin to the Direction Perpendicular to the Surface. <i>Physical Review Letters</i> , 2009, 102, 096805.	2.9	137

#	ARTICLE	IF	CITATIONS
6532	XPS study of nitrogen dioxide adsorption on metal oxide particle surfaces under different environmental conditions. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 8295.	1.3	241
6533	Effect of Pt Clusters on Methanol Adsorption and Dissociation over Perfect and Defective Anatase TiO <sub>2</sub> (101) Surface. <i>Journal of Physical Chemistry C</i> , 2009, 113, 20674-20682.	1.5	24
6534	1,3,4,6,7,9-Hexamethylbenzo[1,2-c:3,4-c'':5,6-c''']trithiophene: a twisted heteroarene. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 2748.	1.5	7
6535	<i>Ab initio</i> study on the thermal properties of the fcc Al <sub>3</sub> Mg and Al <sub>3</sub> Sc alloys. <i>Journal Physics D: Applied Physics</i> , 2009, 42, 225407.	1.3	17
6536	A first-principles study of bulk oxide formation on Pd(100). <i>Journal of Chemical Physics</i> , 2009, 131, 054701.	1.2	53
6537	Correlating Acid Properties and Catalytic Function: A First-Principles Analysis of Alcohol Dehydration Pathways on Polyoxometalates. <i>Journal of Physical Chemistry C</i> , 2009, 113, 1872-1885.	1.5	110
6538	Deriving Carbon Atomic Chains from Graphene. <i>Physical Review Letters</i> , 2009, 102, 205501.	2.9	571
6539	Structure and electronic properties of iron oxide clusters: A first-principles study. <i>Physical Review B</i> , 2009, 80, .	1.1	40
6540	Ca-Coated Boron Fullerenes and Nanotubes as Superior Hydrogen Storage Materials. <i>Nano Letters</i> , 2009, 9, 1944-1948.	4.5	165
6541	Experimental and Density Functional Theory Study of the Tribochemical Wear Behavior of SiO <sub>2</sub> in Humid and Alcohol Vapor Environments. <i>Langmuir</i> , 2009, 25, 13052-13061.	1.6	89
6542	Dislocation theory of chirality-controlled nanotube growth. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 2506-2509.	3.3	297
6543	<i>Ab initio</i> calculations of elastic properties of bcc Fe-Mg and Fe-Cr random alloys. <i>Physical Review B</i> , 2009, 79, .	1.1	73
6544	Theoretical investigation of Hf and Zr defects in c-Ge. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 012206.	0.7	0
6545	First Principles Study on Intrinsic Vacancies in Cubic and Orthorhombic CaTiO <sub>3</sub> . <i>Materials Transactions</i> , 2009, 50, 977-983.	0.4	30
6546	Selective Ionization of 2,4-Xylenol in Mass Spectrometry Using a Tunable Laser and Supersonic Jet Technique. <i>Analytical Sciences</i> , 2009, 25, 599-604.	0.8	11
6547	Micropreparative isolation of Cu(II) complexes of isoniazid and ethambutol and determination of their structures. <i>Journal of Planar Chromatography - Modern TLC</i> , 2009, 22, 83-88.	0.6	5
6548	Stability of ferromagnetic phase in Fe-doped AlH <sub>3</sub> . <i>Europhysics Letters</i> , 2009, 85, 67006.	0.7	3
6549	Stable structure and effects of the substrate Ti pre-treatment on the epitaxial growth of SrTiO <sub>3</sub> on GaAs. <i>Europhysics Letters</i> , 2009, 86, 46008.	0.7	15

#	ARTICLE	IF	CITATIONS
6550	Ab initio quantum chemical calculation as a tool of evaluating diamagnetic susceptibility of magnetically levitating substances. <i>Journal of Physics: Conference Series</i> , 2009, 156, 012022.	0.3	0
6551	Density-Functional-Theory-Based Finite-Element Analysis of Diamond Single Crystal. <i>Journal of Solid Mechanics and Materials Engineering</i> , 2009, 3, 541-551.	0.5	3
6553	Structural stability and decomposition of Mg(BH <sub>4</sub> ) <sub>2</sub> isomorphs. <i>Ab initio free energy study. Journal of Physics Condensed Matter</i> , 2009, 21, 012203.	0.7	57
6554	A Periodic Density Functional Theory Analysis of CO Chemisorption on Pt(111) in the Presence of Uniform Electric Fields. <i>Journal of Physical Chemistry A</i> , 2009, 113, 4125-4133.	1.1	51
6555	Dissociation and thermochemistry of methylsilylanitrile and silylsilylanitrile: implications for the chemistry of silicon in interstellar medium. <i>Molecular Physics</i> , 2009, 107, 157-164.	0.8	0
6556	Electronic Structure of Anthocyanidins Adsorbed on Buckminsterfullerene: First Principles Studies. <i>Journal of the Chinese Chemical Society</i> , 2010, 57, 1212-1216.	0.8	2
6557	Alternating layers of plutonium and lead or indium as surrogate for plutonium. <i>IOP Conference Series: Materials Science and Engineering</i> , 2010, 9, 012098.	0.3	0
6558	Ab Initio Calculations of Crystalline and Amorphous In <sub>2</sub> Se <sub>3</sub> Compounds for Chalcogenide Phase Change Memory. <i>Materials Research Society Symposia Proceedings</i> , 2010, 1251, 34.	0.1	0
6559	Magnetoelastic study in Lu <sub>2</sub> Fe <sub>17</sub> . <i>Journal of Physics: Conference Series</i> , 2010, 200, 022004.	0.3	0
6560	Minimum Energy Motion and Core Structure of Pure Edge and Screw Dislocations in Aluminum. <i>Journal of Computational Science and Technology</i> , 2010, 4, 185-193.	0.4	5
6561	Ab Initio Molecular Dynamics Study of Fe Adsorption on TiN (001) Surface. <i>Materials Transactions</i> , 2010, 51, 2005-2008.	0.4	8
6562	Effect of Zn on the adsorption of CO on Pd(111). <i>Journal of Chemical Physics</i> , 2010, 133, 214702.	1.2	12
6563	Theoretical studies on electronic and magnetic properties of ultrathin Mo nanowires. <i>Journal of Applied Physics</i> , 2010, 107, 024307.	1.1	3
6564	Ab initio study on pressure-induced change of effective Coulomb interaction in superconducting yttrium. <i>Applied Physics Letters</i> , 2010, 96, .	1.5	5
6565	Energetics of Pb heterostructures formation on the Cu (111) in the early stage of the deposition process. <i>Journal of Applied Physics</i> , 2010, 107, 114315.	1.1	3
6566	On Occupied-orbital Dependent Exchange-correlation Functionals: From Local Hybrids to Becke's B05 Model. <i>Zeitschrift Fur Physikalische Chemie</i> , 2010, 224, 545-567.	1.4	8
6567	Influence of gallium (and aluminum) substituted in monoclinic $\beta$ plutonium: A possible structural change induced with increasing content of alloying element. <i>IOP Conference Series: Materials Science and Engineering</i> , 2010, 9, 012085.	0.3	2
6568	Density Functional Theory Study of Gas Phase Hydrolysis of Titanium Tetrachloride. <i>Bulletin of the Chemical Society of Japan</i> , 2010, 83, 1030-1036.	2.0	12



#	ARTICLE	IF	CITATIONS
6569	Estimation of linear thermal expansion coefficient from cohesive energy obtained by ab-initio calculation of metals and ceramics. Journal of the Ceramic Society of Japan, 2010, 118, 241-245.	0.5	17
6570	Melting of MgO Studied Using a Multicanonical Ensemble Method Combined with a First-Principles Calculation. Journal of the Physical Society of Japan, 2010, 79, 034602.	0.7	9
6571	Stabilization Mechanism of Vacancies in Group-III Nitrides: Exchange Splitting and Electron Transfer. Journal of the Physical Society of Japan, 2010, 79, 083705.	0.7	9
6572	Electronic Structures of Tungsten and Molybdenum Carbides as a Fuel Cell Anode Catalyst. Bulletin of the Chemical Society of Japan, 2010, 83, 1501-1503.	2.0	9
6573	Study of H:Si(113)2 $\times$ 2 Structure by Scanning Tunneling Microscopy and <i>Ab Initio</i> Calculation. E-Journal of Surface Science and Nanotechnology, 2010, 8, 261-265.	0.1	2
6574	Interactions of Hydrogen with Solid Surfaces. Journal of the Vacuum Society of Japan, 2010, 53, 592-601.	0.3	2
6575	Ab initio investigation of the clustering of carbon adatoms on Fe(001) and Fe(111) surfaces. Journal of Experimental and Theoretical Physics, 2010, 110, 81-87.	0.2	1
6576	Effect of hydrogen impurity atoms and molecules on the atomic structure of palladium nanocontacts. Physics of the Solid State, 2010, 52, 641-648.	0.2	9
6577	Electronic structure and adhesion on metal-aluminum-oxide interfaces. Physics of the Solid State, 2010, 52, 2589-2595.	0.2	16
6578	Stability of FeAl(110) alloy surface structures: a first-principles study. European Physical Journal B, 2010, 73, 367-373.	0.6	8
6579	Magnetism-induced ballistic conductance changes in palladium nanocontacts. European Physical Journal B, 2010, 75, 57-64.	0.6	9
6580	Electronic structure and magnetic coupling in CaV2O5: spin dimer versus spin ladder. European Physical Journal B, 2010, 75, 179-185.	0.6	2
6581	Atomic and electronic properties of tert-butanol on the Si(001)-(2 $\times$ 1) surface. European Physical Journal B, 2010, 76, 359-363.	0.6	2
6582	The main factors influencing the O vacancy formation on the Ir doped ceria surface: A DFT+U study. European Physical Journal B, 2010, 77, 373-380.	0.6	20
6583	Adsorption and co-adsorption of CH <sub>3</sub> and H on flat and defective nickel (111) surfaces. European Physical Journal B, 2010, 78, 353-358.	0.6	13
6584	Real-space calculations of atomic and molecular polarizabilities using asymptotically correct exchange-correlation potentials. Physical Review A, 2010, 82, .	1.0	8
6585	Heterogeneous nucleation of solid Al from the melt by $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{Al} \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:mtext} \rangle$ Molecular dynamics simulations. Physical Review B, 2010, 82, .	1.1	39
6586	Greatly facilitated oxygen vacancy formation in ceria nanocrystallites. Chemical Communications, 2010, 46, 5936.	2.2	160



#	ARTICLE	IF	CITATIONS
6587	Wurtzite-derived polytypes of kesterite and stannite quaternary chalcogenide semiconductors. Physical Review B, 2010, 82, .	1.1	259
6588	Ultrafast ionization and fragmentation of molecular silane. Physical Review A, 2010, 82, .	1.0	20
6589	Two-component relativistic density functional theory modeling of the adsorption of element 114(eka-lead) on gold. Physical Chemistry Chemical Physics, 2010, 12, 4152.	1.3	28
6590	Mechanism of Hydrodeoxygenation of Acrolein on a Cluster Model of MoO <sub>3</sub> . Journal of Physical Chemistry C, 2010, 114, 13782-13795.	1.5	76
6591	Origin of $\mu$ magn in II-VI and III-V semiconductors by substitutional doping at anion site. Physical Review B, 2010, 81, .		
6592	Electronic structure calculations with the Tran-Blaha modified Becke-Johnson density functional. Physical Review B, 2010, 82, .	1.1	292
6593	Novel properties of graphene nanoribbons: a review. Journal of Materials Chemistry, 2010, 20, 8207.	6.7	369
6594	DFT-Based Coverage-Dependent Model of Pt-Catalyzed NO Oxidation. ChemCatChem, 2010, 2, 1450-1460.	1.8	91
6595	Hydrogenation Reactions on Au/TiC(001): Effects of Au <sub>2</sub> C Interactions on the Dissociation of H <sub>2</sub> . ChemCatChem, 2010, 2, 1219-1222.	1.8	39
6596	Atomistic models of hydrogenated amorphous silicon nitride from first principles. Physical Review B, 2010, 82, .	1.1	22
6597	Electronic and magnetic structure of bulk cobalt: The $\hat{1}\pm$ , $\hat{1}^2$ , and $\hat{1}\mu$ -phases from density functional theory calculations. Journal of Chemical Physics, 2010, 133, 024701.	1.2	83
6598	Crystal and electronic structures of lithium fluorosulphate based materials for lithium-ion batteries. Physical Review B, 2010, 82, .	1.1	24
6599	First-principles studies of electronic, optical, and vibrational properties of LaVO <sub>4</sub> polymorph. Journal of Applied Physics, 2010, 108, .	1.1	59
6600	Crystal Structures and Thermodynamic Investigations of LiK(BH <sub>4</sub> ) <sub>2</sub> , KBH <sub>4</sub> , and NaBH <sub>4</sub> from First-Principles Calculations. Journal of Physical Chemistry C, 2010, 114, 678-686.	1.5	56
6602	First-principles study of iron segregation into silicon $\sim 5$ grain boundary. Journal of Applied Physics, 2010, 107, 093713.	1.1	10
6603	Competing structural ordering tendencies in Heusler-type alloys with high Curie temperatures: $\text{Fe}_{2\text{Mn}}\text{M}_2\text{M}'\text{M}''$ . Physical Review B, 2010, 82, .	1.1	27
6604	Structure and Bonding of $\hat{1}^3\text{-B}_{28}$ : Is the High Pressure Form of Elemental Boron Ionic?. Inorganic Chemistry, 2010, 49, 11270-11275.	1.9	20
6605	Titania-water interactions: a review of theoretical studies. Journal of Materials Chemistry, 2010, 20, 10319.	6.7	255

#	ARTICLE	IF	CITATIONS
6606	Applying ultra-accelerated quantum chemical molecular dynamics technique for the evaluation of ligand protein interactions. <i>Medicinal Chemistry Research</i> , 2010, 19, 1-10.	1.1	4
6607	Density functional calculations of potential energy surface and charge transfer integrals in molecular triphenylene derivative HAT6. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 445-451.	0.5	10
6608	Quantum cluster size and solvent polarity effects on the geometries and Mössbauer properties of the active site model for ribonucleotide reductase intermediate X: a density functional theory study. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 305-317.	0.5	23
6609	Structure and bonding of ethoxy species adsorbed on transition metal surfaces. <i>Theoretical Chemistry Accounts</i> , 2010, 126, 223-229.	0.5	8
6610	Structural and optical properties of a neutral Nickel bisdithiolene complex: density functional versus ab initio methods. <i>Theoretical Chemistry Accounts</i> , 2010, 126, 243-255.	0.5	15
6611	Transport properties of chrysazine-type molecules. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 535-541.	0.5	1
6612	Charge state of metal atoms on oxide supports: a systematic study based on simulated infrared spectroscopy and density functional theory. <i>Theoretical Chemistry Accounts</i> , 2010, 126, 265-273.	0.5	17
6613	Adsorption of tetralin and hydrogenated intermediates and products on the (100) surfaces of Ir, Pt and Pd: a DFT study. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 401-409.	0.5	11
6614	Modulation of the work function of silicon nanowire by chemical surface passivation: a DFT study. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 689-695.	0.5	25
6615	The effects of the introduction of Al atom into monoclinic BiVO <sub>4</sub> : a theoretical prediction. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 751-757.	0.5	21
6616	Effects of carbon on the weak ferromagnetism in doped GaN. <i>Chemical Physics Letters</i> , 2010, 487, 251-255.	1.2	24
6617	Structural and electronic properties of the fully hydrogenated boron nitride sheets and nanoribbons: Insight from first-principles calculations. <i>Chemical Physics Letters</i> , 2010, 488, 67-72.	1.2	60
6618	Spin and band-gap engineering in copper-doped BN sheet. <i>Chemical Physics Letters</i> , 2010, 491, 203-207.	1.2	28
6619	Investigation of ferromagnetism in Al-doped 4H-β-SiC by density functional theory. <i>Chemical Physics Letters</i> , 2010, 496, 276-279.	1.2	29
6620	First principles mechanistic study of borohydride oxidation over the Pt(111) surface. <i>Electrochimica Acta</i> , 2010, 55, 1175-1183.	2.6	66
6621	Spectroscopic and electrochemical properties of heteroleptic cationic copper complexes bis-(diphenylphosphino)alkane-(2,2'-biquinoline)copper(I). Crystal structure of bis(diphenylphosphino)ethane-(2,2'-biquinoline)copper(I) perchlorate. <i>Inorganica Chimica Acta</i> , 2010, 363, 3809-3816.	1.2	12
6622	Understanding the cubic AlN growth plane from first principles. <i>Journal of Crystal Growth</i> , 2010, 312, 2892-2895.	0.7	4
6623	Hydrogenography of Mg Ni <sup>1/2</sup> H gradient thin films: Interplay between the thermodynamics and kinetics of hydrogenation. <i>Acta Materialia</i> , 2010, 58, 658-668.	3.8	29

#	ARTICLE	IF	CITATIONS
6624	Vibrational spectra and structures of urazole and 4-methylurazole: DFT calculations of the normal modes in aqueous solution and in the solid state, and the influence of hydrogen bonding. <i>Chemical Physics</i> , 2010, 373, 219-227.	0.9	7
6625	Thermochemical properties, electronic structure and bonding of mixed lithium boron clusters (BnLi). <i>Tj ETQq1 1 0.784314 rgBT /Over</i>	0.9	38
6626	Dopings in the transition-metal aluminides OsAl <sub>2</sub> to obtain materials with high spin polarization: A first-principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2010, 374, 4909-4914.	0.9	5
6627	Experimental (FT-IR and FT-RS) and theoretical (DFT) studies of molecular structure and internal modes of [Mn(NH <sub>3</sub> ) <sub>6</sub> ](NO <sub>3</sub> ) <sub>2</sub> . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 77, 402-410.	2.0	16
6628	Effects of oxygen vacancy on adhesion of incoherent metal/oxide interface by first-principles calculations. <i>Surface Science</i> , 2010, 604, 196-200.	0.8	6
6629	Density-functional study of the CO adsorption on the ferromagnetic fcc Co(001) film surface. <i>Surface Science</i> , 2010, 604, 265-268.	0.8	4
6630	When does static correlation scale to the high-density limit as exchange does?. <i>Computational and Theoretical Chemistry</i> , 2010, 943, 19-22.	1.5	8
6631	Magnetic, bonding and structural behavior of Ru <sub>12</sub> and Ru <sub>13</sub> clusters: Is Ru <sub>12</sub> magic?. <i>Computational and Theoretical Chemistry</i> , 2010, 954, 109-114.	1.5	12
6632	DFT study of the Jahn-Teller effect in Cu(II) chelate complexes. <i>Computational and Theoretical Chemistry</i> , 2010, 954, 80-85.	1.5	17
6633	Towards a rational design of enantioselective heterogeneous catalysts: Modeling of chiral organotin precursors. <i>Computational and Theoretical Chemistry</i> , 2010, 953, 91-97.	1.5	4
6634	Density functional study of CO binding on small Ag <sub>n</sub> Pd <sub>m</sub> clusters. <i>Computational and Theoretical Chemistry</i> , 2010, 955, 66-70.	1.5	10
6635	Structural, electronic, and magnetic properties of (n+m=5) clusters. <i>Computational and Theoretical Chemistry</i> , 2010, 957, 26-30.	1.5	6
6636	Surface electronic structure of Ti-covered W(111) by photofield emission. <i>Ultramicroscopy</i> , 2010, 111, 5-10.	0.8	0
6637	Reaction of enamines with trifluoromethyl containing carbonyl reagents. <i>Journal of Fluorine Chemistry</i> , 2010, 131, 190-199.	0.9	2
6638	Atomistic properties of helium in hcp titanium: A first-principles study. <i>Journal of Nuclear Materials</i> , 2010, 402, 55-59.	1.3	18
6639	Comparison of empirical interatomic potentials for iron applied to radiation damage studies. <i>Journal of Nuclear Materials</i> , 2010, 406, 19-38.	1.3	217
6640	Ab initio interionic potentials for UN by multiple lattice inversion. <i>Journal of Nuclear Materials</i> , 2010, 404, 6-8.	1.3	7
6641	Development of a pair potential for Fe-He by lattice inversion. <i>Journal of Nuclear Materials</i> , 2010, 405, 156-159.	1.3	21

#	ARTICLE	IF	CITATIONS
6642	First principles study of intrinsic defects in hexagonal tungsten carbide. <i>Journal of Nuclear Materials</i> , 2010, 406, 323-329.	1.3	22
6643	Vacancy formation and solid solubility in the Uâ€“Zrâ€“N system. <i>Journal of Nuclear Materials</i> , 2010, 406, 351-355.	1.3	9
6644	Theoretical study of the Pb(II)â€“catechol system in dilute aqueous solution: Complex structure and metal coordination sphere determination. <i>Journal of Molecular Structure</i> , 2010, 969, 88-96.	1.8	6
6645	Phase stability comparison by first principle calculation and experimental observation of microstructure evolution in a Mgâ€“6Gdâ€“2Zn(wt%) alloy. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2010, 527, 2643-2648.	2.6	8
6646	Bonding and electronic structures in W@Au <sub>12</sub> AE complexes (AE= NO <sup>+</sup> , CO, BF, CNâ€“, or BOâ€“): analogies among ligands isoelectronic to carbon monoxide. <i>Journal of Molecular Modeling</i> , 2010, 16, 9-16.	0.8	10
6647	Combined DFT and NBO study on the electronic basis of Siâ€“N-â€“donor bond. <i>Journal of Molecular Modeling</i> , 2010, 16, 437-446.	0.8	13
6648	Computational and QSAR study of the alkylnaphthyl ketones adsorption on silver-ion stationary phase. <i>Journal of Molecular Modeling</i> , 2010, 16, 513-522.	0.8	4
6649	Theoretical study of hydrogen bonding interactions on MDI-based polyurethane. <i>Journal of Molecular Modeling</i> , 2010, 16, 1391-1399.	0.8	75
6650	Electrochemical reactions at the electrode/solution interface: Theory and applications to water electrolysis and oxygen reduction. <i>Science China Chemistry</i> , 2010, 53, 543-552.	4.2	11
6651	First principles studies on the electronics structures of (Li <sup>1-x</sup> Me <sup>x</sup> )FePO <sub>4</sub> (Me=Na and Be). <i>Science Bulletin</i> , 2010, 55, 3222-3227.	1.7	7
6652	First-principle study on NiSn <sub>0.5</sub> Ti <sub>0.5</sub> phase as electrode materials for lithium ion battery. <i>Science Bulletin</i> , 2010, 55, 3113-3117.	1.7	3
6653	Effect of Nb on plasticity and oxidation behavior of TiAlNb intermetallic compound by density functional theory. <i>Central South University</i> , 2010, 17, 674-682.	0.5	8
6654	Prediction of Glass-Forming Compositions in Metallic Systems: Copper-Based Bulk Metallic Glasses in the Cu-Mg-Ca System. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2010, 41, 1699-1705.	1.1	25
6655	Theory Study of AlCl Disproportionation Reaction Mechanism on Al (110) Surface. <i>Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science</i> , 2010, 41, 137-145.	1.0	7
6656	Weakening of the Cu/Cu <sub>3</sub> Sn(100) Interface by Bi Impurities. <i>Journal of Electronic Materials</i> , 2010, 39, 1277-1282.	1.0	11
6657	Influences of H on the Adsorption of a Single Ag Atom on Si(111)-7x7 Surface. <i>Nanoscale Research Letters</i> , 2010, 5, 143-148.	3.1	4
6658	On the Chemical Origin of the Gap Bowing in (GaAs) <sub>1-x</sub> Ge <sub>2x</sub> Alloys: A Combined DFTâ€“QSGW Study. <i>Nanoscale Research Letters</i> , 2010, 5, 469-477.	3.1	22
6659	Theoretical Investigations into Self-Organized Ordered Metallic Semi-Clusters Arrays on Metallic Substrate. <i>Nanoscale Research Letters</i> , 2010, 5, 1020-1026.	3.1	2

#	ARTICLE	IF	CITATIONS
6660	Structural Growth Sequences and Electronic Properties of Lanthanum-Doped-Gold Clusters. <i>Journal of Cluster Science</i> , 2010, 21, 701-711.	1.7	7
6661	Bimetallic Cobalt/Rhenium Systems: Preferred Position of Rhenium Through an Interdisciplinary Approach. <i>Catalysis Letters</i> , 2010, 135, 21-25.	1.4	11
6662	A first principles investigation of isotactic polypropylene. <i>Journal of Materials Science</i> , 2010, 45, 443-447.	1.7	19
6663	Effect of interface structure on the Ru on HfO <sub>2</sub> work function. <i>Journal of Materials Science</i> , 2010, 45, 4924-4928.	1.7	2
6664	2-Propylamino-5-[4-(2-hydroxy-3,5-dichlorobenzylideneamino) phenyl]-1,3,4-thiadiazole: X-ray and DFT-calculated structures. <i>Structural Chemistry</i> , 2010, 21, 59-65.	1.0	5
6665	First-principles study of electronic structure, absorption spectra, and thermodynamic properties of crystalline 1H-tetrazole and its substituted derivatives. <i>Structural Chemistry</i> , 2010, 21, 847-854.	1.0	16
6666	Different coordination modes of the dimethyldisulfide ligand in trimethylplatinum(IV) complexes. <i>Transition Metal Chemistry</i> , 2010, 35, 19-25.	0.7	1
6667	Theoretical Prediction and Experimental Verification of Stability of Pt <sup>3d</sup> -Pt Subsurface Bimetallic Structures: From Single Crystal Surfaces to Polycrystalline Films. <i>Topics in Catalysis</i> , 2010, 53, 338-347.	1.3	19
6668	Establishing Relationships Between the Geometric Structure and Chemical Reactivity of Alloy Catalysts Based on Their Measured Electronic Structure. <i>Topics in Catalysis</i> , 2010, 53, 348-356.	1.3	60
6669	DFT Versus the "Real World" (or, Waiting for Godft). <i>Topics in Catalysis</i> , 2010, 53, 417-422.	1.3	23
6670	Water Adsorption on TiO <sub>2</sub> . <i>Topics in Catalysis</i> , 2010, 53, 423-430.	1.3	100
6671	An approach based on Density Functional Theory (DFT) calculations to assess the <i>Candida antarctica</i> lipase B selectivity in rutin, isoquercitrin and quercetin acetylation. <i>Journal of Molecular Catalysis B: Enzymatic</i> , 2010, 66, 325-331.	1.8	21
6672	High-pressure meta-stable phase of BeO: A first principle study. <i>Materials Chemistry and Physics</i> , 2010, 124, 768-772.	2.0	7
6673	First-principles calculations of twin-boundary and stacking-fault energies in magnesium. <i>Scripta Materialia</i> , 2010, 62, 646-649.	2.6	141
6674	First-principles understanding of environmental embrittlement of the Ni/Ni <sub>3</sub> Al interface. <i>Scripta Materialia</i> , 2010, 63, 391-394.	2.6	27
6675	Ab initio study of the bonding and elastic properties of Ti <sub>2</sub> CdC. <i>Solid State Sciences</i> , 2010, 12, 144-147.	1.5	31
6676	First-principles study of structural, elastic, electronic and optical properties of perovskites XCaH <sub>3</sub> (X=Cs and Rb) under pressure. <i>Solid State Sciences</i> , 2010, 12, 587-596.	1.5	22
6677	First-principles comparative study of multiferroic compound PbVO <sub>3</sub> . <i>Solid State Sciences</i> , 2010, 12, 938-945.	1.5	21

#	ARTICLE	IF	CITATIONS
6678	The thermal properties of Al <sup>TM</sup> Mg <sup>TM</sup> (TM=Sc, Zr): Ab initio study. Solid State Sciences, 2010, 12, 845-850.	1.5	4
6679	Chemical bonding and elastic properties of Ti <sub>3</sub> AC <sub>2</sub> phases (A=Si, Ge, and Sn): A first-principle study. Solid State Sciences, 2010, 12, 1220-1225.	1.5	57
6680	First-principles study of structural, elastic, electronic and optical properties of rutile GeO <sub>2</sub> and $\hat{1}\pm$ -quartz GeO <sub>2</sub> . Solid State Sciences, 2010, 12, 1748-1755.	1.5	84
6681	A new chromium (III) complex containing N-(2-pyridylmethyl)-2-pyrazinecarboxamide, (NPyPzCa): Synthesis, molecular and crystal structure and theoretical electron density analysis. Solid State Sciences, 2010, 12, 1960-1965.	1.5	3
6682	Effects of Ta content on the phase stability and elastic properties of $\hat{1}^2$ Ti <sup>TM</sup> Ta alloys from first-principles calculations. Solid State Sciences, 2010, 12, 2120-2124.	1.5	25
6683	Descriptors controlling the catalytic activity of metallic surfaces toward water splitting. Journal of Catalysis, 2010, 276, 92-100.	3.1	86
6684	Cell volume effect on the ferroelectric stability of perovskite oxides pbtio <sub>3</sub> and batio <sub>3</sub> from first principle calculation. Chinese Journal of Chemistry, 2010, 21, 1130-1132.	2.6	4
6685	Tuning Adsorption via Strain and Vertical Ligand Effects. ChemPhysChem, 2010, 11, 1518-1524.	1.0	79
6686	Mechanism of Charging of Au Atoms and Nanoclusters on Li Doped SiO <sub>2</sub> /Mo(112) Films. ChemPhysChem, 2010, 11, 412-418.	1.0	14
6687	Ab Initio Molecular Dynamics Simulations of the Adsorption of H <sub>2</sub> on Palladium Surfaces. ChemPhysChem, 2010, 11, 1374-1381.	1.0	48
6688	Theoretical Investigations of the Oxygen Reduction Reaction on Pt(111). ChemPhysChem, 2010, 11, 2779-2794.	1.0	200
6689	Segregation into Layers: A General Problem for Structural Instability under Pressure, Exemplified by SnH <sub>4</sub> . ChemPhysChem, 2010, 11, 3105-3112.	1.0	14
6690	Glycine Dimers: Structure, Stability, and Medium Effects. ChemPhysChem, 2010, 11, 3499-3504.	1.0	38
6691	DFT study of the full catalytic cycle for the propene hydroformylation catalyzed by a heterobimetallic HPt(SnCl <sub>3</sub> )(PH <sub>3</sub> ) <sub>2</sub> model catalyst. Journal of Computational Chemistry, 2010, 31, 1986-2000.	1.5	13
6692	Conformational behavior of simple furanosides studied by optical rotation. Journal of Computational Chemistry, 2010, 31, 2213-2224.	1.5	10
6693	Substituent Effects on Structural, Electronic, and Redox Properties of Bis( <i>N</i> -alkyl-2-oxo-1-naphthalidiminato)copper(II) Complexes Revisited: Inequivalence in Solid and Solution State Structures by Electronic Spectroscopy and X-ray Diffraction Explained by DFT. European Journal of Inorganic Chemistry, 2010, 2010, 1373-1380.	1.0	10
6694	Room-Temperature Ferromagnetic Silver Vanadium Oxide (Ag <sub>1.2</sub> V <sub>3</sub> O <sub>8</sub> ): A Magnetic Semiconductor Nanoring Structure. Advanced Functional Materials, 2010, 20, 3666-3672.	7.8	33
6696	One-Dimensional Ferromagnetically Coupled Bimetallic Chains Constructed with <i>trans</i> -[Ru(acac) <sub>2</sub> (CN) <sub>2</sub> ] <sup>+</sup> : Syntheses, Structures, Magnetic Properties, and Density Functional Theoretical Study. Chemistry - A European Journal, 2010, 16, 3524-3535.	1.7	73



#	ARTICLE	IF	CITATIONS
6697	Probing the Electronic Effect of Carbon Nanotubes in Catalysis: $\text{NH}_3$ Synthesis with Ru Nanoparticles. <i>Chemistry - A European Journal</i> , 2010, 16, 5379-5384.	1.7	164
6698	Aggregation and Contingent Metal/Surface Reactivity of 1,3,8,10-tetraazaperopyrene (TAPP) on Cu(111). <i>Chemistry - A European Journal</i> , 2010, 16, 2079-2091.	1.7	89
6699	Spin Coupling in Roussin's Red and Black Salts. <i>Chemistry - A European Journal</i> , 2010, 16, 10397-10408.	1.7	32
6700	Phenakite-type $\text{BeP}_2\text{N}_4$ : A Possible Precursor for a New Hard Spinel-type Material. <i>Chemistry - A European Journal</i> , 2010, 16, 7208-7214.	1.7	34
6701	Olefin Epoxidation by $\text{H}_2\text{O}_2/\text{MeCN}$ Catalysed by Cyclopentadienyloxidotungsten(VI) and Molybdenum(VI) Complexes: Experiments and Computations. <i>Chemistry - A European Journal</i> , 2010, 16, 9572-9584.	1.7	71
6702	Modular, Homochiral, Porous Coordination Polymers: Rational Design, Enantioselective Guest Exchange Sorption and Ab Initio Calculations of Host-Guest Interactions. <i>Chemistry - A European Journal</i> , 2010, 16, 10348-10356.	1.7	67
6703	Dynamic Calcium Metal-Organic Framework Acts as a Selective Organic Solvent Sponge. <i>Chemistry - A European Journal</i> , 2010, 16, 11632-11640.	1.7	53
6704	Unexpected Deformations Induced by Surface Interaction and Chiral Self-Assembly of $\text{Co}^{\text{II}}$ -Tetraphenylporphyrin ( $\text{Co}^{\text{II}}$ -TPP) Adsorbed on Cu(110): A Combined STM and Periodic DFT Study. <i>Chemistry - A European Journal</i> , 2010, 16, 11641-11652.	1.7	48
6708	Ferroelectricity in Perovskites with $\text{A}^{\text{B}}$ -Site Cations: Toward Near-Room-Temperature Multiferroics. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 1603-1606.	7.2	22
6709	Reduction of a Metal-Organic Framework by an Organometallic Complex: Magnetic Properties and Structure of the Inclusion Compound $[(\text{I}^{\text{V}}\text{Co}_5\text{H}_5)_2\text{Co}_{0.5}]@ \text{MIL-47(V)}$ . <i>Angewandte Chemie - International Edition</i> , 2010, 49, 6212-6215.	7.2	62
6710	The Interplay between Structure and CO Oxidation Catalysis on Metal-Supported Ultrathin Oxide Films. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 4418-4421.	7.2	191
6711	A comparison of experimental and DFT calculations of $^{195}\text{Pt}$ NMR shielding trends for $[\text{PtX}_n\text{Y}_6]^{2+}$ ( $X, Y = \text{Cl}, \text{Br}, \text{F}$ and $\text{I}$ ) anions. <i>Magnetic Resonance in Chemistry</i> , 2010, 48, S38-S47.	1.1	33
6712	Determination of the geometry of acetoxyendynes and acetoxyenyynes by NMR heteronuclear $^{13}\text{C}$ - $^1\text{H}$ scalar couplings and $^{13}\text{C}$ NMR chemical shifts. Structural assignment of the oxylipin natural products peyssonenyynes A and B. <i>Magnetic Resonance in Chemistry</i> , 2010, 48, 543-549.	1.1	12
6713	First-principles calculations of NMR parameters for phosphate materials. <i>Magnetic Resonance in Chemistry</i> , 2010, 48, S142-S150.	1.1	28
6714	Probing the stereo-electronic properties of cationic rhodium complexes bearing chiral diphosphine ligands by $^{103}\text{Rh}$ NMR. <i>Magnetic Resonance in Chemistry</i> , 2010, 48, 848-856.	1.1	16
6715	Spatial and electronic structure of the Ni <sub>3</sub> P surface. <i>Applied Surface Science</i> , 2010, 256, 7692-7695.	3.1	11
6716	Preparation, electronic structure, and photocatalytic properties of Bi <sub>2</sub> O <sub>2</sub> CO <sub>3</sub> nanosheet. <i>Applied Surface Science</i> , 2010, 257, 172-175.	3.1	171
6717	Effect of cation doping on lattice and grain boundary diffusion in superplastic yttria-stabilized tetragonal zirconia. <i>Journal of the European Ceramic Society</i> , 2010, 30, 657-668.	2.8	17



#	ARTICLE	IF	CITATIONS
6718	Detailed first-principles models of hydrogen permeation through PdCu-based ternary alloys. <i>Journal of Membrane Science</i> , 2010, 362, 384-392.	4.1	47
6719	A theoretical study on the adsorption of an all-metal aromatic molecule Na <sub>2</sub> Al <sub>4</sub> on MCM-22 zeolite. <i>Microporous and Mesoporous Materials</i> , 2010, 130, 67-75.	2.2	3
6720	Theoretical calculations of mechanical, electronic, chemical bonding and optical properties of delafossite CuAlO <sub>2</sub> . <i>Physica B: Condensed Matter</i> , 2010, 405, 2028-2033.	1.3	26
6721	Elastic properties of cubic perovskite BaRuO <sub>3</sub> from first-principles calculations. <i>Physica B: Condensed Matter</i> , 2010, 405, 3117-3119.	1.3	14
6722	First principles study on the new sp <sup>3</sup> bonded metallic carbon crystal. <i>Physica B: Condensed Matter</i> , 2010, 405, 3324-3327.	1.3	4
6723	Ab initio molecular dynamics simulations of structural change in liquid Se <sub>30</sub> Te <sub>70</sub> from low- to high-density phases. <i>Physica B: Condensed Matter</i> , 2010, 405, 3342-3349.	1.3	3
6724	Adsorption of S, O, and H on the NiAl(110)-(2 $\times$ 2) surface. <i>Physica B: Condensed Matter</i> , 2010, 405, 4059-4063.	1.3	12
6725	Structural, elastic, electronic, and thermodynamic properties of PrN from first principles calculations. <i>Physica B: Condensed Matter</i> , 2010, 405, 4139-4144.	1.3	15
6726	New hybrid inorganic-organic polymer electrolytes based on Zr(O(CH <sub>2</sub> ) <sub>3</sub> CH <sub>3</sub> ) <sub>4</sub> , glycerol and EMIm-TFSI ionic liquid. <i>Journal of Power Sources</i> , 2010, 195, 341-353.	4.0	29
6727	Structural, electronic and optical properties of orthorhombic CdGeO <sub>3</sub> from first principles calculations. <i>Journal of Solid State Chemistry</i> , 2010, 183, 437-443.	1.4	7
6728	Coordination polymer based on cyano: Synthesis, crystal structure, and fluorescence. <i>Journal of Solid State Chemistry</i> , 2010, 183, 1615-1619.	1.4	6
6729	Pressure-induced structural transformations in lanthanide titanates: La <sub>2</sub> TiO <sub>5</sub> and Nd <sub>2</sub> TiO <sub>5</sub> . <i>Journal of Solid State Chemistry</i> , 2010, 183, 2636-2643.	1.4	33
6730	The adsorption of 1,3-butadiene on Pd/Ni multilayers: The interplay between spin polarization and chemisorption strength. <i>Journal of Solid State Chemistry</i> , 2010, 183, 3086-3092.	1.4	10
6731	The effect of external electric fields on the electronic structure of (5,5)/(10,0) metal-semiconductor single wall carbon nanotube intramolecule junction. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2010, 42, 1590-1596.	1.3	3
6732	Electronic structures and magnetic properties of Zn-doped colossal magnetoresistance materials. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2010, 374, 1555-1559.	0.9	1
6733	Strain-induced structural and direct-to-indirect band gap transition in ZnO nanotubes. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2010, 374, 2846-2849.	0.9	34
6734	A comparative first-principles study of the adsorption of a carbon atom on copper and nickel surfaces. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2010, 374, 4563-4567.	0.9	11
6735	Relativistic electronic structure of cadmium(II) multidecker phthalocyanine compounds. <i>Polyhedron</i> , 2010, 29, 451-455.	1.0	5

#	ARTICLE	IF	CITATIONS
6736	[Cp* <i>Ru</i> (s-indacene) <i>Ru</i> Cp*] and [Cp* <i>Ru</i> (s-indacene) <i>Ru</i> Cp*] <sup>+</sup> : Experimental and theoretical findings concerning the electronic structure of neutral and mixed valence organometallic systems. <i>Polyhedron</i> , 2010, 29, 1137-1143.	1.0	21
6737	A first-principles study on the lower-valence coexisting Cr <sub>2</sub> TiX (X=Al, Ga, Si, Ge, Sn, Sb) Heusler alloys. <i>Journal of Magnetism and Magnetic Materials</i> , 2010, 322, 1-6.	1.0	16
6738	Tuning magnetism of MnO by doping with 2p elements. <i>Journal of Magnetism and Magnetic Materials</i> , 2010, 322, 253-256.	1.0	4
6739	Stability of Ferromagnetism in Fe, Co, and Ni Metals under High Pressure with GGA and GGA+U. <i>Journal of Magnetism and Magnetic Materials</i> , 2010, 322, 653-657.	1.0	42
6740	Magnetic structure of double perovskites Ca <sub>2</sub> MWO <sub>6</sub> (M=Co, Ni): A first principles study. <i>Journal of Magnetism and Magnetic Materials</i> , 2010, 322, L25-L27.	1.0	6
6741	Theoretical study of the electronic and magnetic properties of Co <sub>2</sub> Cr <sub>1-x</sub> V <sub>x</sub> Al. <i>Journal of Magnetism and Magnetic Materials</i> , 2010, 322, 2293-2297.	1.0	14
6742	Non-periodic finite-element formulation of Kohn-Sham density functional theory. <i>Journal of the Mechanics and Physics of Solids</i> , 2010, 58, 256-280.	2.3	101
6743	Ab initio calculations and interatomic potentials for iron and iron alloys: Achievements within the Perfect Project. <i>Journal of Nuclear Materials</i> , 2010, 406, 7-18.	1.3	72
6744	Synthesis and characterization of a dinuclear platinum complex with silsesquioxanate ligand. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 1738-1743.	0.8	7
6745	A density functional theory study of the oxidative addition of methyl iodide to square planar [Rh(acac)(P(OPh) <sub>3</sub> ) <sub>2</sub> ] complex and simplified model systems. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 2126-2133.	0.8	27
6746	Effect of residual stress on the optical properties of CsCl thin films. <i>Journal of Physics and Chemistry of Solids</i> , 2010, 71, 163-169.	1.9	16
6747	Study on the doping stability and electronic structure of wurtzite Zn <sub>1-x</sub> Cd <sub>x</sub> O alloys by first-principle calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2010, 71, 336-339.	1.9	20
6748	Cis-trans isomerism in cobalt(II) complexes with 3-hydroxypicolinic acid. Structural, DFT and thermal studies. <i>Inorganica Chimica Acta</i> , 2010, 363, 1887-1896.	1.2	12
6749	Experimental and theoretical investigations of magnetic properties for two low-dimensional spin systems based on bis(2-thioxo-1,3-dithiole-4,5-dithiolato)nickelate monoanion building blocks. <i>Inorganica Chimica Acta</i> , 2010, 363, 3530-3537.	1.2	3
6750	Hydrogen adsorption on Li metal in boron-substituted graphene: An ab initio approach. <i>International Journal of Hydrogen Energy</i> , 2010, 35, 3583-3587.	3.8	70
6751	Fundamental influence of hydrogen on various properties of $\hat{\pm}$ -titanium. <i>International Journal of Hydrogen Energy</i> , 2010, 35, 3812-3816.	3.8	48
6752	DFT-based FEM analysis of nonlinear effects on indentation process in diamond crystal. <i>International Journal of Mechanical Sciences</i> , 2010, 52, 303-308.	3.6	6
6753	Effects of doping on the electronic properties of LiFePO <sub>4</sub> : A first-principles investigation. <i>Physica B: Condensed Matter</i> , 2010, 405, 803-807.	1.3	63

#	ARTICLE	IF	CITATIONS
6754	Surface structures of Heusler alloys: A first-principles study. <i>Physica B: Condensed Matter</i> , 2010, 405, 1580-1585.	1.3	3
6755	First-principles study of dissociation barriers and electronic structures of monolayer graphite on Ni(111) surface. <i>Physica B: Condensed Matter</i> , 2010, 405, 2852-2856.	1.3	0
6756	Thermal stability and elastic properties of Mg <sub>3</sub> Sb <sub>2</sub> and Mg <sub>3</sub> Bi <sub>2</sub> phases from first-principles calculations. <i>Physica B: Condensed Matter</i> , 2010, 405, 2863-2868.	1.3	60
6757	A study of electronic and optical properties of NaBi(WO <sub>4</sub> ) <sub>2</sub> : A disordered double tungstate crystal. <i>Physica B: Condensed Matter</i> , 2010, 405, 3267-3271.	1.3	10
6758	The electronic and structural properties of $\hat{\Gamma}$ -Pu and PuO from the LSDA (GGA)+U method. <i>Physica B: Condensed Matter</i> , 2010, 405, 3717-3721.	1.3	14
6759	Nitrogen absorption and dissociation on small Tantalum clusters. <i>Physica B: Condensed Matter</i> , 2010, 405, 3940-3942.	1.3	17
6760	The structural, electronic, elastic, vibrational, and thermodynamic properties of HoX (X=Sb, Bi). <i>Physica B: Condensed Matter</i> , 2010, 405, 3977-3985.	1.3	9
6761	First principles calculation of optical properties of BaWO <sub>4</sub> : A study by full potential method. <i>Physica B: Condensed Matter</i> , 2010, 405, 4530-4535.	1.3	19
6762	First principles studies on the structural and electronic properties of Sr <sub>n+1</sub> Ti <sub>n</sub> O <sub>3n+1</sub> (n=1, 2, 3, $\hat{\alpha}$ ~z). <i>Physica B: Condensed Matter</i> , 2010, 405, 4780-4784.	1.3	1
6763	Interaction of CO, CO <sub>2</sub> and CH <sub>4</sub> with mesoporous organosilica: Periodic DFT calculations with dispersion corrections. <i>Microporous and Mesoporous Materials</i> , 2010, 129, 62-67.	2.2	23
6764	Investigation of ruthenium-copper bimetallic catalysts for direct epoxidation of propylene: A DFT study. <i>Journal of Molecular Catalysis A</i> , 2010, 330, 107-111.	4.8	26
6765	First-principles calculations of structural, elastic, electronic and optical properties of XO (X=Ca, Sr) $\Gamma$ 1. <i>Journal of Applied Physics</i> , 2010, 107, 92-101.	1.9	27
6766	A study of atomic interaction between suspended nanoparticles and sodium atoms in liquid sodium. <i>Nuclear Engineering and Design</i> , 2010, 240, 2664-2673.	0.8	10
6767	Density-functional study for the NO <sub>x</sub> (x=1, 2) dissociation mechanism on the Cu(111) surface. <i>Chemical Physics</i> , 2010, 373, 300-306.	0.9	36
6768	Electrochemical and density functional theory study of bis(cyclopentadienyl) mono( $\hat{\Gamma}$ <sup>2</sup> -diketonato) titanium(IV) cationic complexes. <i>Electrochimica Acta</i> , 2010, 56, 257-264.	2.6	28
6769	First principle calculations of core-level binding energy and Auger kinetic energy shifts in metallic solids. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2010, 178-179, 88-99.	0.8	25
6770	Theoretical approximations to X-ray absorption spectroscopy of liquid water and ice. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2010, 177, 135-157.	0.8	132
6771	Selective arylation of aldehydes with di-rhodium(II)/NHC catalysts. <i>Tetrahedron</i> , 2010, 66, 8494-8502.	1.0	30

#	ARTICLE	IF	CITATIONS
6772	Water adsorption and dissociation on the Au(321) stepped surface. Computational and Theoretical Chemistry, 2010, 946, 51-56.	1.5	12
6773	Hydrogen abstraction from biphenyl, acenaphthylene, naphthalene and phenanthrene by atomic hydrogen and methyl radical: DFT and G3(MP2)-RAD data. Computational and Theoretical Chemistry, 2010, 940, 115-118.	1.5	26
6774	Cluster and periodic DFT calculations of adsorption of hydroxyl on the Au(hkl) surfaces. Computational and Theoretical Chemistry, 2010, 946, 43-50.	1.5	28
6775	DFT study of the structure sensitivity for the adsorption of methyl, methoxy, and formate on Ni(111), Ni(100), and Ni(110) surfaces. Computational and Theoretical Chemistry, 2010, 948, 1-10.	1.5	27
6776	Calculation of <sup>59</sup> Co shielding tensor using LF-DFT. Computational and Theoretical Chemistry, 2010, 954, 105-108.	1.5	11
6777	DFT study on the sulfur migration during benzenethiol pyrolysis in coal. Computational and Theoretical Chemistry, 2010, 952, 31-35.	1.5	18
6778	DFT study on the electronic structure, energetics and spectral properties of several bis(organohydrazido(2-)) molybdenum complexes containing substituted phosphines and chloro atoms as ancillary ligands. Computational and Theoretical Chemistry, 2010, 957, 126-132.	1.5	13
6779	A comparative DFT study of atomic and molecular oxygen adsorption on neutral and negatively charged PdxCu3-x (x=0-3) nano-clusters. Computational and Theoretical Chemistry, 2010, 959, 15-21.	1.5	16
6780	A theoretical study of the atomic hydrogen binding on small Ag Cu (n+m-1/2 5) clusters. Computational and Theoretical Chemistry, 2010, 959, 75-79.	1.5	10
6781	A computational study of kinetic phase diagrams for CoPt alloy films during epitaxial growth. Thin Solid Films, 2010, 518, 4860-4867.	0.8	1
6782	Enhancement of optical absorption in Ga-chalcopyrite-based intermediate-band materials for high efficiency solar cells. Solar Energy Materials and Solar Cells, 2010, 94, 1903-1906.	3.0	48
6783	An ab initio study of Co-Cr(V) disorder effects on the electronic structure and magnetic properties of. Solid State Communications, 2010, 150, 109-113.	0.9	3
6784	Structural stability and electronic properties of LiNiN. Solid State Communications, 2010, 150, 669-674.	0.9	8
6785	First principles study of electronic structure and optical properties of double perovskite Ba2(InM)O6 [M, Ta]. Solid State Communications, 2010, 150, 1173-1177.	0.9	18
6786	First-principles investigation on the phase stability and chemical bonding of phase-change random alloys. Solid State Communications, 2010, 150, 1375-1377.	0.9	10
6787	Surface properties of titanium nitride: A first-principles study. Solid State Communications, 2010, 150, 1370-1374.	0.9	31
6788	Structural stability and hydrogen diffusion in alloys. Solid State Communications, 2010, 150, 1715-1718.	0.9	18
6789	First-principles study of structural, electronic and optical properties of orthorhombic. Solid State Communications, 2010, 150, 2032-2035.	0.9	10

#	ARTICLE	IF	CITATIONS
6790	Electronic and magnetic properties of C-doped Mg <sub>3</sub> N <sub>2</sub> : A density functional theory study. <i>Solid State Communications</i> , 2010, 150, 2223-2226.	0.9	5
6791	Ionic conductivity of lithium in spinel-type Li <sub>4/3</sub> Ti <sub>5/3</sub> O <sub>4</sub> –LiMg <sub>1/2</sub> Ti <sub>3/2</sub> O <sub>4</sub> solid-solution system. <i>Solid State Ionics</i> , 2010, 181, 994-1001.	1.3	30
6792	Atomic modification of stepped metal surfaces using vertical single-atom manipulation with a trimer-apex tip: First-principles and semiempirical simulations. <i>Surface and Coatings Technology</i> , 2010, 204, 3254-3257.	2.2	1
6793	Improvement of platinum adhesion to carbon surfaces using PVD coatings. <i>Surface and Coatings Technology</i> , 2010, 205, 306-311.	2.2	17
6794	Reduction of FeO/Pt(111) thin films by exposure to atomic hydrogen. <i>Surface Science</i> , 2010, 604, 11-20.	0.8	58
6795	Unsaturated hydrocarbons adsorbed on low coordinated Pd surface: A periodic DFT study. <i>Surface Science</i> , 2010, 604, 386-395.	0.8	12
6796	Adsorption of Xe atoms on the TiO <sub>2</sub> (110) surface: A density functional study. <i>Surface Science</i> , 2010, 604, 428-434.	0.8	15
6797	Chemisorption of isocyanate (NCO) on the Pd(100) surface at different coverages. <i>Surface Science</i> , 2010, 604, 442-450.	0.8	10
6798	Structural, electronic and energetic properties of water adsorbed on $\beta$ -Si <sub>3</sub> N <sub>4</sub> (0001) surface: First-principles calculations. <i>Surface Science</i> , 2010, 604, 617-622.	0.8	12
6799	Adsorption of molecular SiO <sub>2</sub> on a clean Si(1 0 0) surface. <i>Surface Science</i> , 2010, 604, L21-L25.	0.8	2
6800	Hydrogen adsorption on palladium and palladium hydride at 1 bar. <i>Surface Science</i> , 2010, 604, 718-729.	0.8	158
6801	Methylamine decomposition on nickel surfaces: A density functional theory study. <i>Surface Science</i> , 2010, 604, 779-787.	0.8	21
6802	A theoretical study of Zn adsorption and desorption on a Pd(111) substrate. <i>Surface Science</i> , 2010, 604, 926-931.	0.8	16
6803	A periodic DFT study of water and ammonia adsorption on anatase TiO <sub>2</sub> (001) slab. <i>Surface Science</i> , 2010, 604, 1029-1033.	0.8	68
6804	Isomerization of n-butane on Pt (100): Monomolecular mechanism investigation. <i>Surface Science</i> , 2010, 604, 1040-1043.	0.8	3
6805	Role of sub-surface oxygen in Cu(100) oxidation. <i>Surface Science</i> , 2010, 604, 1425-1431.	0.8	25
6806	A reactive force-field (ReaxFF) Monte Carlo study of surface enrichment and step structure on yttria-stabilized zirconia. <i>Surface Science</i> , 2010, 604, 1438-1444.	0.8	24
6807	Theoretical investigation of the influence of isotope mass on chemicurrents during adsorption of H on K(110). <i>Surface Science</i> , 2010, 604, 1452-1458.	0.8	6

#	ARTICLE	IF	CITATIONS
6808	Adsorption of thin films of titanium on tungsten (111) surface. <i>Surface Science</i> , 2010, 604, 1524-1530.	0.8	4
6809	Near-degenerate stereomorphs of the doubly-chiral hcp-{213̄...1} surface. <i>Surface Science</i> , 2010, 604, 1688-1693.	0.8	1
6810	Effects of bimetallic modification on the decomposition of CH <sub>3</sub> OH and H <sub>2</sub> O on Pt/W(110) bimetallic surfaces. <i>Surface Science</i> , 2010, 604, 1845-1853.	0.8	13
6811	Ab initio study of Yb on the Ge(111)̄(3̄-2) and Si(111)̄(3̄-2) surfaces. <i>Surface Science</i> , 2010, 604, 1899-1905.	0.8	2
6812	First-principles study of solutēvacancy binding in magnesium. <i>Acta Materialia</i> , 2010, 58, 531-540.	3.8	113
6813	The effect of platinum on Al diffusion kinetics in $\hat{1}^2$ -NiAl: Implications for thermal barrier coating lifetime. <i>Acta Materialia</i> , 2010, 58, 2726-2737.	3.8	41
6814	Adsorption of 2-chlorophenol on Cu <sub>2</sub> O(111)̄CuCUS: A first-principles density functional study. <i>Applied Surface Science</i> , 2010, 256, 4764-4770.	3.1	8
6815	Low-coverage alkali metal adsorption on the Ge(001)-p(12) surface. <i>Applied Surface Science</i> , 2010, 256, 4784-4788.	3.1	3
6816	Fluorine, chlorine and iodine adsorption on the Ge(001) surface: Comparative study for the coverage of 0.75 and 1 monolayer. <i>Applied Surface Science</i> , 2010, 256, 4822-4828.	3.1	6
6817	Ferromagnetism driven by cation vacancy in GaN thin films and nanowires. <i>Applied Surface Science</i> , 2010, 256, 6040-6046.	3.1	13
6818	Roles of $\hat{1}^3$ -Fe <sub>2</sub> O <sub>3</sub> in fly ash for mercury removal: Results of density functional theory study. <i>Applied Surface Science</i> , 2010, 256, 6991-6996.	3.1	71
6819	Density functional theory study on adsorption of thiophene on TiO <sub>2</sub> anatase (001) surfaces. <i>Catalysis Today</i> , 2010, 149, 218-223.	2.2	48
6820	Non-equilibrium surface pattern formation during catalytic reactions with nanoscale resolution: Investigations of the electric field influence. <i>Catalysis Today</i> , 2010, 154, 75-84.	2.2	14
6821	Structural and magnetic studies on copper(II) azido complexes. <i>Coordination Chemistry Reviews</i> , 2010, 254, 2933-2958.	9.5	266
6822	Detailed description of the flexible periodic London̄EyrinḡPolanyīSato potential energy function. <i>Chemical Physics</i> , 2010, 367, 136-147.	0.9	24
6823	Electronic and charge-transport properties of 1,1,2,3,4,5-hexaphenylsilole (HPS) crystal from theoretical calculations. <i>Chemical Physics</i> , 2010, 367, 160-166.	0.9	10
6824	NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. <i>Computer Physics Communications</i> , 2010, 181, 1477-1489.	3.0	4,740
6825	Promiscuous DNA alkyladenine glycosylase dramatically favors a bound lesion over undamaged adenine. <i>Biophysical Chemistry</i> , 2010, 152, 118-127.	1.5	9

#	ARTICLE	IF	CITATIONS
6826	First-principles study of transport properties of endohedral Li@C <sub>20</sub> metallofullerene. <i>Current Applied Physics</i> , 2010, 10, 260-265.	1.1	56
6827	DFT and tight binding Monte Carlo calculations related to single-walled carbon nanotube nucleation and growth. <i>Carbon</i> , 2010, 48, 470-478.	5.4	44
6828	First-principles investigation into structural and magnetic properties of binary graphite 3d-transition metal intercalated compounds (XC <sub>6</sub> ; X=Cr, Mn, Fe). <i>Carbon</i> , 2010, 48, 1341-1344.	5.4	7
6829	A theoretical characterization of the interaction of water with oxidized carbonaceous clusters. <i>Carbon</i> , 2010, 48, 1570-1579.	5.4	26
6830	The effect of van der Waals interactions on the properties of intrinsic defects in graphite. <i>Carbon</i> , 2010, 48, 4145-4161.	5.4	37
6831	Influence of $\gamma$ -alumina supports on oxygen binding to Pd, Ag, Pt, and Au. <i>Chemical Physics Letters</i> , 2010, 484, 231-236.	1.2	17
6832	A barrier for the $\text{Al}^{13+}$ reaction and its implication for the chemisorption of $\text{H}_2$ . <i>Chemical Physics Letters</i> , 2010, 489, 16-19.	1.2	11
6833	Study of S <sub>0</sub> and S <sub>1</sub> states of catechol and catechol-Al(III) systems in aqueous solution by TD-DFT methods and electronic spectroscopies. <i>Chemical Physics Letters</i> , 2010, 489, 164-168.	1.2	5
6834	DFT-modeling of the tungsten (V) cofactor of hyperthermophilic <i>Pyrococcus furiosus</i> tungsto-bispterin enzyme via the calculated EPR parameters. <i>Chemical Physics Letters</i> , 2010, 491, 214-217.	1.2	1
6835	Role of hydroxyl groups for the O <sub>2</sub> adsorption on CeO <sub>2</sub> surface: A DFT+U study. <i>Chemical Physics Letters</i> , 2010, 493, 269-272.	1.2	18
6836	Assessment of density functional methods for the study of olefin metathesis catalysed by ruthenium alkylidene complexes. <i>Chemical Physics Letters</i> , 2010, 493, 273-278.	1.2	60
6837	Pressure induced structural changes in the potential hydrogen storage compound ammonia borane: A combined X-ray, neutron and theoretical investigation. <i>Chemical Physics Letters</i> , 2010, 495, 203-207.	1.2	28
6838	Phosphaethyne polymers are analogues of cis-polyacetylene and graphane. <i>Comptes Rendus Chimie</i> , 2010, 13, 1173-1179.	0.2	10
6839	K-shell core-electron binding energies for phosphorus- and sulfur-containing molecules calculated by density functional theory. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2010, 182, 141-144.	0.8	27
6840	$\text{K}_3\text{TaF}_8$ from laboratory X-ray powder data. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2010, 66, i16-i18.	0.4	15
6841	Theoretical investigation on organolanthanide guanidinate complexes. <i>Journal of Rare Earths</i> , 2010, 28, 161-165.	2.5	3
6842	Surface structures of Fe <sub>3</sub> O <sub>4</sub> (111), (110), and (001): A density functional theory study. <i>Journal of Fuel Chemistry and Technology</i> , 2010, 38, 121-128.	0.9	48
6843	The Roles of Intermediate Phases of Li-Si Alloy as Anode Materials for Lithium-Ion Batteries. <i>Rare Metal Materials and Engineering</i> , 2010, 39, 2079-2083.	0.8	17



#	ARTICLE	IF	CITATIONS
6844	Structural models of $\alpha\text{-Si}_3\text{H}$ with a low defect concentration: A first-principles molecular dynamics study. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2010, 207, 605-608.	0.8	2
6845	Density functional calculations of the electronic structure and optical properties of magnesium oxide. <i>Physica Status Solidi (B): Basic Research</i> , 2010, 247, 157-162.	0.7	11
6846	Do the atoms at second layer block the path of vacancies in the bulk? - The DFT study of vacancies below the Mg (0001) surface. <i>Physica Status Solidi (B): Basic Research</i> , 2010, 247, 259-264.	0.7	0
6847	Ab initio calculations of optical spectra of a chiral (4,1) carbon nanotube. <i>Physica Status Solidi (B): Basic Research</i> , 2010, 247, 1814-1821.	0.7	20
6848	Theory of the temperature dependent dielectric function of semiconductors: from bulk to surfaces. Application to GaAs and Si. <i>Physica Status Solidi (B): Basic Research</i> , 2010, 247, 1881-1888.	0.7	15
6849	Theoretical and computational studies of organometallic reactions: successful or not?. <i>Chemical Record</i> , 2010, 10, 29-45.	2.9	31
6850	Adsorption and dissociation of carbon trioxide on Ag(100). <i>International Journal of Quantum Chemistry</i> , 2010, 110, 946-952.	1.0	5
6851	Theoretical determination of lowest structures of all-metal aromatic clusters $M_4L_2$ (M = Al, Ga, In, Tl; L = Li, Na, K, Rb, Cs). <i>International Journal of Quantum Chemistry</i> , 2010, 110, 1127-1135.	1.0	4
6852	Bonding in titanocenyl complexes containing O, $\text{O}^2\text{-cyclic}$ ligands. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 1100-1107.	1.0	4
6853	Comparative theoretical study of small Rh nanoparticles (2 - 8) using DFT methods. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 1152-1164.	1.0	12
6854	The bond bundle in open systems. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 1500-1505.	1.0	34
6855	On the performance of eleven DFT functionals in the description of the vibrational properties of aluminosilicates. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 406-415.	1.0	121
6856	Interaction of atoms with graphenic-type surfaces for the chemistry of the interstellar medium: New properties of H dimers on the surface. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2231-2236.	1.0	10
6857	Performance of 12 DFT functionals in the study of crystal systems: $\text{Al}_2\text{SiO}_5$ orthosilicates and Al hydroxides as a case study. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2260-2273.	1.0	42
6858	The subsystem functional scheme: The Armiento-Mattsson 2005 (AM05) functional and beyond. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2274-2282.	1.0	10
6859	First-principle studies of dissociative adsorption of $\text{H}_2\text{O}$ on NiAl(110) ( $2 \times 2$ ) surface. <i>Surface and Interface Analysis</i> , 2010, 42, 1326-1329.	0.8	3
6860	First-Principles Thermochemistry and Thermodynamic Modeling of the $\text{Al}_2\text{O}_3\text{-Nd}_2\text{O}_3\text{-SiO}_2\text{-Y}_2\text{O}_3$ Pseudoquaternary System. <i>Journal of the American Ceramic Society</i> , 2010, 93, 4158-4167.	1.9	12
6861	$(\text{Ti}_{0.5}\text{Nb}_{0.5})_5\text{AlC}_4$ : A New Layered Compound Belonging to MAX Phases. <i>Journal of the American Ceramic Society</i> , 2010, 93, 3068-3071.	1.9	74

#	ARTICLE	IF	CITATIONS
6862	Composition of cementite in the dependence on the temperature. In situ neutron diffraction study and Ab initio calculations. JETP Letters, 2010, 91, 143-146.	0.4	25
6863	Using first principles to predict bimetallic catalysts for the ammonia decomposition reaction. Nature Chemistry, 2010, 2, 484-489.	6.6	381
6864	State-selective dissociation of a single water molecule on an ultrathin MgO film. Nature Materials, 2010, 9, 442-447.	13.3	171
6865	A Theoretical Investigation of the Structural Properties of Chemically Modified Mo-Si Nanowires. Chinese Journal of Catalysis, 2010, 31, 739-746.	6.9	1
6866	Crystal and Electronic Structures, Photoluminescence Properties of Eu <sup>2+</sup> -Doped Novel Oxynitride Ba <sub>4</sub> Si <sub>6</sub> O <sub>16-3x/2</sub> N <sub>x</sub> . Materials, 2010, 3, 1692-1708.	1.3	27
6867	Theoretical Studies of Substitutionally Doped Single-Walled Nanotubes. Journal of Nanotechnology, 2010, 2010, 1-42.	1.5	12
6868	Taurolidine Antiadhesive Properties on Interaction with E. coli; Its Transformation in Biological Environment and Interaction with Bacteria Cell Wall. PLoS ONE, 2010, 5, e8927.	1.1	29
6869	Native point defects in CaCu <sub>3</sub> Ti <sub>4</sub> O <sub>12</sub> . IOP Conference Series: Materials Science and Engineering, 2010, 8, 012015.	0.3	7
6870	Intramolecular hydroxycarbene C-H insertion: The curious case of (o-methoxyphenyl)hydroxycarbene. Beilstein Journal of Organic Chemistry, 2010, 6, 1061-1069.	1.3	19
6871	Ab initio Study of He Stability in hcp -Ti. Chinese Physics Letters, 2010, 27, 123102.	1.3	3
6872	The Magnetism and Substrate Effects of Co <sub>3</sub> Clusters on Cu(111), Pd(111), Ne(111) and Two Polar ZnO Surfaces. Advanced Materials Research, 0, 154-155, 810-816.	0.3	0
6873	First-Principles Study of Formation and Properties of Fcc-NdO <sub>x</sub> in Nd-Fe-B Sintered Magnets. Materials Science Forum, 2010, 654-656, 1674-1677.	0.3	5
6874	Ab Initio Study of the Structural and Mechanical Properties of Hf-Si-N. Advanced Materials Research, 2010, 139-141, 22-25.	0.3	1
6875	Matrix Coherency Strain and Hardening of Al-Mg-Si. Materials Science Forum, 0, 638-642, 229-234.	0.3	1
6876	The influence of exact exchange corrections in van der Waals layered narrow bandgap black phosphorus. Journal of Physics Condensed Matter, 2010, 22, 015502.	0.7	37
6877	Role of buffer layer in electronic structures of iron phthalocyanine molecules on Au(111). Chinese Physics B, 2010, 19, 097809.	0.7	4
6878	Structural analysis of the antimalarial drug halofantrine by means of Raman spectroscopy and density functional theory calculations. Journal of Biomedical Optics, 2010, 15, 041516.	1.4	47
6879	M atom (M = Cu, Ag and Au) interaction with Ag and Au substrates: a first-principles study using cluster and slab models. Journal of Physics Condensed Matter, 2010, 22, 435001.	0.7	12

#	ARTICLE	IF	CITATIONS
6880	Mechanical and Magnetic Properties of Rh and RhH: First-Principles Calculations. Chinese Physics Letters, 2010, 27, 027101.	1.3	6
6881	Highly Strained Metastable Heterojunction between Wurtzite GaN(0001) and Cubic CrN(111). Journal of the Electrochemical Society, 2010, 157, D577.	1.3	4
6882	New quaternary complex borides, $Ti_9M_2Ru_{18}B_8$ (Cr, Tj ETQq0 0 0 rgBT /Overlock : - Crystalline Materials, 2010, 225, 180-186.	0.4	14
6883	Dynamical stability of body center cubic iron at the Earth's core conditions. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 9962-9964.	3.3	58
6884	Structural, curvature and electronic properties of Rh adsorption on armchair single-walled carbon nanotube. Chinese Physics B, 2010, 19, 097104.	0.7	7
6885	Active Materials Based on Implanted Si for Obtaining Intermediate Band Solar Cells. Advances in Science and Technology, 0, , .	0.2	5
6886	Electronic and Magnetic Properties of Double Perovskite $Ca_2CrSbO_6$ . Communications in Theoretical Physics, 2010, 53, 180-184.	1.1	6
6887	Structural, electronic and magnetic properties of the Mn-Ni(110) (2 Å <sup>-2</sup> ) surface alloy. Chinese Physics B, 2010, 19, 087102.	0.7	4
6888	Ab initio investigations of the charge transport properties of endohedral $M@C_{20}$ ( $M = Na$ and $K$ ) metallofullerenes. Chinese Physics B, 2010, 19, 113402.	0.7	6
6889	First-principle study on phase $Al_{0.8}Ni_3Sn_{0.2}$ in Sn-Ni-Al alloy as anode for lithium ion battery. Chinese Physics B, 2010, 19, 117101.	0.7	8
6890	Dielectric Relaxation and Electronic Structure of Double Perovskite $Ca_2AlNbO_6$ . Integrated Ferroelectrics, 2010, 116, 41-50.	0.3	11
6891	Electronic band transformation from indirect gap to direct gap in Si-H compound. Chinese Physics B, 2010, 19, 077103.	0.7	1
6892	Cathodoluminescence Color Shift in $Zn_{1-x}Mg_xS:Cu,Al$ Powder Phosphors. Journal of the Electrochemical Society, 2010, 157, J164.	1.3	0
6893	Exact nonadditive kinetic potentials for embedded density functional theory. Journal of Chemical Physics, 2010, 133, 084103.	1.2	171
6894	Site preference of Ru in NiAl and valence band structure of NiAl containing Ru: First-principles study and photoelectron spectrum. Philosophical Magazine Letters, 2010, 90, 225-232.	0.5	5
6895	First-principles calculation of electronic and structural properties of $YBa_2Cu_3O_{7-x}$ . Physical Review B, 2010, 82, .		
6896	Characterizing electronic structure motifs in $UH_2$ . Physical Review B, 2010, 82, .	1.1	14
6897	Improving the Electrochemical Activity of $LiMnPO_4$ Via Mn-Site Substitution. Journal of the Electrochemical Society, 2010, 157, A225.	1.3	112

#	ARTICLE	IF	CITATIONS
6898	High-Brightness Photocathodes through Ultrathin Surface Layers on Metals. <i>Physical Review Letters</i> , 2010, 104, 046801.	2.9	26
6899	Statistical average of model orbital potentials for extended systems: Calculation of the optical absorption spectrum of liquid water. <i>Journal of Chemical Physics</i> , 2010, 132, 184513.	1.2	11
6900	Mixed-Valency Signature in Vibrational Inelastic Electron Tunneling Spectroscopy. <i>Physical Review Letters</i> , 2010, 104, 136101.	2.9	39
6901	Mapping antibonding electron states of a Pb adatom on Pb(111). <i>Physical Review B</i> , 2010, 81, .	1.1	12
6902	<i>Ab initio</i> study of solute transition-metal interactions with point defects in bcc Fe. <i>Physical Review B</i> , 2010, 81, .	1.1	191
6903	Structural and dynamical heterogeneity in molten Si-rich oxides. <i>Applied Physics Letters</i> , 2010, 96, 043121.	1.5	6
6904	Effect of adsorbed H atoms on magnetism in monoatomic Fe wires at Ir(100). <i>Physical Review B</i> , 2010, 81, .	1.1	5
6905	<i>Ab initio</i> thermodynamics of deposition growth: Surface terminations of TiC(111) and TiN(111) grown by chemical vapor deposition. <i>Physical Review B</i> , 2010, 82, .	1.1	8
6906	Magnetocrystalline anisotropy energy of Co and Fe adatoms on the (111) surfaces of Pd and Rh. <i>Physical Review B</i> , 2010, 81, .	1.1	82
6907	Asymmetric relief of surface stress induced by a chiral adsorbate: Alaninate adsorption on Cu(110). <i>Physical Review B</i> , 2010, 81, .	1.1	12
6908	Effect of electron correlations on structural phase stability, magnetism, and spin-dependent transport in $\text{CeMnNi}_4$ . <i>Physical Review B</i> , 2010, 81, .	1.1	6
6909	Incipient plasticity of twin and stable/unstable grain boundaries during nanoindentation in copper. <i>Physical Review B</i> , 2010, 82, .	1.1	36
6910	Theory of Fano resonances in graphene: The influence of orbital and structural symmetries on STM spectra. <i>Physical Review B</i> , 2010, 81, .	1.1	79
6911	Response of mechanically strained nanomaterials to irradiation: Insight from atomistic simulations. <i>Physical Review B</i> , 2010, 82, .	1.1	26
6912	Adsorption-enhanced reactivity of the In/Si(001) system. <i>Physical Review B</i> , 2010, 81, .	1.1	14
6913	Reorientable dipolar and anomalous screening in $\text{Cu}_3\text{Ca}$ . <i>Physical Review B</i> , 2010, 81, .	1.1	11
6914	Spin density studies on a heavy $\text{p-O}$ . <i>Physical Review B</i> , 2010, 81, .	1.1	16
6915	Building effective models from sparse but precise data: Application to an alloy cluster expansion model. <i>Physical Review B</i> , 2010, 81, .	1.1	33

#	ARTICLE	IF	CITATIONS
6916	Competing strain effects in reactivity of $\text{LaCoO}_3$ oxygen. Physical Review B, 2010, 82, .	1.1	110
6917	Termination and Verwey transition of the (111) surface of magnetite studied by scanning tunneling microscopy and first-principles calculations. Physical Review B, 2010, 81, .	1.1	49
6918	First-principles study of water adsorption and a high-density interfacial ice structure on $(1\bar{A}-1)\text{-O/Rh}(111)$ . Physical Review B, 2010, 82, .	1.1	2
6919	Magnetoelasticity driven magnetic anisotropy changes in strained $\text{Sr}_2\text{CrReO}_6$ . Physical Review B, 2010, 82, .	1.1	6
6920	Theoretical investigation of intermediate phases between $\text{Li}_2\text{LiNH}_2$ and $\text{Li}_2\text{Li}_2\text{NH}_2$ . Physical Review B, 2010, 81, .	1.1	5
6921	Electronic structure and thermoelectric properties of $\text{PbBi}_2$ related intergrowth compounds. Physical Review B, 2010, 81, .	1.1	56
6922	Binding in alkali and alkaline-earth tetrahydroborates: Special position of magnesium tetrahydroborate. Physical Review B, 2010, 81, .	1.1	33
6923	Chemical reactivity on surfaces: Modeling the imide synthesis from DATP and PTCDA on $\text{Au}(111)$ . Physical Review B, 2010, 81, .	1.1	11
6924	Amorphous defect clusters of pure Si and type inversion in Si detectors. Physical Review B, 2010, 82, .	1.1	12
6925	Doping-dependent thermopower of $\text{PbTe}$ from Boltzmann transport calculations. Physical Review B, 2010, 81, .	1.1	259
6926	Origin of ferromagnetism in molybdenum dioxide from <i>ab initio</i> calculations. Physical Review B, 2010, 81, .	1.1	18
6927	Diffraction of swift atoms after grazing scattering from metal surfaces: $\text{N/Ag}(111)$ system. Physical Review A, 2010, 82, .	1.0	9
6928	Substrate-induced cooperative effects in water adsorption from density functional calculations. Physical Review B, 2010, 82, .	1.1	6
6929	Electronic structure of single-layered undoped cuprates from hybrid density functional theory. Physical Review B, 2010, 81, .	1.1	34
6930	Investigation of protein conformation and interactions with salts via X-ray absorption spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 14008-14013.	3.3	35
6931	<i>Ab initio</i> calculations and ellipsometry measurements of the optical properties of the layered semiconductor $\text{In}_4\text{Mn}_2\text{S}_8$ . Physical Review B, 2010, 81, .	1.1	20
6932	Preparation and photoemission investigation of bulklike $\hat{\pm}\text{-Mn}$ films on $\text{W}(110)$ . Physical Review B, 2010, 81, .	1.1	2
6933	The role of rare earth elements in the structures of FeB-based glass forming liquid alloys. Journal of Applied Physics, 2010, 107, .	1.1	10

#	ARTICLE	IF	CITATIONS
6934	High-pressure phase transformations in carbonates. Physical Review B, 2010, 82, .	1.1	31
6935	First-principles study of structural stability and electronic structure of La-doped Sr <sub>1.9375</sub> La <sub>0.0625</sub> TiO <sub>3.968</sub> . Journal of Applied Physics, 2010, 107, .	1.1	12
6936	Oxidation of pure and potassium-doped NiTi shape memory surface: A density functional theory investigation. Physical Review B, 2010, 82, .	1.1	10
6937	Enhanced electron-mediated ferromagnetism in Co-doped ZnO nanowires. Journal of Applied Physics, 2010, 108, .	1.1	11
6938	Simultaneous Segregation at Coherent and Semicoherent Heterophase Interfaces. Physical Review Letters, 2010, 105, 076102.	2.9	80
6939	Density functional theory study of 3R $\alpha$ and 2H $\alpha$ -CuAlO <sub>2</sub> under pressure. Applied Physics Letters, 2010, 97, 141917.	1.5	15
6940	Soft Bond-Deformation Paths in Superhard $I^3$ -Boron. Physical Review Letters, 2010, 105, 215503.	2.9	55
6941	Electrode material dependent breakdown and recovery in advanced high- $\epsilon$ gate stacks. Applied Physics Letters, 2010, 96, .	1.5	25
6942	Force field experiments of an epitaxial superstructure of 3,4,9,10-perylenetetra-carboxylic-dianhydride on Ag(111). Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics, 2010, 28, C4B6-C4B11.	0.6	4
6943	Initial stages of Mg adsorption on the Si(111)- $7\sqrt{3}\times 7$ surface. Journal of Applied Physics, 2010, 107, 023505.	1.1	0
6944	Vacancy clustering and diffusion in heavily P doped Si. Applied Physics Letters, 2010, 97, 251909.	1.5	6
6945	Highly anisotropic sliding at TiN/Fe interfaces: A first principles study. Journal of Applied Physics, 2010, 108, 113511.	1.1	9
6946	Improvement of the interface integrity between a high-k dielectric film and a metal gate electrode by controlling point defects and residual stress. , 2010, , .		1
6947	A route to strong p-doping of epitaxial graphene on SiC. Applied Physics Letters, 2010, 97, 193304.	1.5	22
6948	Reactive force fields for surface chemical reactions: A case study with hydrogen dissociation on Pd surfaces. Journal of Chemical Physics, 2010, 132, 014704.	1.2	39
6949	Magnetism in two-dimensional BN $\alpha$ . Physical Review B, 2010, 81, .	1.1	7
6950	Reversal of chloride-induced Cu(001) subsurface buckling in the electrochemical environment: An in situ surface x-ray diffraction and density functional theory study. Physical Review B, 2010, 81, .	1.1	43
6951	Doping of cobalt oxide with transition metal impurities: Ab initio study. Physical Review B, 2010, 81, .	1.1	19



#	ARTICLE	IF	CITATIONS
6952	Diffraction of fast atoms during grazing scattering from the surface of an ultrathin silica film on Mo(112). Physical Review B, 2010, 82, .	1.1	59
6953	Oxidation of $\text{Pd}$ on $\text{Si}(111)$ . Physical Review B, 2010, 82, .	1.1	29
6954	Carrier wave effect in nonresonant inelastic scanning tunneling spectroscopy of molecules with delocalized frontier orbitals. Physical Review B, 2010, 81, .	1.1	2
6955	Electronic and magnetic properties of Co and Ni impurities in Cu wires: First-principles investigation of local moment formation in one dimension. Physical Review B, 2010, 82, .	1.1	3
6956	High-Pressure High-Temperature Polymorphism in Ta: Resolving an Ongoing Experimental Controversy. Physical Review Letters, 2010, 104, 255702.	2.9	78
6957	Interaction of a $\frac{1}{2}\langle 111 \rangle$ screw dislocation with Cr precipitates in bcc Fe studied by molecular dynamics. Physical Review B, 2010, 81, .	1.1	44
6958	Diffusion of 1,4-butanedithiol on Au(100) $(1 \times 1)$ : A DFT-based master-equation approach. Physical Review B, 2010, 82, .	1.1	4
6959	Existence of a stable compound in the Au-Ge alloy system. Physical Review B, 2010, 81, .	1.1	6
6960	Defects in carbon implanted silicon calculated by classical potentials and first-principles methods. Physical Review B, 2010, 82, .	1.1	6
6961	First-principles study of 1,4-butanedithiol molecules and radicals adsorbed on unreconstructed Au(111) and Au(100). Physical Review B, 2010, 81, .	1.1	9
6962	Pathways for thermal phosphorus desorption from the silicon (001) surface. Physical Review B, 2010, 82, .	1.1	4
6963	Unusual compression behavior of $\text{TiO}_2$ from first principles. Physical Review B, 2010, 82, .	1.1	28
6964	Origin of Rh and Pd agglomeration on the $\text{CeO}_2$ surface. Physical Review B, 2010, 82, .	1.1	18
6965	Structure and properties of surface and subsurface defects in graphite accounting for van der Waals and spin-polarization effects. Physical Review B, 2010, 82, .	1.1	17
6966	Ab initio study of oxygen reduction mechanism at Pt <sub>4</sub> cluster. Physical Chemistry Chemical Physics, 2010, 12, 614-620.	1.3	45
6967	Assessing a solids-biased density-gradient functional for actinide metals. Physical Review B, 2010, 82, .	1.1	26
6968	Point defect chemistry in amorphous $\text{HfO}_2$ . Density functional theory calculations. Physical Review B, 2010, 81, .	1.1	36
6969	Structural and vibrational study of the negative thermal expansion in liquid $\text{As}_2$ . Physical Review B, 2010, 82, .	1.1	20



#	ARTICLE	IF	CITATIONS
6970	Electronic properties and charge state of gold monomers and chains adsorbed on alumina thin films on NiAl(110). Physical Review B, 2010, 81, .	1.1	32
6971	Correlation energy functional within the $G$ -RPA: Exact forms, approximate forms, and challenges. Physical Review B, 2010, 81, .	1.1	22
6972	Controlling water dissociation on an ultrathin MgO film by tuning film thickness. Physical Review B, 2010, 82, .	1.1	38
6973	Water-induced surface reconstruction of oxygen $A_{12}$ Ru(0001). Physical Review B, 2010, 82, .	1.1	12
6974	Simple model explaining and predicting coverage-dependent atomic adsorption energies on transition metal surfaces. Physical Review B, 2010, 82, .	1.1	62
6975	Anomalies in the response of V, Nb, and Ta to tensile and shear loading: <i>Ab initio</i> density functional theory calculations. Physical Review B, 2010, 81, .	1.1	59
6976	Electronic effects of single H atoms on Ge(001) revisited. Journal of Chemical Physics, 2010, 133, 014703.	1.2	10
6977	Calculation of near K edge x-ray absorption spectra and hydrogen bond network in ice XIII under compression. Journal of Chemical Physics, 2010, 132, 184506.	1.2	7
6978	<i>Ab initio</i> study of the solubility and kinetics of hydrogen in austenitic high Mn steels. Physical Review B, 2010, 81, .	1.1	35
6979	Strong hydrogen trapping at helium in tungsten: Density functional theory calculations. Physical Review B, 2010, 81, .	1.1	83
6980	Cohesive and magnetic properties of grain boundaries in bcc Fe with Cr additions. Physical Review B, 2010, 81, .	1.1	79
6981	A theoretical study of H <sub>2</sub> dissociation on (3 $\bar{1}$ –3)R30 $\hat{A}^{\circ}$ CO/Ru(0001). Journal of Chemical Physics, 2010, 132, 144704.	1.2	4
6982	Elastic constants of $\hat{I}^2$ -eucryptite studied by density functional theory. Physical Review B, 2010, 81, .	1.1	19
6983	Order-disorder phase transition of vacancies in surfaces: The case of Sn/Cu(001)-0.5 ML. Physical Review B, 2010, 82, .	1.1	5
6984	Molecular dynamics study of $H_2$ on H-covered Pd(100). Physical Review B, 2010, 81, .	1.1	4
6985	Density functional study of CO and NO adsorption on Ni-doped MgO(100). Journal of Chemical Physics, 2010, 132, 104701.	1.2	52
6986	Atomic-scale structure and electronic property of the LaAlO <sub>3</sub> /TiO <sub>2</sub> interface. Journal of Applied Physics, 2010, 108, .	1.1	49
6987	Electronic and structural properties of ununquadium from first principles. Physical Review B, 2010, 81, .	1.1	6

#	ARTICLE	IF	CITATIONS
6988	Structural and magnetic properties of $Tc$ metalofullerenes: First-principles predictions. Physical Review B, 2010, 81, .		
6989	Simulating thermal motion in crystalline phase-I ammonia. Journal of Chemical Physics, 2010, 132, 134511.	1.2	15
6990	First-Principles Calculations on $\sqrt{3}$ Grain Boundary Transition Metal Impurities in Multicrystalline Silicon. Japanese Journal of Applied Physics, 2010, 49, 04DP02.	0.8	10
6991	KINETIC ENERGY FUNCTIONALS: EXACT ONES FROM ANALYTIC MODEL WAVE FUNCTIONS AND APPROXIMATE ONES IN ORBITAL-FREE MOLECULAR DYNAMICS. International Journal of Modern Physics B, 2010, 24, 5139-5151.	1.0	1
6992	Adhesion at diamond/metal interfaces: A density functional theory study. Journal of Applied Physics, 2010, 107, .	1.1	46
6993	Comparisons of ZnO codoped by group IIIA elements (Al, Ga, In) and N: a first-principle study. Chinese Physics B, 2010, 19, 117102.	0.7	20
6994	General trend for pressurized superconducting hydrogen-dense materials. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 2793-2796.	3.3	81
6995	Apparent failure of the Born-Oppenheimer static surface model for vibrational excitation of molecular hydrogen on copper. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 20881-20886.	3.3	46
6996	Electron traps and their effect on the surface chemistry of $TiO_2$ (110). Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 2391-2396.	3.3	264
6997	Magnetic phase transformations of face-centered cubic and hexagonal close-packed Co at zero Kelvin. Journal of Physics Condensed Matter, 2010, 22, 096006.	0.7	12
6998	MAGNETIC COUPLING IN PSEUDOMORPHIC 2ML OVERLAYERS AND SANDWICH SUPERLATTICE STRUCTURES OF Cr, Mn, Fe, Co AND Ni ON FCC Cu(001). International Journal of Modern Physics B, 2010, 24, 405-412.	1.0	3
6999	DFT Study of Alkali Metal Atom Adsorption on Defect-Free MgO(001) Surface. Chinese Journal of Chemical Physics, 2010, 23, 538-542.	0.6	7
7000	A Be-W interatomic potential. Journal of Physics Condensed Matter, 2010, 22, 352206.	0.7	26
7001	Effects of Single Vacancy on Electronic and Optical Properties for $\beta$ -Si <sub>3</sub> N <sub>4</sub> . Chinese Journal of Chemical Physics, 2010, 23, 201-206.	0.6	2
7002	Edge versus interior in the chemical bonding and magnetism of zigzag edged triangular graphene molecules. Journal of Chemical Physics, 2010, 133, 044708.	1.2	12
7003	Comparison of bond scission sequence of methanol on tungsten monocarbide and Pt-modified tungsten monocarbide. Journal of Chemical Physics, 2010, 133, 104702.	1.2	26
7004	STUDY OF THE ELECTRONIC AND STRUCTURAL PROPERTIES OF ZnO CLUSTERS. International Journal of Modern Physics B, 2010, 24, 3297-3309.	1.0	3
7005	Kinetics versus thermodynamics in materials modeling: The case of the di-vacancy in iron. Philosophical Magazine, 2010, 90, 2585-2595.	0.7	24

#	ARTICLE	IF	CITATIONS
7006	First-principles study of disordering tendencies in Gd <sub>2</sub> B <sub>2</sub> O <sub>7</sub> ( <i>B</i> = Ti, Sn, Zr) compounds. Chinese Physics B, 2010, 19, 127101.	0.7	6
7007	A Simple Theoretical Method to Predict the Hardness of Pure Metal Crystals. Chinese Physics Letters, 2010, 27, 076201.	1.3	1
7008	<i>Ab initio</i> structure modelling of complex thin-film oxides: thermodynamical stability of TiC/thin-film alumina. Journal of Physics Condensed Matter, 2010, 22, 015004.	0.7	4
7009	Linear complex polarization propagator in a four-component Kohn–Sham framework. Journal of Chemical Physics, 2010, 133, 064105.	1.2	33
7010	Solute Segregation at $\frac{1}{2}(113)[110]$ Grain Boundary and Effect of the Segregation on Grain Boundary Cohesion in Aluminum from First Principles. Materials Science Forum, 2010, 654-656, 942-945.	0.3	5
7011	Nonlinear Time-Dependent Density Functional Theory Studies of Ionization in CO <sub>2</sub> and N <sub>2</sub> by Intense Laser Pulses and Molecular Orbital Reconstruction. Lecture Notes in Computer Science, 2010, , 134-147.	1.0	0
7012	First-principles study of the effect of water on the phase transitions in Mg <sub>2</sub> SiO <sub>4</sub> forsterite. High Pressure Research, 2010, 30, 318-324.	0.4	4
7013	First-principles sliding simulation of Al-terminated $\frac{1}{3}$ pyramidal twin grain boundary in $\pm$ -Al <sub>2</sub> O <sub>3</sub> . Philosophical Magazine Letters, 2010, 90, 159-172.	0.5	6
7014	The influence of hydrogen contamination on the structural stability of CoSn under compression. Journal of Physics Condensed Matter, 2010, 22, 435501.	0.7	3
7015	Compactness Aromaticity of Atoms in Molecules. International Journal of Molecular Sciences, 2010, 11, 1269-1310.	1.8	23
7016	Using and validation of the DFT method for oxygen adsorbed on the iron (100) surface. Institutions of Mining and Metallurgy Transactions Section C: Mineral Processing and Extractive Metallurgy, 2010, 119, 67-70.	0.6	3
7017	Anchoring of a Single Molecular Rotor and Its Array on Metal Surfaces using Molecular Design and Self-Assembly. International Journal of Molecular Sciences, 2010, 11, 656-671.	1.8	9
7018	First-principles studies for CO and O <sub>2</sub> on gold nanocluster. Journal of Chemical Physics, 2010, 132, 244302.	1.2	27
7019	Atomic structure and formation mechanism of identically sized Au clusters grown on Si(111)-(7 $\times$ 7) surface. Journal of Chemical Physics, 2010, 133, 124706.	1.2	20
7020	Nuclear momentum distribution in solid and liquid HF from <i>ab initio</i> calculation. Journal of Chemical Physics, 2010, 133, 144505.	1.2	19
7021	Predicting the melting temperatures of bulk materials. Europhysics Letters, 2010, 91, 46001.	0.7	2
7022	Molecular Modelling of Ground- and Excited-States Vibrations in Organic Conducting Devices: Hexakis(n-hexyloxy)triphenylene (HAT6) as Case Study. Australian Journal of Chemistry, 2010, 63, 388.	0.5	7
7023	Reassessment of the Mg–Ge binary system using CALPHAD supported by first-principles calculation. International Journal of Materials Research, 2010, 101, 1489-1496.	0.1	8

#	ARTICLE	IF	CITATIONS
7024	A First Principles Study on Dissociation and Adsorption Processes of H <sub>2</sub> on Pd <sub>3</sub> Ag(111) Surface. Japanese Journal of Applied Physics, 2010, 49, 115702.	0.8	13
7025	Adsorption of methanol and atomic oxygen on the Pt(100) surface: a first-principles periodic density functional theory study. Physica Scripta, 2010, 81, 045603.	1.2	11
7026	First-principles Study of Field Emissions from Sodium-Encapsulated Boron-Nitride Nanotube in a Perpendicular Geometry. Chinese Journal of Chemical Physics, 2010, 23, 553-557.	0.6	0
7027	Spontaneous spin polarization and charge localization in metal nanowires: the role of a geometric constriction. Journal of Physics Condensed Matter, 2010, 22, 295302.	0.7	7
7028	First-principles analysis of the C-N bond scission of methylamine on Mo-based model catalysts. Journal of Chemical Physics, 2010, 132, 044111.	1.2	13
7029	Thioglycolic acid on the gold (111) surface and Raman vibrational spectra. Journal of Chemical Physics, 2010, 132, 064702.	1.2	6
7030	Towards efficient <i>ab initio</i> calculations of electron scattering by polyatomic molecules: III. Modelling correlation polarization interactions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2010, 43, 175205.	0.6	8
7031	A model bismuth oxide intergranular thin film in a ZnO twist grain boundary. Journal of Physics Condensed Matter, 2010, 22, 145503.	0.7	3
7032	A density-functional study of the adsorption of methane-thiol on the (111) surfaces of the Ni-group metals: II. Vibrational spectroscopy. Journal of Physics Condensed Matter, 2010, 22, 265006.	0.7	68
7033	Efficacy of surface error corrections to density functional theory calculations of vacancy formation energy in transition metals. Journal of Physics Condensed Matter, 2010, 22, 345501.	0.7	17
7034	Entropy effects in hydrocarbon conversion reactions: free-energy integrations and transition-path sampling. Journal of Physics Condensed Matter, 2010, 22, 384201.	0.7	24
7035	Density-functional study of the methoxy intermediates at Cu(111), Cu(110) and Cu(001) surfaces. Journal of Physics Condensed Matter, 2010, 22, 395002.	0.7	5
7036	A density functional study of the adsorption of methane-thiol on the (111) surfaces of the Ni-group metals: I. Molecular and dissociative adsorption. Journal of Physics Condensed Matter, 2010, 22, 265005.	0.7	19
7037	Low-dimensional surface oxides in the oxidation of Rh particles. Journal of Physics Condensed Matter, 2010, 22, 393001.	0.7	13
7038	Atomic structure and adhesion of the Nb(001) interface: a first-principles study. Journal of Physics Condensed Matter, 2010, 22, 085004.	0.7	22
7039	Design of type-II Mg <sub>x</sub> Zn <sub>1-x</sub> O/N/ZnO superlattices for UV photodetector applications. Semiconductor Science and Technology, 2010, 25, 045012.	1.0	1
7040	Elastic properties of Pu metal and Pu-Ga alloys. Physical Review B, 2010, 81, .	1.1	49
7041	Jahn-Teller distortion and magnetic structure in $\text{LaMnO}_3$ . A first-principles theoretical study with full structure optimizations. Physical Review B, 2010, 82, .	1.1	53

#	ARTICLE	IF	CITATIONS
7042	Generalized Gradient Approximation +U Study for Metallization Mechanism of Niobium-Doped Anatase Titanium Dioxide. Japanese Journal of Applied Physics, 2010, 49, 055801.	0.8	21
7043	Resonant Scattering by Realistic Impurities in Graphene. Physical Review Letters, 2010, 105, 056802.	2.9	300
7044	First-principles study of structural, elastic, electronic and optical properties of perovskites hydrides $\text{XLiH}_3$ (X = Ba and Sr) under pressure. EPJ Applied Physics, 2010, 51, 20302.	0.3	13
7045	First Principles Studies of the Effect of Nickel Carbide Catalyst Composition on Carbon Nanotube Growth. Journal of Physical Chemistry C, 2010, 114, 18045-18050.	1.5	26
7046	A DFT study of halogen atoms adsorbed on graphene layers. Nanotechnology, 2010, 21, 485701.	1.3	85
7047	Effect of Waters of Crystallization on Terahertz Spectra: Anhydrous Oxalic Acid and Its Dihydrate. Journal of Physical Chemistry A, 2010, 114, 7127-7138.	1.1	60
7048	First-principles study of defects and adatoms in silicon carbide honeycomb structures. Physical Review B, 2010, 81, .	1.1	344
7049	Codoping synergistic effects in N-doped $\text{SrTiO}_3$ for higher energy conversion efficiency. Physical Chemistry Chemical Physics, 2010, 12, 7612.	1.3	52
7050	DFT-Based Theoretical Calculations of Nb- and W-Doped Anatase $\text{TiO}_2$ : Complex Formation between W Dopants and Oxygen Vacancies. Journal of Physical Chemistry C, 2010, 114, 12777-12783.	1.5	32
7051	Oxidative Decomposition of Methanol on Subnanometer Palladium Clusters: The Effect of Catalyst Size and Support Composition. Journal of Physical Chemistry C, 2010, 114, 10342-10348.	1.5	76
7052	Hydrogen multicenter bond mediated magnetism in Co doped ZnO. Journal of Physics Condensed Matter, 2010, 22, 156001.	0.7	14
7053	First-principles study of the electronic properties of wurtzite, zinc-blende, and twinned InP nanowires. Nanotechnology, 2010, 21, 505709.	1.3	21
7054	Solid-State $^{79/81}\text{Br}$ NMR and Gauge-Including Projector-Augmented Wave Study of Structure, Symmetry, and Hydration State in Alkaline Earth Metal Bromides. Journal of Physical Chemistry A, 2010, 114, 2102-2116.	1.1	43
7055	Time-dependent auxiliary density perturbation theory. Journal of Chemical Physics, 2010, 133, 084102.	1.2	33
7056	Optical to ultraviolet spectra of sandwiches of benzene and transition metal atoms: Time dependent density functional theory and many-body calculations. Journal of Chemical Physics, 2010, 132, 044314.	1.2	40
7057	The electronic structure of the triiodide ion from relativistic correlated calculations: A comparison of different methodologies. Journal of Chemical Physics, 2010, 133, 064305.	1.2	29
7058	Dopant-vacancy binding effects in Li-doped magnesium hydride. Physical Review B, 2010, 82, .	1.1	27
7059	Intrinsic point defects and complexes in the quaternary kesterite semiconductor $\text{Cu}_2\text{MnS}_2$ . Physical Review B, 2010, 81, .	1.1	624

# ARTICLE

IF

CITATIONS

7060 Theoretical study of interface structure and energetics in semicoherent  
 $\langle \text{Fe} \rangle$

#	ARTICLE	IF	CITATIONS
7078	Ab initio study of intrinsic, H, and He point defects in hcp-Er. Journal of Applied Physics, 2010, 107, 054903.	1.1	26
7079	Functionalization of BN honeycomb structure by adsorption and substitution of foreign atoms. Physical Review B, 2010, 82, .	1.1	92
7080	Computational Studies of the Thermochemistry for Conversion of Glucose to Levulinic Acid. Journal of Physical Chemistry B, 2010, 114, 9002-9009.	1.2	107
7081	On the Thermodynamic Stability of $\hat{I}_{\pm}$ -Alkanedithiols Self-Assembled Monolayers on Unreconstructed and Reconstructed Au(111). Langmuir, 2010, 26, 9589-9595.	1.6	12
7082	Theoretical Studies of the Electronic Structure of Compounds of the Actinide Elements. , 2010, , 1893-2012.		8
7083	Far infrared spectra of solid state aliphatic amino acids in different protonation states. Journal of Chemical Physics, 2010, 132, 115105.	1.2	23
7084	Fundamental studies of methanol synthesis from CO <sub>2</sub> hydrogenation on Cu(111), Cu clusters, and Cu/ZnO(0001 $\bar{1}$ , $\bar{1}$ ). Physical Chemistry Chemical Physics, 2010, 12, 9909.	1.3	442
7085	Global Hybrid Functionals: A Look at the Engine under the Hood. Journal of Chemical Theory and Computation, 2010, 6, 3688-3703.	2.3	87
7086	Role of molecular electronic structure in inelastic electron tunneling spectroscopy: $\langle \text{O} \rangle^2$ Ag(110). Physical Review B, 2010, 82, .	1.1	24
7087	Selective synthesis of diameter- and interlayer-controlled carbon nitride nanotubes with hydrogen ensnaring nanopores. Physical Chemistry Chemical Physics, 2010, 12, 7461.	1.3	1
7088	Thiol with an Unusual Adsorption-Desorption Behavior: 6-Mercaptopurine on Au(111). Langmuir, 2010, 26, 17068-17074.	1.6	34
7089	Role of Hydrogen Species in Palladium-Catalyzed Alkyne Hydrogenation. Journal of Physical Chemistry C, 2010, 114, 2293-2299.	1.5	71
7090	Prediction of $^{57}\text{Fe}$ Mössbauer Parameters by Density Functional Theory: A Benchmark Study. Journal of Chemical Theory and Computation, 2010, 6, 3735-3749.	2.3	54
7091	Revisiting Hydrogen Storage in Bulk BC <sub>3</sub> . Journal of Physical Chemistry C, 2010, 114, 3260-3264.	1.5	23
7093	Intrinsic room temperature ferromagnetism in boron-doped ZnO. Applied Physics Letters, 2010, 97, .	1.5	66
7094	Elastic and plastic deformation of graphene, silicene, and boron nitride honeycomb nanoribbons under uniaxial tension: A first-principles density-functional theory study. Physical Review B, 2010, 81, .	1.1	219
7095	Hydrogenation: A Simple Approach To Realize Semiconductor-Half-Metal-Metal Transition in Boron Nitride Nanoribbons. Journal of the American Chemical Society, 2010, 132, 1699-1705.	6.6	277
7096	The feeble role of oxygen vacancies in magnetic coupling in ZnO based dilute magnetic semiconductors. Journal of Physics Condensed Matter, 2010, 22, 486003.	0.7	8



#	ARTICLE	IF	CITATIONS
7097	First-principles study of the structural and elastic properties of Ti <sub>5</sub> Si <sub>3</sub> with substitutions Zr, V, Nb, and Cr. <i>Journal of Materials Research</i> , 2010, 25, 2317-2324.	1.2	18
7098	Surface-passivation-induced metallic and magnetic properties of ZnO graphitic sheet. <i>Applied Physics Letters</i> , 2010, 96, .	1.5	18
7099	Tuning Electronic and Magnetic Properties of Wurtzite ZnO Nanosheets by Surface Hydrogenation. <i>ACS Applied Materials &amp; Interfaces</i> , 2010, 2, 2442-2447.	4.0	79
7100	Quantitative structure-reactivity modeling of copper-catalyzed atom transfer radical polymerization. <i>Polymer Chemistry</i> , 2010, 1, 922.	1.9	15
7101	Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2872-2887.	2.3	1,183
7102	Reversible Bond Formation in a Gold-Atom Organic-Molecule Complex as a Molecular Switch. <i>Physical Review Letters</i> , 2010, 105, 266102.	2.9	142
7103	First Principles Study on Hydrogen Desorption from a Metal (=Al, Ti, Mn, Ni) Doped MgH <sub>2</sub> (110) Surface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 11328-11334.	1.5	69
7104	Ligand Size Effect on Pd Oxidative Addition with Aryl Bromide: A DFT Study. <i>Chinese Journal of Chemical Physics</i> , 2010, 23, 175-179.	0.6	13
7105	Electronic Structure of TiO <sub>2</sub> Surfaces and Effect of Molecular Adsorbates Using Different DFT Implementations. <i>Journal of Physical Chemistry C</i> , 2010, 114, 22659-22670.	1.5	134
7106	van der Waals Interactions in Density-Functional Theory: Intermolecular Complexes. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1081-1088.	2.3	155
7107	Density functional theory investigation of $\langle \mathbf{d} \rangle$ and $\langle \mathbf{d}^2 \rangle$ in $\text{LiMSO}_4\text{F}$ (M = Fe, Co and Ni). <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 15512.	1.1	211
7108	$\text{LiMSO}_4\text{F}$ (M = Fe, Co and Ni): promising new positive electrode materials through the DFT microscope. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 15512.	1.3	65
7109	First-principles study of Fe/MgO based magnetic tunnel junctions with Mg interlayers. <i>Physical Review B</i> , 2010, 82, .	1.1	28
7110	Controllable Modulation of the Electronic Structure of ZnO(10 $\bar{1}$ ...0) Surface by Carboxylic Acids. <i>Journal of Physical Chemistry C</i> , 2010, 114, 3973-3980.	1.5	26
7111	Dramatic reduction of the oxygen vacancy formation energy in ceria particles: a possible key to their remarkable reactivity at the nanoscale. <i>Journal of Materials Chemistry</i> , 2010, 20, 10535.	6.7	192
7112	Elasticity of SrTiO <sub>3</sub> perovskite under high pressure in cubic, tetragonal and orthorhombic phases. <i>Physica Scripta</i> , 2010, 82, 025602.	1.2	37
7113	Reversible high-pressure carbon nanotube vessel. <i>Physical Review B</i> , 2010, 81, .	1.1	7
7114	Computational and Experimental Study of the Structure, Binding Preferences, and Spectroscopy of Nickel(II) and Vanadyl Porphyrins in Petroleum. <i>Journal of Physical Chemistry B</i> , 2010, 114, 2180-2188.	1.2	55

#	ARTICLE	IF	CITATIONS
7115	Electronic and Optical Properties of Cubic SrHfO <sub>3</sub> . Communications in Theoretical Physics, 2010, 54, 908-912.	1.1	14
7116	Embedded ribbons of graphene allotropes: an extended defect perspective. New Journal of Physics, 2010, 12, 125006.	1.2	68
7117	A density functional theory approach to noncovalent interactions via interacting monomer densities. Physical Chemistry Chemical Physics, 2010, 12, 14686.	1.3	9
7118	Binding of Nitric Oxide to a Synthetic Model of Iron-Containing Nitrile Hydratase (Fe-NHase) and Its Photorelease: Relevance to Photoregulation of Fe-NHase by NO. Inorganic Chemistry, 2010, 49, 1854-1864.	1.9	30
7119	Dynamics on Six-Dimensional Potential Energy Surfaces for H <sub>2</sub> /Cu(111): Corrugation Reducing Procedure versus Modified Shepard Interpolation Method and PW91 versus RPBE. Journal of Physical Chemistry C, 2010, 114, 11192-11201.	1.5	53
7120	Oxygen-Induced Transformations of an FeO(111) Film on Pt(111): A Combined DFT and STM Study. Journal of Physical Chemistry C, 2010, 114, 21504-21509.	1.5	90
7121	Growth of Cu Metal Films at Room Temperature Using Catalyzed Reactions. Chemistry of Materials, 2010, 22, 1607-1609.	3.2	17
7122	Atomic and Electronic Structure Investigation and Luminescence Property of Eu <sup>2+</sup> -Doped $\hat{\gamma}$ -SiAlON Green Phosphor: Ab initio Calculations. Japanese Journal of Applied Physics, 2010, 49, 06GJ07.	0.8	5
7123	Molecular Rectifying Diodes Based on an Aluminum/4- $\beta$ -Hydroxy-4-biphenyl Carboxylic Acid/p <sup>+</sup> -Silicon Junction. Journal of Physical Chemistry C, 2010, 114, 20877-20884.	1.5	12
7124	Shutting Down Secondary Reaction Pathways: The Essential Role of the Pyrrolyl Ligand in Improving Silica Supported d <sup>0</sup> -ML <sub>4</sub> Alkene Metathesis Catalysts from DFT Calculations. Journal of the American Chemical Society, 2010, 132, 7750-7757.	6.6	121
7125	Initial Growth of BN on Diamond Substrates: A Theoretical Approach. Journal of Physical Chemistry C, 2010, 114, 11448-11455.	1.5	3
7126	H $\hat{\cdot}$ (H <sub>2</sub> O) <sub>n</sub> Clusters: Microsolvation of the Hydrogen Atom via Molecular ab Initio Gradient Embedded Genetic Algorithm (GEGA). Journal of Physical Chemistry A, 2010, 114, 12591-12599.	1.1	66
7127	Experimental and Theoretical Study of a Tungsten Dihydride Silyl Complex: New Insight into Its Bonding Nature and Fluxional Behavior. Organometallics, 2010, 29, 6267-6281.	1.1	23
7128	Mechanism of Water Splitting and Oxygen-Oxygen Bond Formation by a Mononuclear Ruthenium Complex. Journal of the American Chemical Society, 2010, 132, 120-130.	6.6	133
7129	Poisoning of Pt <sub>3</sub> Co Electrodes: A Combined Experimental and DFT Study. Journal of Physical Chemistry C, 2010, 114, 7822-7830.	1.5	28
7130	Density Functional Theory Study of Surface Carbonate Formation on BaO(001). Journal of Physical Chemistry C, 2010, 114, 1867-1874.	1.5	10
7131	Shear softening in tantalum at megabar pressures. Physical Review B, 2010, 82, .	1.1	24
7132	Discrimination of Chiral Solids: A Terahertz Spectroscopic Investigation of $\langle \text{scp} \rangle$ - and $\langle \text{scp} \rangle$ -Serine. Journal of Physical Chemistry A, 2010, 114, 2945-2953.	1.1	74

#	ARTICLE	IF	CITATIONS
7133	Density Functional Theory Calculations on Ruthenium(IV) Bis(amido) Porphyrins: Search for a Broader Perspective of Heme Protein Compound II Intermediates. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15380-15388.	1.2	10
7134	Low O <sub>2</sub> dissociation barrier on Pt(111) due to adsorbate-adsorbate interactions. <i>Journal of Chemical Physics</i> , 2010, 133, 224701.	1.2	49
7135	Orbital order and partial electronic delocalization in a triangular magnetic metal $\frac{1}{\sqrt{3}} \frac{2}{\sqrt{3}}$ Ag. <i>Physical Review B</i> , 2010, 81, .	1.1	28
7136	Structural Design and Two-Dimensional Conductivity of Sheet-Tube Frameworks. <i>Journal of Physical Chemistry C</i> , 2010, 114, 19673-19677.	1.5	11
7137	A Computational Investigation of the Nitrogen-Boron Interaction in <i>o</i> -( <i>N,N</i> -Dialkylaminomethyl)arylboronate Systems. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12531-12539.	1.1	54
7138	Phase equilibria at Si-HfO <sub>2</sub> from first principles thermodynamics. <i>Physical Review B</i> , 2010, 82, .	1.1	13
7139	Electronic Structure and Redox Properties of the Ti-Doped Zirconia (111) Surface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 15403-15409.	1.5	20
7140	Aromatic Amino Acid Monolayers Sandwiched between Gold and Silver: A Combined Tip-Enhanced Raman and Theoretical Approach. <i>Journal of Physical Chemistry C</i> , 2010, 114, 7412-7420.	1.5	58
7141	A Density Functional Theory Study of Adsorption and Decomposition of Nitroamine Molecules on the Al(111) Surface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 9390-9397.	1.5	23
7142	Prediction for room-temperature half-metallic ferromagnetism in the half-fluorinated single layers of BN and ZnO. <i>Applied Physics Letters</i> , 2010, 97, .	1.5	54
7143	First-Principles Calculations of Hydrogen Generation Due to Water Splitting on Polar GaN Surfaces. <i>Journal of Physical Chemistry C</i> , 2010, 114, 18228-18232.	1.5	41
7144	The CO Formation Reaction Pathway in Steam Methane Reforming by Rhodium. <i>Langmuir</i> , 2010, 26, 16339-16348.	1.6	29
7145	In-Situ Deposition of Alkali and Alkaline Earth Hydride Thin Films To Investigate the Formation of Reactive Hydride Composites. <i>Journal of Physical Chemistry C</i> , 2010, 114, 13895-13901.	1.5	11
7146	Structural Analysis and Electronic Properties of Negatively Charged TCNQ: 2D Networks of (TCNQ) <sub>2</sub> Mn Assembled on Cu(100). <i>Journal of Physical Chemistry C</i> , 2010, 114, 17197-17204.	1.5	28
7147	Possible Reaction Paths of Small Silicon Clusters with Oxygen Explored with Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2010, 114, 13196-13203.	1.5	3
7148	Dissociation Free Energy Profiles for Water and Methanol on TiO <sub>2</sub> Surfaces. <i>Journal of Physical Chemistry C</i> , 2010, 114, 11522-11526.	1.5	36
7149	Coverage Dependence of the Structure of Acrolein Adsorbed on Ag(111). <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 2546-2549.	2.1	17
7150	Ab Initio Study of Bond Characteristics and Magnetic Properties of Mixed-Sandwich V <sub>n</sub> Bz <sub>m</sub> Cp <sub>k</sub> Clusters. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2319-2323.	1.1	30

#	ARTICLE	IF	CITATIONS
7151	Anionic Poly( <i>p</i> -Phenylenevinylene)/Layered Double Hydroxide Ordered Ultrathin Films with Multiple Quantum Well Structure: A Combined Experimental and Theoretical Study. <i>Langmuir</i> , 2010, 26, 7007-7014.	1.6	44
7152	Terahertz Spectroscopic Investigation of S-(+)-Ketamine Hydrochloride and Vibrational Assignment by Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2010, 114, 4364-4374.	1.1	21
7154	Protonated Forms of Monoclinic Zirconia: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 8014-8025.	1.5	17
7155	Stabilizing Monomeric Iron Species in a Porous Silica/Mo(112) Film. <i>ACS Nano</i> , 2010, 4, 863-868.	7.3	11
7156	Thermochemical Properties and Electronic Structure of Boron Oxides $B_nO_m$ ( $n = 5 \times 10^1$ , $m = 1 \times 10^2$ ) and Their Anions. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2893-2912.	1.1	35
7157	Molecular Dynamics Simulations of Folding of Supported Graphene. <i>Journal of Physical Chemistry C</i> , 2010, 114, 22472-22477.	1.5	50
7158	Thermodynamic and Kinetic Control on the Formation of Two Novel Metal-Organic Frameworks Based on the Er(III) Ion and the Asymmetric Dimethylsuccinate Ligand. <i>Inorganic Chemistry</i> , 2010, 49, 5063-5071.	1.9	30
7159	Theoretical Investigations on the Formation and Dehydrogenation Reaction Pathways of $H(NH_2)_2BH_2$ Oligomers: Importance of Dihydrogen Interactions. <i>Inorganic Chemistry</i> , 2010, 49, 7710-7720.	1.9	38
7160	Molecular Geometry of Vanadium Dichloride and Vanadium Trichloride: A Gas-Phase Electron Diffraction and Computational Study. <i>Inorganic Chemistry</i> , 2010, 49, 2816-2821.	1.9	9
7161	Viscosity and mutual diffusion of deuterium-tritium mixtures in the warm-dense-matter regime. <i>Physical Review E</i> , 2010, 82, 036404.	0.8	55
7162	Density Functional Theory Analysis of Structure, Energetics, and Spectroscopy for the Mn <sup>2+</sup> /Fe Active Site of <i>Chlamydia trachomatis</i> Ribonucleotide Reductase in Four Oxidation States. <i>Inorganic Chemistry</i> , 2010, 49, 7266-7281.	1.9	32
7163	Nanoscale Alloying, Phase-Segregation, and Core-Shell Evolution of Gold-Platinum Nanoparticles and Their Electrocatalytic Effect on Oxygen Reduction Reaction. <i>Chemistry of Materials</i> , 2010, 22, 4282-4294.	3.2	205
7164	Heterogeneous nucleation of solid Al from the melt by $TiB_2$ . <i>Physical Review B</i> , 2010, 82, 044107.	1.1	66
7165	An <i>ab initio</i> molecular dynamics study. <i>Physical Review B</i> , 2010, 82, 044107. Understanding the Magic Nature of Ligand-Protected Gold Nanoparticle Au <sub>102</sub> (MBA) <sub>44</sub> . <i>Journal of Physical Chemistry C</i> , 2010, 114, 7548-7552.	1.5	25
7166	Simultaneously Understanding the Geometric and Electronic Structure of Anthraceneselenolate on Au(111): A Combined Theoretical and Experimental Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 2677-2684.	1.5	34
7167	Catalytically Active Structure of Bi Deposited on a Au(111) Electrode for the Hydrogen Peroxide Reduction Reaction. <i>Langmuir</i> , 2010, 26, 4590-4593.	1.6	20
7168	Valence Isomerization of Phosphepines. <i>Organometallics</i> , 2010, 29, 6653-6659.	1.1	15
7169	Calcium Borohydride for Hydrogen Storage: A Computational Study of $Ca(BH_4)_2$ Crystal Structures and the $CaB_2H_x$ Intermediate. <i>Journal of Physical Chemistry C</i> , 2010, 114, 9503-9509.	1.5	26

#	ARTICLE	IF	CITATIONS
7170	Structure of Dimeric Molybdenum(VI) Oxide Species on $\gamma$ -Alumina: A Periodic Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 19406-19414.	1.5	33
7171	A DFT and ab Initio Benchmarking Study of Metal-alkane Interactions and the Activation of Carbon-Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1843-1851.	1.1	32
7172	Band Gap Narrowing versus Formation of Electronic States in the Gap in $\text{NiTiO}_2$ Thin Films. <i>Journal of Physical Chemistry C</i> , 2010, 114, 22546-22557.	1.5	34
7173	Vanadia Aggregates on an Ultrathin Aluminum Oxide Film on NiAl(110). <i>Journal of Physical Chemistry C</i> , 2010, 114, 4983-4994.	1.5	20
7174	Adsorption of Thiophene-Conjugated Sensitizers on $\text{TiO}_2$ Anatase (101). <i>Journal of Physical Chemistry C</i> , 2010, 114, 20240-20248.	1.5	40
7175	Photoelectrochemical Response of $\text{TiVO}_4$ and $\text{InVO}_4$ : $\text{TiVO}_4$ Composite. <i>Chemistry of Materials</i> , 2010, 22, 2555-2562.	3.2	21
7176	Density Functional Theory Study of Ethanol Decomposition on $3\text{Ni}/\gamma\text{-Al}_2\text{O}_3(0001)$ Surface. <i>Langmuir</i> , 2010, 26, 15845-15851.	1.6	13
7177	Coverage Effects on the Palladium-Catalyzed Synthesis of Vinyl Acetate: Comparison between Theory and Experiment. <i>Journal of the American Chemical Society</i> , 2010, 132, 2202-2207.	6.6	59
7178	Structural Transition and Thermal Stability of a Coronene Molecular Monolayer on Cu(110). <i>Journal of Physical Chemistry C</i> , 2010, 114, 11180-11184.	1.5	8
7179	Structure Sensitivity for Forward and Reverse Water-Gas Shift Reactions on Copper Surfaces: A DFT Study. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 3053-3057.	2.1	120
7180	Ab Initio Computational Studies of Mg Vacancy Diffusion in Doped $\text{MgB}_2$ Aimed at Hydriding Kinetics Enhancement of the $\text{LiBH}_4 + \text{MgH}_2$ System. <i>Journal of Physical Chemistry C</i> , 2010, 114, 21801-21807.	1.5	10
7181	Role of Step Sites and Surface Vacancies in the Adsorption and Activation of CO on $\gamma\text{-Fe}_5\text{C}_2$ Surfaces. <i>Journal of Physical Chemistry C</i> , 2010, 114, 7863-7879.	1.5	43
7182	Vibrational Circular Dichroism of Adsorbed Molecules: BINAS on Gold Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2010, 114, 15897-15902.	1.5	50
7183	Use of Metallopeptide Based Mimics Demonstrates That the Metalloprotein Nitrile Hydratase Requires Two Oxidized Cysteines for Catalytic Activity. <i>Inorganic Chemistry</i> , 2010, 49, 9064-9077.	1.9	19
7184	Predicting, Fabricating, and Permeability Testing of Free-Standing Ternary Palladium-Copper-Gold Membranes for Hydrogen Separation. <i>Journal of Physical Chemistry C</i> , 2010, 114, 17173-17180.	1.5	43
7185	Theoretical optoelectronic analysis of $\text{MgIn}_2\text{S}_4$ . <i>Physical Review B</i> , 2010, 81, .	1.1	45
7186	Catalytic activity of small MgO-supported Au clusters towards CO oxidation: A density functional study. <i>Physical Review B</i> , 2010, 81, .	1.1	40
7187	Thermodynamic Properties of $\text{Co}_3\text{O}_4$ and $\text{Sr}_6\text{Co}_5\text{O}_{15}$ from First-Principles. <i>Inorganic Chemistry</i> , 2010, 49, 10291-10298.	1.9	17

#	ARTICLE	IF	CITATIONS
7188	Field Emission Enhancement in Semiconductor Nanofilms by Engineering the Layer Thickness: First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2010, 114, 11584-11587.	1.5	8
7189	Magnetizabilities at Self-Interaction-Corrected Density Functional Theory Level. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3302-3311.	2.3	10
7190	Pseudopotential and full-electron DFT calculations of thermodynamic properties of electrons in metals and semiempirical equations of state. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 505501.	0.7	40
7191	Alumina as a Simultaneous Support and Co Catalyst: Cationic Hafnium Complex Evidenced by Experimental and DFT Analyses. <i>Journal of Physical Chemistry C</i> , 2010, 114, 18516-18528.	1.5	23
7192	Investigating the Anharmonicity of Lattice Vibrations in Water-Containing Molecular Crystals through the Terahertz Spectroscopy of $\alpha$ -Serine Monohydrate. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9570-9578.	1.1	55
7193	Catalytic Action of a Cu(111) Surface on Tetraazaperopyrene Polymerization. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 3266-3270.	2.1	15
7194	DFT-NMR Investigation and $^{51}\text{V}$ QMAS Experiments for Probing Surface OH Ligands and the Hydrogen-Bond Network in a Polyoxovanadate Cluster: The Case of $\text{Cs}_4\text{[H}_2\text{V}_{10}\text{O}_{28}\text{]}\cdot 4\text{H}_2\text{O}$ . <i>Journal of the American Chemical Society</i> , 2010, 132, 4653-4668.	6.6	32
7195	Control of Two-Dimensional Ordering of F16CuPc on Bi/Ag(111): Effect of Interfacial Interactions. <i>Journal of Physical Chemistry C</i> , 2010, 114, 11234-11241.	1.5	15
7196	Gas-Phase Reactions of Uranate Ions, $\text{UO}_2^+$ , $\text{UO}_3^+$ , $\text{UO}_4^+$ , and $\text{UO}_4\text{H}^+$ , with Methanol: a Convergence of Experiment and Theory. <i>Inorganic Chemistry</i> , 2010, 49, 3836-3850.	1.9	27
7197	DFT Investigation of Oligothiophenes on a Si(001) Surface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20068-20075.	1.5	6
7198	Formation Enthalpies of Ions: Routine Prediction Using Atom Equivalents. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2126-2139.	2.3	4
7199	IR Spectroscopic Measurement of Diffusion Kinetics of Chemisorbed Pyridine through $\text{TiO}_2$ Particles. <i>Journal of Physical Chemistry C</i> , 2010, 114, 16649-16659.	1.5	20
7200	Electronic Structure $\rightarrow$ Transport Property Relationships of Polyferrocenylene, Polyferrocenylacetylene, and Polyferrocenylsilane. <i>Journal of Physical Chemistry C</i> , 2010, 114, 9469-9477.	1.5	17
7201	High Photocatalytic Activity of Rutile $\text{TiO}_2$ Induced by Iodine Doping. <i>Journal of Physical Chemistry C</i> , 2010, 114, 6035-6038.	1.5	34
7202	On the Nature and Origin of Si Surface Segregation in Amorphous AuSi Alloys. <i>Journal of Physical Chemistry C</i> , 2010, 114, 3037-3041.	1.5	17
7203	Pentacene Multilayers on Ag(111) Surface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 2724-2729.	1.5	28
7204	Scanning Tunneling Microscopy Investigation of Tris(phthalocyaninato)yttrium Triple-Decker Molecules Deposited on Au(111). <i>Journal of Physical Chemistry C</i> , 2010, 114, 12202-12206.	1.5	24
7205	Structure, Dynamics, and Energetics of Lysobisphosphatidic Acid (LBPA) Isomers. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15712-15720.	1.2	21



#	ARTICLE	IF	CITATIONS
7206	Effects of Morphology on Stability, Electronic, and Optical Properties of Rutile TiO <sub>2</sub> Nanowires. <i>Journal of Physical Chemistry C</i> , 2010, 114, 21013-21019.	1.5	19
7207	Transport Properties of Thiophenes: Insights from Density-Functional Theory Modeling Using Dispersion-Correcting Potentials. <i>Journal of Physical Chemistry C</i> , 2010, 114, 10952-10961.	1.5	7
7208	Photoinduced Fluorescent Cross-Linking of 5-Chloro- and 5-Fluoro-4-thiouridines with Thymidine. <i>Journal of Organic Chemistry</i> , 2010, 75, 621-626.	1.7	13
7209	High Thermoelectric Performance of Ge/Si Core-Shell Nanowires: First-Principles Prediction. <i>Journal of Physical Chemistry C</i> , 2010, 114, 9096-9100.	1.5	36
7210	Density-functional characterization of antiferromagnetism in oxygen-deficient anatase and rutile $\text{TiO}_{2-x}$ . <i>Physical Review B</i> , 2010, 81, .	1.1	135
7211	Density Functional Study of Boron-Doped Anatase TiO <sub>2</sub> . <i>Journal of Physical Chemistry C</i> , 2010, 114, 19830-19834.	1.5	49
7212	Grafting of Lanthanide Complexes on Silica Surfaces: A Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6322-6330.	1.1	29
7213	Diffusivity Control in Molecule-on-Metal Systems Using Electric Fields. <i>Nano Letters</i> , 2010, 10, 1184-1188.	4.5	64
7214	Ab initio thermodynamic and elastic properties of AGaH <sub>4</sub> hydrides (A=Li, Na, K, Rb, and Cs). <i>Physical Review B</i> , 2010, 82, .	1.1	12
7215	First-principles study of La and Sb-doping effects on electronic structure and optical properties of SrTiO <sub>3</sub> . <i>Chinese Physics B</i> , 2010, 19, 017101-8.	0.7	11
7216	Does the MgO(100)-Support Facilitate the Reaction of Nitrogen and Hydrogen Molecules Catalyzed by Zr <sub>2</sub> Pd <sub>2</sub> Clusters? A Computational Study. <i>Inorganic Chemistry</i> , 2010, 49, 2557-2567.	1.9	0
7217	Disappearing and Concomitant Polymorphism of Nickel(II) Complexes with 6-Hydroxypicolinic Acid. Structural and Density Functional Theory Studies. <i>Crystal Growth and Design</i> , 2010, 10, 3685-3693.	1.4	14
7218	Pathways for Oxygen Incorporation in Mixed Conducting Perovskites: A DFT-Based Mechanistic Analysis for (La, Sr)MnO <sub>3-<math>\delta</math></sub> . <i>Journal of Physical Chemistry C</i> , 2010, 114, 3017-3027.	1.5	160
7219	First-Principles Study of Different Polymorphs of Crystalline Zirconium Hydride. <i>Journal of Physical Chemistry C</i> , 2010, 114, 22361-22368.	1.5	75
7220	Structures and Unusual Rearrangements of Coordination Adducts of MX <sub>5</sub> (M = Nb, Ta; X = F, Cl) with Simple Diethers. A Crystallographic, Spectroscopic, and Computational Study. <i>Inorganic Chemistry</i> , 2010, 49, 339-351.	1.9	49
7221	Composition dependent adsorption of multiple CO molecules on binary silver-gold clusters Ag <sub>n</sub> Au <sub>m</sub> <sup>+</sup> (n + m = 5): theory and experiment. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 7865.	1.3	28
7222	Density Functional Study of Hydrogen Binding on Gold and Silver-Gold Clusters. <i>Journal of Physical Chemistry A</i> , 2010, 114, 4917-4923.	1.1	51
7223	Predicting impurity gases and phases during hydrogen evolution from complex metal hydrides using free energy minimization enabled by first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9918.	1.3	20



#	ARTICLE	IF	CITATIONS
7224	Unveiling the atomic and electronic structure of the VN/MgO interface. <i>Physical Review B</i> , 2010, 82, .	1.1	3
7225	Transition-Metal Decoration Enhanced Room-Temperature Hydrogen Storage in a Defect-Modulated Graphene Sheet. <i>Journal of Physical Chemistry C</i> , 2010, 114, 10297-10301.	1.5	135
7226	Trends in the Adsorption of 3d Transition Metal Atoms onto Graphene and Nanotube Surfaces: A DFT Study and Molecular Orbital Analysis. <i>Journal of Physical Chemistry C</i> , 2010, 114, 14141-14153.	1.5	184
7227	Characterization of a new Nb <sup>11</sup> Si <sup>4</sup> silicide (Nb <sub>11</sub> Si <sub>4</sub> ) in Nb <sup>11</sup> Si binary systems. <i>Philosophical Magazine</i> , 2010, 90, 2557-2568.	0.7	12
7228	Ab initio study of formation energy and magnetism of sigma phase in Cr <sup>11</sup> Fe and Cr <sup>11</sup> Co systems. <i>Intermetallics</i> , 2010, 18, 212-220.	1.8	51
7229	Energetic evaluation of Ba <sup>11</sup> and Sr <sup>11</sup> Si clathrate formation at high pressures by first-principle pseudopotential calculations. <i>Intermetallics</i> , 2010, 18, 542-547.	1.8	13
7230	First-principles study of the structural, electronic and elastic properties of W <sub>5</sub> Si <sub>3</sub> . <i>Intermetallics</i> , 2010, 18, 688-693.	1.8	41
7231	Monte-Carlo simulation of atom kinetics in intermetallics: Correcting the jump rates in Ni <sub>3</sub> Al. <i>Intermetallics</i> , 2010, 18, 1091-1098.	1.8	8
7232	Ni and Al diffusion in Ni-rich NiAl and the effect of Pt additions. <i>Intermetallics</i> , 2010, 18, 1470-1479.	1.8	17
7233	Local atomic and electronic structures of equiatomic liquid alloy KSb from 923 to 1773K. <i>Journal of Non-Crystalline Solids</i> , 2010, 356, 8-13.	1.5	4
7234	Correlation between local structure of melts and glass forming ability for Fe <sub>70</sub> EM <sub>10</sub> B <sub>20</sub> (EM = early) Tj ETQq0 0 0 rBT /Overlock 10 Tf	1.5	12
7235	The structure of liquid Mg <sup>11</sup> Cu binary alloys. <i>Journal of Non-Crystalline Solids</i> , 2010, 356, 1587-1592.	1.5	15
7236	Mechanistic Insights into Ferredoxin <sup>11</sup> NADP(H) Reductase Catalysis Involving the Conserved Glutamate in the Active Site. <i>Journal of Molecular Biology</i> , 2010, 397, 814-825.	2.0	22
7237	Phase stability, mechanical property, and electronic structure of Mg <sup>11</sup> Li system. <i>Journal of Alloys and Compounds</i> , 2010, 489, 130-135.	2.8	33
7238	Thermodynamic assessments of Ag <sup>11</sup> Dy and Ag <sup>11</sup> Er binary systems. <i>Journal of Alloys and Compounds</i> , 2010, 489, 146-151.	2.8	6
7239	Sn-flux syntheses, characterizations and bonding analyses of OsB and TiB <sub>2</sub> . <i>Journal of Alloys and Compounds</i> , 2010, 489, 339-342.	2.8	19
7240	First-principles study on the site preference of Dy in B <sub>2</sub> NiAl. <i>Journal of Alloys and Compounds</i> , 2010, 492, 295-299.	2.8	15
7241	First-principles investigation of the structural and mechanical properties of $\beta$ phase in Mg <sup>11</sup> Gd alloy system. <i>Journal of Alloys and Compounds</i> , 2010, 492, 416-420.	2.8	25

#	ARTICLE	IF	CITATIONS
7242	The featured local structural units in liquid Al <sub>80</sub> Si <sub>15</sub> P <sub>5</sub> alloy and their relationship with Si modification. <i>Journal of Alloys and Compounds</i> , 2010, 492, 525-528.	2.8	13
7243	Structural, electronic, and hydriding properties of Li <sub>2</sub> MgSi. <i>Journal of Alloys and Compounds</i> , 2010, 492, 65-68.	2.8	21
7244	Surface complexation of Cu on birnessite ( $\gamma$ -MnO <sub>2</sub> ): Controls on Cu in the deep ocean. <i>Geochimica Et Cosmochimica Acta</i> , 2010, 74, 6721-6730.	1.6	91
7245	Elastic and thermodynamic properties of the Ni-B system studied by first-principles calculations and experimental measurements. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2010, 34, 245-251.	0.7	15
7246	Thermodynamic modeling of the Pd-S system supported by first-principles calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2010, 34, 324-331.	0.7	8
7247	Structure behavior and equation of state (EOS) of Ni <sub>2</sub> P and (Fe <sub>1-x</sub> Ni <sub>x</sub> ) <sub>2</sub> P (allabogdanite) from First-principles calculations. <i>Earth and Planetary Science Letters</i> , 2010, 295, 578-582.	1.8	3
7248	Atomic structures and behaviors of a fcc Cu(111) surface with submonolayer Pb coverage. <i>Computational Materials Science</i> , 2010, 47, 693-697.	1.4	3
7249	The structural, electronic, elastic, phonon, and thermodynamical properties of the SmX (X=P, Sb, Bi) compounds. <i>Computational Materials Science</i> , 2010, 47, 758-768.	1.4	5
7250	First principles study of structural, elastic and electronic properties of ACY <sub>3</sub> (A=Al, In and Tl). <i>Computational Materials Science</i> , 2010, 47, 973-976.	1.4	8
7251	First-principles calculations of structural, electronic and optical properties of tetragonal SnO <sub>2</sub> and SnO. <i>Computational Materials Science</i> , 2010, 47, 1016-1022.	1.4	83
7252	Electronic properties and pressure effect on the structural behaviour of M <sub>2</sub> AC (M=V, Nb and A=P, As). <i>Computational Materials Science</i> , 2010, 48, 174-178.	1.4	5
7253	First-principles calculation and luminescence property of Eux:Si <sub>5</sub> Al <sub>1-x</sub> O <sub>1+x</sub> N <sub>7-x</sub> green phosphor. <i>Computational Materials Science</i> , 2010, 49, S359-S363.	1.4	4
7254	The role of structural variations in the magnetism of Fe/Cu(111): First-principles calculations. <i>Computational Materials Science</i> , 2010, 49, S291-S296.	1.4	5
7255	Hydrogen storage in Al and Ti dispersed on graphene with boron substitution: First-principles calculations. <i>Computational Materials Science</i> , 2010, 49, S297-S301.	1.4	29
7256	Dehydrogenation kinetics of magnesium hydride investigated by DFT and experiment. <i>Computational Materials Science</i> , 2010, 49, S144-S149.	1.4	26
7257	Au-K co-deposition on MgO(2L)/Ag(001): A first principles study. <i>Computational Materials Science</i> , 2010, 48, 719-723.	1.4	0
7258	First-principles study on the structural, mechanical and electronic properties of $\gamma$ and $\gamma$ -3 phases in Inconel 718. <i>Computational Materials Science</i> , 2010, 49, 414-418.	1.4	33
7259	Optical absorption and electron energy loss spectra of single-walled carbon nanotubes. <i>Computational Materials Science</i> , 2010, 49, 450-456.	1.4	38

#	ARTICLE	IF	CITATIONS
7260	General trends in the structural, electronic and elastic properties of the M <sub>3</sub> AlC <sub>2</sub> phases (M =) Tj ETQq0 0 0 rgBT /Oyerlock 10 Tf 50 742	1.4	86
7261	Crystal structure and elastic properties of ZrB compared with ZrB <sub>2</sub> : A first-principles study. Computational Materials Science, 2010, 49, 814-819.	1.4	79
7262	First-principles study of the structural, elastic and electronic properties of HfTaO <sub>3</sub> N. Computational Materials Science, 2010, 50, 114-117.	1.4	1
7263	First-principles study of self-diffusion in hcp Mg and Zn. Computational Materials Science, 2010, 50, 301-307.	1.4	64
7264	First-principles study of electronic and optical properties of Pbnm orthorhombic SrHfO <sub>3</sub> . Computational Materials Science, 2010, 50, 454-458.	1.4	8
7265	First-principles study of NiAl microalloyed with Sc, Y, La and Nd. Computational Materials Science, 2010, 50, 545-549.	1.4	26
7266	Theoretical investigation of moderate misfit and interface energetics in the Fe/VN system. Computational Materials Science, 2010, 50, 550-559.	1.4	23
7267	Equation of state (EOS) and collapse of magnetism in iron-rich meteorites at high pressure by first-principles calculations. Physics of the Earth and Planetary Interiors, 2010, 182, 175-178.	0.7	5
7268	A particularly strong organic acceptor for tuning the hole-injection barriers in modern organic devices. Synthetic Metals, 2010, 160, 1456-1462.	2.1	8
7269	Pentaatomic planar tetracoordinate carbon molecules [XCAI <sub>3</sub> ] <sub>q</sub> [(X,q) = (B,âˆ²), (C,âˆ¹), (N,0)] with Câ€“X multiple bonding. Physical Chemistry Chemical Physics, 2010, 12, 13637.	1.3	39
7270	Tuning the Hydrogen Storage in Magnesium Alloys. Journal of Physical Chemistry Letters, 2010, 1, 1982-1986.	2.1	25
7271	Adsorption of Carbon Dioxide and Nitrogen on Single-Layer Aluminum Nitride Nanostructures Studied by Density Functional Theory. Journal of Physical Chemistry C, 2010, 114, 7846-7849.	1.5	53
7272	Modeling and simulation of nuclear fuel materials. Energy and Environmental Science, 2010, 3, 1406.	15.6	80
7273	First-Principles-Based Kinetic Monte Carlo Simulation of Nitric Oxide Reduction over Platinum Nanoparticles under Lean-Burn Conditions. Industrial & Engineering Chemistry Research, 2010, 49, 10364-10373.	1.8	36
7274	Oxygen activation on gold nanoparticles: separating the influence of particle size, particle shape and support interaction. Dalton Transactions, 2010, 39, 8538.	1.6	134
7275	Water Adsorption on Native and Hydrogenated Diamond (001) Surfaces. Journal of Physical Chemistry C, 2010, 114, 7045-7053.	1.5	47
7276	Structural, electronic, and optical properties of Î±, Î², and Î³-TeO <sub>2</sub> . Journal of Applied Physics, 2010, 107, .	1.1	39
7277	Search and Characterization of Transition State Structures in Crystalline Systems Using Valence Coordinates. Journal of Chemical Theory and Computation, 2010, 6, 1341-1350.	2.3	19

#	ARTICLE	IF	CITATIONS
7278	Solid-State <sup>127</sup> I NMR and GIPAW DFT Study of Metal Iodides and Their Hydrates: Structure, Symmetry, and Higher-Order Quadrupole-Induced Effects. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10810-10823.	1.1	63
7279	Effect of substrate strain on calculated magnetic properties and magnetic anisotropy energy of CoO. <i>Physical Review B</i> , 2010, 81, .	1.1	21
7280	Charge effect in S enhanced CO adsorption: A theoretical study of CO on Au, Ag, Cu, and Pd (111) surfaces coadsorbed with S, O, Cl, and Na. <i>Journal of Chemical Physics</i> , 2010, 133, 094703.	1.2	29
7281	Dynamics simulation of N <sub>2</sub> scattering onto W(100,110) surfaces: A stringent test for the recently developed flexible periodic Londonâ€“Eyringâ€“Polanyiâ€“Sato potential energy surface. <i>Journal of Chemical Physics</i> , 2010, 132, 204501.	1.2	27
7282	First principles prediction of the third conformer of hydrogenated BN sheet. <i>Physica Status Solidi - Rapid Research Letters</i> , 2010, 4, 368-370.	1.2	32
7283	Atomistic modeling of interfaces and their impact on microstructure and properties. <i>Acta Materialia</i> , 2010, 58, 1117-1151.	3.8	430
7284	Second-generation charge-optimized many-body potential for $\text{Si}$ amorphous silica. <i>Physical Review B</i> , 2010, 82, .	1.1	80
7285	Structures and Chemical Ordering of Small Cu <sup>+</sup> Ag Clusters. <i>Journal of Physical Chemistry C</i> , 2010, 114, 13255-13266.	1.5	91
7286	Electronic Structure of an Iron-Porphyrin <sup>+</sup> Nitrene Complex. <i>Inorganic Chemistry</i> , 2010, 49, 243-248.	1.9	18
7287	The Effect of CO and H Chemisorption on the Chemical Ordering of Bimetallic Clusters. <i>Journal of Physical Chemistry C</i> , 2010, 114, 19678-19686.	1.5	47
7288	First-principles prediction of partitioning of alloying elements between cementite and ferrite. <i>Acta Materialia</i> , 2010, 58, 6276-6281.	3.8	84
7289	JuNoLo â€“ JÃ¼lich nonlocal code for parallel post-processing evaluation of vdW-DF correlation energy. <i>Computer Physics Communications</i> , 2010, 181, 371-379.	3.0	40
7290	A DFT study of PtAu bimetallic clusters adsorbed on MgO/Ag(100) ultrathin films. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6352.	1.3	12
7291	Palladium Complexes of the Heterodiphosphine $\text{C}_6\text{H}_4(\text{CH}_2)_2\text{P}(\text{tBu})_2(\text{CH}_2)_2\text{PPh}_2$ Are Highly Selective and Robust Catalysts for the Hydromethoxycarbonylation of Ethene. <i>Organometallics</i> , 2010, 29, 2292-2305.	1.1	49
7292	Electron-poor antimonides: complex framework structures with narrow band gaps and low thermal conductivity. <i>Dalton Transactions</i> , 2010, 39, 1036-1045.	1.6	27
7293	CO and NO complexes of Fe(II) and Co(II) porphyrins. <i>Journal of Coordination Chemistry</i> , 2010, 63, 2854-2867.	0.8	7
7294	Modeling surface segregation phenomena in the (111) surface of ordered Pt <sub>3</sub> Ti crystal. <i>Journal of Chemical Physics</i> , 2010, 133, 114701.	1.2	25
7295	Catalytic Reduction of NO <sub>2</sub> with Hydrogen on Pt Field Emitter Tips: Kinetic Instabilities on the Nanoscale. <i>Langmuir</i> , 2010, 26, 16381-16391.	1.6	20

#	ARTICLE	IF	CITATIONS
7296	A quantum chemistry investigation on the structure of lanthanide triflates Ln(OTf) <sub>3</sub> where Ln = La, Ce, Nd, Eu, Gd, Er, Yb and Lu. Dalton Transactions, 2010, 39, 3673.	1.6	13
7297	Stability and mechanical properties of BC <sub>x</sub> crystals: the role of B–B bonds and boron concentration. Journal of Physics Condensed Matter, 2010, 22, 215401.	0.7	4
7298	Structural and Electronic Properties of Li-Ion Battery Cathode Material FeF <sub>3</sub> . Journal of Physical Chemistry C, 2010, 114, 16813-16817.	1.5	59
7299	Structure and optical properties of high light output halide scintillators. Physical Review B, 2010, 82, .	1.1	155
7300	Molecular structures and activity of organic depressants for marmatite, jamesonite and pyrite flotation. Transactions of Nonferrous Metals Society of China, 2010, 20, 1993-1999.	1.7	29
7301	First-principles Calculation Assisted Thermodynamic Modeling of Ti-Co-Cu Ternary System. Journal of Materials Science and Technology, 2010, 26, 317-326.	5.6	4
7302	Achieving Ferromagnetism in Single-Crystalline ZnS Wurtzite Nanowires via Chromium Doping. Journal of Physical Chemistry C, 2010, 114, 12099-12103.	1.5	31
7303	Origin of the Different Activity and Selectivity toward Hydrogenation of Single Metal Au and Pt on TiO <sub>2</sub> and Bimetallic Au <sup>~</sup> Pt/TiO <sub>2</sub> Catalysts. Langmuir, 2010, 26, 16607-16614.	1.6	77
7304	Band gap tuning in GaN through equibiaxial in-plane strains. Applied Physics Letters, 2010, 96, .	1.5	76
7305	Density functional theory study of ZnX(X=O, S, Se, Te) under uniaxial strain. Physical Review B, 2010, 81, .	1.1	66
7306	The fascinating physics of carbon surfaces: first-principles study of hydrogen on C(0001), C(110) and graphene. Journal Physics D: Applied Physics, 2010, 43, 374016.	1.3	16
7307	Accurate dispersion interactions from standard density-functional theory methods with small basis sets. Physical Chemistry Chemical Physics, 2010, 12, 6092.	1.3	52
7308	THE CHEMICAL BONDING OF Re <sub>3</sub> Cl <sub>9</sub> AND REVEALED BY THE ADAPTIVE NATURAL DENSITY PARTITIONING ANALYSES. Comments on Inorganic Chemistry, 2010, 31, 2-12.	3.0	55
7309	Tunable properties of Pt <sub>x</sub> Fe <sub>1-x</sub> electrocatalysts and their catalytic activity towards the oxygen reduction reaction. Nanoscale, 2010, 2, 573.	2.8	40
7310	Theoretical Confirmation of the Enhanced Facility to Increase Oxygen Vacancy Concentration in TiO <sub>2</sub> by Iron Doping. Journal of Physical Chemistry C, 2010, 114, 6511-6517.	1.5	78
7311	Adsorption and Electronic Structure of Single C <sub>60</sub> F <sub>18</sub> Molecule on Si(111)-7 $\times$ 7 Surface. Fullerenes Nanotubes and Carbon Nanostructures, 2010, 18, 369-375.	1.0	2
7312	Quantum Chemistry on Graphics Processing Units. Annual Reports in Computational Chemistry, 2010, , 21-35.	0.9	24
7313	Magnetic anisotropy of Fe and Co ultrathin films deposited on Rh(111) and Pt(111) substrates: An experimental and first-principles investigation. Physical Review B, 2010, 82, .	1.1	106

#	ARTICLE	IF	CITATIONS
7314	Scalar and Spin-Orbit Relativistic Corrections to the NICS and the Induced Magnetic Field: The case of the $E_{12}^{2+}$ Spherenes (E = Ge, Sn, Pb). <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2701-2705.	2.3	44
7315	Structure and stability of aluminium doped lithium clusters ( $LiAlO_n$ , $n = 1-8$ ): a case of the phenomenological shell model. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 11477.	1.3	11
7316	Structures and Stability of Metal Amidoboranes (MAB): Density Functional Calculations. <i>Communications in Theoretical Physics</i> , 2010, 53, 1167-1171.	1.1	2
7317	On the Origin of the Inverted Stability Order of the Reverse-Keggin $[(MnO_4)(CH_3)_3]_{12}Sb_{12}O_{24}]^{6-}$ : A DFT Study of $I_{\pm}^2$ , $I_{\pm}^3$ , $I_{\pm}^1$ , and $I_{\mu}$ Isomers. <i>Inorganic Chemistry</i> , 2010, 49, 5472-5481.	1.9	14
7318	Quantitative Characteristics of Qualitative Localized Bonding Patterns. <i>Journal of Physical Chemistry A</i> , 2010, 114, 3074-3079.	1.1	3
7319	Rhodium atoms confined in boron nitride nanotubes: Density functional calculations. <i>Europhysics Letters</i> , 2010, 90, 47003.	0.7	2
7320	Gaining Insights into the Energetics of $FePO_4$ Polymorphs. <i>Chemistry of Materials</i> , 2010, 22, 994-1001.	3.2	20
7321	ELECTRONIC AND THERMOELECTRIC PROPERTIES OF PURE AND ALLOYS $In_2O_3$ TRANSPARENT CONDUCTORS. <i>Modern Physics Letters B</i> , 2010, 24, 2251-2265.	1.0	5
7322	Structure and Reactivity of Aluminum Oxide Supported Nickel Clusters. <i>Journal of Physical Chemistry C</i> , 2010, 114, 22155-22158.	1.5	8
7323	The Vibrational Spectrum of Parabanic Acid by Inelastic Neutron Scattering Spectroscopy and Simulation by Solid-State DFT. <i>Journal of Physical Chemistry A</i> , 2010, 114, 3630-3641.	1.1	6
7324	X-ray snapshots for metalloporphyrin axial ligation. <i>Chemical Science</i> , 2010, 1, 642.	3.7	40
7325	Defect physics of the kesterite thin-film solar cell absorber $Cu_2ZnSnS_4$ . <i>Applied Physics Letters</i> , 2010, 96, .	1.5	454
7326	<i>Ab initio</i> studies on atomic and electronic structures of black phosphorus. <i>Journal of Applied Physics</i> , 2010, 107, .	1.1	235
7327	First-principles study of structural, elastic, lattice dynamical and thermodynamical properties of $GdX$ (X = Bi, Sb). <i>Philosophical Magazine</i> , 2010, 90, 1833-1852.	0.7	9
7328	A theoretical insight into the catalytic effect of a mixed-metal oxide at the nanometer level: The case of the highly active metal/CeO <sub>x</sub> /TiO <sub>2</sub> (110) catalysts. <i>Journal of Chemical Physics</i> , 2010, 132, 104703.	1.2	93
7329	Structure and mechanical properties of cubic BC <sub>2</sub> N crystals within a random solid solution model. <i>Diamond and Related Materials</i> , 2010, 19, 1419-1422.	1.8	15
7330	Detection of Weak Intramolecular Interactions in $Ru_3(CO)_{12}$ by Topological Analysis of Charge Density Distributions. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9368-9373.	1.1	17
7331	Hydrogen Rotational and Translational Diffusion in Calcium Borohydride from Quasielastic Neutron Scattering and DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20249-20257.	1.5	23







#	ARTICLE	IF	CITATIONS
7350	A molecular simulation analysis of producing monatomic carbon chains by stretching ultranarrow graphene nanoribbons. <i>Nanotechnology</i> , 2010, 21, 265702.	1.3	25
7351	Carbon- <sup>13</sup> Chlorine Bond Scission in Li-Doped Single-Walled Carbon Nanotubes: Reaction of CH <sub>3</sub> Cl and Lithium. <i>Journal of Physical Chemistry C</i> , 2010, 114, 17148-17158.	1.5	9
7352	Adsorption Species of Ethyl Benzoate in MgCl <sub>2</sub> -Supported Ziegler-Natta Catalysts. A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 429-435.	1.5	44
7353	Unusual Physical and Chemical Properties of Ni in Ce <sub>1-x</sub> Ni <sub>x</sub> O <sub>2-y</sub> Oxides: Structural Characterization and Catalytic Activity for the Water Gas Shift Reaction. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12689-12697.	1.5	151
7354	Computer simulations of structures and properties of the biomaterial hydroxyapatite. <i>Journal of Materials Chemistry</i> , 2010, 20, 5376.	6.7	72
7355	Pd(ii)-promoted direct cross-coupling reaction of arenes via highly regioselective aromatic C-H activation: a theoretical study. <i>Dalton Transactions</i> , 2010, 39, 3279.	1.6	55
7356	High-Pressure Phases of Calcium: Density-Functional Theory and Diffusion Quantum Monte Carlo Approach. <i>Physical Review Letters</i> , 2010, 105, 235503.	2.9	37
7357	Orbitally controlled Kondo effect of Co adatoms on graphene. <i>Physical Review B</i> , 2010, 81, .	1.1	132
7358	A density functional theory study of CO <sub>2</sub> and N <sub>2</sub> adsorption on aluminium nitride single walled nanotubes. <i>Journal of Materials Chemistry</i> , 2010, 20, 10426.	6.7	62
7359	Atomic Charges Derived from Electrostatic Potentials for Molecular and Periodic Systems. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10225-10233.	1.1	70
7360	Computational studies on the interactions among redox couples, additives and TiO <sub>2</sub> : implications for dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 14609.	1.3	32
7361	Theoretical study of physisorption of nucleobases on boron nitride nanotubes: a new class of hybrid nano-biomaterials. <i>Nanotechnology</i> , 2010, 21, 165703.	1.3	127
7362	Scaling Behavior of Electronic Excitations in Assemblies of Molecules with Degenerate Ground States. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2213-2220.	1.1	3
7363	Magnetic Properties of Transition-Metal-Doped Tubular Gold Clusters: M@Au <sub>24</sub> (M = V, Cr, Mn, Fe, Co). <i>Journal of Physical Chemistry B</i> , 2010, 14, 7843-7855.	1.1	35
7364	Endohedrally Doped Golden Fullerenes [X@Au <sub>32</sub> ] (X = Li, Na, K, Rb, Cs). <i>Journal of Physical Chemistry B</i> , 2010, 14, 10000-10006.	1.5	26
7365	Ethylene Epoxidation on a Au Nanoparticle versus a Au(111) Surface: A DFT Study. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 739-742.	2.1	40
7366	Role of Adsorbed H, C, O, and CO on the Atomic Structure of Free and MgO(100)-Supported Ir <sub>4</sub> Clusters: An ab Initio Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 15653-15660.	1.5	7
7367	Preferential CO Oxidation in Hydrogen: Reactivity of Core-Shell Nanoparticles. <i>Journal of the American Chemical Society</i> , 2010, 132, 7418-7428.	6.6	258

#	ARTICLE	IF	CITATIONS
7369	Towards an understanding of the vibrational mode specificity for dissociative chemisorption of CH <sub>4</sub> on Ni(111): a 15 dimensional study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 7654.	1.3	36
7370	The interaction of NO <sub>x</sub> on Ni(111) surface investigated with quantum-chemical calculations. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13707.	1.3	12
7371	STM fingerprint of molecule-atom interactions in a self-assembled metal-organic surface coordination network on Cu(111). <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8815.	1.3	62
7372	Adsorption and activation of O <sub>2</sub> at Au chains on MgO/Mo thin films. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1483.	1.3	29
7373	Pt promotion and spill-over processes during deposition and desorption of upd-H <sub>ad</sub> and OH <sub>ad</sub> on Pt <sub>x</sub> Ru <sub>1-x</sub> /Ru(0001) surface alloys. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10388.	1.3	29
7374	First-principles investigation of electron-induced cross-linking of aromatic self-assembled monolayers on Au(111). <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1578.	1.3	10
7375	Surface reconstructions and relaxation effects in a centre-symmetrical crystal: the {00.1} form of calcite (CaCO <sub>3</sub> ). <i>CrystEngComm</i> , 2010, 12, 3626.	1.3	38
7376	Six-dimensional dynamics study of reactive and non reactive scattering of H <sub>2</sub> from Cu(111) using a chemically accurate potential energy surface. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6499.	1.3	88
7377	Adsorption of glycine on the anatase (101) surface: an ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 11033.	1.3	38
7378	Nature and role of surface carbonates and bicarbonates in CO oxidation over RuO <sub>2</sub> . <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6367.	1.3	24
7379	Adsorption-induced structural changes of gold cations from two- to three-dimensions. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 3038.	1.3	20
7380	The maximum number of carbonyl groups around an Ru <sub>6</sub> C polyhedral cluster: hexanuclear ruthenium carbonyl carbides. <i>Dalton Transactions</i> , 2010, 39, 10697.	1.6	8
7381	Gold carbenes via 1,2-dialkoxycyclopropane ring-opening: a mass spectrometric and DFT study of the reaction pathways. <i>Chemical Communications</i> , 2010, 46, 3899.	2.2	51
7382	Dynamics of dissociative adsorption of hydrogen on a CO-precovered Ru(0001) surface: a comparison of theoretical and experimental results. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1331-1340.	1.3	17
7383	Monitoring the interaction of adsorbates on metal surfaces by surface site engineering: the case of ethoxy on Cu, Pd, Ag and Au regular and stepped surfaces. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6492.	1.3	11
7384	On the calculation of the vibrational frequencies of polycyclic aromatic hydrocarbons. <i>Molecular Physics</i> , 2010, 108, 2647-2654.	0.8	29
7385	Ab Initio Simulations of Li/Pyrite-MS <sub>2</sub> (M=Fe, Ni) Battery Cells. <i>Journal of the Electrochemical Society</i> , 2010, 157, A630.	1.3	31
7386	Stabilization of a Complex Perovskite Superstructure under Ambient Conditions: Influence of Cation Composition and Ordering, and Evaluation as an SOFC Cathode. <i>Chemistry of Materials</i> , 2010, 22, 6598-6615.	3.2	19

#	ARTICLE	IF	CITATIONS
7387	Combined Experimental and Theoretical Investigation of Three-Dimensional, Nitrogen-Doped, Gallium Cluster Anions. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11070-11077.	1.1	17
7388	Electronic Conductivity and Stability of Doped Titania (Ti <sub>1-x</sub> M <sub>x</sub> O <sub>2</sub> , M = Nb, Ru, and Ta) A Density Functional Theory-Based Comparison. <i>Journal of Physical Chemistry C</i> , 2010, 114, 13162-13167.	1.5	26
7389	On the SmCo Dimer: A Detailed Density Functional Theory Analysis. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1897-1905.	1.1	1
7390	Direct Measurement of the Attractive Interaction Forces on F <sup>0</sup> Color Centers on MgO(001) by Dynamic Force Microscopy. <i>ACS Nano</i> , 2010, 4, 2510-2514.	7.3	29
7391	Density functional theory study of the high- and low-temperature phases of cubic iron sulfide. <i>Physical Review B</i> , 2010, 82, .	1.1	13
7392	Two-dimensional carbon semiconductor: Density functional theory calculations. <i>Physical Review B</i> , 2010, 82, .	1.1	79
7393	Static equation of state of bcc iron. <i>Physical Review B</i> , 2010, 82, .	1.1	35
7394	Magnetism in binary and encapsulated Co-Mn clusters. <i>Physical Review B</i> , 2010, 82, .	1.1	7
7395	Ultrathin Mn layers on Rh(001): Investigations using scanning tunneling microscopy and density functional calculations. <i>Physical Review B</i> , 2010, 82, .	1.1	9
7396	Formation of a reliable intermediate band in Si heavily coimplanted with chalcogens (S, Se, Te) and group III elements (B, Al). <i>Physical Review B</i> , 2010, 82, .	1.1	83
7397	Gold cluster beyond hollow cage: A double shell structure of Au <sub>58</sub> . <i>Journal of Chemical Physics</i> , 2010, 132, 104301.	1.2	22
7398	Spin-orbit effects in structural and electronic properties for the solid state of the group-14 elements from carbon to superheavy element 114. <i>Physical Review B</i> , 2010, 82, .	1.1	61
7399	First-principles study of charge-density waves on Cu surfaces covered by In, Pb, and Bi atoms: Analysis of electronic structure and surface phonons. <i>Physical Review B</i> , 2010, 82, .	1.1	1
7400	Density Functional Dependence in the Theoretical Analysis of the Terahertz Spectrum of the Illicit Drug MDMA (Ecstasy). <i>IEEE Sensors Journal</i> , 2010, 10, 478-484.	2.4	18
7401	Shape memory effects and pseudoelasticity in bcc metallic nanowires. <i>Journal of Applied Physics</i> , 2010, 108, .	1.1	45
7402	The first-order structural phase transition of YSb. <i>Canadian Journal of Physics</i> , 2010, 88, 591-596.	0.4	1
7403	The crystal structure and superconducting properties of monatomic bromine. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 015702.	0.7	10
7404	Magnetic effects of defect pair formation in ZnO. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 436002.	0.7	52

#	ARTICLE	IF	CITATIONS
7405	̂-Bonding in the [Pd4(̂4-C9H9)(̂4-C8H8)] <sup>+</sup> sandwich complex. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 12050.	1.3	36
7406	Influence of dopants Ti and Ni on bonding interactions and dehydrogenation properties of lithium alanate. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10942.	1.3	10
7407	First-principles investigations of GaAs (112)-(2&#x00D7;2) surface reconstruction. , 2010, , .		1
7408	Adsorption and binding of capping molecules for highly luminescent CdSe nanocrystals â€“ DFT simulation studies. <i>Nanoscale</i> , 2010, 2, 2679.	2.8	13
7409	Enantiospecific adsorption of amino acids on hydroxylated quartz (101̂,0). <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8024.	1.3	31
7410	Influence of clustering and molecular orbital shapes on the ionization enhancement in ammonia. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 12231.	1.3	19
7411	Non-reactive scattering of N2 from the W(110) surface studied with different exchangeâ€“correlation functionals. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 4357.	1.3	20
7412	Hydrogen dissociation on Cu(111): the influence of lattice motion. Part I. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 4552.	1.3	53
7413	Epitaxial growth of diindenoperylene ultrathin films on Ag(111) investigated by LT-STM and LEED. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20933.	1.3	17
7414	A luminescent gold(i)â€“copper(i) cluster with unprecedented carbon-centered trigonal prismatic hexagold. <i>Chemical Communications</i> , 2011, 47, 4739.	2.2	58
7415	An infrared study of solid glycine in environments of astrophysical relevance. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 12268.	1.3	43
7416	Silica hollow nanospheres as new nanoscaffold materials to enhance hydrogen releasing from ammonia borane. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18592.	1.3	37
7417	Mechanism of Mycolic Acid Cyclopropane Synthase: A Theoretical Study. <i>Biochemistry</i> , 2011, 50, 1505-1513.	1.2	25
7418	Mechanisms of Ion-Beam Modification of Terthiophene Oligomers from Atomistic Simulations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23936-23945.	1.5	6
7419	Perpendicular growth of carbon chains on graphene from first-principles. <i>Physical Review B</i> , 2011, 83, .	1.1	44
7420	Interaction between NO and Na, O, S, Cl on Au and Pd(111) surfaces. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14466.	1.3	10
7421	State-resolved THz spectroscopy and dynamics of crystalline peptideâ€“water systems. <i>Faraday Discussions</i> , 2011, 150, 175.	1.6	16
7422	Examining the robustness of first-principles calculations for metal hydride reaction thermodynamics by detection of metastable reaction pathways. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 21520.	1.3	14

#	ARTICLE	IF	CITATIONS
7423	Tracking thermally-activated transformations in a nanostructured metal/oxide/metal system. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 17171.	1.3	6
7424	Investigation of hydrogen absorption in Li <sub>7</sub> VN <sub>4</sub> and Li <sub>7</sub> MnN <sub>4</sub> . <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 8889.	1.3	6
7425	Reaction-Induced Magnetic Transition in Mn <sub>2</sub> Dimers. <i>Journal of Physical Chemistry A</i> , 2011, 115, 549-555.	1.1	11
7426	Replacing Platinum with Tungsten Carbide (WC) for Reforming Reactions: Similarities in Ethanol Decomposition on Ni/Pt and Ni/WC Surfaces. <i>ACS Catalysis</i> , 2011, 1, 390-398.	5.5	44
7427	Interplay between structure, stoichiometry and properties of technetium nitrides. <i>Dalton Transactions</i> , 2011, 40, 6738.	1.6	20
7428	Calculation of isotropic Compton profiles with Gaussian basis sets. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 5630.	1.3	16
7429	The isomeric effect on the adjacent Si dimer didechlorination of trans and iso-dichloroethylene on Si(100)-2 $\times$ 1. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 7121.	1.3	2
7430	The effect of phonon modes on the H <sub>2</sub> ( $\nu$ , $j$ )/D <sub>2</sub> ( $\nu$ , $j$ ) $\hat{\epsilon}$ Cu(111) scattering processes. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 10100.	1.3	17
7431	NXA <sub>3</sub> <sup>+</sup> (X = N, P, As): penta-atomic planar tetracoordinate nitrogen with N $\hat{\epsilon}$ X multiple bonding. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 5960.	1.3	26
7432	Synthesis and structures of the [benzamidinato] <sub>3</sub> $\hat{\epsilon}$ complexes Li <sub>3</sub> (tmeda)(L <sub>1</sub> ) <sub>2</sub> and [Li(thf) <sub>4</sub> ][Li <sub>5</sub> (L <sub>2</sub> )(OEt <sub>2</sub> ) <sub>2</sub> ] [L <sub>1</sub> = N(SiMe <sub>3</sub> )C(Ph)N(SiMe <sub>3</sub> ) and L <sub>2</sub> = N(SiMe <sub>3</sub> )C(C <sub>6</sub> H <sub>4</sub> -4)NPh]. <i>Dalton Transactions</i> , 2011, 40, 3047.	1.6	3
7433	Theoretical study of the vibrational properties of NaAlH <sub>4</sub> with AlH <sub>3</sub> vacancies. <i>Faraday Discussions</i> , 2011, 151, 243.	1.6	2
7434	Weak Intermolecular Interactions in an Ionically Bound Molecular Adsorbate: Cyclopentadienyl/Cu(111). <i>Physical Review Letters</i> , 2011, 106, 186101.	2.9	20
7435	CO <sub>2</sub> adsorption by nitrogen-doped carbon nanotubes predicted by density-functional theory with dispersion-correcting potentials. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2780-2787.	1.3	31
7436	Energetics and structure of single Ti defects and their influence on the decomposition of NaAlH <sub>4</sub> . <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 552-562.	1.3	9
7437	NMR, DFT and luminescence studies of the complexation of Zn(ii) with 8-hydroxyquinoline-5-sulfonate. <i>Dalton Transactions</i> , 2011, 40, 11732.	1.6	23
7438	DFT study of the Ring Opening Polymerization of $\hat{\mu}$ -caprolactone by grafted lanthanide complexes: 1 $\hat{\epsilon}$ Effect of the grafting mode on the reactivity of borohydride complexes. <i>Dalton Transactions</i> , 2011, 40, 11211.	1.6	24
7439	Modulation of the photophysics of 2-(4 $\hat{\epsilon}$ -N,N-dimethylaminophenyl)imidazo-[4,5-b]pyridine by long chain N-alkylations. <i>Photochemical and Photobiological Sciences</i> , 2011, 10, 939-946.	1.6	13
7440	Constructing simple yet accurate potentials for describing the solvation of HCl/water clusters in bulk helium and nanodroplets. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14550.	1.3	13

#	ARTICLE	IF	CITATIONS
7441	Continuum electrostatic investigations of charge transfer processes in biological molecules using a microstate description. <i>Faraday Discussions</i> , 2011, 148, 173-193.	1.6	18
7442	Interface-Dependent Spin-Reorientation Energy Barrier in Fe/MgO(001) Thin Film. <i>IEEE Electron Device Letters</i> , 2011, 32, 1287-1289.	2.2	8
7443	DFT study of the Ring Opening Polymerization of $\epsilon$ -caprolactone by grafted lanthanide complexes: 2 $\epsilon$ Effect of the initiator ligand. <i>Dalton Transactions</i> , 2011, 40, 11228.	1.6	23
7444	On the PES for the interaction of an H atom with an H chemisorbate on a graphenic platelet. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 17579.	1.3	13
7445	Reductive coupling of carbon monoxide by U(iii) complexes—a computational study. <i>Dalton Transactions</i> , 2011, 40, 11080.	1.6	22
7446	Conformational analysis and UV/Vis spectroscopic properties of a rotaxane-based molecular machine in acetonitrile dilute solution: when simulations meet experiments. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2342-2349.	1.3	38
7447	The mechanism of the water-gas shift reaction on Cu/TiO <sub>2</sub> (110) elucidated from application of density-functional theory. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20393.	1.3	20
7448	Mössbauer properties of the diferric cluster and the differential iron(ii)-binding affinity of the iron sites in protein R2 of class Ia Escherichia coli ribonucleotide reductase: a DFT/electrostatics study. <i>Dalton Transactions</i> , 2011, 40, 11164.	1.6	12
7449	A new photocatalyst: Bi <sub>2</sub> TiO <sub>4</sub> F <sub>2</sub> nanoflakes synthesized by a hydrothermal method. <i>Dalton Transactions</i> , 2011, 40, 12670.	1.6	25
7450	Towards the computational modelling of polyoxoanions on metal surfaces: IR spectrum characterisation of [SiW <sub>12</sub> O <sub>40</sub> ] <sup>4-</sup> on Ag(111). <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 15143.	1.3	21
7451	Cluster or periodic, static or dynamic—the challenge of calculating the g tensor of the solid-state glycine radical. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18638.	1.3	18
7452	The active site structure of nitrated and oxynitrated graphite as a cathode catalyst in a fuel cell. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2659-2662.	1.3	13
7453	Fe—H/D stretching and bending modes in nuclear resonant vibrational, Raman and infrared spectroscopies: Comparisons of density functional theory and experiment. <i>Faraday Discussions</i> , 2011, 148, 409-420.	1.6	29
7454	Effective increasing of optical absorption and energy conversion efficiency of anatase TiO <sub>2</sub> nanocrystals by hydrogenation. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18063.	1.3	92
7455	Indole-substituted nickel dithiolene complexes in electronic and optoelectronic devices. <i>Journal of Materials Chemistry</i> , 2011, 21, 15422.	6.7	29
7456	Theory of gold on ceria. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 22-33.	1.3	108
7457	The Adsorption Properties of Cu and Ni on the Ceria(111) Surface. <i>Advanced Materials Research</i> , 2011, 213, 166-171.	0.3	5
7458	Lithium cluster anions: Photoelectron spectroscopy and <i>ab initio</i> calculations. <i>Journal of Chemical Physics</i> , 2011, 134, 044322.	1.2	38



#	ARTICLE	IF	CITATIONS
7459	Phase stability, point defects, and elastic properties of W-V and W-Ta alloys. <i>Physical Review B</i> , 2011, 84, .	1.1	139
7460	Strain-tunable band gap of hydrogenated bilayer graphene. <i>New Journal of Physics</i> , 2011, 13, 063047.	1.2	19
7461	Pressure induced structural transformation in $Gd_2Ti_2O_7$ and $Gd_2Zr_2O_7$ . <i>Journal of Physics Condensed Matter</i> , 2011, 23, 035501.	0.7	19
7462	Study of 40-atom Pt-Au clusters using a combined empirical potential-density functional approach. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2011, 467, 2004-2019.	1.0	35
7463	First principles study of the electric field effect on magnetization and magnetic anisotropy of FeCo/MgO(001) thin film. <i>Applied Physics Letters</i> , 2011, 99, .	1.5	57
7464	First-Principles Study of $H^+$ Intercalation in Layer-Structured $LiCoO_2$ . <i>Journal of Physical Chemistry C</i> , 2011, 115, 12672-12676.	1.5	70
7465	Persistent Covalency and Planarity in the $BAl_6^{2+}$ and $LiBAl_6^{+}$ ( $n = 0-6$ ) Cluster Ions. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2046-2051.	2.1	33
7466	Quantum Proton Transfer in Hydrated Sulfuric Acid Clusters: A Perspective from Semiempirical Path Integral Simulations. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11486-11494.	1.1	20
7467	Deposition of Nonstoichiometric Tritungsten Oxides on the $TiO_2(110)$ Surface: A Possible Way to Stabilize the Unstable Clusters in the Gas Phase. <i>Journal of Physical Chemistry C</i> , 2011, 115, 15335-15344.	1.5	8
7468	Half-Metallic Dirac Point in B-Edge Hydrogenated BN Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2011, 115, 17252-17254.	1.5	38
7469	Molecular Structures, Acid-Base Properties, and Formation of Group 6 Transition Metal Hydroxides. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8072-8103.	1.5	54
7470	Structural, Elastic Constant, and Vibrational Properties of Wurtzite Gallium Nitride: A First-Principles Approach. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14502-14509.	1.1	13
7471	Interaction of BrPDI, BrGly, and BrAsp with the Rutile $TiO_2(110)$ Surface for Photovoltaic and Photocatalytic Applications: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 9220-9226.	1.5	7
7472	The high-pressure structural transition in MnS: an <i>ab initio</i> study. <i>Molecular Physics</i> , 2011, 109, 251-256.	0.8	6
7473	Electronic structure and phonons in $La_{2-x}CoMnO_6$ : A ferromagnetic insulator driven by Coulomb-assisted spin-orbit coupling. <i>Physical Review B</i> , 2011, 84, .	1.1	64
7474	CO Oxidation on Inverse $CeO_2/Cu(111)$ Catalysts: High Catalytic Activity and Ceria-Promoted Dissociation of $O_2$ . <i>Journal of the American Chemical Society</i> , 2011, 133, 3444-3451.	6.6	241
7475	Structural and thermodynamic properties of liquid Na-Li and Ca-Li alloys at high pressure. <i>Physical Review B</i> , 2011, 83, .	1.1	18
7476	Tunable band gap $Cu_2ZnSnS_4(1-x)$ nanocrystals: experimental and first-principles calculations. <i>CrystEngComm</i> , 2011, 13, 2222.	1.3	75



#	ARTICLE	IF	CITATIONS
7477	<i>o</i> -Iminobenzosemiquinonate and <i>o</i> -Imino- <i>p</i> -methylbenzosemiquinonate Anion Radicals Coupled VO <sup>2+</sup> Stabilization. <i>Inorganic Chemistry</i> , 2011, 50, 2488-2500.	1.9	31
7478	Stability of the hydrogen-storage compound Li <sub>6</sub> Mg(NH) <sub>4</sub> from first principles. <i>Physical Review B</i> , 2011, 83, .	1.1	2
7479	Hybrid DFT Functional-Based Static and Molecular Dynamics Studies of Excess Electron in Liquid Ethylene Carbonate. <i>Journal of the Electrochemical Society</i> , 2011, 158, A400.	1.3	71
7480	Understanding Acetaldehyde Thermal Chemistry on the TiO <sub>2</sub> (110) Rutile Surface: From Adsorption to Reactivity. <i>Journal of Physical Chemistry C</i> , 2011, 115, 2819-2825.	1.5	22
7481	CO Adsorption on Noble Metal Clusters: Local Environment Effects. <i>Journal of Physical Chemistry C</i> , 2011, 115, 5637-5647.	1.5	45
7482	Phonon, IR, and Raman Spectra, NMR Parameters, and Elastic Constant Calculations for AlH <sub>3</sub> Polymorphs. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10708-10719.	1.1	20
7483	How Do Surface and Edge Effects Alter the Electronic Properties of GaN Nanoribbons?. <i>Journal of Physical Chemistry C</i> , 2011, 115, 1724-1731.	1.5	41
7484	Kinetic Modeling of the Free-Radical Process during the Initiated Thermal Cracking of Normal Alkanes with 1-Nitropropane as an Initiator. <i>Industrial &amp; Engineering Chemistry Research</i> , 2011, 50, 9054-9062.	1.8	18
7485	Methyl iodide oxidative addition to [Rh(acac)(CO)(PPh <sub>3</sub> )]: an experimental and theoretical study of the stereochemistry of the products and the reaction mechanism. <i>Dalton Transactions</i> , 2011, 40, 8226.	1.6	26
7486	Interaction of Water with FeO(111)/Pt(111): Environmental Effects and Influence of Oxygen. <i>Journal of Physical Chemistry C</i> , 2011, 115, 19328-19335.	1.5	39
7487	Preserving Charge and Oxidation State of Au(III) Ions in an Agent-Functionalized Nanocrystal Model System. <i>ACS Nano</i> , 2011, 5, 6480-6486.	7.3	26
7488	Complete Structural Characterization of Ni <sub>3</sub> Si <sub>2</sub> O <sub>5</sub> (OH) <sub>4</sub> Nanotubes: Theoretical and Experimental Comparison. <i>Journal of Physical Chemistry C</i> , 2011, 115, 11442-11446.	1.5	35
7489	Light- and Heavy-Atom Tunneling in Rearrangement Reactions of Cyclopropylcarbenes. <i>Organic Letters</i> , 2011, 13, 3526-3529.	2.4	48
7490	Theoretical Thermochemistry for Organic Molecules: Development of the Generalized Connectivity-Based Hierarchy. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2094-2103.	2.3	77
7491	Asymmetric saddling of single porphyrin molecules on Au(111). <i>Physical Review B</i> , 2011, 83, .	1.1	26
7492	Site Substitution of Ti in NaAlH <sub>4</sub> and Na <sub>3</sub> AlH <sub>6</sub> . <i>Journal of Physical Chemistry C</i> , 2011, 115, 21454-21464.	1.5	19
7493	Density Functional Theory Study of Acetaldehyde Hydrodeoxygenation on MoO <sub>3</sub> . <i>Journal of Physical Chemistry C</i> , 2011, 115, 8155-8164.	1.5	64
7494	Impurity Concentration Dependence of Optical Absorption for Phosphorus-Doped Anatase TiO <sub>2</sub> . <i>Journal of Physical Chemistry C</i> , 2011, 115, 8184-8188.	1.5	56

#	ARTICLE	IF	CITATIONS
7495	Computational Mechanistic Study on C <sub>p</sub> *Ir Complex-Mediated Acceptorless Alcohol Dehydrogenation: Bifunctional Hydrogen Transfer vs $\beta$ -H Elimination. <i>Organometallics</i> , 2011, 30, 2349-2363.	1.1	74
7496	Theoretical Study of Pt(PR <sub>3</sub> ) <sub>2</sub> (AlCl <sub>3</sub> ) (R = H, Me, Ph, or Cy) Including an Unsupported Bond between Transition Metal and Non-transition Metal Elements: Geometry, Bond Strength, and Prediction. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8520-8527.	1.1	9
7497	Temperature Behavior of the AlH <sub>3</sub> Polymorph by in Situ Investigation Using High Resolution Raman Scattering. <i>Journal of Physical Chemistry A</i> , 2011, 115, 691-699.	1.1	7
7498	Interplay between Layer-Resolved Chemical Composition and Electronic Structure in a Sn/Pt(110) Surface Alloy. <i>Journal of Physical Chemistry C</i> , 2011, 115, 14264-14269.	1.5	14
7499	Chemical storage of hydrogen in few-layer graphene. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 2674-2677.	3.3	229
7500	Orthogonal Interactions of CO Molecules on a One-Dimensional Substrate. <i>ACS Nano</i> , 2011, 5, 8877-8883.	7.3	24
7501	Reaction of NO on Ni <sup>0</sup> Pt Bimetallic Surfaces Investigated with Theoretical Calculations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 7538-7544.	1.5	18
7502	Electronic Communications in (Z)-Bis(ferrocenyl)ethylenes with Electron-Withdrawing Substituents. <i>Organometallics</i> , 2011, 30, 3037-3046.	1.1	54
7503	Mapping Complex Chiral Adlayers: A Truly Random 2-D Solid Solution of ( <i>R,S</i> )-3-Pyrroline-2-Carboxylic Acid on Cu(110). <i>Journal of Physical Chemistry C</i> , 2011, 115, 1180-1185.	1.5	12
7504	Behavior of Ag <sub>3</sub> Clusters Inside a Nanometer-Sized Space of ZSM-5 Zeolite. <i>Inorganic Chemistry</i> , 2011, 50, 6533-6542.	1.9	24
7505	Stress and structure at the NiO/Ag(001) interface. <i>Physical Review B</i> , 2011, 84, .	1.1	13
7506	Dissociative Adsorption of Nitric Oxide on Fullerene Functionalized with a Scandium Metal Atom: A Quantum Chemical Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 12054-12063.	1.5	9
7507	Experimental and theoretical studies of ammonia decomposition activity on Fe-Pt, Co-Pt, and Cu-Pt bimetallic surfaces. <i>Journal of Chemical Physics</i> , 2011, 134, 184701.	1.2	34
7508	First-Principles Investigation of High-Order Oxidation of Chromium and Neptunium: $UO_3$ and $NpO_3$	1.1	43
7509	First-Principles Study of Silicon Nanowire Approaching the Bulk Limit. <i>Nano Letters</i> , 2011, 11, 4794-4799.	4.5	40
7510	Adsorption and Reaction of Furfural and Furfuryl Alcohol on Pd(111): Unique Reaction Pathways for Multifunctional Reagents. <i>ACS Catalysis</i> , 2011, 1, 1272-1283.	5.5	145
7511	Growth and Structural Properties of Mg <sub>N</sub> ( $N = 10 \text{--} 56$ ) Clusters: Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12307-12314.	1.1	52
7512	DFT Calculations for Intermediate and Active States of the Diiron Center with a Tryptophan or Tyrosine Radical in <i>Escherichia coli</i> Ribonucleotide Reductase. <i>Inorganic Chemistry</i> , 2011, 50, 2302-2320.	1.9	26

#	ARTICLE	IF	CITATIONS
7513	The role of electron localization in the atomic structure of transition-metal 13-atom clusters: the example of Co <sub>13</sub> , Rh <sub>13</sub> , and Hf <sub>13</sub> . <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 17242.	1.3	43
7514	A density functional theory study of Mn nanowires on the Si(001) surface. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 305003.	0.7	7
7515	Role of Geometric Relaxation in Oxygen Binding to Metal Nanoparticles. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1237-1240.	2.1	21
7516	Alkanethiol Adsorption on Platinum: Chain Length Effects on the Quality of Self-Assembled Monolayers. <i>Journal of Physical Chemistry C</i> , 2011, 115, 17788-17798.	1.5	34
7517	Dissociative Chemisorption of Hydrazine on an Fe{211} Surface. <i>Journal of Physical Chemistry C</i> , 2011, 115, 17812-17828.	1.5	30
7518	Vacancy Diffusion in NaAlH <sub>4</sub> and Na <sub>3</sub> AlH <sub>6</sub> . <i>Journal of Physical Chemistry C</i> , 2011, 115, 21465-21472.	1.5	28
7519	Energetics of Oxidation in MoS <sub>2</sub> Nanoparticles by Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2011, 115, 10606-10616.	1.5	55
7520	Relative Stabilities of Low Index and Stepped CeO <sub>2</sub> Surfaces from Hybrid and GGA + <i>U</i> Implementations of Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2011, 115, 3716-3721.	1.5	58
7521	TD-CI Simulation of the Electronic Optical Response of Molecules in Intense Fields II: Comparison of DFT Functionals and EOM-CCSD. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11832-11840.	1.1	42
7522	Reactivity of C Scission on Ni-Based Core/Shell Bimetallic Surfaces Investigated with Quantum-Chemical Calculations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 19231-19238.	1.5	2
7523	Oxygen Reduction Reaction on Metal-Terminated MnCr <sub>2</sub> O <sub>4</sub> Nano-octahedron Catalyzing MnS Dissolution in an Austenitic Stainless Steel. <i>Journal of Physical Chemistry C</i> , 2011, 115, 4127-4133.	1.5	4
7524	Oxygen-Stabilized Rh Adatoms: OD Oxides on a Vicinal Surface. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2747-2751.	2.1	5
7525	Potential Energy Surface for (Retro-)Cyclopropanation: Metathesis with a Cationic Gold Complex. <i>Journal of the American Chemical Society</i> , 2011, 133, 12162-12171.	6.6	72
7526	Methane Dissociation on High and Low Indices Rh Surfaces. <i>Journal of Physical Chemistry C</i> , 2011, 115, 13027-13034.	1.5	35
7527	Heat-to-Connect: Surface Commensurability Directs Organometallic One-Dimensional Self-Assembly. <i>ACS Nano</i> , 2011, 5, 9093-9103.	7.3	64
7528	Theoretical Study of Photoinduced Epoxidation of Olefins Catalyzed by Ruthenium Porphyrin. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4774-4785.	1.1	16
7529	Rh-Decorated Cu Alloy Catalyst for Improved C <sub>2</sub> Oxygenate Formation from Syngas. <i>Journal of Physical Chemistry C</i> , 2011, 115, 18247-18256.	1.5	62
7530	DFT Study on Amino-Phospholipids Surface-Mediated Decomposition of Hydrogen Peroxide. <i>Journal of Physical Chemistry C</i> , 2011, 115, 22945-22953.	1.5	8

#	ARTICLE	IF	CITATIONS
7531	Vibrational Analysis of the Hydrogen-Bond Symmetrization in Ice. <i>Journal of Physical Chemistry B</i> , 2011, 115, 71-74.	1.2	12
7532	Theoretical Study of Magnetic Properties of Oxovanadium(IV) Complex Self-Assemblies with Tetradentate Schiff Base Ligands. <i>Journal of Physical Chemistry B</i> , 2011, 115, 8465-8473.	1.2	8
7533	Influence of Flipping Si Dimers on the Dissociation Pathways of Water Molecules on Si(001). <i>Journal of Physical Chemistry C</i> , 2011, 115, 24800-24803.	1.5	12
7534	Magnetism and bonding in graphene nanodots with H modified interior, edge, and apex. <i>Journal of Chemical Physics</i> , 2011, 135, 084707.	1.2	4
7535	Pathways of Methanol Steam Reforming on PdZn and Comparison with Cu. <i>Journal of Physical Chemistry C</i> , 2011, 115, 20583-20589.	1.5	60
7536	Synthesis of Optically Pure <i>trans</i> -Sulfanyl Amines Mediated by a Remote Sulfinyl Group. <i>Organic Letters</i> , 2011, 13, 4534-4537.	2.4	13
7537	Ab Initio Molecular Dynamics Study of Temperature Effects on the Structure and Stability of Energetic Solid Silver Azide. <i>Journal of Physical Chemistry C</i> , 2011, 115, 20782-20787.	1.5	24
7538	Effect of Surface Modes on the Six-Dimensional Molecule-Surface Scattering Dynamics of H <sub>2</sub> -Cu(100) and D <sub>2</sub> -Cu(111) Systems. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5256-5273.	1.1	17
7539	Understanding the Interaction of the Porphyrin Macrocycle to Reactive Metal Substrates: Structure, Bonding, and Adatom Capture. <i>ACS Nano</i> , 2011, 5, 1831-1838.	7.3	58
7540	Theoretical Studies on Thermochemistry for Conversion of 5-Chloromethylfurfural into Valuable Chemicals. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13628-13641.	1.1	25
7541	Folding and Unfolding Movements in a [2]Pseudorotaxane. <i>Journal of Organic Chemistry</i> , 2011, 76, 138-144.	1.7	39
7542	New Nickel Gallium Boride, B <sub>14</sub> Ga <sub>3</sub> Ni <sub>27</sub> : Synthesis and Crystal Structure. <i>Inorganic Chemistry</i> , 2011, 50, 3907-3912.	1.9	9
7543	Theoretical Study of the Interaction of CO on TiC(001) and Au Nanoparticles Supported on TiC(001): Probing the Nature of the Au/TiC Interface. <i>Journal of Physical Chemistry C</i> , 2011, 115, 22495-22504.	1.5	17
7544	Atomistic Design of High Thermoelectricity on Si/Ge Superlattice Nanowires. <i>Journal of Physical Chemistry C</i> , 2011, 115, 20696-20702.	1.5	30
7545	First-Principles Study of Water Dissociation on PdZn near Surface Alloys. <i>Journal of Physical Chemistry C</i> , 2011, 115, 18752-18760.	1.5	21
7546	Glycolaldehyde as a Probe Molecule for Biomass Derivatives: Reaction of C=OH and C=O Functional Groups on Monolayer Ni Surfaces. <i>Journal of the American Chemical Society</i> , 2011, 133, 20528-20535.	6.6	42
7547	First Principles Study of Steam Carbon Reaction on $\hat{\Gamma}$ -Fe(111) Surface. <i>Journal of Physical Chemistry C</i> , 2011, 115, 12068-12076.	1.5	9
7548	New Insights into the Strain Coupling to Surface Chemistry, Electronic Structure, and Reactivity of La <sub>0.7</sub> Sr <sub>0.3</sub> MnO <sub>3</sub> . <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 801-807.	2.1	145



#	ARTICLE	IF	CITATIONS
7567	Effect of impurities on the mechanical and electronic properties of Au, Ag, and Cu monatomic chain nanowires. <i>Physical Review B</i> , 2011, 84, .	1.1	30
7568	Role of metal oxide support in redox reactions of iron oxide for chemical looping applications: experiments and density functional theory calculations. <i>Energy and Environmental Science</i> , 2011, 4, 3661.	15.6	138
7569	Parameter estimation by Density Functional Theory for a lattice-gas model of Br and Cl chemisorption on Ag (100). <i>Journal of Electroanalytical Chemistry</i> , 2011, 662, 130-136.	1.9	8
7570	Theoretical study on the effective methanol decomposition on Pd(111) surface facilitated in alkaline medium. <i>Journal of Electroanalytical Chemistry</i> , 2011, 662, 251-256.	1.9	15
7571	Superhydrogenated PAHs: Catalytic formation of H <sub>2</sub> . <i>EAS Publications Series</i> , 2011, 46, 453-460.	0.3	7
7572	Antifungal Activity of Resveratrol against <i>Botrytis cinerea</i> Is Improved Using 2-Furyl Derivatives. <i>PLoS ONE</i> , 2011, 6, e25421.	1.1	56
7573	First-principles investigation of the stability of MN and CrMN precipitates under coherency strains in $\hat{\pm}$ -Fe (M=V, Nb, Ta). <i>Journal of Applied Physics</i> , 2011, 109, .	1.1	17
7574	Properties of Carbon Nanotubes: An ab Initio Study Using Large Gaussian Basis Sets and Various DFT Functionals. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8876-8885.	1.5	42
7575	Photophysical properties of Kuratowski-type coordination compounds [MII <sub>2</sub> Zn <sub>4</sub> Cl <sub>4</sub> (Me <sub>2</sub> bta) <sub>6</sub> ] (MII = Zn) <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5</i>	1.6	29
7576	Effects of strain, <i>d</i> -band filling, and oxidation state on the bulk electronic structure of cubic <i>3d</i> perovskites. <i>Journal of Chemical Physics</i> , 2011, 135, 104702.	1.2	18
7578	Transition States and Energetics of Nucleophilic Additions of Thiols to Substituted $\hat{\pm}$ , $\hat{1}^2$ -Unsaturated Ketones: Substituent Effects Involve Enone Stabilization, Product Branching, and Solvation. <i>Journal of Organic Chemistry</i> , 2011, 76, 5074-5081.	1.7	84
7579	Characterization of Surface Hydride Hafnium Complexes on Alumina by a Combination of Experiments and DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 6757-6763.	1.5	15
7580	Vapor Pressures and Sublimation Enthalpies of Nickelocene and Cobaltocene Measured by Thermogravimetry. <i>Journal of Chemical &amp; Engineering Data</i> , 2011, 56, 5008-5018.	1.0	28
7581	Mechanism of Methanol Synthesis on Cu through CO <sub>2</sub> and CO Hydrogenation. <i>ACS Catalysis</i> , 2011, 1, 365-384.	5.5	990
7582	Investigation of the structure and photoluminescence properties of Eu <sup>3+</sup> ion-activated Y <sub>6</sub> WxMo <sub>1</sub> <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5</i>	8.7	57
7583	Ab initio study of lithium-doped graphane for hydrogen storage. <i>Europhysics Letters</i> , 2011, 96, 27013.	0.7	48
7584	Atomic and Electronic Structures of M (=Ni, Fe, NiFe, or FeNi) Adlayer-Modified $\hat{\pm}$ -Al <sub>2</sub> O <sub>3</sub> (0001) Catalyst Interface. <i>Journal of Physical Chemistry C</i> , 2011, 115, 13796-13803.	1.5	6
7585	Clean Coupling of Unfunctionalized Porphyrins at Surfaces To Give Highly Oriented Organometallic Oligomers. <i>Journal of the American Chemical Society</i> , 2011, 133, 12031-12039.	6.6	133



#	ARTICLE	IF	CITATIONS
7586	Functionalization of Single-Layer MoS <sub>2</sub> Honeycomb Structures. Journal of Physical Chemistry C, 2011, 115, 13303-13311.	1.5	484
7587	Pathways for methanol steam reforming involving adsorbed formaldehyde and hydroxyl intermediates on Cu(111): density functional theory studies. Physical Chemistry Chemical Physics, 2011, 13, 9622.	1.3	61
7588	Ab Initio Calculation of the Adhesion and Ideal Shear Strength of Planar Diamond Interfaces with Different Atomic Structure and Hydrogen Coverage. Langmuir, 2011, 27, 6862-6867.	1.6	83
7589	Accurate Band Gaps for Semiconductors from Density Functional Theory. Journal of Physical Chemistry Letters, 2011, 2, 212-217.	2.1	444
7590	Mechanism of $\gamma$ -Al <sub>2</sub> O <sub>3</sub> Support in CO <sub>2</sub> Reforming of CH <sub>4</sub> A Density Functional Theory Study. Journal of Physical Chemistry C, 2011, 115, 225-233.	1.5	23
7591	Third conformer of graphene: A first-principles density functional theory study. Physical Review B, 2011, 83, .	1.1	57
7592	Stabilization Principles for Polar Surfaces of ZnO. ACS Nano, 2011, 5, 5987-5994.	7.3	144
7593	Nanocrystals of CeVO <sub>4</sub> Doped by Metallic Heteroions. Inorganic Chemistry, 2011, 50, 6189-6194.	1.9	28
7594	Nitrogen and sulfur co-doped TiO <sub>2</sub> nanosheets with exposed {001} facets: synthesis, characterization and visible-light photocatalytic activity. Physical Chemistry Chemical Physics, 2011, 13, 4853-4861.	1.3	282
7595	Surface Related Emission in CdS Quantum Dots. DFT Simulation Studies. Journal of Physical Chemistry C, 2011, 115, 20856-20863.	1.5	32
7596	On the Mechanism and Rate of Spontaneous Decomposition of Amino Acids. Journal of Physical Chemistry B, 2011, 115, 13624-13632.	1.2	21
7597	Width- and Edge-Dependent Stability, Electronic Structures, and Magnetic Properties of Graphene-Like and Wurtzite ZnS Nanoribbons. Journal of Physical Chemistry C, 2011, 115, 4466-4475.	1.5	17
7598	Molecular dynamics study of the adhesion of Cu/SiO <sub>2</sub> interfaces using a variable-charge interatomic potential. Physical Review B, 2011, 83, .	1.1	47
7599	Trends in Aromatic Oxidation Reactions Catalyzed by Cytochrome P450 Enzymes: A Valence Bond Modeling. Journal of Chemical Theory and Computation, 2011, 7, 327-339.	2.3	53
7600	Energetics and Mechanism for H <sub>2</sub> S Adsorption by Ceria-Lanthanide Mixed Oxides: Implications for the Desulfurization of Biomass Gasifier Effluents. Journal of Physical Chemistry C, 2011, 115, 24178-24188.	1.5	24
7602	Structural and Electronic Properties of (Al <sub>2</sub> O <sub>3</sub> ) <sub>n</sub> Clusters with $n = 10$ from First Principles Calculations. Journal of Physical Chemistry C, 2011, 115, 18111-18121.	1.5	60
7603	Ab initio study of stability and migration of H and He in hcp-Sc. Journal of Physics Condensed Matter, 2011, 23, 035701.	0.7	11
7604	Formation of Superoxide Anions on Ceria Nanoparticles by Interaction of Molecular Oxygen with Ce <sup>3+</sup> Sites. Journal of Physical Chemistry C, 2011, 115, 5817-5822.	1.5	107



#	ARTICLE	IF	CITATIONS
7605	DFT investigations on the ring-opening polymerization of cyclic carbonates catalyzed by zinc- $\beta$ -diiminate complexes. <i>Polymer Chemistry</i> , 2011, 2, 2564.	1.9	21
7606	Investigation of Formation Mechanism of Pt(111) Nanoparticle Layers Grown on Ru(0001) Core. <i>Langmuir</i> , 2011, 27, 1131-1135.	1.6	7
7607	Selective Hydrogenolysis of Polyols and Cyclic Ethers over Bifunctional Surface Sites on Rhodium-Rhenium Catalysts. <i>Journal of the American Chemical Society</i> , 2011, 133, 12675-12689.	6.6	439
7608	Electronic Structure, Effective Masses and Optical Properties of Monoclinic $\text{HfO}_2$ from First-Principles Calculations. <i>Advanced Materials Research</i> , 0, 216, 341-344.	0.3	4
7609	Coverage effects in the adsorption of $\text{H}_2$ on Pd(100) studied by <i>ab initio</i> molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2011, 135, 174707.	1.2	35
7610	Theoretical investigations into the enantiomeric and racemic forms of $\beta$ -(trifluoromethyl)lactic acid. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 811-817.	1.3	17
7611	O K-energy loss near-edge structure change induced by tantalum impurity in monoclinic hafnium oxide. <i>Journal of Applied Physics</i> , 2011, 109, 053723.	1.1	3
7612	Simulation of absorption of femtosecond laser pulses in solid-density copper. <i>High Energy Density Physics</i> , 2011, 7, 361-370.	0.4	35
7613	Vibrational properties of the $\text{LiNbO}_3$ z-surfaces. <i>IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control</i> , 2011, 58, 1751-1756.	1.7	9
7614	Understanding Structure, Size, and Charge Effects for the $\text{H}_2$ Dissociation Mechanism on Planar Gold Clusters. <i>Journal of Physical Chemistry C</i> , 2011, 115, 47-57.	1.5	19
7615	Strain-induced band-gap deformation of H/F passivated graphene and $\text{h-BN}$ sheet. <i>Physical Review B</i> , 2011, 84, .	1.1	45
7616	Density Functional Calculation of Intermolecular Potentials. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6888-6891.	1.1	0
7617	Graphitic GaN-ZnO and corresponding nanotubes. <i>Journal of Materials Chemistry</i> , 2011, 21, 17071.	6.7	5
7618	Mechanism of the phase transitions in MnAs. <i>Physical Review B</i> , 2011, 83, .	1.1	27
7619	Decomposition Pathways of Glycerol via C-H, O-H, and C-C Bond Scission on Pt(111): A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 19702-19709.	1.5	151
7620	High- $T_c$ Ferromagnetism Emerging from Magnetic Degeneracy in Cupric Oxide. <i>Physical Review Letters</i> , 2011, 106, 026401.	1.9	69
7621	Ground states of group-IV nanostructures: Magic structures of diamond and silicon nanocrystals. <i>Physical Review B</i> , 2011, 83, .	1.1	13
7622	Optical and Electronic Properties of Wurtzite Structure $\text{Zn}_{1-x}\text{Mg}_x\text{O}$ Alloys. <i>Chinese Physics Letters</i> , 2011, 28, 117101.	1.3	11

#	ARTICLE	IF	CITATIONS
7623	Surface Electronic Structure Transitions at High Temperature on Perovskite Oxides: The Case of Strained La <sub>0.8</sub> Sr <sub>0.2</sub> CoO <sub>3</sub> Thin Films. Journal of the American Chemical Society, 2011, 133, 17696-17704.	6.6	148
7624	Tailoring Homochirality at Surfaces: Going Beyond Molecular Handedness. Journal of the American Chemical Society, 2011, 133, 15992-16000.	6.6	33
7625	Methyl Formate Pathway in Methanol Steam Reforming on Copper: Density Functional Calculations. ACS Catalysis, 2011, 1, 1263-1271.	5.5	47
7626	Enhanced one dimensional mobility of oxygen on strained LaCoO <sub>3</sub> (001) surface. Journal of Materials Chemistry, 2011, 21, 18983.	6.7	64
7627	Chirality and Rotation of Asymmetric Surface-Bound Thioethers. Journal of Physical Chemistry C, 2011, 115, 897-901.	1.5	29
7628	Diffraction and reactive scattering of H <sub>2</sub> from Ru(0001): experimental and theoretical study. Physical Chemistry Chemical Physics, 2011, 13, 8583.	1.3	32
7629	First-principles study of diffusion of interstitial and vacancy in $\hat{\pm}$ U $\hat{\epsilon}$ Zr. Journal of Physics Condensed Matter, 2011, 23, 205402.	0.7	26
7630	Group-VII point defects in ZnSe. Physical Review B, 2011, 84, .	1.1	14
7631	Theoretical Study of Electrochemical Processes on Pt $\hat{\epsilon}$ Ni Alloys. Journal of Physical Chemistry C, 2011, 115, 10640-10650.	1.5	79
7632	Accurate Conformational Energy Differences of Carbohydrates: A Complete Basis Set Extrapolation. Journal of Chemical Theory and Computation, 2011, 7, 988-997.	2.3	26
7633	Gas-Phase and Ar-Matrix SQM Scaling Factors for Various DFT Functionals with Basis Sets Including Polarization and Diffuse Functions. Journal of Physical Chemistry A, 2011, 115, 4640-4649.	1.1	47
7634	NMR shielding tensors from auxiliary density functional theory. Journal of Chemical Physics, 2011, 134, 124108.	1.2	22
7635	Electronic and optical properties of potential solar absorber Cu <sub>3</sub> PSe <sub>4</sub> . Applied Physics Letters, 2011, 99, .	1.5	25
7636	An <i>ab initio</i> study of the effect of charge localization on oxygen defect formation and migration energies in magnesium oxide. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2011, 467, 2054-2065.	1.0	28
7637	Electron Localization in Defective Ceria Films: A Study with Scanning-Tunneling Microscopy and Density-Functional Theory. Physical Review Letters, 2011, 106, 246801.	2.9	158
7638	Bias in bonding behavior among boron, carbon, and nitrogen atoms in ion implanted <i>a</i> -BN, <i>a</i> -BC, and diamond like carbon films. Journal of Applied Physics, 2011, 110, .	1.1	20
7639	Experimental and computational study of crystalline formic acid composed of the higher-energy conformer. Journal of Chemical Physics, 2011, 134, 054506.	1.2	10
7640	Magnetoelastic coupling in $\hat{\pm}$ iron investigated within an <i>ab initio</i> spin spiral approach. Physical Review B, 2011, 84, .	1.1	39

#	ARTICLE	IF	CITATIONS
7641	First-principles study on the interaction of H interstitials with grain boundaries in $\text{Fe}$ . Physical Review B, 2011, 84, .	1.1	211
7642	Crystal structure and dynamics of $\text{Mg}(\text{ND}_3)_6\text{Cl}_2$ . Physical Chemistry Chemical Physics, 2011, 13, 7644.	1.3	9
7643	Electronic Structure and Thermochemical Properties of Small Neutral and Cationic Lithium Clusters and Boron-Doped Lithium Clusters: $\text{Li}_n$ and $\text{Li}_n\text{B}$ ( $n = 1\text{--}8$ ). Journal of Physical Chemistry A, 2011, 115, 7673-7686.	1.1	31
7644	Chemical Bonding and Aromaticity in Trinuclear Transition-Metal Halide Clusters. Inorganic Chemistry, 2011, 50, 1039-1046.	1.9	24
7645	Interatomic potential for the Al-Cu system. Physical Review B, 2011, 83, .	1.1	123
7646	First-Principles Study of the Local Magnetic Moment on a N-Doped $\text{Cu}_2\text{O}$ (111) Surface. Chinese Physics Letters, 2011, 28, 127102.	1.3	1
7647	Selective Americium(III) Complexation by Dithiophosphinates: A Density Functional Theoretical Validation for Covalent Interactions Responsible for Unusual Separation Behavior from Trivalent Lanthanides. Inorganic Chemistry, 2011, 50, 3913-3921.	1.9	75
7648	Electronic and optical properties of $\text{MgZnO}$ and $\text{CdZnO}$ from <i>ab initio</i> calculations. New Journal of Physics, 2011, 13, 085012.	1.2	60
7649	A First-Principles Model for Hydrogen Uptake Promoted by Sulfur on Ni(111). Journal of the Electrochemical Society, 2011, 158, F36.	1.3	17
7650	Physical and chemical properties of a Ga-doped ZnO crystal. Physica Scripta, 2011, 83, 065604.	1.2	11
7651	A comparative study of quantum transport properties of silver and copper nanowires using first principles calculations. Journal of Physics Condensed Matter, 2011, 23, 085501.	0.7	28
7652	Rigorous formulation of two-parameter double-hybrid density-functionals. Journal of Chemical Physics, 2011, 135, 244106.	1.2	43
7653	Thermal Dehydration and Vibrational Spectra of Hydrated Sodium Metaborates. Industrial & Engineering Chemistry Research, 2011, 50, 7746-7752.	1.8	30
7654	On the dissociation of molecular hydrogen by Au supported on transition metal carbides: choice of the most active support. Physical Chemistry Chemical Physics, 2011, 13, 6865.	1.3	31
7655	Temperature-induced martensitic phase transitions in gum-metal approximants: First-principles investigations for $\text{Ti}_3\text{Nb}$ . Physical Review B, 2011, 84, .	1.1	41
7656	Dithizone and Its Oxidation Products: A DFT, Spectroscopic, and X-ray Structural Study. Journal of Physical Chemistry A, 2011, 115, 14637-14646.	1.1	29
7657	First Principles Studies of the Effect of Ostwald Ripening on Carbon Nanotube Chirality Distributions. ACS Nano, 2011, 5, 771-779.	7.3	27
7658	Effects of rhenium alloying on adhesion of Mo/HfC and Mo/ZrC interfaces: A first-principles study. Journal of Applied Physics, 2011, 110, .	1.1	14

#	ARTICLE	IF	CITATIONS
7659	Sensitivity of Boron Nitride Nanotubes toward Biomolecules of Different Polarities. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2442-2447.	2.1	149
7660	Improved visible-light photocatalysis of nano-Bi <sub>2</sub> Sn <sub>2</sub> O <sub>7</sub> with dispersed s-bands. <i>Journal of Materials Chemistry</i> , 2011, 21, 3872.	6.7	92
7661	First-principles study of misfit strain-stabilized ferroelectric SnTiO <sub>3</sub> . <i>Physical Review B</i> , 2011, 84, .	1.1	49
7662	Ab initio calculation of the geometric, electronic and magnetic properties of neutral and anionic Au <sub>n</sub> Pd <sub>(n-1)</sub> clusters. <i>Molecular Physics</i> , 2011, 109, 1485-1494. <sup>0.8</sup>		12
7663	Near-Infrared Absorption and Polarized Luminescent Ultrathin Films Based on Sulfonated Cyanines and Layered Double Hydroxide. <i>Journal of Physical Chemistry C</i> , 2011, 115, 7939-7946.	1.5	24
7664	High-Pressure Study of Lithium Azide from Density-Functional Calculations. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4521-4529.	1.1	32
7665	New insight into mechanisms in water-gas-shift reaction on Au/CeO <sub>2</sub> (111): A density functional theory and kinetic study. <i>Faraday Discussions</i> , 2011, 152, 121.	1.6	85
7666	Implementation of screened hybrid functionals based on the Yukawa potential within the LAPW basis set. <i>Physical Review B</i> , 2011, 83, .	1.1	159
7667	Electronic and Structural Properties of WO <sub>3</sub> : A Systematic Hybrid DFT Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8345-8353.	1.5	250
7668	Novel Sn <sub>x</sub> Se <sub>1-x</sub> nanocrystals with tunable band gap: experimental and first-principles calculations. <i>Journal of Materials Chemistry</i> , 2011, 21, 12605.	6.7	40
7669	Structure and Properties of Single Crystalline CaMg <sub>2</sub> Bi <sub>2</sub> , EuMg <sub>2</sub> Bi <sub>2</sub> , and YbMg <sub>2</sub> Bi <sub>2</sub> . <i>Inorganic Chemistry</i> , 2011, 50, 11127-11133.	1.9	74
7670	Evaluating the C, N, and F Pairwise Codoping Effect on the Enhanced Photoactivity of ZnWO <sub>4</sub> : The Charge Compensation Mechanism in Donor-Acceptor Pairs. <i>Journal of Physical Chemistry C</i> , 2011, 115, 15516-15524.	1.5	20
7671	Improving the Carbon Resistance of Ni-Based Steam Reforming Catalyst by Alloying with Rh: A Computational Study Coupled with Reforming Experiments and EXAFS Characterization. <i>ACS Catalysis</i> , 2011, 1, 574-582.	5.5	67
7672	Calibration of DFT Functionals for the Prediction of <sup>57</sup> Fe Mössbauer Spectral Parameters in Iron-Nitrosyl and Iron-Sulfur Complexes: Accurate Geometries Prove Essential. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3232-3247.	2.3	70
7673	Excited States and Absorption Spectra of UF <sub>6</sub> : A RASPT2 Theoretical Study with Spin-Orbit Coupling. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3223-3231.	2.3	19
7674	Methods for Computing Accurate Atomic Spin Moments for Collinear and Noncollinear Magnetism in Periodic and Nonperiodic Materials. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4146-4164.	2.3	77
7675	Kinetically Controlled Autocatalytic Chemical Process for Bulk Production of Bimetallic Core-Shell Structured Nanoparticles. <i>ACS Nano</i> , 2011, 5, 9370-9381.	7.3	67
7676	Dual Coordination Modes of Ethylene-Linked NP <sub>2</sub> Ligands in Cobalt(II) and Nickel(II) Iodides. <i>Inorganic Chemistry</i> , 2011, 50, 10213-10224.	1.9	24

#	ARTICLE	IF	CITATIONS
7677	Methyl Chloride Reactions on Lithiated Carbon Nanotubes: Lithium as Both Reactant and Catalyst. <i>Journal of Physical Chemistry C</i> , 2011, 115, 11694-11700.	1.5	8
7678	Normal Mode Analysis in Zeolites: Toward an Efficient Calculation of Adsorption Entropies. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1090-1101.	2.3	94
7679	Spin-crossover in cyanide-based bimetallic coordination polymers—insight from first-principles calculations. <i>Journal of Materials Chemistry</i> , 2011, 21, 13832.	6.7	20
7680	Density Functional Modeling of the Interactions of Platinum Clusters with CeO <sub>2</sub> Nanoparticles of Different Size. <i>Journal of Physical Chemistry C</i> , 2011, 115, 16081-16086.	1.5	40
7681	Density Functional Theory (DFT) Study on the Dehydration of Cellulose. <i>Energy &amp; Fuels</i> , 2011, 25, 2664-2670.	2.5	67
7682	CO Adsorption on Anatase Nanocrystals: A Combined Experimental and Periodic DFT Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 7694-7700.	1.5	83
7683	A density functional study of atomic oxygen and water molecule adsorption on Ni(111) and chromium-substituted Ni(111) surfaces. <i>Applied Surface Science</i> , 2011, 258, 442-447.	3.1	62
7684	Adsorption and dissociation of O <sub>2</sub> on CuCl(111) surface: A density functional theory study. <i>Applied Surface Science</i> , 2011, 258, 408-413.	3.1	12
7685	Guaiacol derivatives and inhibiting species adsorption over MoS <sub>2</sub> and CoMoS catalysts under HDO conditions: A DFT study. <i>Catalysis Communications</i> , 2011, 12, 901-905.	1.6	74
7686	High-pressure structural phase transitions and mechanical properties of calcite rock. <i>Computational Materials Science</i> , 2011, 50, 852-857.	1.4	28
7687	Ab initio investigation of Al/Mo <sub>2</sub> B interfacial adhesion. <i>Computational Materials Science</i> , 2011, 50, 880-885.	1.4	40
7688	Structural and lattice dynamical properties of Zintl NaIn and NaTl compounds. <i>Computational Materials Science</i> , 2011, 50, 1070-1076.	1.4	25
7689	First-principles studies of typical long-period superstructures Al <sub>5</sub> Ti <sub>3</sub> , h-Al <sub>2</sub> Ti and r-Al <sub>2</sub> Ti in Al-rich TiAl alloys. <i>Computational Materials Science</i> , 2011, 50, 1467-1476.	1.4	28
7690	Ab initio study of structural, elastic and vibrational properties of praseodymium chalcogenides. <i>Computational Materials Science</i> , 2011, 50, 1958-1964.	1.4	5
7691	Phonon and thermodynamic properties of Al—Mn compounds: A first-principles study. <i>Computational Materials Science</i> , 2011, 50, 2096-2103.	1.4	23
7692	Dependence of pressure on elastic, electronic and optical properties of CeO <sub>2</sub> and ThO <sub>2</sub> : A first principles study. <i>Computational Materials Science</i> , 2011, 50, 2280-2286.	1.4	36
7693	Optical properties of $\hat{1}\pm$ , $\hat{1}^2$ and $\hat{1}\%$ structure of Titanium: Ab initio approach. <i>Computational Materials Science</i> , 2011, 50, 2549-2553.	1.4	8
7694	Magnetic properties for the transition-metal aluminides XAl <sub>2</sub> (X=V, Cr, Mn, and Co): A first-principles study. <i>Computational Materials Science</i> , 2011, 50, 2433-2438.	1.4	7

#	ARTICLE	IF	CITATIONS
7695	Structural, elastic, and thermodynamic properties of ZnSexTe1-x: A first-principles study. Computational Materials Science, 2011, 50, 2745-2749.	1.4	7
7696	The energetic and structural properties of bcc NiCu, FeCu alloys: A first-principles study. Computational Materials Science, 2011, 50, 2586-2591.	1.4	40
7697	Self-diffusion in Zn4Sb3 from first-principles molecular dynamics. Computational Materials Science, 2011, 50, 2663-2665.	1.4	11
7698	Mechanical properties and defective effects of bcc V4Cr4Ti and V5Cr5Ti alloys by first-principles simulations. Computational Materials Science, 2011, 50, 2727-2731.	1.4	22
7699	First-principles study of structural, elastic, electronic and optical properties of orthorhombic NaAlF4. Computational Materials Science, 2011, 50, 2822-2827.	1.4	38
7700	Sign-changeable spin-filter efficiency and giant magnetoresistance in seamless graphene nanoribbon junctions. Computational Materials Science, 2011, 50, 2886-2890.	1.4	6
7701	Stacking faults in B2-structured magnesium alloys from first principles calculations. Computational Materials Science, 2011, 50, 3198-3207.	1.4	11
7702	A comparison of density functional theory (DFT) methods for estimating the singlet-triplet (S0-T1) excitation energies of benzene and polyacenes. Computational and Theoretical Chemistry, 2011, 976, 105-112.	1.1	36
7703	Structural and electronic properties of phosphorus-doped titanium clusters: A DFT study. Computational and Theoretical Chemistry, 2011, 977, 50-54.	1.1	9
7704	Singlet-triplet (S0-T1) excitation energies of the [4n] rectangular graphene nanoribbon series (n=2-6): A comparative theoretical study. Computational and Theoretical Chemistry, 2011, 977, 163-167.	1.1	13
7705	Adsorption of hydrogen, chlorine, and sulfur atoms on Cr2O3(001) surfaces: A density functional theory investigation. Corrosion Science, 2011, 53, 3612-3622.	3.0	17
7706	Structural stability of intermetallic phases in the Ga-Ti system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2011, 35, 133-141.	0.7	7
7707	Formation of Carbon Clusters in the Initial Stage of Chemical Vapor Deposition Graphene Growth on Ni(111) Surface. Journal of Physical Chemistry C, 2011, 115, 17695-17703.	1.5	119
7708	Oxidovanadium(IV) Schiff Base Complex Derived from Vitamin B6: Synthesis, Characterization, and Insulin Enhancing Properties. Inorganic Chemistry, 2011, 50, 4349-4361.	1.9	66
7709	Hydrogen electrocatalysis on overlayers of rhodium over gold and palladium substrates: more active than platinum?. Physical Chemistry Chemical Physics, 2011, 13, 16437.	1.3	29
7710	Optical gap and native point defects in kaolinite studied by the GGA-PBE, HSE functional, and GW approaches. Physical Review B, 2011, 84, .	1.1	40
7711	First-principles investigations of electronic and magnetic properties of SrTiO3(001) surfaces with adsorbed ethanol and acetone molecules. Physical Review B, 2011, 83, .	1.1	18
7712	DFT Studies of the Interactions of a Graphene Layer with Small Water Aggregates. Journal of Physical Chemistry A, 2011, 115, 12348-12356.	1.1	73



#	ARTICLE	IF	CITATIONS
7713	Theoretical study of metallasilatranes; Bonding nature and prediction of new metallasilatrane. Collection of Czechoslovak Chemical Communications, 2011, 76, 619-629.	1.0	8
7714	Electron Densities and Related Properties from the ab-initio Simulation of Crystalline Solids. , 2011, , 79-132.		3
7715	Large-scale screening of metal hydrides for hydrogen storage from first-principles calculations based on equilibrium reaction thermodynamics. Physical Chemistry Chemical Physics, 2011, 13, 7218.	1.3	30
7716	A multifaceted approach to hydrogen storage. Physical Chemistry Chemical Physics, 2011, 13, 16955.	1.3	64
7717	Electrical Characteristics of Cobalt Phthalocyanine Complexes Adsorbed on Graphene. Journal of Physical Chemistry C, 2011, 115, 16052-16062.	1.5	38
7718	Low-Temperature Growth of Graphene by Chemical Vapor Deposition Using Solid and Liquid Carbon Sources. ACS Nano, 2011, 5, 3385-3390.	7.3	353
7719	Crystal structure of the mirror symmetry 10H-type long-period stacking order phase in Mg-Y-Zn alloy. Journal of Alloys and Compounds, 2011, 509, 669-674.	2.8	24
7720	Structural, electronic and optical properties of BiFeO <sub>3</sub> studied by first-principles. Journal of Alloys and Compounds, 2011, 509, 1901-1905.	2.8	98
7721	Synthesis of Li <sub>2</sub> MgIr and LiMgIrH <sub>6</sub> : Guidance from DFT. Journal of Alloys and Compounds, 2011, 509, 3203-3207.	2.8	1
7722	Thermodynamic optimization of the Cu-Nd system. Journal of Alloys and Compounds, 2011, 509, 2679-2683.	2.8	20
7723	Synthesis and hydriding behavior of Li <sub>2</sub> MgPt. Journal of Alloys and Compounds, 2011, 509, 2650-2653.	2.8	2
7724	Chemical trends of the band gaps of idealized crystal of semiconducting silicon clathrates, M <sub>8</sub> Si <sub>38</sub> A <sub>8</sub> (M = Na, K, Rb, Cs; A = Ga, Al, In), predicted by first-principle pseudopotential calculations. Journal of Alloys and Compounds, 2011, 509, 3924-3930.	2.8	20
7725	Thermodynamic assessment of Au-La and Au-Er binary systems. Journal of Alloys and Compounds, 2011, 509, 4439-4444.	2.8	9
7726	First-principles calculations of elemental crystalline boron phases under high pressure: Orthorhombic B <sub>28</sub> and tetragonal B <sub>48</sub> . Journal of Alloys and Compounds, 2011, 509, 5219-5229.	2.8	57
7727	Phase stability of magnesium-rare earth binary systems from first-principles calculations. Journal of Alloys and Compounds, 2011, 509, 6899-6907.	2.8	59
7728	First-principles study of lattice dynamics and thermodynamic properties of LiInX <sub>2</sub> (X=S, Se, Te). Journal of Alloys and Compounds, 2011, 509, 9733-9741.	2.8	22
7729	First-principles phase stability calculations and estimation of finite temperature effects on pseudo-binary Mg <sub>6</sub> (PdxNi <sub>1-<math>\hat{x}</math>) compounds. Intermetallics, 2011, 19, 502-510.</sub>	1.8	11
7730	The new intermetallic compound Ga <sub>5</sub> Pt:Structure from a twinned crystal. Intermetallics, 2011, 19, 518-525.	1.8	6



#	ARTICLE	IF	CITATIONS
7731	Native Defect Concentrations in NaAlH <sub>4</sub> and Na <sub>3</sub> AlH <sub>6</sub> . Journal of Physical Chemistry C, 2011, 115, 21443-21453.	1.5	27
7732	Dynamics of the [4Fe-4S] Cluster in <i>Pyrococcus furiosus</i> D14C Ferredoxin via Nuclear Resonance Vibrational and Resonance Raman Spectroscopies, Force Field Simulations, and Density Functional Theory Calculations. Biochemistry, 2011, 50, 5220-5235.	1.2	38
7733	Phonons of the anomalous element cerium. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 9342-9345.	3.3	47
7734	Ammonia decomposition activity on monolayer Ni supported on Ru, Pt and WC substrates. Surface Science, 2011, 605, 2055-2060.	0.8	22
7735	Spontaneous formation of highly dispersed spheroidal metallic silver nanoparticles in surfactant-free N,N-dimethylacetamide. Synthetic Metals, 2011, 161, 1517-1521.	2.1	15
7736	First-principles calculation of structural and elastic properties of Pd <sub>3</sub> -xRh <sub>x</sub> V alloys. Transactions of Nonferrous Metals Society of China, 2011, 21, 388-394.	1.7	9
7737	Density functional theory study of influence of impurity on electronic properties and reactivity of pyrite. Transactions of Nonferrous Metals Society of China, 2011, 21, 1887-1895.	1.7	53
7738	First-principles study of phase stability and electronic properties of RhZr. Transactions of Nonferrous Metals Society of China, 2011, 21, 2301-2305.	1.7	4
7739	A first-principles study on electronic structure and elastic properties of Al <sub>4</sub> Sr, Mg <sub>2</sub> Sr and Mg <sub>23</sub> Sr <sub>6</sub> phases. Transactions of Nonferrous Metals Society of China, 2011, 21, 2677-2683.	1.7	10
7740	First-principles Study of NiAl Alloyed with Rare Earth Element Ce. Journal of Materials Science and Technology, 2011, 27, 719-724.	5.6	23
7741	Mechanical Properties and Defective Effects of 316LN Stainless Steel by First-Principles Simulations. Journal of Materials Science and Technology, 2011, 27, 1029-1033.	5.6	12
7742	The origin of p-type conduction in Li-N codoped ZnO: An ab initio calculation study. Journal of Applied Physics, 2011, 110, 013711.	1.1	20
7743	An ab initio molecular dynamics study of iron phases at high pressure and temperature. Journal of Physics Condensed Matter, 2011, 23, 485402.	0.7	19
7744	Electronic Structure and Reactivity of Ce- and Zr-Doped TiO <sub>2</sub> : Assessing the Reliability of Density Functional Theory Approaches. Journal of Physical Chemistry C, 2011, 115, 12995-13007.	1.5	78
7745	Computational Molecular Engineering for Nanodevices and Nanosystems. , 2011, , 347-383.		0
7746	Molecular Models of the Stabilization of Bivalent Metal Cations in Zeolite Catalysts. , 2011, , 579-643.		1
7747	Electrostatic studies of $\pi$ - $\pi$ interaction for benzene stacking on a graphene layer. Applied Physics Letters, 2011, 99, .	1.5	41
7748	Theoretical Study of the Interstitial Oxygen Atom in Anatase and Rutile TiO <sub>2</sub> : Electron Trapping and Elongation of the r(O <sup>••</sup> O) Bond. Journal of Physical Chemistry C, 2011, 115, 8265-8273.	1.5	44

#	ARTICLE	IF	CITATIONS
7749	Receptor design and extraction of inorganic fluoride ion from aqueous medium. Chemical Communications, 2011, 47, 7398.	2.2	49
7750	Computational Investigation of CO Adsorption and Oxidation on Iron-Modified Cerium Oxide. Journal of Physical Chemistry C, 2011, 115, 14745-14753.	1.5	63
7751	Density Functional Study on the Morphology and Photoabsorption of CdSe Nanoclusters. Journal of Physical Chemistry C, 2011, 115, 16782-16796.	1.5	104
7752	Fabrication and enhanced visible-light photocatalytic activity of carbon self-doped TiO <sub>2</sub> sheets with exposed {001} facets. Journal of Materials Chemistry, 2011, 21, 1049-1057.	6.7	390
7753	Hydride-Assisted Hydrogenation of Ti-Doped NaH/Al: A Density Functional Theory Study. Journal of Physical Chemistry C, 2011, 115, 2522-2528.	1.5	11
7754	First-principles study of the biomineral hydroxyapatite. Physical Review B, 2011, 84, .	1.1	91
7755	An unsymmetrical behavior of reactant units in the Kolbe-Schmitt reaction. Theoretical Chemistry Accounts, 2011, 130, 891-900.	0.5	2
7756	An examination of density functional theories on isomerization energy calculations of organic molecules. Theoretical Chemistry Accounts, 2011, 130, 851-857.	0.5	24
7757	Theoretical studies on nitrogen rich energetic azoles. Journal of Molecular Modeling, 2011, 17, 1507-1515.	0.8	49
7758	Structural and electronic properties of 0.5 ML sulfur adsorbed on the GaP(001) surface. Journal of Materials Science, 2011, 46, 1635-1639.	1.7	0
7759	Electronic coupling in iron oxide-modified TiO <sub>2</sub> leads to a reduced band gap and charge separation for visible light active photocatalysis. Physical Chemistry Chemical Physics, 2011, 13, 18194.	1.3	50
7760	Formation and Mobility of Li Point Defects in LiBO <sub>2</sub> : A First-Principles Investigation. Journal of Physical Chemistry C, 2011, 115, 12343-12349.	1.5	15
7761	Adsorption of R <sup>+</sup> OH Molecules on TiO <sub>2</sub> Surfaces at the Solid-Liquid Interface. Langmuir, 2011, 27, 2411-2419.	1.6	27
7762	Concise relation of substitution energy to macroscopic deformation in a deformed system. Physical Review B, 2011, 84, .	1.1	7
7763	A Comparative Study of Lattice Dynamics of Three- and Two-Dimensional MoS <sub>2</sub> . Journal of Physical Chemistry C, 2011, 115, 16354-16361.	1.5	298
7764	Compositional dependence of structural and electronic properties of Cu <sub>2</sub> ZnSn(S,Se)S <sub>4</sub>		399
7765	Adsorption Behavior of 4-Methoxypyridine on Gold Nanoparticles. Langmuir, 2011, 27, 7258-7264.	1.6	18
7766	Novel [4 + 2] cycloaddition reactions of alkyne and enyne key-units: Direct access to bicyclic aromatic and heteroaromatic products. A theoretical mechanistic study. Chemical Science, 2011, 2, 2332-2341.	3.7	15

#	Abstracts	IF	CITATIONS
7767	Properties of single quintuple Bi <sub>2</sub> Te <sub>3</sub> and Bi <sub>3</sub> Te <sub>2</sub> Computational design and characterisation of artificial enzymes for Kemp elimination. Molecular Simulation, 2011, 37, 557-571.	1.1	68
7769	Engineering quantum anomalous/valley Hall states in graphene via metal-atom adsorption: An ab-initio study. Physical Review B, 2011, 84, .	1.1	217
7770	Bond-Order Potential for Erbium-Hydride System. Journal of Physical Chemistry C, 2011, 115, 25097-25104.	1.5	9
7771	Understanding Ti intermediate-band formation in partially inverse thiospinel MgIn <sub>2</sub> S <sub>4</sub> through many-body approaches. Physical Review B, 2011, 84, .	1.1	14
7772	Combined ATR-FTIR and DFT Study of Cyclohexanone Adsorption on Hydrated TiO <sub>2</sub> Anatase Surfaces. Journal of Physical Chemistry C, 2011, 115, 14164-14172.	1.5	23
7773	Theoretical investigation of gold clusters supported on graphene sheets. New Journal of Chemistry, 2011, 35, 2153.	1.4	31
7774	Electronic structure and chemical bonding of the electron-poor II-V semiconductors ZnSb and ZnAs. Physical Review B, 2011, 84, .	1.1	34
7775	Influence of Doping Effect on Zinc Oxide by First-Principles Studies. Journal of Physical Chemistry C, 2011, 115, 7706-7716.	1.5	29
7776	Electronic Structure and Magnetic Anisotropy in Ni/Cu(001) from Angle-Resolved Photoemission Spectroscopy. Journal of the Physical Society of Japan, 2011, 80, 064706.	0.7	1
7777	Towards a scalable and accurate quantum approach for describing vibrations of molecule-metal interfaces. Beilstein Journal of Nanotechnology, 2011, 2, 427-447.	1.5	18
7778	Electronic Structure of the Cubic Compounds ReGa <sub>3</sub> (Re = Er, Tm, Yb, and Lu). Advances in Condensed Matter Physics, 2011, 2011, 1-14.	0.4	4
7780	The stability and work function of TaC <sub>x</sub> N <sub>1-x</sub> alloy surfaces. Journal of Applied Physics, 2011, 109, .	1.1	6
7781	Catalytic Reactions on Model Gold Surfaces: Effect of Surface Steps and of Surface Doping. Catalysts, 2011, 1, 40-51.	1.6	8
7782	Coinage metal (4, 4) nanotubes, simulated by first-principles calculations. Journal of Chemical Physics, 2011, 134, 244504.	1.2	7
7783	Layered transition-metal permanent-magnet structures. Journal of Applied Physics, 2011, 109, .	1.1	2
7784	Characterization of K <sub>4</sub> Nb <sub>6</sub> O <sub>17</sub> synthesized by a sol-gel method for H <sub>2</sub> evolution. Journal of the Chinese Institute of Engineers, Series A/Chung-kuo Kung Ch'eng Hsueh K'uan, 2011, 34, 3-9.	0.6	4
7785	Zr segregation and associated Al vacancies in alumina grain boundaries. Journal of the Ceramic Society of Japan, 2011, 119, 840-844.	0.5	14

#	ARTICLE	IF	CITATIONS
7786	Dependence of Structural and Electronic Properties of Uranium Monochalcogenides on Exchangeâ€‘Correlation Energy Functionals. Journal of the Physical Society of Japan, 2011, 80, 084603.	0.7	1
7787	The effects of Bi alloying in Cu delafossites: A density functional theory study. Journal of Applied Physics, 2011, 109, .	1.1	17
7788	Anisotropy of zigzag chains of palladium. Journal of Applied Physics, 2011, 109, 07E322.	1.1	4
7789	Surface structures and magnetic anisotropies of a Fe/Pt (001) surface: An ab initio study. Journal of Applied Physics, 2011, 109, 07B764.	1.1	7
7790	Scaling of flat band potential and dielectric constant as a function of Ta concentration in Ta-TiO2 epitaxial films. AIP Advances, 2011, 1, 022151.	0.6	17
7791	Spatial imaging of individual vibronic states in the interior of single molecules. Journal of Chemical Physics, 2011, 135, 014705.	1.2	22
7792	Effective coordination concept applied for phase change (GeTe) <sub>m</sub> (Sb <sub>2</sub> Te <sub>3</sub> ) <sub>n</sub> compounds. Journal of Applied Physics, 2011, 109, .	1.1	83
7793	Chemical speciation of adsorbed glycine on metal surfaces. Journal of Chemical Physics, 2011, 135, 034703.	1.2	20
7794	Atomic and electronic properties of P/Si(111)-(2x1) surface. EPJ Applied Physics, 2011, 56, 31302.	0.3	1
7795	Structural and electronic characterization of (2,33) bar-shaped stacking fault in 4H-SiC epitaxial layers. Applied Physics Letters, 2011, 98, .	1.5	21
7796	First Principles Investigation on the Modifications of the 4H-SiC Band Structure Due to the (4,4) and (3,5) Stacking Faults. Applied Physics Express, 2011, 4, 025802.	1.1	22
7797	Differential adsorption of complex organic molecules isomers at interstellar ice surfaces. Astronomy and Astrophysics, 2011, 532, A12.	2.1	49
7798	Growth and structure of an ultrathin tin oxide film on Rh(111). Journal of Applied Physics, 2011, 109, .	1.1	7
7799	Interface-dependent magnetic anisotropy of Fe/BaTiO <sub>3</sub> : A first principles study. Journal of Applied Physics, 2011, 109, 07D909.	1.1	8
7800	The interstellar carbonaceous aromatic matter as a trap for molecular hydrogen. Monthly Notices of the Royal Astronomical Society, 2011, 412, 2729-2734.	1.6	10
7801	Phase Stability, Electronic Structure, Compressibility, Elastic and Optical Properties of a Newly Discovered $\text{Ti}_3\text{SnC}_2$ : A Firstâ€‘Principle Study. Journal of the American Ceramic Society, 2011, 94, 3907-3914.	1.9	27
7802	Europiumâ€‘Doped $\text{LaSi}_3\text{N}_5$ Ternary Nitride: Synthesis, Spectroscopy, Computed Electronic Structure and Band Gaps. Journal of the American Ceramic Society, 2011, 94, 4345-4351.	1.9	13
7803	Support nanostructure boosts oxygen transfer to catalytically active platinum nanoparticles. Nature Materials, 2011, 10, 310-315.	13.3	748

#	ARTICLE	IF	CITATIONS
7804	Study on interactions between Cadmium and defects in Cd-doped ZnO by first-principle calculations. <i>Solid State Sciences</i> , 2011, 13, 384-387.	1.5	33
7805	The structural phase transition and elastic properties of zirconia under high pressure from first-principles calculations. <i>Solid State Sciences</i> , 2011, 13, 938-943.	1.5	14
7806	First-principles calculations of the structural, elastic, electronic, chemical bonding and optical properties of zinc-blende and rocksalt GeC. <i>Solid State Sciences</i> , 2011, 13, 2177-2184.	1.5	11
7807	Density functional predictions of new silicon allotropes: Electronic properties and potential applications to Li-battery anode materials. <i>Solid State Communications</i> , 2011, 151, 1228-1230.	0.9	19
7808	First-principles study of martensitic transformation of IrTi alloy. <i>Solid State Communications</i> , 2011, 151, 1433-1436.	0.9	6
7809	Defects in ion-implanted hcp-titanium: A first-principles study of electronic structures. <i>Solid State Communications</i> , 2011, 151, 1889-1893.	0.9	4
7810	A theoretical study of the influence of dopant concentration on the hydration properties of yttrium-doped barium cerate. <i>Solid State Ionics</i> , 2011, 204-205, 27-34.	1.3	23
7811	CFx thin solid films deposited by high power impulse magnetron sputtering: Synthesis and characterization. <i>Surface and Coatings Technology</i> , 2011, 206, 646-653.	2.2	43
7812	First-principles calculations of vacancy formation in In-free photovoltaic semiconductor Cu <sub>2</sub> ZnSnSe <sub>4</sub> . <i>Thin Solid Films</i> , 2011, 519, 7513-7516.	0.8	38
7813	New semiconducting silicides assembled from transition-metal-encapsulating Si clusters. <i>Thin Solid Films</i> , 2011, 519, 8456-8460.	0.8	10
7814	The structure of Tiâ€“Siâ€“N superhard nanocomposite coatings: ab initio study. <i>Thin Solid Films</i> , 2011, 520, 876-880.	0.8	13
7815	Interaction of gas molecules with crystalline polymer separation membranes: Atomic-scale modeling and first-principles calculations. <i>Journal of Membrane Science</i> , 2011, 384, 176-183.	4.1	5
7816	Ni/boride interfaces and environmental embrittlement in Ni-based superalloys: A first-principles study. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2011, 530, 373-377.	2.6	10
7817	Ab initio modeling of oxygen impurity atom incorporation into uranium mononitride surface and sub-surface vacancies. <i>Journal of Nuclear Materials</i> , 2011, 416, 200-204.	1.3	33
7818	Simulation of defect evolution in electron-irradiated dilute FeCr alloys. <i>Journal of Nuclear Materials</i> , 2011, 417, 1078-1081.	1.3	9
7819	Atomistic modelling of the Feâ€“Crâ€“C system. <i>Journal of Nuclear Materials</i> , 2011, 415, 316-319.	1.3	3
7820	First principles study of hydrogen behaviors in hexagonal tungsten carbide. <i>Journal of Nuclear Materials</i> , 2011, 418, 233-238.	1.3	12
7821	First-principles based microkinetic modeling of borohydride oxidation on a Au(111) electrode. <i>Journal of Power Sources</i> , 2011, 196, 9228-9237.	4.0	95

#	ARTICLE	IF	CITATIONS
7822	Spectroscopic characterization, X-ray structure, antimicrobial activity and DFT calculations of novel dipicolinate copper(II) complex with 2,6-pyridinedimethanol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 84, 168-177.	2.0	32
7823	Ab initio study on preferred growth of ZnO. <i>Scripta Materialia</i> , 2011, 64, 483-485.	2.6	29
7824	First-principles study of long-period stacking ordered-like multi-stacking fault structures in pure magnesium. <i>Scripta Materialia</i> , 2011, 64, 942-945.	2.6	47
7825	Structural, electronic and energetic properties of GaN[0 0 1]/Ga <sub>2</sub> O <sub>3</sub> [1 0 0] heterojunctions: A first-principles density functional theory study. <i>Scripta Materialia</i> , 2011, 65, 465-468.	2.6	5
7826	The effect of alloying elements on grain boundary and bulk cohesion in aluminum alloys: An ab initio study. <i>Scripta Materialia</i> , 2011, 65, 926-929.	2.6	56
7827	Hydrogen sensing and mechanism of M-doped SnO <sub>2</sub> (M = Cr <sup>3+</sup> , Cu <sup>2+</sup> and Pd <sup>2+</sup> ) nanocomposite. <i>Sensors and Actuators B: Chemical</i> , 2011, 160, 455-462.	4.0	129
7828	Electronic and optical properties of BAs under pressure. <i>Physica B: Condensed Matter</i> , 2011, 406, 4272-4277.	1.3	24
7829	Structural and electronic properties of U <sub>2</sub> Ti: A first principles study. <i>Physica B: Condensed Matter</i> , 2011, 406, 4317-4321.	1.3	12
7830	Transition metal encapsulated hydrogenated silicon nanotubes: Silicon-based half-metal. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2011, 375, 4209-4213.	0.9	9
7831	Electron transport through molecular junctions. <i>Physics Reports</i> , 2011, 509, 1-87.	10.3	161
7832	First principles predictions on mechanical and physical properties of HoX (X=As, P). <i>Materials Chemistry and Physics</i> , 2011, 125, 887-894.	2.0	10
7833	Ideal mechanical strength and interface cohesion property of Ir-base superalloys from first principles calculation. <i>Materials Chemistry and Physics</i> , 2011, 126, 284-288.	2.0	14
7834	FP-LAPW study of the fundamental properties of the cubic spinel CdAl <sub>2</sub> O <sub>4</sub> . <i>Materials Research Bulletin</i> , 2011, 46, 2252-2260.	2.7	27
7835	Why is metallic Pt the best catalyst for methoxy decomposition?. <i>Journal of Natural Gas Chemistry</i> , 2011, 20, 90-98.	1.8	11
7836	Metal catalyzed ethylene epoxidation: A comparative density functional theory study. <i>Journal of Natural Gas Chemistry</i> , 2011, 20, 303-310.	1.8	5
7837	Theoretical studies of adsorption property on Ir <sub>4</sub> /MgO and Ir <sub>4</sub> / $\gamma$ -Al <sub>2</sub> O <sub>3</sub> . <i>Journal of Natural Gas Chemistry</i> , 2011, 20, 595-602.	1.8	0
7838	Structure and Magnetic Properties of $\text{LiFePO}_4$ Under Pressure. <i>IEEE Transactions on Magnetics</i> , 2011, 47, 3817-3820.	1.2	4
7839	Hydrodeoxygenation pathways catalyzed by MoS <sub>2</sub> and NiMoS active phases: A DFT study. <i>Journal of Catalysis</i> , 2011, 279, 276-286.	3.1	118

#	ARTICLE	IF	CITATIONS
7840	Spectroscopy, microscopy and theoretical study of NO adsorption on MoS <sub>2</sub> and Co-MoS <sub>2</sub> hydrotreating catalysts. <i>Journal of Catalysis</i> , 2011, 279, 337-351.	3.1	64
7841	Free-energy profiles along reduction pathways of MoS <sub>2</sub> M-edge and S-edge by dihydrogen: A first-principles study. <i>Journal of Catalysis</i> , 2011, 280, 178-195.	3.1	117
7842	Oxide clusters as source of the third oxygen atom for the formation of carbonates in alkaline earth dehydrated zeolites. <i>Journal of Catalysis</i> , 2011, 281, 212-221.	3.1	18
7843	Effect of water on the stability of Mo and CoMo hydrodeoxygenation catalysts: A combined experimental and DFT study. <i>Journal of Catalysis</i> , 2011, 282, 155-164.	3.1	153
7844	Selectivity of chemisorbed oxygen in C-H bond activation and CO oxidation and kinetic consequences for CH <sub>4</sub> -O <sub>2</sub> catalysis on Pt and Rh clusters. <i>Journal of Catalysis</i> , 2011, 283, 10-24.	3.1	81
7845	Mechanism for the water-gas shift reaction on monofunctional platinum and cause of catalyst deactivation. <i>Journal of Catalysis</i> , 2011, 282, 278-288.	3.1	58
7846	Interaction of valine and valine radicals with single-walled carbon nanotube (5,0). <i>Chemical Physics Letters</i> , 2011, 511, 299-303.	1.2	11
7847	DFT study of influences of As, Co and Ni impurities on pyrite (100) surface oxidation by O <sub>2</sub> molecule. <i>Chemical Physics Letters</i> , 2011, 511, 389-392.	1.2	30
7848	CF: A first-principles study of structural patterns arising during synthetic growth. <i>Chemical Physics Letters</i> , 2011, 516, 62-67.	1.2	44
7849	Formation of novel ene-yne substituted $\eta^2$ -diketonato ruthenium(III) complexes by the Heck-like reactions on coordinated ligand. <i>Inorganica Chimica Acta</i> , 2011, 374, 654-659.	1.2	2
7850	Oxidative addition of methyl iodide to [Rh(CH <sub>3</sub> COCHCOCH <sub>3</sub> )(CO)(P(OCH <sub>2</sub> ) <sub>3</sub> CCH <sub>3</sub> )]. <i>Inorganica Chimica Acta</i> , 2011, 375, 128-134.	1.2	10
7851	Preparation, structural, spectroscopic, thermal and DFT characterization of cadmium(II) complexes with quinaldic acid. <i>Inorganica Chimica Acta</i> , 2011, 378, 154-162.	1.2	14
7852	Prediction of crystal structure, lattice dynamical, and mechanical properties of CaB <sub>2</sub> H <sub>2</sub> . <i>International Journal of Hydrogen Energy</i> , 2011, 36, 10149-10158.	3.8	16
7853	Hydrogen adsorption around lithium atoms anchored on graphene vacancies. <i>International Journal of Hydrogen Energy</i> , 2011, 36, 13657-13662.	3.8	40
7854	Surface diffusion coefficient determination by uniaxial tensile strain in Pb/Cu(111) surface systems. <i>Current Applied Physics</i> , 2011, 11, S400-S403.	1.1	4
7855	A density functional theory study on CO <sub>2</sub> capture and activation by graphene-like boron nitride with boron vacancy. <i>Catalysis Today</i> , 2011, 175, 271-275.	2.2	80
7856	Formation of oxygen active species in Ag-modified CeO <sub>2</sub> catalyst for soot oxidation: A DFT study. <i>Catalysis Today</i> , 2011, 177, 31-38.	2.2	61
7857	Synergy between ionic-covalent bonds and van der Waals interactions in SAMs formation: A first-principles study of adsorption of carboxylic acids on the Zn-ZnO(0001) surface. <i>Catalysis Today</i> , 2011, 177, 39-49.	2.2	34



#	ARTICLE	IF	CITATIONS
7858	Simple rules for the understanding of Heusler compounds. Progress in Solid State Chemistry, 2011, 39, 1-50.	3.9	1,742
7859	Reassignment of the Vibrational Spectra of Carbonates, Formates, and Related Surface Species on Ceria: A Combined Density Functional and Infrared Spectroscopy Investigation. Journal of Physical Chemistry C, 2011, 115, 23435-23454.	1.5	294
7860	Size effects on silver nanoparticles' properties. Nanotechnology, 2011, 22, 275708.	1.3	19
7861	Methanol conversion over TiO <sub>2</sub> -anatase supported oxomolybdate catalysts: an integrated <i>operando</i> DFT modeling approach. Phase Transitions, 2011, 84, 700-713.	0.6	8
7862	Using first-principles metadynamics simulation to predict new phases and probe the phase transition of NaAlH <sub>4</sub> . Journal of Physics Condensed Matter, 2011, 23, 345401.	0.7	3
7863	Unexpected Direct Reduction Mechanism for Hydrogenation of Ketones Catalyzed by Iron PNP Pincer Complexes. Inorganic Chemistry, 2011, 50, 12836-12843.	1.9	71
7864	Reactivity of Chemisorbed Oxygen Atoms and Their Catalytic Consequences during CH <sub>4</sub> -O <sub>2</sub> Catalysis on Supported Pt Clusters. Journal of the American Chemical Society, 2011, 133, 15958-15978.	6.6	184
7865	PH-Controlled Construction of Cu(I) Coordination Polymers: In Situ Transformation of Ligand, Network Topologies, and Luminescence and UV-vis-NIR Absorption Properties. Inorganic Chemistry, 2011, 50, 11403-11411.	1.9	56
7867	Structural and thermal properties of LaMnO <sub>3</sub> from neutron diffraction and first principles studies. Journal of Physics Condensed Matter, 2011, 23, 245402.	0.7	12
7868	V-doped SnS <sub>2</sub> : a new intermediate band material for a better use of the solar spectrum. Physical Chemistry Chemical Physics, 2011, 13, 20401.	1.3	80
7869	Ab Initio Molecular Dynamics Simulations of the Cooperative Adsorption of Hydrazine and Water on Copper Surfaces: Implications for Shape Control of Nanoparticles. Chemistry of Materials, 2011, 23, 2718-2728.	3.2	15
7870	Alkyne Insertion into the M- $\eta^5$ -P and M- $\eta^5$ -H Bonds (M=Pd, Ni, Pt, and Rh): A Theoretical Mechanistic Study of the C- $\eta^5$ -P and C- $\eta^5$ -H Bond Formation Steps. Chemistry - an Asian Journal, 2011, 6, 1423-1430.	1.7	47
7871	Density Functional Characterization of Pure and Alkaline Earth Metal-Doped Bi <sub>12</sub> GeO <sub>20</sub> , Bi <sub>12</sub> SiO <sub>20</sub> , and Bi <sub>12</sub> TiO <sub>20</sub> Photocatalysts. ChemCatChem, 2011, 3, 378-385.	1.8	21
7872	CO+NO versus CO+O <sub>2</sub> Reaction on Monolayer FeO(111) Films on Pt(111). ChemCatChem, 2011, 3, 671-674.	1.8	29
7873	DFT Comparison of <i>in situ</i> Nitrosodimethylamine Decomposition Pathways Over Ni and Pd. ChemCatChem, 2011, 3, 898-903.	1.8	11
7874	Mechanical and Electronic Properties of MoS <sub>2</sub> Nanoribbons and Their Defects. Journal of Physical Chemistry C, 2011, 115, 3934-3941.	1.5	427
7875	Electronic properties of the partially hydrogenated armchair carbon nanotubes. Physical Review B, 2011, 84, .	1.1	16
7876	Modelling charge transfer reactions with the frozen density embedding formalism. Journal of Chemical Physics, 2011, 135, 234103.	1.2	87

#	ARTICLE	IF	CITATIONS
7877	Effect of coverage by carbon on the possibility of forming an interstitial solid solution in Fe(001) and Fe(111) subsurface layers. <i>Physics of the Solid State</i> , 2011, 53, 599-605.	0.2	3
7878	Structural, vibrational and thermodynamic properties of Mg <sub>2</sub> FeH <sub>6</sub> complex hydride. <i>European Physical Journal B</i> , 2011, 79, 283-288.	0.6	13
7879	Interaction between stacking faults in pure Mg. <i>European Physical Journal B</i> , 2011, 82, 143-146.	0.6	12
7880	A matrix method for the calculation of nonlocal exchange potential and spin-orbit coupling in the first-principles calculation method. <i>European Physical Journal B</i> , 2011, 84, 29-35.	0.6	3
7881	Structural and electronic properties of Ni <sub>5</sub> Nb <sub>3</sub> Zr <sub>5</sub> clusters as a local structural unit of Ni-Nb-Zr glassy alloys. <i>European Physical Journal D</i> , 2011, 63, 177-181.	0.6	6
7882	Phase Transitions of AlFeO <sub>3</sub> and GaFeO <sub>3</sub> from the Chiral Orthorhombic (<math>Pna2_1</math>) Structure to the Rhombohedral (<math>R\bar{3}c</math>) Structure. <i>Inorganic Chemistry</i> , 2011, 50, 9527-9532.	1.9	51
7883	Coordination-driven self-assembly of thiocyanate complexes of Co(ii), Ni(ii) and Cu(ii) with picolinamide: a structural and DFT study. <i>CrystEngComm</i> , 2011, 13, 5863.	1.3	35
7884	Understanding the Electronic Structure of 4d Metal Complexes: From Molecular Spinors to L-Edge Spectra of a di-Ru Catalyst. <i>Journal of the American Chemical Society</i> , 2011, 133, 15786-15794.	6.6	50
7885	Bixbyite-Type V <sub>2</sub> O <sub>3</sub> —A Metastable Polymorph of Vanadium Sesquioxide. <i>Inorganic Chemistry</i> , 2011, 50, 6762-6766.	1.9	36
7886	Hydrogen effect on shearing and cleavage of Al: A first-principles study. <i>Physical Review B</i> , 2011, 84, .	1.1	15
7887	Synthesis, Structure, and Bonding Nature of Ethynediyl-Bridged Bis(silylene) Dinuclear Complexes of Tungsten and Molybdenum. <i>Organometallics</i> , 2011, 30, 4515-4531.	1.1	22
7888	Radiation-induced damage and evolution of defects in Mo. <i>Physical Review B</i> , 2011, 84, .	1.1	53
7889	Effect of vacancy defect on electrical properties of chiral single-walled carbon nanotube under external electrical field. <i>Chinese Physics B</i> , 2011, 20, 017302.	0.7	9
7890	Nanovoids in thermoelectric $\hat{1}^2$ -Zn <sub>4</sub> Sb <sub>3</sub> : A possibility for nanoengineering via Zn diffusion. <i>Acta Materialia</i> , 2011, 59, 5266-5275.	3.8	35
7891	Polymorphism of newly discovered Ti <sub>4</sub> GaC <sub>3</sub> : A first-principles study. <i>Acta Materialia</i> , 2011, 59, 5523-5533.	3.8	39
7892	Precipitates in Al—Cu alloys revisited: Atom-probe tomographic experiments and first-principles calculations of compositional evolution and interfacial segregation. <i>Acta Materialia</i> , 2011, 59, 6187-6204.	3.8	206
7893	Local electronic structure of LiFePO <sub>4</sub> nanoparticles in aged Li-ion batteries. <i>Acta Materialia</i> , 2011, 59, 6917-6926.	3.8	19
7894	The structure and the properties of S-phase in AlCuMg alloys. <i>Acta Materialia</i> , 2011, 59, 7396-7405.	3.8	93

#	ARTICLE	IF	CITATIONS
7895	Dielectric properties of organosilicons from first principles. <i>Journal of Materials Science</i> , 2011, 46, 90-93.	1.7	14
7896	Phase equilibria and thermodynamic modeling in the Ge-Zr binary system. <i>Journal of Materials Science</i> , 2011, 46, 1405-1413.	1.7	3
7897	First-principles calculation of grain boundary energy and grain boundary excess free volume in aluminum: role of grain boundary elastic energy. <i>Journal of Materials Science</i> , 2011, 46, 4199-4205.	1.7	47
7898	Geometrical and Electronic Properties of the Clusters of C <sub>20</sub> Cage Doped with Alkali Metal Atoms. <i>Journal of Cluster Science</i> , 2011, 22, 31-39.	1.7	29
7899	Acrolein Adsorption on Gold Clusters, A Theoretical Study of Conjugation Effect on C=C and C=O Interaction with Au Clusters. <i>Catalysis Letters</i> , 2011, 141, 996-1003.	1.4	7
7900	Electronic structure effects on stability and quantum conductance in 2D gold nanowires. <i>Journal of Nanoparticle Research</i> , 2011, 13, 5225-5238.	0.8	6
7901	Vibrational analysis and thermodynamic properties of C <sub>120</sub> nanotorus: a DFT study. <i>Journal of Nanoparticle Research</i> , 2011, 13, 6649-6659.	0.8	5
7902	Gold Nanoparticles on Yttrium Modified Titania: Support Properties and Catalytic Activity. <i>Topics in Catalysis</i> , 2011, 54, 219-228.	1.3	25
7903	Structural change from doping the gold cluster. <i>Journal of Molecular Modeling</i> , 2011, 17, 955-959.	0.8	1
7904	Light activation of the isomerization and deprotonation of the protonated Schiff base retinal. <i>Journal of Molecular Modeling</i> , 2011, 17, 2539-2547.	0.8	15
7905	Adsorption mechanism of single guanine and thymine on single-walled carbon nanotubes. <i>Journal of Molecular Modeling</i> , 2011, 17, 2773-2780.	0.8	12
7906	Computational analysis of tris(1,2-ethanediamine) cobalt(III) complex ion: calculation of the <sup>59</sup> Co shielding tensor using LF-DFT. <i>Monatshefte für Chemie</i> , 2011, 142, 593-597.	0.9	11
7907	Hydrogenation mechanism in lanthanum-activated magnesium films. <i>Applied Physics A: Materials Science and Processing</i> , 2011, 102, 739-745.	1.1	3
7908	Antisite defects and Mg doping in LiFePO <sub>4</sub> : a first-principles investigation. <i>Applied Physics A: Materials Science and Processing</i> , 2011, 104, 529-537.	1.1	47
7909	Atomic shell structure based on inhomogeneity measures of the electron density. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 39-46.	0.5	20
7910	DFT and kinetics study of O/O <sub>2</sub> mixtures reacting over a graphite (0001) basal surface. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 683-694.	0.5	34
7911	A density functional theory study of the "mythic" Lindlar hydrogenation catalyst. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 663-673.	0.5	130
7912	Performance of density functional theory on homogeneous gold catalysis. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 647-661.	0.5	81

#	ARTICLE	IF	CITATIONS
7913	Rare earth element doping effect on the bonding and the transport property of $\hat{\Gamma}$ -MoN. Theoretical Chemistry Accounts, 2011, 128, 285-293.	0.5	4
7914	Improved valence basis sets for divalent lanthanide 4f-in-core pseudopotentials. Theoretical Chemistry Accounts, 2011, 129, 367-379.	0.5	9
7915	Geometries, electronic structures, and excited states of UN <sub>2</sub> , NUO <sup>+</sup> , and UO <sub>2</sub> <sup>2+</sup> : a combined CCSD(T), RAS/CASPT2 and TDDFT study. Theoretical Chemistry Accounts, 2011, 129, 467-481.	0.5	39
7916	The geometric, energetic, and electronic properties of charged phosphorus-doped silicon clusters, PSi <sub>n</sub> <sup>+</sup> /PSi <sub>n</sub> <sup>-</sup> (n=8). Theoretical Chemistry Accounts, 2011, 130, 1009-1022.	0.5	7
7917	What is the best density functional to describe water clusters: evaluation of widely used density functionals with various basis sets for (H <sub>2</sub> O) <sub>n</sub> (n=10). Theoretical Chemistry Accounts, 2011, 130, 341-352.	0.5	46
7918	Structural and electronic properties of tungsten trioxides: from cluster to solid surface. Theoretical Chemistry Accounts, 2011, 130, 103-114.	0.5	28
7919	Density functional theory study on quasi-three-dimensional oxidized platinum surface: phase transition between $\hat{\Gamma}$ -PtO <sub>2</sub> -like and $\hat{\Gamma}^2$ -PtO <sub>2</sub> -like structures. Theoretical Chemistry Accounts, 2011, 130, 1031-1038.	0.5	5
7920	High-pressure transitions in bulk mercury: a density functional study. Theoretical Chemistry Accounts, 2011, 130, 455-462.	0.5	12
7921	Biradical processes in reactions between benzyne and tropone. Theoretical Chemistry Accounts, 2011, 130, 981-990.	0.5	10
7922	Ground-state properties of the retinal molecule: from quantum mechanical to classical mechanical computations of retinal proteins. Theoretical Chemistry Accounts, 2011, 130, 1169-1183.	0.5	15
7923	First principles calculation of the elastic constants and phonon modes of UO <sub>2</sub> using GGA + U with orbital occupancy control. Journal of Nuclear Materials, 2011, 412, 301-307.	1.3	31
7924	H <sub>2</sub> O chemisorption and H <sub>2</sub> oxidation on yttria-stabilized zirconia: Density functional theory and temperature-programmed desorption studies. Journal of Power Sources, 2011, 196, 7188-7194.	4.0	25
7925	Structure and magnetic properties of the Al <sub>1-x</sub> Ga <sub>x</sub> FeO <sub>3</sub> family of oxides: A combined experimental and theoretical study. Journal of Solid State Chemistry, 2011, 184, 494-501.	1.4	47
7926	Microstructure investigation and first-principle analysis of die-cast AZ91 alloy with calcium addition. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2011, 528, 5283-5288.	2.6	18
7927	Exploring the interaction between the boron nitride nanotube and biological molecules. Computer Physics Communications, 2011, 182, 39-42.	3.0	45
7928	Intercalation of P atoms in Fullerene-like CP. Chemical Physics Letters, 2011, 501, 400-403.	1.2	43
7929	Applications and validations of the Minnesota density functionals. Chemical Physics Letters, 2011, 502, 1-13.	1.2	662
7930	Fullerene-like CS <sub>x</sub> : A first-principles study of synthetic growth. Chemical Physics Letters, 2011, 506, 86-91.	1.2	46

#	ARTICLE	IF	CITATIONS
7931	Cu-doped ceria: Oxygen vacancy formation made easy. <i>Chemical Physics Letters</i> , 2011, 510, 60-66.	1.2	53
7932	Theoretical study of the influence of Na on CO adsorption and dissociation on Pd(111): Long-range or short-range interactions between co-adsorbates?. <i>Chemical Physics Letters</i> , 2011, 511, 33-38.	1.2	11
7933	Lateral interaction and structures in Cl adlayers on the Ag(111) surface. <i>Chemical Physics</i> , 2011, 383, 35-40.	0.9	6
7934	The electronic structure and reflectivity of PEDOT:PSS from density functional theory. <i>Chemical Physics</i> , 2011, 384, 44-51.	0.9	102
7935	Density functional theory study of $3R\bar{4}$ and $2H\bar{4}$ CuAlO <sub>2</sub> in tensile stress. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2011, 375, 1608-1611.	0.9	12
7936	Experimental and theoretical investigations of benzamide oxime. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 245-253.	2.0	24
7937	Characterization of pentacarbonyl(4-methylpyridine)chromium(0) complex using density functional theory (DFT) and Hartree-Fock (HF) computational methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 1715-1721.	2.0	9
7938	Direct imaging of molecular orbitals of metal phthalocyanines on metal surfaces with an O <sub>2</sub> -functionalized tip of a scanning tunneling microscope. <i>Nano Research</i> , 2011, 4, 523-530.	5.8	27
7939	Ab initio molecular dynamic simulation on the elasticity of Mg <sub>3</sub> Al <sub>2</sub> Si <sub>3</sub> O <sub>12</sub> pyrope. <i>Journal of Earth Science (Wuhan, China)</i> , 2011, 22, 169-175.	1.1	13
7940	First-principles calculations and experimental studies of Sn-Zn alloys as negative electrode materials for lithium-ion batteries. <i>Rare Metals</i> , 2011, 30, 160-165.	3.6	11
7941	Effect of Fe ternary addition on ductility of NiAl intermetallic alloy. <i>Rare Metals</i> , 2011, 30, 316-319.	3.6	4
7942	Theoretical study of NO adsorption on gold surfaces. <i>Science China Chemistry</i> , 2011, 54, 194-199.	4.2	10
7943	A first-principle study of the structural and electronic properties of amorphous Cu-Zr alloys. <i>Science China: Physics, Mechanics and Astronomy</i> , 2011, 54, 249-255.	2.0	10
7944	First-principles study of He point-defects in HCP rare-earth metals. <i>Science China: Physics, Mechanics and Astronomy</i> , 2011, 54, 827-830.	2.0	6
7945	First-principles investigation of the effects of B impurities on the mechanical properties of NiAl intermetallics. <i>Science China: Physics, Mechanics and Astronomy</i> , 2011, 54, 809-814.	2.0	4
7946	Elastic and thermodynamic properties of TiC from first-principles calculations. <i>Science China: Physics, Mechanics and Astronomy</i> , 2011, 54, 2196-2201.	2.0	28
7947	Electronic origin of the anomalous solid solution hardening of Y and Gd in Mg: A first-principles study. <i>Science Bulletin</i> , 2011, 56, 1038-1042.	1.7	20
7948	First-principles calculations of the $\hat{I}^2\hat{a}^2$ -Mg <sub>7</sub> Gd precipitate in Mg-Gd binary alloys. <i>Science Bulletin</i> , 2011, 56, 1142-1146.	1.7	25

#	ARTICLE	IF	CITATIONS
7949	Mechanism and kinetics for methanol synthesis from CO <sub>2</sub> /H <sub>2</sub> over Cu and Cu/oxide surfaces: Recent investigations by first-principles-based simulation. <i>Frontiers of Chemistry in China: Selected Publications From Chinese Universities</i> , 2011, 6, 164-172.	0.4	10
7950	Metal-decorated defective BN nanosheets as hydrogen storage materials. <i>Frontiers of Physics</i> , 2011, 6, 224-230.	2.4	7
7951	First-principles study on adsorption of Au atom on hydroxylated SiO <sub>2</sub> surface. <i>Journal Wuhan University of Technology, Materials Science Edition</i> , 2011, 26, 1184-1188.	0.4	3
7952	Self-Diffusion Coefficient of fcc Mg: First-Principles Calculations and Semi-Empirical Predictions. <i>Journal of Phase Equilibria and Diffusion</i> , 2011, 32, 128-137.	0.5	13
7953	First-principles calculation of structural and thermodynamic properties of titanium boride. <i>Central South University</i> , 2011, 18, 1773-1779.	0.5	28
7954	A one-dimensional extremely covalent material: monatomic carbon linear chain. <i>Nanoscale Research Letters</i> , 2011, 6, 577.	3.1	24
7955	Charge-density distribution in hydrogen methylphosphonates of calcium and lithium. <i>Acta Crystallographica Section B: Structural Science</i> , 2011, 67, 399-408.	1.8	14
7956	First-principles study on the structural, phonon, and thermodynamic properties of the ternary carbides in Ti-Al-C system. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2011, 208, 1879-1884.	0.8	23
7957	Adsorption of Sn on the Ge(111)-√3×√3 surface studied by <i>ab initio</i> density functional theory. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 2142-2146.	0.7	1
7958	Electronic structure, effective masses, mechanical and thermoacoustic properties of cubic HfO <sub>2</sub> under pressure. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 950-955.	0.7	6
7959	Variation of hydrogen adsorption with increasing Li doping on carbon nanotubes. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 1420-1424.	0.7	14
7960	Structural and mechanical properties of dolomite rock under high pressure conditions: A first-principles study. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 1894-1900.	0.7	18
7961	Effect of chirality and curvature of single-walled carbon nanotubes on the adsorption of uracil. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 1431-1436.	0.7	13
7962	Elastic properties and electronic structures of Mg <sub>1-x</sub> Ce <sub>x</sub> intermetallic compounds from first-principles calculations. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 2097-2102.	0.7	7
7963	From electrons to materials. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 2213-2221.	0.7	4
7964	Effects of Y and Zn atoms on the elastic properties of Mg solid solution from first-principles calculations. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 2809-2815.	0.7	12
7965	Advances and applications in the <i>IREBALL</i> <i>ab initio</i> tight-binding molecular dynamics formalism. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 1989-2007.	0.7	207
7966	Structures and Properties Prediction of HMX/TATB Co-Crystal. <i>Propellants, Explosives, Pyrotechnics</i> , 2011, 36, 416-423.	1.0	57



#	ARTICLE	IF	CITATIONS
7967	A computational study of $Ci\Xi_iX$ ( $X = H, C, F, Cl$ ) bond dissociation enthalpies (BDEs) in polyhalogenated methanes and ethanes. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 65-73.	0.9	18
7968	Electron correlation and the stability of substituted alkenes. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 1222-1228.	0.9	5
7969	Density functional study of $Ag_nPd$ and $Ag_nPdH$ clusters. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2428-2435.	1.0	28
7970	Density functional theory study of the structure and energetics of negatively charged oligopyrroles. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2295-2305.	1.0	56
7971	Interaction of the $Mn^{2+}$ , $Co^{2+}$ , $Ni^{2+}$ , and $Zn^{2+}$ with prion protein HGGGW pentapeptide model. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1152-1162.	1.0	8
7972	Advances in local hybrid exchange-correlation functionals: from thermochemistry to magnetic resonance parameters and hyperpolarizabilities. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2625-2638.	1.0	42
7973	On the shape dependence of cluster (hyper)polarizabilities. A combined ab initio and DFT study on large fullerene-like gallium arsenide semiconductor clusters. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 788-796.	1.0	14
7974	The effect of the iterative triple and quadruple cluster amplitudes on the adiabatic potential curve in the coupled cluster calculations of the ground electronic state of the Yb dimer. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 3793-3798.	1.0	8
7975	The effect of ionization and $CH_3$ ligand for hydrogen storage in Co and Ni based organometallic compounds. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 4443-4451.	1.0	4
7976	A DFT/TDDFT study of porphyrazines and phthalocyanine oxo-titanium derivatives as potential dyes in solar cells. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 4186-4196.	1.0	17
7977	Vinyl Chloride Selectivity during Epoxidation on Oxygen Pre-adsorbed Ag(100): A Density-Functional Theory Study. <i>Chinese Journal of Catalysis</i> , 2011, 32, 451-455.	6.9	3
7978	DFT-aided interpretation of the Raman spectra of the polymorphic forms of $Y_2Si_2O_7$ . <i>Journal of Raman Spectroscopy</i> , 2011, 42, 78-85.	1.2	36
7979	A single-crystal Raman and infrared study of the nonlinear optical crystal MBANP. <i>Journal of Raman Spectroscopy</i> , 2011, 42, 1174-1184.	1.2	12
7980	Understanding the Terahertz Spectra of Crystalline Pharmaceuticals: Terahertz Spectroscopy and Solid-State Density Functional Theory Study of (S)-(+)-Ibuprofen and (R)-(-)-Ibuprofen. <i>Journal of Pharmaceutical Sciences</i> , 2011, 100, 1116-1129.	1.6	65
7981	Surface-Modified Low-Temperature Solid Oxide Fuel Cell. <i>Advanced Functional Materials</i> , 2011, 21, 4684-4690.	7.8	67
7982	Fabrication of an anionic polythiophene/layered double hydroxide ultrathin film showing red luminescence and reversible pH photoresponse. <i>AIChE Journal</i> , 2011, 57, 1926-1935.	1.8	16
7983	A tale of two vacancies. <i>Annalen Der Physik</i> , 2011, 523, 129-136.	0.9	8
7984	Spectroscopic, Electrochemical, and DFT Studies of Oxo-Centered Triruthenium Cluster Complexes with a Bis(tridentate) Triazine Ligand. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 2306-2316.	1.0	11



#	ARTICLE	IF	CITATIONS
7985	Li <sub>2</sub> Sr <sub>4</sub> [Si <sub>2</sub> N <sub>5</sub> ]N - A Layered Lithium Nitridosilicate Nitride. European Journal of Inorganic Chemistry, 2011, 2011, 2118-2123.	1.0	8
7986	Zn <sup>II</sup> 2,2',6',2'-terpyridine-Based Complex as Fluorescent Chemosensor for PPI, AMP and ADP. European Journal of Inorganic Chemistry, 2011, 2011, 3050-3058.	1.0	63
7987	A Convenient Road to 1-Chloropentacycloundecanes - A Joint Experimental and Computational Investigation. European Journal of Organic Chemistry, 2011, 2011, 2554-2561.	1.2	12
7988	Optimizing the Electrocatalytic Activity of Surface Confined Co Macrocyclics for the Electrooxidation of Thiocyanate at pH 4. Electroanalysis, 2011, 23, 711-718.	1.5	2
7989	Novel Aspects of the Conduction Mechanisms of Electrolytes Containing Tetrahedral Moieties. Fuel Cells, 2011, 11, 38-43.	1.5	15
7990	Outer Helmholtz Plane of the Electrical Double Layer Formed at the Solid Electrode-Liquid Interface. ChemPhysChem, 2011, 12, 1430-1434.	1.0	85
7991	The Prominent Enhancing Effect of the Cation-Interaction on the Halogen-Hydride Halogen Bond in M <sup>1+</sup> ...C <sub>6</sub> H <sub>5</sub> X...HM <sup>2+</sup> . ChemPhysChem, 2011, 12, 2289-2295.	1.0	41
7992	Electronic Structures and Thermochemical Properties of the Small Silicon-Doped Boron Clusters B <sub>n</sub> Si (=1-7) and Their Anions. ChemPhysChem, 2011, 12, 2948-2958.	1.0	40
7993	Nitrogen-Doped Carbon Nanotubes: Growth, Mechanism and Structure. ChemPhysChem, 2011, 12, 2995-3001.	1.0	26
7994	Electronic Properties of Vanadium-Doped TiO <sub>2</sub> . ChemPhysChem, 2011, 12, 3467-3473.	1.0	25
7995	Copper Seed Layer Deposition by a New Liquid Precursor. Chemical Vapor Deposition, 2011, 17, 65-68.	1.4	5
7996	Structural, electronic, bonding, and elastic properties of NH <sub>3</sub> BH <sub>3</sub> : A density functional study. Journal of Computational Chemistry, 2011, 32, 1734-1742.	1.5	37
7997	Harmonic vibrational frequencies: Scale factors for pure, hybrid, hybrid meta, and double-hybrid functionals in conjunction with correlation consistent basis sets. Journal of Computational Chemistry, 2011, 32, 2339-2347.	1.5	61
7998	Density functional study of neutral and anionic AlO <sub>n</sub> and ScO <sub>n</sub> with high oxygen content. Journal of Computational Chemistry, 2011, 32, 2974-2982.	1.5	21
7999	New insights in quantum chemical topology studies using numerical grid-based analyses. Journal of Computational Chemistry, 2011, 32, 3207-3217.	1.5	47
8000	Density functional theory-based electrochemical models for the oxygen reduction reaction: Comparison of modeling approaches for electric field and solvent effects. Journal of Computational Chemistry, 2011, 32, 3399-3408.	1.5	61
8003	Activation of Oxygen on MgO: O <sub>2</sub> <sup>•-</sup> Radical Ion Formation on Thin, Metal-Supported MgO(001) Films. Angewandte Chemie - International Edition, 2011, 50, 2635-2638.	7.2	101
8004	An Iridium-Stabilized, Formally Uncharged Te <sub>10</sub> Molecule with 3-Center-4-Electron Bonding. Angewandte Chemie - International Edition, 2011, 50, 9987-9990.	7.2	17

#	ARTICLE	IF	CITATIONS
8005	Geometrically Specific Imino Complexes of the $[\text{Re}_6(\mu_3\text{Se})_8]^{2+}$ Core-Containing Clusters. Chemistry - A European Journal, 2011, 17, 580-587.		18
8006	Hierarchical $\text{TiO}_2$ Microspheres: Synergetic Effect of {001} and {101} Facets for Enhanced Photocatalytic Activity. Chemistry - A European Journal, 2011, 17, 15032-15038.	1.7	180
8007	Is Electronegativity a Useful Descriptor for the Pseudo-Alkali Metal $\text{NH}_4$ ?. Chemistry - A European Journal, 2011, 17, 13197-13205.	1.7	16
8008	Novel Au-TiC catalysts for CO oxidation and desulfurization processes. Catalysis Today, 2011, 166, 2-9.	2.2	37
8009	Structure evolution of Pt-3d transition metal alloys under reductive and oxidizing conditions and effect on the CO oxidation: a first-principles study. Catalysis Today, 2011, 165, 89-95.	2.2	33
8010	Adsorption of selenium atoms at the Si(111)-7 $\times$ 7 surface: A combination of scanning tunnelling microscopy and density functional theory studies. Chemical Physics, 2011, 382, 41-46.	0.9	9
8011	An experimental and theoretical examination of the effect of sulfur on the pyrolytically grown carbon nanotubes from sucrose-based solid state precursors. Carbon, 2011, 49, 508-517.	5.4	20
8012	The effect of cluster thickness on the adsorption of $\text{CH}_4$ on Pd. Computational and Theoretical Chemistry, 2011, 963, 236-244.	1.1	14
8013	DFT investigation of CO oxidation over Mg exchanged periodic zeolite models. Computational and Theoretical Chemistry, 2011, 964, 108-115.	1.1	16
8014	Levels of theory modifications and their effects on 1JCH SSCCs calculations: A factorial design analysis. Computational and Theoretical Chemistry, 2011, 964, 116-120.	1.1	6
8015	Density functional study of NO binding on small Ag <sub>n</sub> Pd <sub>m</sub> ( $n+m \leq 25$ ) clusters. Computational and Theoretical Chemistry, 2011, 964, 298-303.	1.1	13
8016	MESP: An efficient method to validate an ONIOM partition for the modelization of phosphine ligands commonly used in the Pauson-Khand reaction. Computational and Theoretical Chemistry, 2011, 965, 231-235.	1.1	0
8017	DFT study on the one-electron reduction of $\text{CF}_3\text{X}$ (X=Cl, Br, I) molecules. Computational and Theoretical Chemistry, 2011, 966, 340-351.	1.1	5
8018	Theoretical investigation of the interaction of oxygen with pure and K-doped NiTi shape memory surface alloys. Computer Physics Communications, 2011, 182, 1979-1983.	3.0	5
8019	Speeding up plane-wave electronic-structure calculations using graphics-processing units. Computer Physics Communications, 2011, 182, 1421-1427.	3.0	48
8020	Energetics and concentration of defects in $\text{Gd}_2\text{Ti}_2\text{O}_7$ and $\text{Gd}_2\text{Zr}_2\text{O}_7$ pyrochlore at high pressure. Acta Materialia, 2011, 59, 1607-1618.	3.8	34
8021	Material transfer mechanisms between aluminum and fluorinated carbon interfaces. Acta Materialia, 2011, 59, 2601-2614.	3.8	49
8022	The equilibrium morphology of WC particles - A combined ab initio and experimental study. Acta Materialia, 2011, 59, 3748-3757.	3.8	52

#	ARTICLE	IF	CITATIONS
8023	First-principles lattice dynamics and heat capacity of BiFeO <sub>3</sub> . <i>Acta Materialia</i> , 2011, 59, 4229-4234.	3.8	55
8024	Structures of CoAl(111) surface: A first principles study. <i>Applied Surface Science</i> , 2011, 257, 3341-3345.	3.1	1
8025	Adsorption and dissociation of O <sub>2</sub> on the Cu <sub>2</sub> O(111) surface: Thermochemistry, reaction barrier. <i>Applied Surface Science</i> , 2011, 257, 4787-4794.	3.1	85
8026	Adsorption of water on TiN (1 0 0), (1 1 0) and (1 1 1) surfaces: A first-principles study. <i>Applied Surface Science</i> , 2011, 257, 6462-6467.	3.1	18
8027	Density functional theory study of selenium adsorption on Fe(110). <i>Applied Surface Science</i> , 2011, 257, 6878-6883.	3.1	5
8028	Density functional theory study of the chemisorption of CO on Ir/MgO(100). <i>Applied Surface Science</i> , 2011, 257, 6986-6990.	3.1	2
8029	Theoretical study of H <sub>2</sub> dissociation on a ZrO <sub>2</sub> cluster. <i>Chemical Physics Letters</i> , 2011, 503, 12-17.	1.2	10
8030	The role of Ru atoms toward the dehydrogenation of ethanol on Ru/ZrO <sub>2</sub> (111) surface. <i>Chemical Physics Letters</i> , 2011, 501, 315-318.	1.2	2
8031	Chemisorbed atomic oxygen inducing Pd segregation in PdAu(1 1 1) alloy: Energetic and electronic DFT analysis. <i>Chemical Physics Letters</i> , 2011, 503, 97-100.	1.2	35
8032	DFT study on the NO oxidation on a flat gold surface model. <i>Chemical Physics Letters</i> , 2011, 503, 129-133.	1.2	17
8033	DFT determination of ammonia adsorption configurations on the Pt{100} (1 $\bar{1}$ -1) surface at low coverage. <i>Chemical Physics Letters</i> , 2011, 505, 21-25.	1.2	5
8034	W4-11: A high-confidence benchmark dataset for computational thermochemistry derived from first-principles W4 data. <i>Chemical Physics Letters</i> , 2011, 510, 165-178.	1.2	353
8035	Structures and energies of iron promoted $\gamma$ -Al <sub>2</sub> O <sub>3</sub> surface: A computational study. <i>Chemical Physics Letters</i> , 2011, 510, 224-227.	1.2	23
8036	Acetate and phosphate anion adsorption linear sweep voltammograms simulated using density functional theory. <i>Electrochimica Acta</i> , 2011, 56, 3996-4006.	2.6	32
8037	Lithium ion diffusion in Li <sub>4+x</sub> Ti <sub>5</sub> O <sub>12</sub> : From ab initio studies. <i>Electrochimica Acta</i> , 2011, 56, 6084-6088.	2.6	46
8038	The extraordinary stability imparted to silver monolayers by chloride. <i>Electrochimica Acta</i> , 2011, 56, 1652-1661.	2.6	17
8039	A model for the electrical double layer combining integral equation techniques with quantum density functional theory. <i>Electrochimica Acta</i> , 2011, 56, 7298-7302.	2.6	10
8040	Electronic structures of LaB <sub>6</sub> and CeB <sub>6</sub> single crystals: X-ray absorption near-edge structure studies at the B K-edge and the La and Ce giant resonance. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2011, 184, 188-191.	0.8	10

#	ARTICLE	IF	CITATIONS
8041	Elasticity, electronic structure, chemical bonding and optical properties of monoclinic ZrO <sub>2</sub> from first-principles. <i>Physica B: Condensed Matter</i> , 2011, 406, 345-350.	1.3	32
8042	Impedance spectroscopy study and ground state electronic properties of In(Mg <sub>1/2</sub> Ti <sub>1/2</sub> )O <sub>3</sub> . <i>Physica B: Condensed Matter</i> , 2011, 406, 1081-1087.	1.3	5
8043	First-principles study of structural, mechanical, electronic and optical properties of 3R- and 2H-CuGaO <sub>2</sub> . <i>Physica B: Condensed Matter</i> , 2011, 406, 3377-3382.	1.3	13
8044	Structural and electronic properties of neutral clusters Ga <sub>12</sub> X (X=C, Si, Ge, Sn, and Pb) and their anions from first principles. <i>Physica B: Condensed Matter</i> , 2011, 406, 3498-3501.	1.3	4
8045	Density functional investigation of structural, electronic and optical properties of Ge-doped ZnO. <i>Physica B: Condensed Matter</i> , 2011, 406, 3926-3930.	1.3	6
8046	Computational insights into interactions between Hg species and $\hat{\pm}$ -Fe <sub>2</sub> O <sub>3</sub> (001). <i>Fuel</i> , 2011, 90, 1840-1846.	3.4	52
8047	Density functional theory studies on a designed photoactive {FeNO} <sub>6</sub> nitrosyl and the corresponding photoinactive {FeNO} <sub>7</sub> species: Insight into the origin of NO photolability. <i>Inorganica Chimica Acta</i> , 2011, 367, 194-198.	1.2	6
8048	Decomposition of lithium magnesium aluminum hydride. <i>International Journal of Hydrogen Energy</i> , 2011, 36, 7602-7611.	3.8	12
8049	First-principles electronic-structure calculations on the stability and oxygen conductivity in Ba <sub>0.5</sub> Sr <sub>0.5</sub> Co <sub>0.8</sub> Fe <sub>0.2</sub> O <sub>3-<math>\delta</math></sub> . <i>Journal of Membrane Science</i> , 2011, 366, 92-96.	4.1	23
8050	Electronic structure of MoO <sub>2</sub> . DFT periodic and cluster model studies. <i>Applied Catalysis A: General</i> , 2011, 391, 137-143.	2.2	30
8051	Structural and electronic properties of atomic oxygen adsorption on Pt(111): A density-functional theory study. <i>Applied Surface Science</i> , 2011, 257, 3047-3054.	3.1	23
8052	Effect of donor (I) or acceptor (N) co-doping on Cr doped (ZnTe) <sub>12</sub> clusters. <i>Journal of Magnetism and Magnetic Materials</i> , 2011, 323, 166-174.	1.0	2
8053	Reactivity of TpMe <sub>2</sub> Ir(C <sub>2</sub> H <sub>4</sub> )(DMAD) with carboxylic acids. A DFT study on geometrical isomers and structural characterization. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 748-757.	0.8	0
8054	Ab initio study of 5d-shells Ir substitution for Fe-based SmOFe <sub>1-x</sub> Ir <sub>x</sub> As. <i>Journal of Physics and Chemistry of Solids</i> , 2011, 72, 329-332.	1.9	0
8055	First-principle study of structural and electronic properties of ternary layered Ta <sub>2</sub> AlC. <i>Journal of Physics and Chemistry of Solids</i> , 2011, 72, 954-956.	1.9	13
8056	Structural, thermodynamic and optical properties of MgF <sub>2</sub> studied from first-principles theory. <i>Journal of Solid State Chemistry</i> , 2011, 184, 343-350.	1.4	75
8057	Structural, optoelectronic, infrared and Raman spectra of orthorhombic SrSnO <sub>3</sub> from DFT calculations. <i>Journal of Solid State Chemistry</i> , 2011, 184, 921-928.	1.4	85
8058	Electronic origins for sulfur interactions with palladium alloys for hydrogen-selective membranes. <i>Journal of Membrane Science</i> , 2011, 375, 96-103.	4.1	24

#	ARTICLE	IF	CITATIONS
8059	The geometric structure and electronic properties of Fe <sub>3</sub> O <sub>3</sub> + clusters. <i>Physica B: Condensed Matter</i> , 2011, 406, 200-204.	1.3	8
8060	Ab initio study of PrAg intermetallic compound. <i>Physica B: Condensed Matter</i> , 2011, 406, 388-392.	1.3	2
8061	Plane-wave pseudopotential study for the structural stability of Hf: The role of spin-orbit interaction. <i>Physica B: Condensed Matter</i> , 2011, 406, 1744-1748.	1.3	16
8062	The structural, elastic and thermodynamic properties of the cotunnite-type phase of Hafnia under high pressure from first-principles calculations. <i>Physica B: Condensed Matter</i> , 2011, 406, 2501-2508.	1.3	3
8063	Aluminum and nitrogen impurities in Wurtzite ZnO: first-principles studies. <i>Physica B: Condensed Matter</i> , 2011, 406, 3125-3129.	1.3	38
8064	Effect of the encapsulation of Li atom on the electronic transport properties of C <sub>20</sub> F <sub>20</sub> cage. <i>Physica B: Condensed Matter</i> , 2011, 406, 3442-3445.	1.3	5
8065	Structural, elastic and electronic properties of a new ternary-layered Ti <sub>2</sub> SiN. <i>Physica B: Condensed Matter</i> , 2011, 406, 3847-3850.	1.3	12
8066	Capturing the spin state diversity of iron(III)-aryl porphyrins: OLYP is better than TPSSh. <i>Journal of Inorganic Biochemistry</i> , 2011, 105, 84-91.	1.5	40
8067	A mesh-free convex approximation scheme for Kohn-Sham density functional theory. <i>Journal of Computational Physics</i> , 2011, 230, 5226-5238.	1.9	27
8068	Enthalpies of sublimation of ferrocene and nickelocene measured by calorimetry and the method of Langmuir. <i>Journal of Chemical Thermodynamics</i> , 2011, 43, 1738-1747.	1.0	20
8069	First approach to studies of sulphur electron DOS in prostate cancer cell lines and tissues studied by XANES. <i>Radiation Physics and Chemistry</i> , 2011, 80, 1104-1108.	1.4	3
8070	Study on the interactions between ginsenosides and lysozyme under acidic condition by ESI-MS and molecular docking. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 78, 676-680.	2.0	8
8071	Synthesis, FTIR, FT-Raman, UV-visible, ab initio and DFT studies on benzohydrazide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 486-496.	2.0	43
8072	Spectroscopic and quantum chemical studies on 4-acryloyl morpholine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 1386-1394.	2.0	7
8073	A combined experimental and theoretical quantum chemical studies on 4-morpholinecarboxaldehyde. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 1395-1401.	2.0	3
8074	Electronic and magnetic properties of metal atom adsorption on SWNT. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2011, 43, 889-892.	1.3	6
8075	Molecular and electronic structures of Mn-doped tris-8-hydroxyquinolate gallium: DFT calculation and experiment. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2011, 43, 1470-1474.	1.3	10
8076	First principles investigation on carbon nanostructures functionalized with borane: An analysis on their hydrogen storage capacity. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2011, 43, 1528-1534.	1.3	9

#	ARTICLE	IF	CITATIONS
8077	Geometries, stabilities, and electronic properties of gold-magnesium (AuMg) bimetallic clusters. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2011, 375, 1877-1882.	0.9	20
8078	Characterization of [Rh(PhCOCHCOCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> )(CO) <sub>2</sub> ] by X-ray crystallography, a computational and a statistical study. <i>Polyhedron</i> , 2011, 30, 660-665.	1.0	10
8079	Relativistic scalar and spin-orbit density functional calculations of the electronic structure, NICS index and ELF function of the [Re <sub>2</sub> (CO) <sub>8</sub> ( $\eta^4$ -BiPh) <sub>2</sub> ] and [Re <sub>2</sub> (CO) <sub>8</sub> ( $\eta^4$ -BiPh <sub>2</sub> ) <sub>2</sub> ] clusters. <i>Polyhedron</i> , 2011, 30, 846-850.	1.0	14
8080	Are closed clusters expected from the (n+1) skeletal electron pairs rule in alanes and gallanes? A DFT structural study of AnHn+2 (A=Al, Ga, and n=4-6). <i>Polyhedron</i> , 2011, 30, 1080-1084.	1.0	6
8081	Further insights into the chemistry of niobium and tantalum pentahalides with 1,2-dialkoxyalkanes: Synthesis of bromo- and iodoalkoxides, spectroscopic and computational studies. <i>Polyhedron</i> , 2011, 30, 1412-1419.	1.0	14
8082	REPRINT OF: Surface electronic structure of Ti-covered W(111) by photofield emission. <i>Ultramicroscopy</i> , 2011, 111, 386-391.	0.8	0
8083	Effect of Mo addition on microstructure and vacuum arc characteristics of CuCr50 alloy. <i>Vacuum</i> , 2011, 85, 943-948.	1.6	50
8084	Bonding character of lithium atoms adsorbed on a graphene layer. <i>Solid State Communications</i> , 2011, 151, 529-531.	0.9	9
8085	Structural, elastic and electronic properties of transition metal carbides TMC (TM=Ti, Zr, Hf and Ta) from first-principles calculations. <i>Solid State Communications</i> , 2011, 151, 602-606.	0.9	92
8086	An ab initio study of the structural, electronic, and thermodynamic properties of Ti <sub>6</sub> Si <sub>2</sub> B and Ti <sub>6</sub> Ge <sub>2</sub> B with Fe <sub>2</sub> P-type structure. <i>Solid State Communications</i> , 2011, 151, 1018-1021.	0.9	8
8087	Electronic and magnetic properties of silicon adsorption on graphene. <i>Solid State Communications</i> , 2011, 151, 1128-1130.	0.9	16
8088	Preferred orientation, phase transition and hardness for sputtered zirconium nitride films grown at different substrate biases. <i>Surface and Coatings Technology</i> , 2011, 205, 2865-2870.	2.2	42
8089	Density functional study of copper segregation in aluminum. <i>Surface Science</i> , 2011, 605, 341-350.	0.8	24
8090	DFT calculations of point defects on UN(001) surface. <i>Surface Science</i> , 2011, 605, 396-400.	0.8	26
8091	High resolution scanning-tunneling-microscopy imaging of individual molecular orbitals by eliminating the effect of surface charge. <i>Surface Science</i> , 2011, 605, 415-418.	0.8	27
8092	Chemisorption on cobalt surfaces: The effect of subsurface rhenium atoms from quantum chemical cluster model calculations. <i>Surface Science</i> , 2011, 605, 513-519.	0.8	3
8093	A theoretical study of CO adsorption on FeCo(100) and the effect of alloying. <i>Surface Science</i> , 2011, 605, 681-688.	0.8	34
8094	Initial steps in methanol steam reforming on PdZn and ZnO surfaces: Density functional theory studies. <i>Surface Science</i> , 2011, 605, 750-759.	0.8	58



#	ARTICLE	IF	CITATIONS
8095	Decomposition of NH <sub>3</sub> on Ir(110): A first-principle study. Surface Science, 2011, 605, 802-807.	0.8	20
8096	Surface reactions of AsH <sub>3</sub> , H <sub>2</sub> Se, and H <sub>2</sub> S on the Zn <sub>2</sub> TiO <sub>4</sub> (010) surface. Surface Science, 2011, 605, 818-823.	0.8	10
8097	Symmetrical transition of an atomic arrangement for 2D Bi films on Rh(111). Surface Science, 2011, 605, 844-847.	0.8	7
8098	Understanding 4-bromostyrene Adsorption on the Si(001)-(1 $\times$ 1)-2 surface: A density functional theory study. Surface Science, 2011, 605, 1056-1061.	0.8	1
8099	DFT study of isocyanate chemisorption on Cu(100). Surface Science, 2011, 605, 1202-1208.	0.8	10
8100	Adsorption of water molecule on (001) and (110) surfaces of MgH <sub>2</sub> . Surface Science, 2011, 605, 1224-1229.	0.8	3
8101	Structural dependence of intermediate species for the hydrogen evolution reaction on single crystal electrodes of Pt. Surface Science, 2011, 605, 1462-1465.	0.8	31
8102	Dissolution, diffusion and permeation behavior of hydrogen in vanadium: a first-principles investigation. Journal of Physics Condensed Matter, 2011, 23, 135501.	0.7	23
8103	Density Functional Theory Investigation on the Dissociation and Adsorption Processes of N <sub>2</sub> on Pd(111) and Pd <sub>3</sub> Ag(111) Surfaces. Japanese Journal of Applied Physics, 2011, 50, 045701.	0.8	4
8104	Electronic Structures and Magnetism of Al/Fe(001) Thin-Film Systems: First-Principles Calculations. Japanese Journal of Applied Physics, 2011, 50, 01BF03.	0.8	0
8105	Using First-principles Models to Advance Development of Metal Membranes for High Temperature Hydrogen Purification. Membrane Science and Technology, 2011, , 309-331.	0.5	1
8106	Ab initio Study of Atomic Hydrogen on ZnO Surfaces. Applied Physics Express, 2011, 4, 125601.	1.1	9
8107	The effect of phonon modes on the D <sub>2</sub> ( $\nu=0, j=0$ ) $\rightarrow$ Cu(111) scattering processes. Physica Scripta, 2011, 84, 028105.	1.2	8
8108	Theoretical Simulation of Deformed Carbon Nanotubes with Adsorbed Metal Atoms: Enhanced Reactivity by Deformation. Japanese Journal of Applied Physics, 2011, 50, 105101.	0.8	1
8109	Atomic-Scale Investigation on the Ti/Fe(001) Interface Structure: Molecular Dynamics Simulations and Ab initio Calculations. Japanese Journal of Applied Physics, 2011, 50, 01BE07.	0.8	1
8110	Mechanism for Lower Resistivity of Niobium-Doped Anatase Titanium Dioxide Obtained in Oxygen-Reduced Atmosphere: Investigation by Generalized Gradient Approximation + U Method. Japanese Journal of Applied Physics, 2011, 50, 041102.	0.8	1
8111	First-principles study of native and extrinsic point defects in cubic boron nitride. Physica Scripta, 2011, 83, 045605.	1.2	3
8112	Reactive force field simulation of proton diffusion in BaZrO <sub>3</sub> using an empirical valence bond approach. Journal of Physics Condensed Matter, 2011, 23, 334213.	0.7	31



#	ARTICLE	IF	CITATIONS
8113	First-principle description of magnonic Pd <sub>n</sub> Fe <sub>m</sub> multilayers. Journal of Applied Physics, 2011, 109, 07C110.	1.1	2
8114	Unexpected relationship between interlayer distances and surface/cleavage energies in $\hat{\Gamma}$ -TiAl: density functional study. Journal of Physics Condensed Matter, 2011, 23, 265009.	0.7	18
8115	Carbon release by selective alloying of transition metal carbides. Journal of Physics Condensed Matter, 2011, 23, 355401.	0.7	15
8116	SO <sub>x</sub> on ceria from adsorbed SO <sub>2</sub> . Journal of Chemical Physics, 2011, 134, 184703.	1.2	32
8117	Six-dimensional quasiclassical and quantum dynamics of H <sub>2</sub> dissociation on the c(2 $\sqrt{3}$ $\times$ 2)-Ti/Al(100) surface. Journal of Chemical Physics, 2011, 134, 114708.	1.2	13
8118	Effects of O in a binary-phase TiAl <sub>3</sub> Al alloy: from site occupancy to interfacial energetics. Journal of Physics Condensed Matter, 2011, 23, 225504.	0.7	22
8119	Communication: The reason why +c ZnO surface is less stable than $\hat{a}$ 'c ZnO surface: First-principles calculation. Journal of Chemical Physics, 2011, 135, 241103.	1.2	6
8120	Equilibrium compositional distribution in freestanding ternary semiconductor quantum dots: The case of In <sub>x</sub> Ga <sub>1-x</sub> As. Journal of Chemical Physics, 2011, 135, 234701.	1.2	5
8121	Structural and zero-point vibrational effects on the electric dipole moments and static dipole polarizabilities of sodium clusters. Physical Review B, 2011, 84, .	1.1	23
8122	Scattered surface charge density: A tool for surface characterization. Physical Review B, 2011, 84, .	1.1	7
8123	First principles potential for the acetylene dimer and refinement by fitting to experiments. Journal of Chemical Physics, 2011, 135, 234306.	1.2	36
8124	Influence of hydrogen impurities on atomic and electronic structure of palladium nanowires and nanocontacts. Physical Review B, 2011, 84, .	1.1	9
8125	Quantum molecular dynamics simulations of transport properties in liquid and dense-plasma plutonium. Physical Review E, 2011, 83, 026404.	0.8	38
8126	Nanodopant-Induced Band Modulation in $\langle \text{AgPb} \rangle_m \langle \text{SbTe} \rangle_n$ Thermoelectrics. Physical Review Letters, 2011, 106, 206601.	2.9	18
8127	Effects of N doping on the electronic properties of a small carbon atomic chain with distinct $\langle s \rangle_p \langle mn \rangle_2$ A first-principles study. Physical Review B, 2011, 84, .	1.1	39
8128	Adsorption and dissociation of NO on Ir(100): A first-principles study. Journal of Chemical Physics, 2011, 135, 204707.	1.2	19
8129	Binding configuration, electronic structure, and magnetic properties of metal phthalocyanines on a Au(111) surface studied with <i>ab initio</i> calculations. Physical Review B, 2011, 84, .	1.1	66
8130	Elastic properties of Ca-based metallic glasses predicted by first-principles simulations. Physical Review B, 2011, 84, .	1.1	21

#	ARTICLE	IF	CITATIONS
8131	A multinuclear solid-state magnetic resonance and GIPAW DFT study of anhydrous calcium chloride and its hydrates. Canadian Journal of Chemistry, 2011, 89, 754-763.	0.6	20
8132	Combined <i>ab initio</i> and classical potential simulation study on silicon carbide precipitation in silicon. Physical Review B, 2011, 84, .	1.1	19
8133	Influence of the electronic structure on tunneling through ferroelectric insulators: Application to BaTiO <sub>3</sub> and PbTiO <sub>3</sub>	1.1	17
8134	Density functional calculations for $\text{La}_2\text{O}_3$	1.1	14
8135	Screening and band structure effects on quasi-one-dimensional transport in periodically modulated graphene. Physical Review B, 2011, 84, .	1.1	5
8136	Strain-induced formation of ultrathin mixed-oxide films. Physical Review B, 2011, 83, .	1.1	34
8137	Anomalous Lattice Dynamics near the Ferroelectric Instability in PbTe. Physical Review Letters, 2011, 107, 175503.	2.9	97
8138	First-principles calculation of current density in molecular devices. Physical Review B, 2011, 84, .	1.1	18
8139	High-resolution core-level spectroscopy study of the ultrathin aluminum oxide film on NiAl(110). Physical Review B, 2011, 83, .	1.1	19
8140	Band structure modulation of ZnSe/ZnTe nanowires under strain. Physical Review B, 2011, 84, .	1.1	9
8141	Effect of carbon/hydrogen species incorporation on electronic structure of anatase-TiO <sub>2</sub> . Journal of Applied Physics, 2011, 110, .	1.1	18
8142	Effective work function of metals interfaced with dielectrics: A first-principles study of the Pt-HfO <sub>2</sub> interface. Physical Review B, 2011, 83, .	1.1	27
8143	Pressure-induced changes in the electronic structure of americium metal. Physical Review B, 2011, 84, .	1.1	22
8144	Density functional study of weak ferromagnetism in a thick BiCrO <sub>3</sub> film. Journal of Applied Physics, 2011, 109, 103905.	1.1	6
8145	Catalytic effect of near-surface alloying on hydrogen interaction on the aluminum surface. Physical Review B, 2011, 83, .	1.1	18
8146	First-principles study of the adsorption of Au atoms and Au <sub>2</sub> and Au <sub>3</sub> clusters on Fe-O/P(111). Physical Review B, 2011, 84, .	1.1	20
8147	Strong spin-orbit effects in small Pt clusters: Geometric structure, magnetic isomers and anisotropy. Journal of Chemical Physics, 2011, 134, 034107.	1.2	79
8148	Intrinsic ambient ferromagnetism in ZnO:Co induced by Eu codoping. Journal of Applied Physics, 2011, 109, 013909.	1.1	25

#	ARTICLE	IF	CITATIONS
8149	Optical response of the sodium alanate system: $\langle \mathbf{G} \rangle$ calculations and thin film measurements. Physical Review B, 2011, 83, .	1.1	20
8150	First-principles study of elastic properties of Cr- and Fe-rich Fe-Cr alloys. Physical Review B, 2011, 84, .	1.1	49
8151	Barium titanate ground- and excited-state properties from first-principles calculations. Physical Review B, 2011, 83, .	1.1	85
8152	First-Principles Calculations, Electrochemical and X-ray Absorption Studies of Li-Ni-PO <sub>4</sub> Surface-Treated Li <sub>2</sub> MnO <sub>3</sub> (1-x)LiMO <sub>2</sub> (M = Mn, Ni, Co) Electrodes for Li-Ion Batteries. Journal of the Electrochemical Society, 2011, 159, A121-A127.	1.3	38
8153	Correlation factors for interstitial-mediated self-diffusion in the diamond lattice: Kinetic lattice Monte Carlo approach. Physical Review B, 2011, 83, .	1.1	5
8154	Atomistic mechanisms of moisture-induced fracture at copper-silica interfaces. Applied Physics Letters, 2011, 99, 133103.	1.5	8
8155	Modulated Na <sub>2</sub> Ti <sub>4</sub> O <sub>9</sub> :Zr Nanobelt via Site-Specific Zr Doping. Applied Physics Express, 2011, 4, 085003.	1.1	3
8156	Mo- and N-doped BiNbO <sub>4</sub> for photocatalysis applications. Applied Physics Letters, 2011, 99, .	1.5	47
8157	Intrinsic defects and krypton impurity atoms in hcp titanium: A first-principles study. Physical Review B, 2011, 83, .	1.1	11
8158	Sodium overlayers on low-index tungsten surfaces: Field and photofield emission currents and surface electronic structures. Physical Review B, 2011, 83, .	1.1	1
8159	First-principles prediction of the thermodynamic stability of xenon in monoclinic, tetragonal, and yttrium-stabilized cubic ZrO <sub>2</sub> . Physical Review B, 2011, 83, .	1.1	14
8160	Two-Site Kondo Effect in Atomic Chains. Physical Review Letters, 2011, 107, 106804.	2.9	58
8161	Effect of pressure on phase stability in Fe-Cr alloys. Physical Review B, 2011, 84, .	1.1	20
8162	First-principles study of the solid solution of hydrogen in lanthanum. Physical Review B, 2011, 84, .	1.1	5
8163	<i>Ab initio</i> study of point defects in the strongly correlated system CoO. Physical Review B, 2011, 84, .	1.1	13
8164	Theoretical analysis of the crystal structure, band-gap energy, polarization, and piezoelectric properties of ZnO-BeO solid solutions. Physical Review B, 2011, 84, .	1.1	22
8165	Energetics and kinetics of the $\langle \mathbf{T} \rangle$ ( $\langle \mathbf{T} \rangle$ ) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 112		

#	ARTICLE	IF	CITATIONS
8167	Blueshifting the Onset of Optical UV Absorption for Water under Pressure. Physical Review Letters, 2011, 106, 187403.	2.9	30
8168	Adsorbate modification of the structural, electronic, and magnetic properties of ferromagnetic fcc{110}surfaces. Physical Review B, 2011, 83, .	1.1	7
8169	Correlation energy functional from jellium surface analysis. Physical Review B, 2011, 84, .	1.1	39
8170	Spectral Functions of Isolated Ce Adatoms on Paramagnetic Surfaces. Physical Review Letters, 2011, 107, 026801.	2.9	10
8171	Superconducting high-pressure phase of platinum hydride from first principles. Physical Review B, 2011, 84, .	1.1	47
8172	Ab initio nuclear momentum distributions in lithium hydride: Assessing nonadiabatic effects. Physical Review B, 2011, 83, .	1.1	31
8173	Defect energetics in SrTiO <sub>3</sub> symmetric tilt grain boundaries. Physical Review B, 2011, 83, .	1.1	58
8174	Water Interaction with native defects on rutile TiO <sub>2</sub> nanowire: Ab initio calculations. Applied Physics Letters, 2011, 98, 083115.	1.5	12
8175	Water Interaction with native defects on rutile TiO <sub>2</sub> nanowire: Ab initio calculations. Applied Physics Letters, 2011, 98, 083115.	1.5	12
8176	Effect of carbon concentration on shear modulus of (W <sub>1/2</sub> Al <sub>1/2</sub> )CZ. Journal of Applied Physics, 2011, 109, 073519.	1.1	1
8177	First principles study on the switching mechanism in Resistance Random Access Memory devices. , 2011, , .		0
8178	Glass-forming ability and atomic-level structure of the ternary Ag-Ni-Zr metallic glasses studied by molecular dynamics simulations. Journal of Applied Physics, 2011, 109, 053505.	1.1	7
8179	FeP(Im) <sup>+</sup> AB bonding energies evaluated with a large number of density functionals (Pâ€‰=â€‰porphine,) Tj ETQq 0 0 0 rgBT /Overloc	0.8	13
8180	Theoretical study of C <sub>60</sub> as catalyst for dehydrogenation in LiBH <sub>4</sub> . Nanotechnology, 2011, 22, 335401.	1.3	24
8181	The Configuration and Evolution of Ti-Si-N Island on TiN (&lt;i>001</i>) Surface: &lt;i>Ab Initio</i> Study. Advanced Materials Research, 0, 295-297, 301-306.	0.3	1
8182	First-Principle Calculation on Lithium Insertion of NiSn <sub>3</sub> Sb <sub>4</sub> Alloy. Advanced Materials Research, 0, 268-270, 881-885.	0.3	0
8183	First-Principles Calculations on Structural, Electronic, and Optical Properties of 2H-CuAlO <sub>2</sub> . Advanced Materials Research, 2011, 197-198, 487-490.	0.3	1
8184	The Effect of Vacancy on the Phase Stability of TiNi Shape Memory Alloy from First-Principle Calculation. Materials Science Forum, 2011, 687, 528-532.	0.3	1

#	ARTICLE	IF	CITATIONS
8185	Ferromagnetism and Electronic Structure in Nitrogen-Doped ZnO Nanowire: First-Principle Calculation. <i>Applied Mechanics and Materials</i> , 2011, 130-134, 1435-1438.	0.2	0
8186	Study on the Electron Excitation for Polychlorinated Dibenzo-P-Dioxins and Several Aromatic Substances by DFT Method. <i>Advanced Materials Research</i> , 2011, 282-283, 17-20.	0.3	0
8187	First-Principles Study on Mechanical Properties of IVB-Group Transition-Metal Nitrides TiN, ZrN, and HfN. <i>Advanced Materials Research</i> , 0, 415-417, 1451-1456.	0.3	1
8188	Ab Initio Structure Characterization for the Amorphous Assembly of Si Clusters Encapsulating Transition Metal. <i>Materials Research Society Symposia Proceedings</i> , 2011, 1321, 307.	0.1	0
8189	First-principles study of electronic properties and stability of Nb <sub>5</sub> SiB <sub>2</sub> (001) surface. <i>Chinese Physics B</i> , 2011, 20, 037101.	0.7	6
8190	First-Principles Study of Structural, Electronic, Elastic, Phonon, and Thermodynamical Properties of the Niobium Carbide. <i>Solid State Phenomena</i> , 0, 171, 67-77.	0.3	14
8191	Amphoteric behavior of Ge in GaAs: an LDA analysis. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2011, 19, 035001.	0.8	4
8192	Crystalline InGaZnO Density of States and Energy Band Structure Calculation Using Density Function Theory. <i>Japanese Journal of Applied Physics</i> , 2011, 50, 091102.	0.8	14
8193	Effects of Mg Addition on Thickness of Galvalume Coating: A First-Principles Study. <i>Advanced Materials Research</i> , 0, 291-294, 125-128.	0.3	1
8194	Ab initio Study of the Hydrogen Molecule on ZnO Surfaces. <i>Materials Research Society Symposia Proceedings</i> , 2011, 1327, 80401.	0.1	0
8195	The Electronic and Magnetic Properties of Chemically Decorated Boron Nitride Sheet. <i>Applied Mechanics and Materials</i> , 2011, 130-134, 1439-1443.	0.2	0
8196	Computational Studies of the NiTi Alloy System: Bulk, Supercell, and Surface Calculations. <i>Materials Research Society Symposia Proceedings</i> , 2011, 1295, 15.	0.1	3
8197	Phase separation and surface segregation in ceria-zirconia solid solutions. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2011, 467, 1925-1938.	1.0	45
8198	Study of Silicon-metal Interaction in Adsorption Process: An Ab-initio Approach. <i>Materials Research Society Symposia Proceedings</i> , 2011, 1305, 1.	0.1	0
8199	Electronic structure of twinned ZnS nanowires. <i>Chinese Physics B</i> , 2011, 20, 067101.	0.7	5
8200	LiNbO <sub>3</sub> ; linear and nonlinear optical response from first-principles calculations. , 2011, , .		0
8201	Cation binding to 15-TBA quadruplex DNA is a multiple-pathway cation-dependent process. <i>Nucleic Acids Research</i> , 2011, 39, 9789-9802.	6.5	64
8202	The geometric, electronic and magnetic properties of (M <sup>n+</sup> ) <sub>6</sub> clusters: a density functional theory study. <i>Molecular Physics</i> , 2011, 109, 1889-1899.	0.8	2

#	ARTICLE	IF	CITATIONS
8203	Theoretical study on the gas and solution phase enthalpies, free energies and equilibrium constants for the isomerisation of [1.1]paracyclophane derivatives as potential molecular switches. <i>Molecular Simulation</i> , 2011, 37, 369-378.	0.9	0
8204	Localised Phonon Modes at LiNbO <sub>3</sub> (0001) Surfaces. <i>Ferroelectrics</i> , 2011, 419, 1-8.	0.3	11
8205	Effect of impurities on structural, cohesive and magnetic properties of grain boundaries in $\hat{1}\pm$ -Fe. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2011, 19, 025001.	0.8	56
8206	Adsorption and Diffusion of Li and Ni on Graphene with Boron Substitution for Hydrogen Storage: Ab-initio Method. <i>Japanese Journal of Applied Physics</i> , 2011, 50, 06GJ02.	0.8	2
8207	Reactive Ability and Bong Strength Analysis on Al(OH) <sub>3</sub> Crystals with Three Different Crystalline. <i>Advanced Materials Research</i> , 0, 396-398, 614-619.	0.3	0
8208	Magnetism and Substrate Effects of Mn Clusters on Cu(111), Pd(111) and Ne(111). <i>Chinese Physics Letters</i> , 2011, 28, 057501.	1.3	2
8209	Ab initio studies on the mechanic and magnetic properties of PdH x. <i>Chinese Physics B</i> , 2011, 20, 026201.	0.7	7
8210	Chemical and topological short-range order evolution of Mg <sub>65</sub> Cu <sub>25</sub> Gd <sub>10</sub> alloy in the process of rapid solidification. <i>Journal of Applied Physics</i> , 2011, 109, 093519.	1.1	9
8211	Effect of Doping on the Thermoelectric Properties of Thallium Tellurides Using First Principles Calculations. <i>Solid State Phenomena</i> , 0, 172-174, 985-989.	0.3	2
8212	Computational Evaluation of Adhesion and Mechanical Properties of Nanolayered Erosion-Resistant Coatings for Gas Turbines. <i>Journal of Engineering for Gas Turbines and Power</i> , 2011, 133, .	0.5	17
8213	Dependence of the electrical properties of defective single-walled carbon nanotubes on the vacancy density. <i>Chinese Physics B</i> , 2011, 20, 087303.	0.7	3
8214	Half metallicity and electronic structures in armchair BCN-hybrid nanoribbons. <i>Journal of Chemical Physics</i> , 2011, 134, 074708.	1.2	17
8215	Electronic structures and thermodynamic stabilities of aluminum-based deuterides from first principles calculations. <i>Chinese Physics B</i> , 2011, 20, 017102.	0.7	2
8216	Cation mixing (Li <sub>0.5</sub> Fe <sub>0.5</sub> ) <sub>2</sub> SO <sub>4</sub> F cathode material for lithium-ion batteries. <i>Chinese Physics B</i> , 2011, 20, 126101.	0.7	9
8217	LOW TEMPERATURE SYNTHESIS AND ELECTRONIC PROPERTIES OF NTC TEMPERATURE SENSOR SPINEL-TYPE OXIDES NANOPOWDERS. <i>International Journal of Nanoscience</i> , 2011, 10, 479-486.	0.4	4
8218	Atomic-scale insight and design principles for turbine engine thermal barrier coatings from theory. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 5480-5487.	3.3	37
8219	First-Principles Calculations of Structural, Elastic and Electronic Properties of Tetragonal HfO <sub>2</sub> under Pressure. <i>Communications in Theoretical Physics</i> , 2011, 56, 779-784.	1.1	7
8220	First Principles Calculations of Defect Formation in In-Free Photovoltaic Semiconductors Cu <sub>2</sub> ZnSnS <sub>4</sub> and Cu <sub>2</sub> ZnSnSe <sub>4</sub> . <i>Japanese Journal of Applied Physics</i> , 2011, 50, 04DP07.	0.8	83



#	ARTICLE	IF	CITATIONS
8221	Controllability of Electrical Conductivity by Oxygen Vacancies and Charge Carrier Trapping at Interface between CoO and Electrodes. Japanese Journal of Applied Physics, 2011, 50, 071101.	0.8	6
8222	PHYSISORPTION TO CHEMISORPTION TRANSFORMATION OF A H <sub>2</sub> MOLECULE ON B-DOPED FULLERENE C <sub>59</sub> B. Journal of Theoretical and Computational Chemistry, 2011, 10, 839-847.	1.8	5
8223	EFFECTS OF SULFUR SUBSTITUTIONAL IMPURITIES ON $\langle \text{font} \rangle \text{ZnO} \langle /font \rangle$ STRUCTURE USING DENSITY FUNCTIONAL THEORY. International Journal of Nanoscience, 2011, 10, 381-390.	0.4	1
8224	FIRST-PRINCIPLES STUDY OF THE ADSORPTION AND DIFFUSION OF O <sub>2</sub> ON A Si(001) SURFACE. Surface Review and Letters, 2011, 18, 315-321.	0.5	2
8225	Size-dependent elastic properties of single-walled ZnO nanotubes: A first-principles study. Journal of Applied Physics, 2011, 109, .	1.1	11
8226	A density functional theory study of the adsorption of uracil on the Au(100) surface. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2011, 467, 1959-1969.	1.0	11
8227	On the formation of hydrogen gas on copper in anoxic water. Journal of Chemical Physics, 2011, 135, 084709.	1.2	24
8228	The mechanical, electronic structure and thermodynamic properties of B <sub>2</sub> -based AgRE studied from first-principles. Physica Scripta, 2011, 83, 045301.	1.2	12
8229	AB INITIO CALCULATIONS OF ELECTRONIC STRUCTURE AND OPTICAL SPECTRA OF (13-0) CARBON NANOTUBE. International Journal of Nanoscience, 2011, 10, 587-590.	0.4	19
8230	Hydrogen Storage on Platinum-Decorated Carbon Nanotubes with Boron, Nitrogen Dopants or Sidewall Vacancies. Journal of Nano Research, 2011, 15, 29-40.	0.8	10
8231	Electric-field effects on magnetic anisotropy in Pd/Fe/Pd(O <sub>2</sub> ) surface. Journal Physics D: Applied Physics, 2011, 44, 064005.	1.3	23
8232	Mechanical and thermal properties of methane clathrate hydrates as an alternative energy resource. Journal of Renewable and Sustainable Energy, 2011, 3, 063110.	0.8	26
8233	Density functional study of the magnetic properties of Bi <sub>4</sub> Mn clusters: Discrepancy between theory and experiment. Journal of Chemical Physics, 2011, 134, 034307.	1.2	0
8234	Triplet states of zigzag edged hexagonal graphene molecules C <sub>6m</sub> * <sub>2</sub> H <sub>6m</sub> (m= 1, 2, 3, $\infty$ ) and carbon based magnetism. Journal of Chemical Physics, 2011, 134, 124706.	1.2	12
8235	Intrinsic stability and hydrogen affinity of pure and bimetallic nanowires. Journal of Chemical Physics, 2011, 134, 174106.	1.2	3
8236	Rare earth chalcogenide Ce <sub>3</sub> Te <sub>4</sub> as high efficiency high temperature thermoelectric material. Applied Physics Letters, 2011, 98, .	1.5	18
8237	The identification of a solvated electron pair in the gaseous clusters of Na <sup>+</sup> (H <sub>2</sub> O) <sub>n</sub> and Li <sup>+</sup> (H <sub>2</sub> O) <sub>n</sub> . Journal of Chemical Physics, 2011, 135, 064309.	1.2	5
8238	Stabilizing the defect-induced dilute magnetic semiconductors: Li-doping in GaN with Ga vacancies. Europhysics Letters, 2011, 93, 57006.	0.7	7



#	ARTICLE	IF	CITATIONS
8239	Response of fcc metals and $\text{L}_{12}$ and $\text{D}_{022}$ -type trialuminides to uniaxial loading along [100] and [001]: ab initio DFT calculations. Philosophical Magazine, 2011, 91, 491-516.	0.7	11
8240	First-Principles Study of Electronic Structure of V-Si-N Nanocomposite Thin Film. Advanced Materials Research, 2012, 476-478, 2374-2378.	0.3	0
8241	Interface Effect on Properties of Fe/BaTiO <sub>3</sub> /Fe Junction. Advanced Materials Research, 0, 465, 244-247.	0.3	0
8242	Effect of Nb Doping on Electronic and Magnetic Properties of Heusler Alloy $\text{Ti}_2\text{NiAl}$ with Hg <sub>2</sub> CuTi-Type Structure. Advanced Materials Research, 2012, 535-537, 1295-1298.	0.3	1
8243	Onset of Coulomb explosion in small silicon clusters exposed to strong-field laser pulses. New Journal of Physics, 2012, 14, 055014.	1.2	11
8244	A comparative density functional study of the high-pressure phases of solid ZnX, CdX, and HgX (X = S, Tl, Pb, Bi, Te, Se, Sn, Ge, Si, C). Tj ETQq1 1 0,784314.rgBT /Over	1.2	16
8245	First-Principles Study on Electronic Structure of Gd-Doped HfO <sub>2</sub> High k Gate Dielectrics. Integrated Ferroelectrics, 2012, 134, 3-9.	0.3	8
8246	Ab Initio Study on the Structural and Magnetic Properties of Co-Pd and Co-Pt Linear and Zigzag Nanowires. Integrated Ferroelectrics, 2012, 136, 132-138.	0.3	1
8247	Activation of Propane C-H and C-C Bonds by Gas-Phase Pt Atom: A Theoretical Study. International Journal of Molecular Sciences, 2012, 13, 9278-9297.	1.8	15
8248	Stability, interaction and influence of domain boundaries in Ge/Si(111)-5 Å–5. Journal of Physics Condensed Matter, 2012, 24, 445003.	0.7	3
8249	Surface structure and phase transition of K adsorption on Au(111): By ab initio atomistic thermodynamics. Journal of Chemical Physics, 2012, 136, 044510.	1.2	7
8251	Non-empirical improvement of PBE and its hybrid PBE0 for general description of molecular properties. Journal of Chemical Physics, 2012, 136, 104108.	1.2	78
8252	Molecular perspective of MoS <sub>2</sub> /Co unsupported catalyst using computer assisted TEM simulations. Materials Research Society Symposia Proceedings, 2012, 1373, 173.	0.1	1
8253	Geometrical Structures and Electronic Properties of Copper-Doped Aluminum Clusters. Chinese Journal of Chemical Physics, 2012, 25, 169-176.	0.6	13
8254	Density Functional Theory and Ab Initio Molecular Dynamics Study of the Effect of Ti and Zr Transition Metals in $\text{D}_{03}$ Fe <sub>3</sub> Al. Materials Science Forum, 0, 706-709, 1095-1099.	0.3	0
8255	A reactive force field for lithium–aluminum silicates with applications to eucryptite phases. Modelling and Simulation in Materials Science and Engineering, 2012, 20, 015002.	0.8	51
8256	Electronic effects on the melting of small gallium clusters. Journal of Chemical Physics, 2012, 137, 144307.	1.2	30
8257	Effect of C doping on the structural and electronic properties of LiFePO <sub>4</sub> : A first-principles investigation. Chinese Physics B, 2012, 21, 097401.	0.7	10

#	ARTICLE	IF	CITATIONS
8258	<i>Ab initio</i> study of H and He migrations in $\hat{f}^2$ -phase Sc, Y, and Er hydrides. Chinese Physics B, 2012, 21, 056601.	0.7	9
8259	First-principles calculation of structural and electronic properties of pyrochlore $\text{Lu}_2\text{Sn}_2\text{O}_7$ . Chinese Physics B, 2012, 21, 027103.	0.7	1
8260	Electronic structures and vibrational properties of coronene on Ru(0001): first-principles study. Chinese Physics B, 2012, 21, 036801.	0.7	4
8261	Anchoring platinum on graphene using metallic adatoms: a first principles investigation. Journal of Physics Condensed Matter, 2012, 24, 225003.	0.7	17
8262	The Role of Na and Mg Doping on the Electronic Conductivity of $\text{LiFePO}_4$ : First-Principles Investigations. Advanced Materials Research, 0, 629, 64-69.	0.3	0
8263	Models of Mixed Metal-Oxide Interfaces for Atomistic Materials Simulations. Materials Research Society Symposia Proceedings, 2012, 1444, 57.	0.1	0
8264	A density functional study of $\text{Cl-C}_4$ alkyl adsorption on Cu(111). Journal of Chemical Physics, 2012, 136, 204710.	1.2	13
8265	Conductance of single-atom magnetic junctions: A first-principles study. Applied Physics Letters, 2012, 101, .	1.5	4
8266	Surface Stabilities of Various Crystal Faces of $\text{CuInSe}_2$ and Related Compounds by First-Principles Calculation. Japanese Journal of Applied Physics, 2012, 51, 10NC22.	0.8	4
8267	First-principles study on the incipient oxidization of Nb(110). Journal of Physics Condensed Matter, 2012, 24, 225005.	0.7	5
8268	Long-range correlation energies from frequency-dependent weighted exchange-hole dipole polarisabilities. Journal of Chemical Physics, 2012, 136, 014104.	1.2	15
8269	Probing the structural and electronic properties of $\text{Ag}_n\text{H}^+$ ( $n = 1-3$ ) using photoelectron imaging and theoretical calculations. Journal of Chemical Physics, 2012, 136, 184312.	1.2	11
8270	Infrared absorption of trans-1-chloromethylallyl and trans-1-methylallyl radicals produced in photochemical reactions of trans-1,3-butadiene and $\text{C}_2$ in solid para-hydrogen. Journal of Chemical Physics, 2012, 137, 084310.	1.2	21
8271	Organic salts as super-high rate capability materials for lithium-ion batteries. Applied Physics Letters, 2012, 100, .	1.5	33
8272	The origin of the conductivity maximum in molten salts. I. Bismuth chloride. Journal of Chemical Physics, 2012, 136, 124504.	1.2	16
8273	Communication: Effect of the orbital-overlap dependence in the meta generalized gradient approximation. Journal of Chemical Physics, 2012, 137, 051101.	1.2	122
8274	Vibrational deexcitation and rotational excitation of $\text{H}_2$ and $\text{D}_2$ scattered from Cu(111): Adiabatic versus non-adiabatic dynamics. Journal of Chemical Physics, 2012, 137, 064707.	1.2	40
8275	Validation of the reaction thermodynamics associated with $\text{NaSc}(\text{BH}_4)_4$ from first-principles calculations: Detecting metastable paths and identifying the minimum free energy path. Journal of Chemical Physics, 2012, 137, 084111.	1.2	4

#	ARTICLE	IF	CITATIONS
8276	Uranyl ion interaction at the water/NiO(100) interface: A predictive investigation by first-principles molecular dynamic simulations. Journal of Chemical Physics, 2012, 137, 164701.	1.2	7
8277	Plasmon resonances in linear noble-metal chains. Journal of Chemical Physics, 2012, 137, 194307.	1.2	35
8278	Potential energy surface of H2O on Al{111} and Rh{111} from theoretical methods. Journal of Chemical Physics, 2012, 137, 204702.	1.2	11
8279	Structural and optoelectronic properties, and infrared spectrum of cubic BaSnO3 from first principles calculations. Journal of Applied Physics, 2012, 112, .	1.1	54
8280	First-principles Study of Geometric and Electronic Structures of Si(111)- $\sqrt{3}\times\sqrt{3}$ -In Surface Reconstruction. Chinese Journal of Chemical Physics, 2012, 25, 403-408.	0.6	8
8281	Heredity of medium-range order structure from melts to amorphous solids. Journal of Applied Physics, 2012, 112, .	1.1	17
8282	Hydrogen induced stabilization of meta-stable Mg-Ti. Applied Physics Letters, 2012, 100, 111902.	1.5	7
8283	Spin densities from subsystem density-functional theory: Assessment and application to a photosynthetic reaction center complex model. Journal of Chemical Physics, 2012, 136, 194104.	1.2	35
8284	Magnetizability tensors from auxiliary density functional theory. Journal of Chemical Physics, 2012, 137, 094113.	1.2	11
8285	Infrared spectroscopy of copper-resveratrol complexes: A joint experimental and theoretical study. Journal of Chemical Physics, 2012, 137, 024307.	1.2	46
8286	Effects of biaxial strains on the magnetic properties of Co-graphene heterojunctions. Journal of Applied Physics, 2012, 111, .	1.1	3
8287	Defect and solute properties in dilute Fe-Cr-Ni austenitic alloys from first principles. Physical Review B, 2012, 85, .	1.1	61
8288	Tuning the adatom-surface and interadatom interactions in hydrogenated graphene by charge doping. Physical Review B, 2012, 86, .	1.1	20
8289	Stabilization and growth of non-native nanocrystals at low and atmospheric pressures. Journal of Chemical Physics, 2012, 136, 044703.	1.2	11
8290	Interplay of localized and itinerant character of Ru ions: $Tl_{2-x}Ru_xO_7$	1.1	5
8291	Energy-resolved spin-polarized tunneling and exchange coupling of Co and Cr atoms on Fe islands on W(110). Physical Review B, 2012, 85, .	1.1	10
8292	Hydrogen-induced disruption of the ZnO(0001) polar surface. Physical Review B, 2012, 86, .	1.1	12
8293	Anharmonic phonons of NaZr $_{2-x}$ (PO) $_2$ (0 < x < 1). Physical Review B, 2012, 86, .	1.1	43

#	ARTICLE	IF	CITATIONS
8294	Critical reinvestigation of vibronic couplings in picene from view of vibronic coupling density analysis. <i>Physical Review B</i> , 2012, 85, .	1.1	6
8295	Joint density functional theory of the electrode-electrolyte interface: Application to fixed electrode potentials, interfacial capacitances, and potentials of zero charge. <i>Physical Review B</i> , 2012, 86, .	1.1	257
8296	Formation of NaCl-Type Monodeuteride LaD by the Disproportionation Reaction of $\text{LaD}_2$ . <i>Physical Review Letters</i> , 2012, 108, 205501.	2.9	24
8297	Large organic molecule chemisorption on the SiC(0001) surface. <i>Physical Review B</i> , 2012, 85, .	1.1	18
8298	Theoretical study of the temperature dependence of the magnon dispersion relation in transition-metal wires and monolayers. <i>Physical Review B</i> , 2012, 86, .	1.1	7
8299	Energetics and approximate quasiparticle electronic structure of low-index surfaces of SnO <sub>2</sub> . <i>Physical Review B</i> , 2012, 86, .	1.1	31
8300	The electronic and optical properties of Eu/Si-codoped anatase TiO <sub>2</sub> photocatalyst. <i>Applied Physics Letters</i> , 2012, 100, 102105.	1.5	16
8301	Band bending and surface defects in $\text{In}^2\text{-Ga}_2\text{O}_3$ . <i>Applied Physics Letters</i> , 2012, 100, .	1.5	82
8302	LiB and its boron-deficient variants under pressure. <i>Physical Review B</i> , 2012, 86, .	1.1	23
8303	Control of graphene nanoribbon vacancies by Fe and N dopants: Implications for catalysis. <i>Applied Physics Letters</i> , 2012, 101, 064102.	1.5	37
8304	Theory of orthogonal interactions of CO molecules on a one-dimensional substrate. <i>Physical Review B</i> , 2012, 85, .	1.1	6
8305	Quantum Monte Carlo study of small aluminum clusters Al <sub>n</sub> . <i>Physical Review B</i> , 2012, 85, .	1.1	44
8306	Tuning the catalytic property of nitrogen-doped graphene for cathode oxygen reduction reaction. <i>Physical Review B</i> , 2012, 85, .	1.1	81
8307	Antiferromagnetism in Cr <sub>3</sub> Al and relation to semiconducting behavior. <i>Physical Review B</i> , 2012, 85, .	1.1	31
8308	Electronic and vibrational properties of vanadium-carbide nanowires. <i>Journal of Applied Physics</i> , 2012, 112, .	1.1	3
8309	Unraveling the polar state in TMITF <sub>2</sub> -PF <sub>6</sub> organic crystals. <i>Physical Review B</i> , 2012, 85, .	1.1	13
8310	Tunable UV Absorption and Mobility of Yttrium-Doped ZnO using First-Principles Calculations. <i>Chinese Physics Letters</i> , 2012, 29, 117101.	1.3	9
8311	Competition between Electron and Phonon Excitations in the Scattering of Nitrogen Atoms and Molecules off Tungsten and Silver Metal Surfaces. <i>Physical Review Letters</i> , 2012, 108, 096101.	2.9	79

#	ARTICLE	IF	CITATIONS
8312	Adsorbate-induced segregation: First-principles study for C/Pt25Rh75(100). Physical Review B, 2012, 86, . Surface properties of the clean and Au/Pd covered Fe	1.1	10
8313	xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>O<mml:math /><mml:mn>4</mml:mn></mml:msub></mml:math>(111): DFT and DFT+ xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>U</mml:mi></mml:math>	1.1	68
8314	Electronic and optical properties of free-standing and supported vanadium nanowires. Journal of Applied Physics, 2012, 111, 093506.	1.1	8
8315	Polarization of poly(vinylidene fluoride) and poly(vinylidene fluoride-trifluoroethylene) thin films revealed by emission spectroscopy with computational simulation during phase transition. Journal of Applied Physics, 2012, 111, .	1.1	32
8316	Role of heteroepitaxial misfit strains on the band offsets of Zn1 $\hat{x}$ BexO/ZnO quantum wells: A first-principles analysis. Journal of Applied Physics, 2012, 111, 113714.	1.1	16
8317	Structure, electronic, and CV properties of hydroxy-naphthaldehyde Schiff-base copper(II) complexes derived from alkyl amines: X-ray structure of bis(n-i-propyl-3-hydroxy-2-naphthaldiminato)copper(II). Journal of Coordination Chemistry, 2012, 65, 3752-3765.	0.8	3
8318	Nanoscale thermal stabilization via permutational premelting. Physical Review B, 2012, 85, .	1.1	11
8319	Epitaxial growth mechanisms of graphene and effects of substrates. Physical Review B, 2012, 85, .	1.1	39
8320	Polarization-dependent methanol adsorption on lithium niobate Z-cut surfaces. Physical Review B, 2012, 86, .	1.1	19
8321	Structure of nanoscale copper precipitates in neutron-irradiated Fe-Cu-C alloys. Physical Review B, 2012, 85, .	1.1	17
8322	Chemical ordering in Cr3Al and relation to semiconducting behavior. Physical Review B, 2012, 86, .	1.1	6
8323	<i>Ab initio</i> atomistic thermodynamics study of the early stages of Cu(100) oxidation. Physical Review B, 2012, 86, .	1.1	42
8324	Theoretical study on the effects of nitrogen and methyl substitution on tris-(8-hydroxyquinoline) aluminum: An efficient exciton blocking layer for organic photovoltaic cells. Journal of Chemical Physics, 2012, 137, 034704.	1.2	8
8325	STABILITIES AND FRAGMENTATION BEHAVIORS OF Ag <sub>n</sub> CLUSTERS (n = 2 $\hat{e}$ 34). Journal of Theoretical and Computational Chemistry, 2012, 11, 953-964.	1.8	8
8326	H <sub>2</sub> ADSORPTION ON LiB (001) SURFACE: A FIRST PRINCIPLES CALCULATION. Journal of Theoretical and Computational Chemistry, 2012, 11, 781-790.	1.8	3
8327	Pressure dependence of the optical properties of $\hat{f}_1\pm, \hat{f}_2$ and $\hat{f}_0$ phases of titanium. Physica Scripta, 2012, 86, 055602.	1.2	2
8328	A first-principles study of the magnetic properties in boron-doped ZnO. Chinese Physics B, 2012, 21, 047504.	0.7	12
8329	THE ELECTRONIC CORRELATION EFFECT FROM WEAK TO STRONG IN THE THREE DIMENSIONAL ELECTRON GAS. International Journal of Modern Physics B, 2012, 26, 1250065.	1.0	2

#	ARTICLE	IF	CITATIONS
8330	Low-lying planar isomers of neutral and charged B <sub>22</sub> clusters. Journal of Physics B: Atomic, Molecular and Optical Physics, 2012, 45, 225101.	0.6	17
8331	<i>Ab initio</i> kinetic Monte Carlo model of ionic conduction in bulk yttria-stabilized zirconia. Modelling and Simulation in Materials Science and Engineering, 2012, 20, 065006.	0.8	12
8332	Predictions of Surface Electrochemistry of Saturated and Alkaline NH <sub>4</sub> Cl Solutions Interacting with Fe(110) from Ab Initio Calculations. Corrosion, 2012, 68, 591-599.	0.5	19
8333	Surface properties of clean and Au or Pd covered hematite (Î±-Fe <sub>2</sub> O <sub>3</sub> ) (0001). Journal of Physics Condensed Matter, 2012, 24, 095003.	0.7	50
8334	The thickness, electric field, and strain effects on the magnetic anisotropy of FeCo/MgO(001) thin films: A first principles study. Journal of Applied Physics, 2012, 111, 07C109.	1.1	25
8335	Study on electronic structure and optical properties of the filled skutterudite CeFe <sub>4</sub> P <sub>12</sub> . , 2012, , .		0
8336	First-Principles Investigation of the Luminescence Mechanism of Eu <sup>2+</sup> in M <sub>2</sub> SiO <sub>4</sub> :Eu <sup>2+</sup> (M = Ba, Sr). ECS Journal of Solid State Science and Technology, 2012, 1, R87-R91.	0.9	17
8337	First-Principles Study on the Ideal Strengths of Typical Hcp Metals. Advanced Materials Research, 2012, 476-478, 2523-2529.	0.3	5
8338	Hydrogen Chemisorption on Co(0001) Surface: A DFT Study. Advanced Materials Research, 2012, 571, 48-55.	0.3	0
8339	Polymorphism, Hydrogen Bond Properties, and Vibrational Structure of 1H-Pyrrolo[3,2-h]Quinoline Dimers. Journal of Atomic, Molecular, and Optical Physics, 2012, 2012, 1-11.	0.5	3
8340	LDA and GGA Investigations of Some Ground-State Properties and the Compton Profile of Copper with the All-Electron MAPW Method. ISRN Materials Science, 2012, 2012, 1-13.	1.0	2
8341	Differential adsorption of complex organic molecule isomers on interstellar ice surfaces. EAS Publications Series, 2012, 58, 349-352.	0.3	0
8342	The effects of Na on high pressure phases of CuIn <sub>0.5</sub> Ga <sub>0.5</sub> Se <sub>2</sub> from <i>ab initio</i> calculation. Journal of Physics Condensed Matter, 2012, 24, 095802.	0.7	6
8343	Dynamical reaction pathways in Eley-Rideal recombination of nitrogen from W(100). Journal of Chemical Physics, 2012, 137, 064709.	1.2	24
8344	First-principles study of the electronic and optical properties of the (Y, N)-codoped anatase TiO <sub>2</sub> photocatalyst. Chinese Physics B, 2012, 21, 033103.	0.7	14
8345	Electronic and Spin Structure of Metal Phthalocyanines. Solid State Phenomena, 2012, 190, 141-144.	0.3	4
8346	First-Principles Study of Hydrogen Impact on the Formation and Migration of Helium Interstitial Defects in <i>hcp</i> Titanium. Chinese Physics Letters, 2012, 29, 013102.	1.3	6
8347	First Principle Study of Dynamical Properties of a New Perovskite Material Based on GeTiO <sub>3</sub> . Advanced Materials Research, 2012, 501, 352-356.	0.3	8



#	ARTICLE	IF	CITATIONS
8348	Scanning Tunneling Microscopy and ab initio Studies of Precursor States of Ga-Induced Cluster on Si(001) Surface. <i>Hyomen Kagaku</i> , 2012, 33, 467-472.	0.0	0
8349	Prediction of glass-forming ability and characterization of atomic structure of the Co-Ni-Zr metallic glasses by a proposed long range empirical potential. <i>Journal of Applied Physics</i> , 2012, 111, 033521.	1.1	4
8350	Direct observation of the cleavage plane of sapphire by in-situ indentation TEM. <i>Journal of the Ceramic Society of Japan</i> , 2012, 120, 473-477.	0.5	8
8351	Segregation of Alkali and Alkaline Earth Metals at $\sigma_{11}(113)[110]$ Grain Boundary in Aluminum from First-Principles Calculations. <i>Materials Transactions</i> , 2012, 53, 1699-1705.	0.4	16
8352	First-principles calculation of grain boundary excess volume and free volume in nanocrystalline and ultrafine-grained aluminum. <i>Keikinzoku/Journal of Japan Institute of Light Metals</i> , 2012, 62, 464-471.	0.1	2
8353	New Growth Mechanism of Cubic Rh Clusters Composed of 8–12 Atoms Found by the Method of Euclidean Designs. <i>Materials Transactions</i> , 2012, 53, 459-462.	0.4	3
8354	Hybrid Functional Study of the Structural and Electronic Properties of Co and Ni. <i>Journal of the Physical Society of Japan</i> , 2012, 81, 114715.	0.7	16
8355	Ferromagnetism and Orbital Order in a Topological Ferroelectric. <i>Physical Review Letters</i> , 2012, 109, 217202.	2.9	21
8356	Role of correlation and relativistic effects in MAX phases. <i>Journal of Materials Science</i> , 2012, 47, 7615-7620.	1.7	16
8357	Changes in a nanoparticle's spectroscopic signal mediated by the local environment. <i>Nanotechnology</i> , 2012, 23, 485202.	1.3	3
8358	Making C–C Bonds with Gold: Identification of Selective Gold Sites for Homo- and Cross-Coupling Reactions between Iodobenzene and Alkynes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 24855-24867.	1.5	65
8359	Phonons in lanthanum manganite: Inelastic neutron scattering and density functional theory studies. <i>Physical Review B</i> , 2012, 86, .	1.1	2
8360	Selectivity of Palladium–Cobalt Surface Alloy toward Oxygen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2012, 116, 6200-6207.	1.5	24
8361	<i>Ab initio</i> investigation of graphene-based one-dimensional superlattices and their interfaces. <i>Physical Review B</i> , 2012, 86, .	1.1	13
8362	Properties of atoms under pressure: Bonded interactions of the atoms in three perovskites. <i>Journal of Chemical Physics</i> , 2012, 137, 164313.	1.2	12
8363	Mechanism of Morphology Transformation of Tetragonal Phase $\text{LaVO}_4$ Nanocrystals Controlled by Surface Chemistry: Experimental and Theoretical Insights. <i>Crystal Growth and Design</i> , 2012, 12, 5042-5050.	1.4	22
8364	Discoloration of the smalt pigment: experimental studies and ab initio calculations. <i>Journal of Analytical Atomic Spectrometry</i> , 2012, 27, 1941.	1.6	21
8365	Transferable Potentials for Phase Equilibria—United Atom Description of Five- and Six-Membered Cyclic Alkanes and Ethers. <i>Journal of Physical Chemistry B</i> , 2012, 116, 11234-11246.	1.2	106



#	ARTICLE	IF	CITATIONS
8366	Effects of surface chemistry on the morphology transformation of ZnWO <sub>4</sub> nanocrystals: investigated from experiment and theoretical calculations. CrystEngComm, 2012, 14, 920-928.	1.3	14
8367	Detailed QM/MM study of the Electron Paramagnetic Resonance Parameters of Nitrosyl Myoglobin. Journal of Chemical Theory and Computation, 2012, 8, 563-574.	2.3	23
8368	Complex Surface Chemistry of 4-Mercaptopyridine Self-Assembled Monolayers on Au(111). Langmuir, 2012, 28, 6839-6847.	1.6	45
8369	Syntheses, Thermal Reactivities, and Computational Studies of Aryl-Fused Quinoxalenediynes: Effect of Extended Benzannelation on Bergman Cyclization Energetics. Journal of Organic Chemistry, 2012, 77, 10329-10339.	1.7	23
8370	Computational Insights on the Isomerization of Photochromic Oxazines. Journal of Physical Chemistry A, 2012, 116, 11888-11895.	1.1	19
8371	Gas-Induced Formation of Cu Nanoparticle as Catalyst for High-Purity Straight and Helical Carbon Nanofibers. ACS Nano, 2012, 6, 8611-8619.	7.3	50
8372	Lattice electrical resistivity of magnetic bcc iron from first-principles calculations. Physical Review B, 2012, 85, .	1.1	42
8373	van der Waals Interaction Energies of Small Fragments of P, As, Sb, S, Se, and Te: Comparison of Complete Basis Set Limit CCSD(T) and DFT with Approximate Dispersion. Journal of Chemical Theory and Computation, 2012, 8, 2301-2309.	2.3	6
8374	Interaction between graphene and the surface of SiO <sub>2</sub> . Journal of Physics Condensed Matter, 2012, 24, 305004.	0.7	69
8375	Molecular dynamics study of Co-Au and Ag-Au bimetallic atomic chain formation. European Physical Journal B, 2012, 85, 1.	0.6	19
8376	Environment-dependent surface structures and stabilities of SnO <sub>2</sub> from the first principles. Journal of Applied Physics, 2012, 111, .	1.1	32
8377	Catalytic Oxygen Activation on Helical Gold Nanowires. Journal of Physical Chemistry C, 2012, 116, 11189-11194.	1.5	13
8378	Atomic Hydrogen Activated TiO <sub>2</sub> Nanocluster: DFT Calculations. Journal of Physical Chemistry C, 2012, 116, 18139-18145.	1.5	25
8379	Bromination of Double-Walled Carbon Nanotubes. Chemistry of Materials, 2012, 24, 2708-2715.	3.2	76
8380	DFT investigation of molybdenum (oxo)carbide formation from MoO <sub>3</sub> . Structural Chemistry, 2012, 23, 1417-1424.	1.0	8
8381	High-pressure temperature phase diagram and the equation of state of beryllium. Physical Review B, 2012, 86, .	1.1	36
8382	Carbon-supported Pd-Co as cathode catalyst for APPEMFCs and validation by DFT. Physical Chemistry Chemical Physics, 2012, 14, 9683.	1.3	45
8383	Interaction of the Gold(I) Cation Au(PMe <sub>3</sub> ) <sub>3</sub> <sup>+</sup> with Unsaturated Hydrocarbons. Organometallics, 2012, 31, 1935-1942.	1.1	49

#	ARTICLE	IF	CITATIONS
8384	An alternative approach: a highly selective dual responding fluoride sensor having active methylene group as binding site. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 2263.	1.5	20
8385	Models for incomplete nucleophilic attack on a protonated carbonyl group and electron-deficient alkenes: salts and zwitterions from 1-dimethylamino-naphthalene-8-carbaldehyde. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 7763.	1.5	11
8386	Energetic Driving Force of H Spillover between Rhodium and Titania Surfaces: A DFT View. <i>Journal of Physical Chemistry C</i> , 2012, 116, 25362-25367.	1.5	18
8387	A new insight into the initial step in the Fischer-Tropsch synthesis: CO dissociation on Ru surfaces. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 16686.	1.3	28
8388	Formation of twins in sapphire under shock wave loading: Atomistic simulations. <i>Journal of Applied Physics</i> , 2012, 111, .	1.1	16
8389	Analysis of structural and electronic properties of Pr <sub>2</sub> NiO <sub>4</sub> through first-principles calculations. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 405504.	0.7	13
8390	Linear and nonlinear optical response of LiNbO <sub>3</sub> calculated from first principles. <i>IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control</i> , 2012, 59, 1929-1933.	1.7	9
8391	Metavanadate at the Active Site of the Phosphatase VHZ. <i>Journal of the American Chemical Society</i> , 2012, 134, 14298-14301.	6.6	9
8392	Density functional theory embedding for correlated wavefunctions: Improved methods for open-shell systems and transition metal complexes. <i>Journal of Chemical Physics</i> , 2012, 137, 224113.	1.2	104
8393	Ligand Bond Energies in <i>cis</i> - and <i>trans</i> -[L-Pd(PH <sub>3</sub> ) <sub>3</sub> Cl] <sup>2+</sup> Complexes from Coupled Cluster Theory (CCSD(T)) and Density Functional Theory. <i>Inorganic Chemistry</i> , 2012, 51, 13195-13203.	1.9	17
8394	DFVB: A Density-Functional-Based Valence Bond Method. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1608-1615.	2.3	38
8395	Adsorption studies of C <sub>6</sub> H <sub>6</sub> on Cu (111), Ag (111), and Au (111) within dispersion corrected density functional theory. <i>Journal of Chemical Physics</i> , 2012, 137, 134703.	1.2	40
8396	Generalization of Natural Bond Orbital Analysis to Periodic Systems: Applications to Solids and Surfaces via Plane-Wave Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1902-1911.	2.3	177
8397	Chemical and optical properties of carbon-doped TiO <sub>2</sub> : A density-functional study. <i>Applied Physics Letters</i> , 2012, 100, 102114.	1.5	54
8399	C-[o-(p-Tolyl)sulfinyl]phenylnitrones. Synthesis and Reactivity in [3+2] Dipolar Cycloadditions. <i>Heterocycles</i> , 2012, 84, 913.	0.4	3
8400	Ferric Complexes of 3-Hydroxy-4-pyridinones Characterized by Density Functional Theory and Raman and UV-vis Spectroscopies. <i>Inorganic Chemistry</i> , 2012, 51, 4473-4481.	1.9	23
8401	Theoretical Study of Near-Edge X-ray Absorption Fine Structure Spectra of Metal Phthalocyanines at C and N K-Edges. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2885-2894.	1.1	38
8402	First-Principles Calculations on Structure, Elastic and Thermodynamic Properties of Al <sub>2</sub> X (X=Sc, Y) under Pressure. <i>Journal of Materials Science and Technology</i> , 2012, 28, 155-163.	5.6	28

#	ARTICLE	IF	CITATIONS
8403	Quantum-chemical calculations of NMR chemical shifts of organic molecules: VI. Accuracy of DFT calculations of <sup>29</sup> Si chemical shifts of four-coordinate silicon compounds. Russian Journal of Organic Chemistry, 2012, 48, 1518-1525.	0.3	9
8404	First Principles Study toward CO Adsorption on Au/Ni Surface Alloys. ChemPhysChem, 2012, 13, 3909-3915.	1.0	10
8405	The Interaction of Noble Metal With La <sub>1-x</sub> Sr <sub>x</sub> MnO <sub>3</sub> (001) Surface and Catalytic Role for Oxygen Adsorption: A Density Functional Theory Study. Fuel Cells, 2012, 12, 1048-1055.	1.5	0
8406	Elastic constants of La, LaH <sub>2</sub> , and LaH <sub>3</sub> . Monatshefte für Chemie, 2012, 143, 1325-1328.	0.9	4
8407	Equilibrium geometries, stabilities, and electronic properties of the cationic Au <sub>n</sub> Be <sup>+</sup> (n=1-8) clusters: comparison with pure gold clusters. Journal of Molecular Modeling, 2012, 18, 3553-3562.	0.8	12
8408	Architectures, electronic structures, and stabilities of Cu-doped Ge <sub>n</sub> clusters: density functional modeling. Journal of Molecular Modeling, 2012, 18, 3887-3902.	0.8	47
8409	Tuning electronic structure and photophysical properties of [Ir(ppy) <sub>2</sub> (py) <sub>2</sub> ] <sup>+</sup> by substituents binding in pyridyl ligand: a computational study. Journal of Molecular Modeling, 2012, 18, 4615-4624.	0.8	3
8410	Vacancy-Driven Surface Segregation in Ni <sub>x</sub> Mg <sub>1-x</sub> O(100) Solid Solutions from First Principles Calculations. Catalysis Letters, 2012, 142, 1211-1217.	1.4	11
8411	Polarization, piezoelectric properties, and elastic coefficients of In <sub>x</sub> Ga <sub>1-x</sub> N solid solutions from first principles. Journal of Materials Science, 2012, 47, 7587-7593.	1.7	7
8412	Emergence of Magnetism in Doped Two-Dimensional Honeycomb Structures of III-V Binary Compounds. Journal of Superconductivity and Novel Magnetism, 2012, 25, 2533-2537.	0.8	12
8413	Oxygen- and nitrogen-chemisorbed carbon nanostructures for Z-scheme photocatalysis applications. Journal of Nanoparticle Research, 2012, 14, 1.	0.8	8
8414	First principles-based adsorption comparison of group IV elements (C, Si, Ge, and Sn) on Au(111)/Ag(111) surface. Journal of Nanoparticle Research, 2012, 14, 1.	0.8	1
8415	Double layers of H <sub>2</sub> adsorption on an AlN sheet induced by electric field. Journal of Nanoparticle Research, 2012, 14, 1.	0.8	1
8416	New insight into the CO formation mechanism during formic acid oxidation on Pt(111). Catalysis Communications, 2012, 29, 82-86.	1.6	33
8417	Adsorbate-induced segregation in a PdAg membrane model system: Pd <sub>3</sub> Ag(111). Catalysis Today, 2012, 193, 111-119.	2.2	42
8418	Role of passivated Na <sup>+</sup> F <sup>-</sup> pairs in enhancing photoactivity of ZnWO <sub>4</sub> (010) surface: Emphasis on correlation between codoping forms and compensation mechanisms. Chemical Engineering Journal, 2012, 211-212, 168-178.	6.6	9
8419	Structural determination of stable MoO <sub>x</sub> monolayers on O/Cu <sub>3</sub> Au(100): DFT calculations. Chemical Physics, 2012, 406, 47-49.	0.9	1
8420	Effects of S-containing ligands on the structure and electronic properties of CdnSen/CdnTen nanoparticles (n=3, 4, 6, and 9). Chemical Physics, 2012, 407, 97-109.	0.9	12

#	ARTICLE	IF	CITATIONS
8421	Characterization of Ptn (n=2-12) clusters through global reactivity descriptors and vibrational spectroscopy, a theoretical study. Computational Materials Science, 2012, 53, 18-24.	1.4	33
8422	Bipolarons and polaron pairs in oligopyrrole dications. Computational and Theoretical Chemistry, 2012, 993, 7-12.	1.1	9
8423	First crystallographic report on a novel 2D layer of water pentagons: L5(7) water motif enclathrating [Co(cyclam)Cl <sub>2</sub> ]. Inorganic Chemistry Communication, 2012, 24, 157-161.	1.8	1
8424	Ab-initio study of the effect of rare-earth elements on the stacking faults of Mg solid solutions. Intermetallics, 2012, 29, 21-26.	1.8	58
8425	Investigation in the Ga-rich side of the Mn-Ga system: Synthesis and crystal structure of MnGa <sub>4</sub> and MnGa <sub>5</sub> <sup>x</sup> (x=1/4, 0.15). Intermetallics, 2012, 29, 147-154.	1.8	9
8426	Effects of transition metals in a binary-phase TiAl-Ti3Al alloy: From site occupancy, interfacial energetics to mechanical properties. Intermetallics, 2012, 31, 105-113.	1.8	29
8427	First-principles study of doping effect on the phase transition of zinc oxide with transition metal doped. Journal of Alloys and Compounds, 2012, 541, 250-255.	2.8	32
8428	A first principles analysis of the hydrogenation of C1C4 aldehydes and ketones over Ru(0001). Journal of Catalysis, 2012, 295, 31-44.	3.1	48
8429	Atomic-scale insight into adsorption of sterically hindered dibenzothiophenes on MoS <sub>2</sub> and Co-MoS hydrotreating catalysts. Journal of Catalysis, 2012, 295, 146-154.	3.1	116
8430	First-principles study of electronic structure and elasticity of UAl <sub>x</sub> (x=1,2,3) system. Physica B: Condensed Matter, 2012, 407, 748-755.	1.3	9
8431	Crystal structure determination of nanolaminated Ti5Al2C3 by combined techniques of XRPD, TEM and ab initio calculations. Journal of Advanced Ceramics, 2012, 1, 268-273.	8.9	18
8432	Probing the structural and electronic properties of Al-doped small niobium clusters. Chemical Physics Letters, 2012, 554, 231-235.	1.2	15
8433	A joint experimental and theoretical determination of the structures of oxidized and reduced molecules. Electrochemistry Communications, 2012, 23, 83-86.	2.3	20
8434	Structural Role of Counterions Adsorbed on Self-Assembled Peptide Nanotubes. Journal of the American Chemical Society, 2012, 134, 723-733.	6.6	41
8435	Density functional theory model study of size and structure effects on water dissociation by platinum nanoparticles. Journal of Chemical Physics, 2012, 137, 034701.	1.2	56
8436	Cauchy pressure and the generalized bonding model for nonmagnetic bcc transition metals. Physical Review B, 2012, 86, .	1.1	64
8437	Ab Initio Analysis of the Interactions of GaN Clusters with Oxygen and Water. Journal of Physical Chemistry C, 2012, 116, 12079-12092.	1.5	7
8438	Thermochemical Parameters and Growth Mechanism of the Boron-Doped Silicon Clusters, Si <sub>n</sub> B <sub>q</sub> with n = 1-10 and q = 1, 0, +1. Journal of Physical Chemistry C, 2012, 116, 20086-20098.	1.5	37

#	ARTICLE	IF	CITATIONS
8439	Ideal strength and structural instability of aluminum at finite temperatures. <i>Physical Review B</i> , 2012, 86, .	1.1	24
8440	Computational Evidence for $\hat{\pm}$ -Nitrosamino Radical as Initial Metabolite for Both the P450 Dealkylation and Denitrosation of Carcinogenic Nitrosamines. <i>Journal of Physical Chemistry B</i> , 2012, 116, 903-912.	1.2	39
8441	First principles study of Al and Ni segregation to the $\hat{\pm}$ -Fe/Cu (100) coherent interface and their effects on the interfacial cohesion. <i>Computational Materials Science</i> , 2012, 63, 329-335.	1.4	32
8442	First-principles studies of structural, mechanical, electronic, optical properties and pressure-induced phase transition of CuInO <sub>2</sub> polymorph. <i>Physica B: Condensed Matter</i> , 2012, 407, 4665-4670.	1.3	6
8443	Spin orbital effect in lanthanides doped silicon cage clusters. <i>Chemical Physics Letters</i> , 2012, 550, 134-137.	1.2	17
8444	Prediction of chemical and electrochemical oxidation potentials of $\hat{\pm}$ -diketonatobis(triphenylphosphite)rhodium(I) complexes: A DFT study. <i>Inorganica Chimica Acta</i> , 2012, 392, 30-37.	1.2	9
8445	DFT study on electronic structure and optical properties of N-doped, S-doped, and N/S co-doped SrTiO <sub>3</sub> . <i>Physica B: Condensed Matter</i> , 2012, 407, 4649-4654.	1.3	26
8446	First-principles study on the atomic and electronic structures of graphene-protected magnetic Fe/Ni(111) thin film. <i>Current Applied Physics</i> , 2012, 12, S37-S40.	1.1	1
8447	Electronic Structure and Half-Metallic Properties of Cubic Perovskite BaRu <sub>1-x</sub> Ti <sub>x</sub> O <sub>3</sub> System. <i>Key Engineering Materials</i> , 0, 519, 174-178.	0.4	0
8448	Origin of the anomalous magnetic behavior of the Fe <sub>13</sub> clusters. <i>Physical Review B</i> , 2012, 86, .	1.1	26
8449	Transition-metal dispersion on carbon-doped boron nitride nanostructures: Applications for high-capacity hydrogen storage. <i>Physical Review B</i> , 2012, 86, .	1.1	45
8450	Dynamics of H <sub>2</sub> dissociation on the 1/2 ML c(2 $\sqrt{2}$ )-Ti/Al(100) surface. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 3234.	1.3	14
8451	Anomalous decrease in structural disorder due to charge redistribution in Cr-doped Li <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> negative-electrode materials for high-rate Li-ion batteries. <i>Energy and Environmental Science</i> , 2012, 5, 9903.	15.6	143
8452	Decomposition of methylamine on nitrogen atom modified Mo(100): a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 6869.	1.3	10
8453	Oxidation mechanism of the intermetallic compound Ti <sub>3</sub> Al from ab initio thermodynamics. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11160.	1.3	26
8454	Cation interdiffusion model for enhanced oxygen kinetics at oxide heterostructure interfaces. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 2606.	1.3	52
8455	Spectroscopic and magnetic properties of an iodo CoI tripodal phosphine complex. <i>Dalton Transactions</i> , 2012, 41, 11788.	1.6	6
8456	Computationally efficient determination of hydrogen isotope effects on the thermodynamic stability of metal hydrides. <i>Physical Review B</i> , 2012, 86, .	1.1	11

#	ARTICLE	IF	CITATIONS
8457	Energetics and electronic structure of GaN codoped with Eu and Si. <i>Physical Review B</i> , 2012, 85, .	1.1	24
8458	Predictions of Sulfur Resistance in Metal Membranes for H <sub>2</sub> Purification Using First-Principles Calculations. <i>Industrial &amp; Engineering Chemistry Research</i> , 2012, 51, 301-309.	1.8	6
8459	A density functional theory investigation of the molecular and dissociative adsorption of hydrazine on defective copper surfaces. <i>Journal of Materials Chemistry</i> , 2012, 22, 23210.	6.7	25
8460	Dissociative and non-dissociative adsorption dynamics of N <sub>2</sub> on Fe(110). <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7471.	1.3	37
8461	Theoretical study on the charge transport property of Pt(CNtBu) <sub>2</sub> (CN) <sub>2</sub> nanowires induced by Pt <sup>+</sup> -Pt interactions. <i>Dalton Transactions</i> , 2012, 41, 7272.	1.6	13
8462	Inverse NiO <sub>x</sub> /Cu Catalyst with High Activity toward Water-Gas Shift. <i>Journal of Physical Chemistry C</i> , 2012, 116, 16089-16092.	1.5	19
8463	Oxidation of Magnesia-Supported Pd <sub>30</sub> Nanoclusters and Catalyzed CO Combustion: Size-Selected Experiments and First-Principles Theory. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9594-9607.	1.5	40
8464	Synthesis of Oxorhenium Acetyl and Benzoyl Complexes Incorporating Diamidopyridine Ligands: Implications for the Mechanism of CO Insertion. <i>Organometallics</i> , 2012, 31, 4295-4301.	1.1	20
8465	Influence of Electric Field on SERS: Frequency Effects, Intensity Changes, and Susceptible Bonds. <i>Journal of the American Chemical Society</i> , 2012, 134, 4646-4653.	6.6	41
8466	The paradox of an insulating contact between a chemisorbed molecule and a wide band gap semiconductor surface. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 1700-1705.	1.3	18
8467	Octahedrality versus tetrahedrality in stoichiometric ceria nanoparticles. <i>Chemical Communications</i> , 2012, 48, 4199.	2.2	25
8468	Method/basis set dependence of NICS values among metallic nano-clusters and hydrocarbons. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 3471.	1.3	16
8469	How to get superhard MnB <sub>2</sub> : a first-principles study. <i>Journal of Materials Chemistry</i> , 2012, 22, 17630.	6.7	9
8470	Tin oxide-surface modified anatase titanium(IV) dioxide with enhanced UV-light photocatalytic activity. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 705-711.	1.3	36
8471	Photoelectron imaging and theoretical calculations of gold-silver hydrides: comparing the characteristics of Au, Ag and H in small clusters. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11666.	1.3	9
8472	Investigation of spin-flip reactions of Nb + CH <sub>3</sub> CN by relativistic density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 6833.	1.3	9
8473	Promoters in the hydrogenation of alkynes in mixtures: insights from density functional theory. <i>Chemical Communications</i> , 2012, 48, 1379-1391.	2.2	183
8474	Strain-induced modulation of mechanical properties and electronic structure of edge-modification graphene nanoribbons. , 2012, , .		1



#	ARTICLE	IF	CITATIONS
8475	MASS-RADIUS RELATIONSHIPS FOR EXOPLANETS. <i>Astrophysical Journal</i> , 2012, 744, 59.	1.6	134
8476	<sup>17</sup> O NMR Gives Unprecedented Insights into the Structure of Supported Catalysts and Their Interaction with the Silica Carrier. <i>Journal of the American Chemical Society</i> , 2012, 134, 9263-9275.	6.6	93
8477	Information-Theoretic Approach for the Discovery of Design Rules for Crystal Chemistry. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1812-1820.	2.5	40
8478	Photoelectron Imaging and Theoretical Calculations of Bimetallic Clusters: AgCu <sup>+</sup> , AgCu <sub>2</sub> <sup>+</sup> , and Ag <sub>2</sub> Cu <sup>+</sup> . <i>Journal of Physical Chemistry A</i> , 2012, 116, 10365-10370.	1.1	12
8479	Hindered Rotational Energy Barriers of BH <sub>4</sub> <sup>+</sup> Tetrahedra in Î <sup>2</sup> -Mg(BH <sub>4</sub> ) <sub>2</sub> from Quasielastic Neutron Scattering and DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 2013-2023.	1.5	43
8480	Environment-Controlled Tethering by Aggregation and Growth of Phosphonic Acid Monolayers on Silicon Oxide. <i>Langmuir</i> , 2012, 28, 8046-8051.	1.6	73
8481	Ab Initio Studies of Ag-S Bond Formation during the Adsorption of <i>l</i> -Cysteine on Ag(111). <i>Langmuir</i> , 2012, 28, 11472-11480.	1.6	30
8482	Role of Multivalent Pr in the Formation and Migration of Oxygen Vacancy in Pr-Doped Ceria: Experimental and First-Principles Investigations. <i>Chemistry of Materials</i> , 2012, 24, 4261-4267.	3.2	86
8483	Influence of impurities on phase stability of martensites in titanium. <i>Philosophical Magazine</i> , 2012, 92, 2272-2285.	0.7	4
8484	An Extended Charge Equilibration Method. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2506-2511.	2.1	253
8485	Structures of uranyl peroxide hydrates: a first-principles study of studtite and metastudtite. <i>Dalton Transactions</i> , 2012, 41, 9748.	1.6	58
8486	Influence of Ni on the lattice stability of Fe-Ni alloys at multimegabar pressures. <i>Physical Review B</i> , 2012, 86, .	1.1	1
8487	Special Chemical Properties of RuO <sub>x</sub> Nanowires in RuO <sub>x</sub> /TiO <sub>2</sub> (110): Dissociation of Water and Hydrogen Production. <i>Journal of Physical Chemistry C</i> , 2012, 116, 4767-4773.	1.5	25
8488	First-Principles Study on Cd Doping in Cu <sub>2</sub> ZnSnS <sub>4</sub> and Cu <sub>2</sub> ZnSnSe <sub>4</sub> . <i>Japanese Journal of Applied Physics</i> , 2012, 51, 10NC11.	0.8	32
8489	Ligand Field Effect at Oxide-Metal Interface on the Chemical Reactivity of Ultrathin Oxide Film Surface. <i>Journal of the American Chemical Society</i> , 2012, 134, 10554-10561.	6.6	23
8490	Synthesis and Structure of an Intramolecularly Coordinated Diaryltelluronic Acid and Its Dimethyl Ester. <i>Organometallics</i> , 2012, 31, 289-293.	1.1	14
8491	Shape-Selective Methylation of 2-Methylnaphthalene with Methanol over H-ZSM-5 Zeolite: A Computational Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 4071-4082.	1.5	37
8492	Adsorption of Pt and Bimetallic PtAu Clusters on the Partially Reduced Rutile (110) TiO <sub>2</sub> Surface: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 5735-5746.	1.5	40



#	ARTICLE	IF	CITATIONS
8493	Photocatalytic Activities of Tin(IV) Oxide Surface-Modified Titanium(IV) Dioxide Show a Strong Sensitivity to the TiO <sub>2</sub> Crystal Form. <i>Journal of Physical Chemistry C</i> , 2012, 116, 12621-12626.	1.5	42
8494	Role of $\pi$ -Acceptor Effects in Controlling the Lability of Novel Monofunctional Pt(II) and Pd(II) Complexes: Crystal Structure of [Pt(triipyridinedimethane)Cl]Cl. <i>Inorganic Chemistry</i> , 2012, 51, 1516-1529.	1.9	48
8495	Structure and Energetics of Nanometer Size Clusters of Sulfuric Acid with Ammonia and Dimethylamine. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1030-1040.	1.1	65
8496	Computational studies of graphene growth mechanisms. <i>Physical Review B</i> , 2012, 85, .	1.1	20
8497	Ag and N acceptors in ZnO: An <i>ab initio</i> study of acceptor pairing, doping efficiency, and the role of hydrogen. <i>Physical Review B</i> , 2012, 85, .	1.1	13
8498	Insight into the SBU Condensation in Mg Coordination and Supramolecular Frameworks: A Combined Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2012, 134, 4762-4771.	6.6	24
8499	Drug nano-domains in spray-dried ibuprofen-silica microspheres. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12285.	1.3	16
8500	Evaluation of Electrokinetic Parameters for All DNA Bases with Sputter Deposited Nanocarbon Film Electrode. <i>Analytical Chemistry</i> , 2012, 84, 10607-10613.	3.2	18
8501	Silicon-Containing Multidecker Organometallic Complexes and Nanowires: A Density Functional Theory Study. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 151-156.	2.1	8
8502	Assessment of Density Functional Theory in Predicting Structures and Free Energies of Reaction of Atmospheric Prenucleation Clusters. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2071-2077.	2.3	168
8503	Successive hydrogenation starting from the edge(s): an effective approach to fine-tune the electronic and magnetic behaviors of SiC nanoribbons. <i>Journal of Materials Chemistry</i> , 2012, 22, 24166.	6.7	32
8504	Effects of N-Substitution on Phosphorescence Efficiency and Color Tuning of a Series of Ir(III) Complexes with a Phosphite Tripod Ligand: A DFT/TDDFT Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 26496-26506.	1.5	39
8505	Ab initiointeratomic potentials for low-energy He ion/atom scattering. <i>Radiation Effects and Defects in Solids</i> , 2012, 167, 666-675.	0.4	2
8506	Kinetic-Dynamic Properties of Different Monomers and Two-Dimensional Homoepitaxy Growth on the Zn-Polar (0001) ZnO Surface. <i>Crystal Growth and Design</i> , 2012, 12, 2850-2855.	1.4	4
8507	Theoretical Study of the Role of a Metal-Cation Ensemble at the Oxide-Metal Boundary on CO Oxidation. <i>Journal of Physical Chemistry C</i> , 2012, 116, 7491-7498.	1.5	59
8508	Adsorption, Dissociation, and Hydrogenation of CO <sub>2</sub> on WC(0001) and WC-Co Alloy Surfaces Investigated with Theoretical Calculations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 13202-13209.	1.5	27
8509	Structure and Defect Chemistry of Low- and High-Temperature Phases of LiBH <sub>4</sub> . <i>Journal of Physical Chemistry C</i> , 2012, 116, 13488-13496.	1.5	25
8510	Are Deposited Bimetallic Clusters More Effective for SO <sub>3</sub> Decomposition? A Systematic Study Using First Principles Theory. <i>Journal of Physical Chemistry C</i> , 2012, 116, 25594-25601.	1.5	10

#	ARTICLE	IF	CITATIONS
8511	Synergistic Effects in La/N Codoped TiO <sub>2</sub> Anatase (101) Surface Correlated with Enhanced Visible-Light Photocatalytic Activity. <i>Langmuir</i> , 2012, 28, 5882-5891.	1.6	42
8512	Surface Dependence of CO <sub>2</sub> Adsorption on Zn <sub>2</sub> GeO <sub>4</sub> . <i>Langmuir</i> , 2012, 28, 10415-10424.	1.6	71
8513	First-principles study of structural, magnetic, and electronic properties of small Fe-Rh alloy clusters. <i>Physical Review B</i> , 2012, 85, .	1.1	42
8514	Ultrafast Observation of a Solvent Dependent Spin State Equilibrium in CpCo(CO). <i>Journal of the American Chemical Society</i> , 2012, 134, 3120-3126.	6.6	26
8515	An exploration of the potential energy surface of the seven atom silver cluster and a carbon monoxide ligand. <i>European Physical Journal D</i> , 2012, 66, 1.	0.6	3
8516	Slab Thickness Effects for the Clean and Adsorbed Ge(001) Surface with Comparison to Si(001). <i>Journal of Physical Chemistry C</i> , 2012, 116, 6615-6622.	1.5	11
8517	Chemically Doped Radial Junction Characteristics in Silicon Nanowires. <i>Nano Letters</i> , 2012, 12, 6133-6138.	4.5	5
8518	The electronic and optical properties of carbon-doped SrTiO <sub>3</sub> : Density functional characterization. <i>AIP Advances</i> , 2012, 2, .	0.6	34
8519	Controlled, Low-Coverage Metal Oxide Activation of Silicon for Organic Functionalization: Unraveling the Phosphonate Bond. <i>Langmuir</i> , 2012, 28, 17494-17505.	1.6	40
8520	Thermodynamics and elastic properties of Ta from first-principles calculations. <i>Chinese Physics B</i> , 2012, 21, 127102.	0.7	7
8521	Li, Al, and Ni Substitutional Doping in MgO Ultrathin Films on Metals: Work Function Tuning via Charge Compensation. <i>Journal of Physical Chemistry C</i> , 2012, 116, 5781-5786.	1.5	30
8522	Crystal and Electronic Structures of Neptunium Nitrides Synthesized Using a Fluoride Route. <i>Journal of the American Chemical Society</i> , 2012, 134, 3111-3119.	6.6	20
8523	On the Need for Spin Polarization in Heterogeneously Catalyzed Reactions on Nonmagnetic Metallic Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1737-1743.	2.3	21
8524	First-principles study of the effect of iron on the crystal structure, stability and chemical bonding in the I <sup>2</sup> -based AlCu ordered I <sup>2</sup> -phase and the pretransition state of a solid solution. <i>Philosophical Magazine</i> , 2012, 92, 1649-1662.	0.7	5
8525	Tailoring Electronic Structure Through Alloying: The Ag <sub>n</sub> Cu <sub>34-n</sub> (n= 0-34) Nanoparticle Family. <i>Journal of Physical Chemistry C</i> , 2012, 116, 281-291.	1.5	31
8526	Acetone-Assisted Oxygen Vacancy Diffusion on TiO <sub>2</sub> (110). <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2970-2974.	2.1	18
8527	Stable Subnanometer Cobalt Oxide Clusters on Ultrananocrystalline Diamond and Alumina Supports: Oxidation State and the Origin of Sintering Resistance. <i>Journal of Physical Chemistry C</i> , 2012, 116, 24027-24034.	1.5	24
8528	Structural properties of PbVO <sub>3</sub> perovskites under hydrostatic pressure conditions up to 10.6 GPa. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 435403.	0.7	16

#	ARTICLE	IF	CITATIONS
8529	Porous Alumina Protective Coatings on Palladium Nanoparticles by Self-Poisoned Atomic Layer Deposition. <i>Chemistry of Materials</i> , 2012, 24, 2047-2055.	3.2	110
8530	Variable-Temperature Scanning Tunneling Microscopy and Computational Studies Examining Water and Potassium Adsorption on Au(100). <i>Journal of Physical Chemistry C</i> , 2012, 116, 555-562.	1.5	5
8531	On the Mechanisms of Carbon Formation Reaction on Ni(111) Surface. <i>Journal of Physical Chemistry C</i> , 2012, 116, 16522-16531.	1.5	19
8532	Interface atomic structures and magnetic anisotropy of Fe and Pd/Fe monatomic films on Pd(001). <i>Physical Review B</i> , 2012, 85, .	1.1	6
8533	Investigation of Spin-Flip Reactions of Zr + CH <sub>3</sub> CN by Relativistic Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5019-5025.	1.1	8
8534	Analysis of Charge Transfer for in Situ Li Intercalated Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 11364-11369.	1.5	25
8535	Ethanol and Water Adsorption on Close-Packed 3d, 4d, and 5d Transition-Metal Surfaces: A Density Functional Theory Investigation with van der Waals Correction. <i>Journal of Physical Chemistry C</i> , 2012, 116, 24695-24705.	1.5	103
8536	Application of <sup>204</sup> mPb Perturbed Angular Correlation of <sup>137</sup> La Spectroscopy in Coordination Chemistry. <i>Inorganic Chemistry</i> , 2012, 51, 1992-1994.	1.9	1
8537	Mesityltellurenyl Cations Stabilized by Triphenylpnictogens [MesTe(EPh <sub>3</sub> )] <sup>+</sup> (E) Tj ETQq0,0,0 rgBT /Overlock 1	1.9	44
8538	Oxygen Vacancy-Assisted Coupling and Enolization of Acetaldehyde on CeO <sub>2</sub> (111). <i>Journal of the American Chemical Society</i> , 2012, 134, 18034-18045.	6.6	97
8539	Kinetics and Mechanisms for the Adsorption, Dissociation, and Diffusion of Hydrogen in Ni and Ni/YSZ Slabs: A DFT Study. <i>Langmuir</i> , 2012, 28, 5596-5605.	1.6	34
8540	First-principles study of lithium ion migration in lithium transition metal oxides with spinel structure. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 13963.	1.3	64
8541	Computational Investigation of the Mechanism for the Activation of CO by Oxorhenium Complexes. <i>Organometallics</i> , 2012, 31, 4055-4062.	1.1	19
8542	On the Reaction Mechanism of Acetaldehyde Decomposition on Mo(110). <i>ACS Catalysis</i> , 2012, 2, 468-478.	5.5	16
8543	Role of NH <sub>3</sub> in the Dehydrogenation of Calcium Amidoborane Ammoniate and Magnesium Amidoborane Ammoniate: A First-Principles Study. <i>Inorganic Chemistry</i> , 2012, 51, 76-87.	1.9	14
8544	Sulfidization of Au(111) from Thioacetic Acid: An Experimental and Theoretical Study. <i>Langmuir</i> , 2012, 28, 15278-15285.	1.6	16
8545	Nuclear Quadrupole Coupling Constants for N <sub>2</sub> O: Experiment and Theory. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9769-9776.	1.1	4
8546	Ab Initio Density Functional Calculations of Adsorption of Transition Metal Atoms on $\gamma$ -Al <sub>2</sub> O <sub>3</sub> (010) Surface. <i>Journal of Physical Chemistry C</i> , 2012, 116, 5628-5636.	1.5	30

#	ARTICLE	IF	CITATIONS
8547	An ab initio molecular dynamics study: liquid-Al/solid-TiB <sub>2</sub> interfacial structure during heterogeneous nucleation. Journal Physics D: Applied Physics, 2012, 45, 455307.	1.3	23
8548	Extending the Density Functional Tight Binding Method to Carbon Under Extreme Conditions. Journal of Physical Chemistry C, 2012, 116, 2198-2204.	1.5	29
8549	New Investigations on the Surface Reactivity of Layered Lithium Oxides. Journal of Physical Chemistry C, 2012, 116, 20332-20341.	1.5	27
8550	Inner-Sphere Activation, Outer-Sphere Catalysis: Theoretical Study on the Mechanism of Transfer Hydrogenation of Ketones Using Iron(II) PNNP Eneamido Complexes. Organometallics, 2012, 31, 7375-7385.	1.1	79
8551	Reinterpreting the Role of the Catalyst Formal Potential. The case of Thiocyanate Electrooxidation Catalyzed by CoN <sub>4</sub> -Macrocyclic Complexes. Journal of Physical Chemistry C, 2012, 116, 7091-7098.	1.5	13
8552	Building Principles and Structural Motifs in TiO <sub>x</sub> Ultrathin Films on a (111) Substrate. Journal of Physical Chemistry C, 2012, 116, 13302-13306.	1.5	30
8553	Anti-Kubas Type Interaction in Hydrogen Storage on a Li Decorated BHNH Sheet: A First-Principles Based Study. Journal of Physical Chemistry C, 2012, 116, 3840-3844.	1.5	35
8554	CO Oxidation Mechanism on Tungsten Nanoparticle. Journal of Physical Chemistry C, 2012, 116, 18803-18815.	1.5	10
8555	First-Principles Assessment of the Reactions of Boric Acid on NiO(001) and ZrO <sub>2</sub> (1̄1...11) Surfaces. Journal of Physical Chemistry C, 2012, 116, 10113-10119.	1.5	7
8556	H <sub>2</sub> Diffraction from a Strained Pseudomorphic Monolayer of Cu Deposited on Ru(0001). Journal of Physical Chemistry C, 2012, 116, 13671-13678.	1.5	15
8557	Photoluminescence Properties, Molecular Structures, and Theoretical Study of Heteroleptic Silver(I) Complexes Containing Diphosphine Ligands. Inorganic Chemistry, 2012, 51, 5805-5813.	1.9	69
8558	Lewis Acido-Basic Interactions between CO <sub>2</sub> and MgO Surface: DFT and DRIFT Approaches. Journal of Physical Chemistry C, 2012, 116, 6645-6654.	1.5	154
8559	Density Functional Theory and ab Initio Studies of the Structure and Energetics of Digallium Tetraoxide, Ga <sub>2</sub> O <sub>4</sub> , in the Gas Phase. Journal of Physical Chemistry A, 2012, 116, 3215-3223.	1.1	7
8560	1D Hydrogen Bond Chain on Pt(211) Stepped Surface Observed by O K-NEXAFS Spectroscopy. Journal of Physical Chemistry C, 2012, 116, 13980-13984.	1.5	19
8561	Structure of Isolated Molybdenum(VI) and Molybdenum(IV) Oxide Species on Silica: Periodic and Cluster DFT Studies. Journal of Physical Chemistry C, 2012, 116, 5571-5584.	1.5	60
8562	Ultrafast Studies of Stannane Activation by Triplet Organometallic Photoproducts. Organometallics, 2012, 31, 3947-3957.	1.1	11
8563	Assessment of Theoretical Procedures for Calculating Barrier Heights for a Diverse Set of Water-Catalyzed Proton-Transfer Reactions. Journal of Physical Chemistry A, 2012, 116, 4211-4221.	1.1	92
8564	Tuning Structural and Mechanical Properties of Two-Dimensional Molecular Crystals: The Roles of Carbon Side Chains. Nano Letters, 2012, 12, 1229-1234.	4.5	27

#	ARTICLE	IF	CITATIONS
8565	Hydrogen Interaction with the Al Surface Promoted by Subsurface Alloying with Transition Metals. <i>Journal of Physical Chemistry C</i> , 2012, 116, 18663-18668.	1.5	19
8566	Density Functional Theory Study of Oxygen Reduction Activity on Ultrathin Platinum Nanotubes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 16499-16510.	1.5	18
8567	Anosovite-Type $V_3O_5$ : A New Binary Oxide of Vanadium. <i>Inorganic Chemistry</i> , 2012, 51, 8524-8529.	1.9	14
8568	Size-Selected Monodisperse Nanoclusters on Supported Graphene: Bonding, Isomerism, and Mobility. <i>Nano Letters</i> , 2012, 12, 5907-5912.	4.5	76
8569	Catalytic Reactivity of CuNi Alloys toward $H_2O$ and CO Dissociation for an Efficient Water-Gas Shift: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 745-752.	1.5	71
8570	Role of Fluorine Interactions in the Self-Assembly of a Functionalized Anthradithiophene Monolayer on Au(111). <i>Journal of Physical Chemistry C</i> , 2012, 116, 21465-21471.	1.5	9
8571	$Au_{10}^{2+}$ : A Tetrahedral Cluster Exhibiting Spherical Aromaticity. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3335-3337.	2.1	25
8572	Substrate Induced Thermal Decomposition of Perfluoro-Pentacene Thin Films on the Coinage Metals. <i>Journal of Physical Chemistry C</i> , 2012, 116, 24098-24106.	1.5	22
8573	Density Functional Theory Study on the Role of Ceria Addition in $Ti_xCe_{1-x}O_2$ Adsorbents for Thiophene Adsorption. <i>Journal of Physical Chemistry C</i> , 2012, 116, 3457-3466.	1.5	25
8574	The Importance of Attractive Three-Point Interaction in Enantioselective Surface Chemistry: Stereospecific Adsorption of Serine on the Intrinsically Chiral Cu <sub>531</sub> Surface. <i>Journal of the American Chemical Society</i> , 2012, 134, 9615-9621.	6.6	47
8575	Stabilizing Gold Adatoms by Thiophenyl Derivatives: A Possible Route toward Metal Redispersion. <i>Journal of the American Chemical Society</i> , 2012, 134, 11161-11167.	6.6	16
8576	Influence of Crystal Structure of Bulk Phase on the Stability of Nanoscale Phases: Investigation on $MgH_2$ Derived Nanostructures. <i>Journal of Physical Chemistry C</i> , 2012, 116, 18965-18972.	1.5	30
8577	Computational Differentiation of Brønsted Acidity Induced by Alkaline Earth or Rare Earth Cations in Zeolites. <i>Inorganic Chemistry</i> , 2012, 51, 12165-12175.	1.9	9
8578	Atomic-Scale Study of Ambient-Pressure Redox-Induced Changes for an Oxide-Supported Submonolayer Catalyst: $VO_x/Ir-TiO_2(110)$ . <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2845-2850.	2.1	20
8579	Si/Ge Double-Layered Nanotube Array as a Lithium Ion Battery Anode. <i>ACS Nano</i> , 2012, 6, 303-309.	7.3	225
8580	Dynamics of Nitrogen Scattering off N-Covered Ag(111). <i>Journal of Physical Chemistry C</i> , 2012, 116, 21903-21912.	1.5	14
8581	Bonding and Charge Transfer in Metal-Organic Coordination Networks on Au(111) with Strong Acceptor Molecules. <i>Journal of Physical Chemistry C</i> , 2012, 116, 24558-24565.	1.5	112
8582	Influence of Dipole-Dipole Interactions on Coverage-Dependent Adsorption: CO and NO on Pt(111). <i>Langmuir</i> , 2012, 28, 8408-8417.	1.6	67

#	ARTICLE	IF	CITATIONS
8583	Melanin films on Au(1 1 1): Adsorption and molecular conductance. <i>Organic Electronics</i> , 2012, 13, 1844-1852.	1.4	4
8584	Carbon monoxide sensing mechanism of highly oriented TiO <sub>2</sub> from first principles. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2012, 44, 1567-1571.	1.3	13
8585	Effect of Ti on the gas sensing characteristic of (Ti <sub>0.5</sub> Sn <sub>0.5</sub> )O <sub>2</sub> solid solutions. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2012, 44, 2143-2151.	1.3	4
8586	First-principles study of nitrogen-doped CuAlO <sub>2</sub> . <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012, 376, 2613-2616.	0.9	16
8587	Understanding the chiral selectivity of gold nanotubes. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012, 376, 2707-2711.	0.9	6
8588	Three iodometalate organic-inorganic hybrid materials based on methylene blue cation: Syntheses, structures, properties and DFT calculations. <i>Solid State Sciences</i> , 2012, 14, 1226-1232.	1.5	25
8589	First principles study on electronic properties and occupancy sites of molybdenum doped into LiFePO <sub>4</sub> . <i>Solid State Communications</i> , 2012, 152, 1577-1580.	0.9	23
8590	First-principles studies on the structural and electronic properties of Li-ion battery cathode material CuF <sub>2</sub> . <i>Solid State Communications</i> , 2012, 152, 1703-1706.	0.9	20
8591	First principles study of the structural, elastic, electronic and optical properties of CaSrTt (Tt=Si, Ge). <i>Journal of Applied Physics</i> , 2012, 112, 083701.	0.9	4
8592	Detailed insights into the structural properties and oxygen-pathways in orthorhombic Ba <sub>0.5</sub> Sr <sub>0.5</sub> Co <sub>0.8</sub> Fe <sub>0.2</sub> O <sub>3</sub> by electronic-structure theory. <i>Solid State Ionics</i> , 2012, 222-223, 53-58.	1.3	20
8593	Quintuple-period Si atomic wires with alternative double and triple modulations by metal: Mg/Si(557). <i>Surface Science</i> , 2012, 606, 57-61.	0.8	1
8594	Ionic and radical adsorption on the Au(hkl) surfaces: A DFT study. <i>Surface Science</i> , 2012, 606, 69-77.	0.8	32
8595	Formation of a missing row reconstruction on a Cu(100) surface: An atom scale density functional theory based study. <i>Surface Science</i> , 2012, 606, 192-201.	0.8	11
8596	Stress-driven structural transformation of Sb-passivated Si(114). <i>Surface Science</i> , 2012, 606, 312-319.	0.8	5
8597	Coverage-dependent molecular tilt of carbon monoxide chemisorbed on Pt{110}: A combined LEED and DFT structural analysis. <i>Surface Science</i> , 2012, 606, 383-393.	0.8	10
8598	Passivation effect of allylamine molecule on the electronic structure of a Si(001) (2 $\times$ 1) surface. <i>Surface Science</i> , 2012, 606, 470-474.	0.8	3
8599	Relative stability of armchair, zigzag and reczag graphene edges on the Ru(0001) surface. <i>Surface Science</i> , 2012, 606, 485-489.	0.8	10
8600	Structural and electronic properties of cobalt carbide Co <sub>2</sub> C and its surface stability: Density functional theory study. <i>Surface Science</i> , 2012, 606, 598-604.	0.8	79



#	ARTICLE	IF	CITATIONS
8601	Hydrogen adsorption, absorption and diffusion on and in transition metal surfaces: A DFT study. <i>Surface Science</i> , 2012, 606, 679-689.	0.8	380
8602	pH-dependent structure and energetics of H <sub>2</sub> O/MgO(100). <i>Surface Science</i> , 2012, 606, 902-907.	0.8	23
8603	Interplay between metal-free phthalocyanine molecules and Au(110) substrates. <i>Surface Science</i> , 2012, 606, 1120-1125.	0.8	20
8604	Stability of small chemical groups on hexagonal-SiC(0001) surfaces: A theoretical study. <i>Surface Science</i> , 2012, 606, 1195-1202.	0.8	2
8605	Atomistic simulations of the adsorption and migration barriers of Cu adatoms on ZnO surfaces using COMB potentials. <i>Surface Science</i> , 2012, 606, 1280-1288.	0.8	27
8606	Structure and properties of a model oxide-supported catalyst under redox conditions: WO <sub>x</sub> /Fe <sub>2</sub> O <sub>3</sub> (0001). <i>Surface Science</i> , 2012, 606, 1367-1381.	0.8	6
8607	Pt-chain induced formation of Ge nanowires on the Ge(001) surface. <i>Surface Science</i> , 2012, 606, 1405-1411.	0.8	8
8608	Interfacial structure of Co porphyrins on Au(111) electrode: Interaction of porphyrin molecules with substrate. <i>Surface Science</i> , 2012, 606, 1560-1564.	0.8	8
8609	Atomic and molecular adsorption on Pd(111). <i>Surface Science</i> , 2012, 606, 1670-1679.	0.8	119
8610	The structure of epitaxial V <sub>2</sub> O <sub>3</sub> films and their surfaces: A medium energy ion scattering study. <i>Surface Science</i> , 2012, 606, 1716-1727.	0.8	16
8611	Graphene nanodots with intrinsically magnetic protrusions. <i>Journal of Chemical Physics</i> , 2012, 136, 064706.	1.2	5
8612	Spin-filtering and switching effects of a single-molecule magnet Mn(dmit) <sub>2</sub> . <i>Journal of Applied Physics</i> , 2012, 111, 043713.	1.1	13
8613	Role of Explicit Solvents in Palladium(II)-Catalyzed Alkoxylation of Arenes: An Interesting Paradigm for Preferred Outer-Sphere Reductive Elimination over Inner-Sphere Pathway. <i>Organometallics</i> , 2012, 31, 6466-6481.	1.1	42
8614	State-of-the-art and challenges in theoretical simulations of heterogeneous catalysis at the microscopic level. <i>Catalysis Science and Technology</i> , 2012, 2, 2405.	2.1	38
8615	Highly corrosion resistant platinum-niobium oxide-carbon nanotube electrodes for the oxygen reduction in PEM fuel cells. <i>Energy and Environmental Science</i> , 2012, 5, 6156.	15.6	94
8616	Guided Self-Assembly of Metal Atoms on Silicon Using Organic-Molecule Templating. <i>Journal of the American Chemical Society</i> , 2012, 134, 15312-15317.	6.6	17
8617	Modified embedded atom method potential for Al, Si, Mg, Cu, and Fe alloys. <i>Physical Review B</i> , 2012, 85, .	1.1	267
8618	Simulation of crack propagation in alumina with <i>ab initio</i> based polarizable force field. <i>Journal of Chemical Physics</i> , 2012, 136, 084707.	1.2	18



#	ARTICLE	IF	CITATIONS
8619	Vibrational Spectra of Water Solutions of Azoles from QM/MM Calculations: Effects of Solvation. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10160-10171.	1.1	14
8620	Diffusion quantum Monte Carlo study of the equation of state and point defects in aluminum. <i>Physical Review B</i> , 2012, 85, .	1.1	38
8621	Computational study of the adsorption and dissociation of phenol on Pt and Rh surfaces. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 5849.	1.3	74
8622	Towards chemically accurate simulation of molecule-surface reactions. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14966.	1.3	80
8623	A Density Functional with Spherical Atom Dispersion Terms. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4989-5007.	2.3	463
8624	Does dehydrocyclization of 4-benzoylthiosemicarbazides in acetic acid lead to s-triazoles or thiadiazoles?. <i>Structural Chemistry</i> , 2012, 23, 1441-1448.	1.0	5
8625	First-principles study of bubble nucleation and growth behaviors in $\delta$ -U-Zr. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 415404.	0.7	16
8626	How low can you go? Minimum energy pathways for O <sub>2</sub> dissociation on Pt(111). <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 16677.	1.3	50
8627	Self-Assembled Monolayer Induced Au(111) and Ag(111) Reconstructions: Work Functions and Interface Dipole Formation. <i>Journal of Physical Chemistry C</i> , 2012, 116, 7826-7837.	1.5	64
8628	Lattice dynamics, thermodynamics and elastic properties of monoclinic Li <sub>2</sub> CO <sub>3</sub> from density functional theory. <i>Acta Materialia</i> , 2012, 60, 5204-5216.	3.8	64
8629	The effect of native point defect thermodynamics on off-stoichiometry in $\delta$ -Mg <sub>17</sub> Al <sub>12</sub> . <i>Acta Materialia</i> , 2012, 60, 5135-5142.	3.8	18
8630	Effect of H <sub>2</sub> O on catalytic performance of manganese oxides in NO reduction by NH <sub>3</sub> . <i>Applied Catalysis A: General</i> , 2012, 437-438, 139-148.	2.2	30
8631	First-principles study on the catalytic role of Ag in the oxygen adsorption of LaMnO <sub>3</sub> (001) surface. <i>Applied Surface Science</i> , 2012, 258, 2602-2606.	3.1	15
8632	Adsorption of ammonia on vanadium-antimony mixed oxides. <i>Applied Surface Science</i> , 2012, 258, 3617-3623.	3.1	10
8633	The dehydrogenation of CH <sub>4</sub> on Rh(111), Rh(110) and Rh(100) surfaces: A density functional theory study. <i>Applied Surface Science</i> , 2012, 258, 3714-3722.	3.1	61
8634	Reaction mechanism for CO oxidation on Cu(311): A density functional theory study. <i>Applied Surface Science</i> , 2012, 258, 3980-3985.	3.1	7
8635	First-principles study of boron, carbon and nitrogen adsorption on WC(100) surface. <i>Applied Surface Science</i> , 2012, 258, 4581-4587.	3.1	34
8636	First-principles study of the adsorption of lysine on hydroxyapatite (100) surface. <i>Applied Surface Science</i> , 2012, 258, 4911-4916.	3.1	38

#	ARTICLE	IF	CITATIONS
8637	Grain-size effect on the preferred orientation of TiC/ $\sqrt{3}$ -C:H thin films. <i>Applied Surface Science</i> , 2012, 258, 6800-6806.	3.1	8
8638	Periodic DFT study of adsorption of nitroamine molecule on $\sqrt{3}$ -Al <sub>2</sub> O <sub>3</sub> (001) surface. <i>Applied Surface Science</i> , 2012, 258, 7334-7342.	3.1	13
8639	Insight into the adsorption and dissociation of CH <sub>4</sub> on Pt(hkl) surfaces: A theoretical study. <i>Applied Surface Science</i> , 2012, 258, 7154-7160.	3.1	49
8640	Theoretical prediction of hydrogen storage on Li decorated planar boron sheets. <i>Applied Surface Science</i> , 2012, 258, 8874-8879.	3.1	29
8641	Electronic and magnetic properties of semiconducting nanoclusters and large organic molecules: Features interesting for spintronics. <i>Journal of Magnetism and Magnetic Materials</i> , 2012, 324, 3597-3600.	1.0	3
8642	Carbonate adsorption in the NaKA zeolite as the reason of higher CO <sub>2</sub> uptake relative to N <sub>2</sub> . <i>Microporous and Mesoporous Materials</i> , 2012, 162, 98-104.	2.2	20
8643	Ethanol gas sensing property and mechanism of ZnSnO <sub>3</sub> doped with Ti ions. <i>Materials Science in Semiconductor Processing</i> , 2012, 15, 319-325.	1.9	18
8644	Theoretical approaches to graphene and graphene-based materials. <i>Nano Today</i> , 2012, 7, 180-200.	6.2	122
8645	Energetics of Ti and Zr transition metals in D0 <sub>3</sub> -Fe <sub>3</sub> Al and its $\sqrt{5}$ (310) [001] grain boundary. <i>Intermetallics</i> , 2012, 22, 251-254.	1.8	7
8646	First-principles investigation on shear deformation of a TiAl/Ti <sub>3</sub> Al interface and effects of oxygen. <i>Intermetallics</i> , 2012, 22, 41-46.	1.8	21
8647	First principle study of the effect of Ti and Zr transition metals located in bulk D0 <sub>3</sub> Fe <sub>3</sub> Al and $\sqrt{5}$ (310)[001] grain boundary. <i>Intermetallics</i> , 2012, 28, 1-10.	1.8	4
8648	Site occupation behavior of sulfur and phosphorus in NiAl, TiAl and FeAl. <i>Intermetallics</i> , 2012, 28, 156-163.	1.8	10
8649	Magnetism-induced ductility in NiAl intermetallic alloys with Fe additions: Theory and experiment. <i>Journal of Alloys and Compounds</i> , 2012, 519, 101-105.	2.8	8
8650	Core-shell VPO <sub>4</sub> /C anode materials for Li ion batteries: Computational investigation and sol-gel synthesis. <i>Journal of Alloys and Compounds</i> , 2012, 522, 167-171.	2.8	33
8651	The structural phase transition and elastic properties of IrN under high pressure from first-principles calculations. <i>Journal of Alloys and Compounds</i> , 2012, 537, 216-220.	2.8	12
8652	Aerobic epoxidation of propene over silver (111) and (100) facet catalysts. <i>Journal of Catalysis</i> , 2012, 292, 138-147.	3.1	56
8653	Spectroscopic and structural characterization of Cr(II)/SiO <sub>2</sub> active site precursors in model Phillips polymerization catalysts. <i>Journal of Catalysis</i> , 2012, 293, 1-12.	3.1	56
8654	Periodic trends of oxygen vacancy formation and C-H bond activation over transition metal-doped CeO <sub>2</sub> (1 1 1) surfaces. <i>Journal of Catalysis</i> , 2012, 293, 103-115.	3.1	139

#	ARTICLE	IF	CITATIONS
8655	Theoretical studies on the multiple metal-metal bonds in the bimetallic molecules and the ultrashort V-Mn bonds in the complexes. <i>Journal of Organometallic Chemistry</i> , 2012, 717, 108-115.	0.8	10
8656	Reactivity of [Rh( $\eta^2$ -diketonato)(cod)] complexes: A DFT approach. <i>Journal of Organometallic Chemistry</i> , 2012, 719, 8-13.	0.8	11
8657	First principles study of the structural stability of intermetallic compounds in the Si-Zr system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2012, 36, 118-126.	0.7	19
8658	Thermodynamic description of the Ge-Na and Ge-K systems using the CALPHAD approach supported by first-principles calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2012, 37, 72-76.	0.7	11
8659	First-principles calculations of phase stability in the Ti-Zr-Si ternary system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2012, 37, 94-99.	0.7	15
8660	Influence of interstitial beryllium on properties of ZnO: A first-principle research. <i>Computational Materials Science</i> , 2012, 61, 127-133.	1.4	11
8661	First-principles study of the Al(001)/Al <sub>3</sub> Ti(001) interfacial properties. <i>Computational Materials Science</i> , 2012, 62, 136-141.	1.4	30
8662	The formation of FeZn <sub>13</sub> phase from atomic cluster during hot dip galvanizing. <i>Computational Materials Science</i> , 2012, 63, 214-217.	1.4	3
8663	Isomerization energies of tetrahedranes to 1,3-cyclobutadienes: A challenge for theoretical methods. <i>Computational and Theoretical Chemistry</i> , 2012, 979, 1-9.	1.1	8
8664	Density-functional theory investigation of oxidative corrosion of UO <sub>2</sub> . <i>Computational and Theoretical Chemistry</i> , 2012, 987, 90-102.	1.1	25
8665	Singlet-triplet excitation energies of naphthyl cations: High level composite method calculations suggest a singlet ground state. <i>Computational and Theoretical Chemistry</i> , 2012, 983, 69-75.	1.1	9
8666	Energy dissipation channels in the adsorption of N on Ag(111). <i>Computational and Theoretical Chemistry</i> , 2012, 990, 126-131.	1.1	28
8667	Molecular dynamics simulations based on reactive force-fields for surface chemical reactions. <i>Computational and Theoretical Chemistry</i> , 2012, 990, 152-158.	1.1	9
8668	Density functional study of NO <sub>x</sub> binding on small Au <sub>n</sub> Cu <sub>m</sub> (n+m=5) clusters. <i>Computational and Theoretical Chemistry</i> , 2012, 993, 90-96.	1.1	7
8669	Activation of C-H and C-C bonds of ethane by gas-phase Pt atom: Potential energy surface and reaction mechanism. <i>Computational and Theoretical Chemistry</i> , 2012, 994, 112-120.	1.1	16
8670	Libxc: A library of exchange and correlation functionals for density functional theory. <i>Computer Physics Communications</i> , 2012, 183, 2272-2281.	3.0	419
8671	Magnetism in graphene induced by hydrogen adsorbates. <i>Chemical Physics Letters</i> , 2012, 541, 70-74.	1.2	27
8672	Impact energy dependence of defect formation in single-walled carbon nanotubes. <i>Chemical Physics Letters</i> , 2012, 541, 92-95.	1.2	5

#	ARTICLE	IF	CITATIONS
8673	Jahn-Teller distortion, ferromagnetic coupling, and electron delocalization in a high-spin Fe <sup>2+</sup> Fe bonded dimer. <i>Comptes Rendus Chimie</i> , 2012, 15, 192-201.	0.2	18
8674	Electronic fine structure calculation of [Gd(DOTA)(H <sub>2</sub> O)] <sup>3+</sup> using LF-DFT: The zero field splitting. <i>Comptes Rendus Chimie</i> , 2012, 15, 250-254.	0.2	13
8675	Models for the trinuclear copper(II) cluster in the particulate methane monooxygenase from methanotrophic bacteria: Synthesis, spectroscopic and theoretical characterization of trinuclear copper(II) complexes. <i>Comptes Rendus Chimie</i> , 2012, 15, 214-224.	0.2	3
8676	First-principles study of electronic structure and metal-insulator transition of plutonium dihydride and trihydride. <i>Computational Materials Science</i> , 2012, 51, 127-134.	1.4	30
8677	Thermal stability and elastic properties of Mg <sub>2</sub> X (X = Si, Ge, Sn, Pb) phases from first-principle calculations. <i>Computational Materials Science</i> , 2012, 51, 409-414.	1.4	86
8678	Formaldehyde on TiO <sub>2</sub> anatase (1 0 1): A DFT study. <i>Computational Materials Science</i> , 2012, 51, 389-395.	1.4	55
8679	The electronic, elastic and structural properties of Pd-Zr intermetallic. <i>Computational Materials Science</i> , 2012, 51, 1-6.	1.4	21
8680	First-principles calculations on the crystal, electronic structures and elastic properties of Ag-rich $\beta$ phase approximants in Al-Ag alloys. <i>Computational Materials Science</i> , 2012, 51, 415-421.	1.4	4
8681	Improved Finnis-Sinclair potential for bcc vanadium solid. <i>Computational Materials Science</i> , 2012, 53, 101-104.	1.4	8
8682	DFT study of the coverage effects for Al adsorption on Si(111) surfaces. <i>Computational Materials Science</i> , 2012, 53, 382-387.	1.4	4
8683	Ab initio study of defect properties in YPO <sub>4</sub> . <i>Computational Materials Science</i> , 2012, 54, 170-175.	1.4	10
8684	First-principles study of grain boundary embrittlement in Fe-Ni-S alloy. <i>Computational Materials Science</i> , 2012, 55, 17-22.	1.4	16
8685	Hybrid density-functional calculations of structural, elastic and electronic properties for a series of cubic perovskites CsMF <sub>3</sub> (M=Ca, Cd, Hg, and Pb). <i>Computational Materials Science</i> , 2012, 58, 101-112.	1.4	28
8686	Cation distribution and mixing thermodynamics in Fe/Ni thiospinels. <i>Geochimica Et Cosmochimica Acta</i> , 2012, 88, 275-282.	1.6	21
8687	Periodic Trends in Adsorption and Activation Energies for Heterometallic Diffusion on (100) Transition Metal Surfaces. <i>Journal of Physical Chemistry C</i> , 2012, 116, 22469-22475.	1.5	8
8688	Bifunctional anode catalysts for direct methanol fuel cells. <i>Energy and Environmental Science</i> , 2012, 5, 8335.	15.6	157
8689	Origin of enhanced water adsorption at $\sqrt{11} \times \sqrt{0}$ step edge on rutile TiO <sub>2</sub> (110) surface. <i>Journal of Chemical Physics</i> , 2012, 137, 114707.	1.2	8
8690	In- and Out-Dependent Interactions of Iron with Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 16461-16466.	1.5	30

#	ARTICLE	IF	CITATIONS
8691	First-principles study of electronic and optical properties of cubic perovskite CsSrF <sub>3</sub> . <i>Materials Science-Poland</i> , 2012, 30, 359-367.	0.4	31
8692	Crystalline and magnetic anisotropy of the $3d$ -transition metal monoxides MnO, FeO, CoO, and NiO. <i>Physical Review B</i> , 2012, 86, .	1.1	97
8693	Graphene Oxide: An Ideal Support for Gold Nanocatalysts. <i>Journal of Physical Chemistry C</i> , 2012, 116, 22336-22340.	1.5	54
8694	Adsorption and Decomposition Mechanism of 1,1-Diamino-2,2-dinitroethylene on Al(111) Surface by Periodic DFT Calculations. <i>Chinese Journal of Chemistry</i> , 2012, 30, 2539-2548.	2.6	19
8695	Initial Decomposition of Methanol and Water on In <sub>2</sub> O <sub>3</sub> (110): A Periodic DFT Study. <i>Chinese Journal of Chemistry</i> , 2012, 30, 2036-2040.	2.6	13
8696	Structural Insight into the Prolyl Hydroxylase PHD2: A Molecular Dynamics and DFT Study. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 4973-4985.	1.0	5
8697	Accelerating VASP electronic structure calculations using graphic processing units. <i>Journal of Computational Chemistry</i> , 2012, 33, 2581-2589.	1.5	143
8698	Gettering of transition metals by porous silicon in epitaxial silicon solar cells. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2012, 209, 1866-1871.	0.8	23
8699	Electronic structure, phonon spectra, and anisotropy of electron-phonon interaction in scandium. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 2118-2124.	0.7	3
8700	Alloy solid solution strengthening of Mg alloys: Valence effect. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 2089-2095.	0.7	15
8701	Density functional theory simulation of the L <sub>2,3</sub> XANES spectra. <i>JETP Letters</i> , 2012, 95, 504-510.	0.4	3
8702	Molecular structure, quantum chemical investigation, and thermal behavior of (DNAZ-CO) <sub>2</sub> . <i>Journal of Structural Chemistry</i> , 2012, 53, 534-541.	0.3	6
8703	An ab-initio study of silicon adsorption on metallic surfaces (Au/Ag): Novel perspective to explore chemical bonding. <i>European Physical Journal B</i> , 2012, 85, 1.	0.6	1
8704	First-principles calculation of phase equilibrium of V-Nb, V-Ta, and Nb-Ta alloys. <i>Physical Review B</i> , 2012, 85, .	1.1	46
8705	Thermodynamic and Kinetic Stabilities of Active Site Protonation States of Class C $\beta$ -Lactamase. <i>Journal of Physical Chemistry B</i> , 2012, 116, 4741-4753.	1.2	13
8706	Hydrogen Shift Reactions of Rhenium Hydrido Carbyne Complexes. <i>Organometallics</i> , 2012, 31, 1817-1824.	1.1	17
8707	Adsorption of NO on the Rh <sub>13</sub> , Pd <sub>13</sub> , Ir <sub>13</sub> , and Pt <sub>13</sub> Clusters: A Density Functional Theory Investigation. <i>Journal of Physical Chemistry C</i> , 2012, 116, 20540-20549.	1.5	33
8708	Self-organization of extraframework cations in zeolites. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2012, 468, 2070-2086.	1.0	73

#	ARTICLE	IF	CITATIONS
8709	Influence of Pressure on the Structural, Electronic and Mechanical Properties of Cubic SrHfO <sub>3</sub> : A First-Principles Study. Chinese Physics Letters, 2012, 29, 127103.	1.3	3
8710	First-principles study of optical properties in Ca-doped ZnO alloys. Open Physics, 2012, 10, .	0.8	3
8711	Carbon dioxide capture by aminoalkyl imidazolium-based ionic liquid: a computational investigation. Physical Chemistry Chemical Physics, 2012, 14, 4589.	1.3	27
8712	Spin-wave method for the total energy of paramagnetic state. Physical Review B, 2012, 85, .	1.1	57
8713	First-Principles Study of Electronic Structure and Optical Properties of Cubic Perovskite CsCaF <sub>3</sub> . Chinese Physics Letters, 2012, 29, 117102.	1.3	32
8714	Computations of 36 Tautomer/Isomer Equilibria of Different Lactams. Journal of Physical Chemistry A, 2012, 116, 6885-6893.	1.1	11
8715	Hole mediated coupling in Sr <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> for visible light photocatalysis. Physical Chemistry Chemical Physics, 2012, 14, 4891.	1.3	28
8716	An interpretation of the absorption and emission spectra of the gold dimer using modern theoretical tools. Physical Chemistry Chemical Physics, 2012, 14, 8732.	1.3	22
8717	Prediction of orientational phase transition in boron carbide. Solid State Sciences, 2012, 14, 1648-1652.	1.5	31
8718	The Chemistry of Water on $\gamma$ -Alumina: Kinetics and Nuclear Quantum Effects from First Principles. Journal of Physical Chemistry C, 2012, 116, 26829-26840.	1.5	26
8719	Density Functional Theory Study of N $\equiv$ CN and O $\equiv$ CN Bond Cleavage by an Iron Silyl Complex. Organometallics, 2012, 31, 3995-4005.	1.1	19
8720	Interplay between Chemical and Magnetic Order in FeRh Clusters. Journal of Physical Chemistry C, 2012, 116, 17228-17238.	1.5	26
8721	Quantum Monte Carlo investigations of adsorption energetics on graphene. Journal of Physics Condensed Matter, 2012, 24, 395002.	0.7	8
8722	Density functional theory study of CO <sub>2</sub> capture with transition metal oxides and hydroxides. Journal of Chemical Physics, 2012, 136, 064516.	1.2	26
8723	Incorporation, valence state, and electronic structure of Mn and Cr in bulk single crystal $\gamma$ -Ga <sub>2</sub> O <sub>3</sub> . Journal of Applied Physics, 2012, 111, 123716.	1.1	40
8724	Structural and magnetic properties of LiNi <sub>0.5</sub> Mn <sub>1.5</sub> O <sub>4</sub> and LiNi <sub>0.5</sub> Mn <sub>1.5</sub> O <sub>4</sub> $\cdot$ $\frac{1}{2}$ spinels: A first-principles study. Chinese Physics B, 2012, 21, 128202.	0.7	17
8725	The solvation of two electrons in the gaseous clusters of Na <sup>+</sup> (NH <sub>3</sub> ) <sub>n</sub> and Li <sup>+</sup> (NH <sub>3</sub> ) <sub>n</sub> . Journal of Chemical Physics, 2012, 136, 124314.	1.2	5
8726	Structural and Electronic Properties of Bare and Capped Cd <sub>n</sub> Se <sub>n</sub> /Cd <sub>n</sub> Te <sub>n</sub> Nanoparticles ( $n = 6, 9$ ). Journal of Physical Chemistry C, 2012, 116, 6817-6830.	1.5	31

#	ARTICLE	IF	CITATIONS
8727	Geometry, Orbital Interaction, and Oxygen Chemisorption Properties of Chromium-Doped Nickel Clusters. <i>Journal of Physical Chemistry C</i> , 2012, 116, 13353-13367.	1.5	17
8728	Screened hybrid density functional study on Sr <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> for visible light photocatalysis. <i>Applied Physics Letters</i> , 2012, 100, .	1.5	31
8729	Correction to DFT interaction energies by an empirical dispersion term valid for a range of intermolecular distances. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 3414.	1.3	10
8730	Platinum-Based Nanoalloys Pt <sub>x</sub> TM <sub>55-x</sub> (TM = Co, Rh, Au): A Density Functional Theory Investigation. <i>Journal of Physical Chemistry C</i> , 2012, 116, 18432-18439.	1.5	65
8731	Optical absorption spectra of gold clusters Au <sub>n</sub> (n = 4, 6, 8, 12, 20) from long-range corrected functionals with optimal tuning. <i>Journal of Chemical Physics</i> , 2012, 137, 114302.	1.2	60
8732	Propene Epoxidation with H <sub>2</sub> /H <sub>2</sub> O/O <sub>2</sub> Mixtures Over Gold Atoms Supported on Defective Graphene: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 19355-19362.	1.5	26
8733	Theoretical Study of the Oxidation of Formic Acid on the PtAu(111) Surface in the Continuum Water Solution Phase. <i>Journal of Physical Chemistry C</i> , 2012, 116, 24143-24150.	1.5	17
8734	Dimeric Gold Bis(carbene) Complexes by Transmetalation in Water. <i>Organometallics</i> , 2012, 31, 619-626.	1.1	65
8735	Mechanism of Ammonia Decomposition and Oxidation on Ir(100): A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 24035-24045.	1.5	47
8736	Adsorption of Small Palladium Clusters on the $\sqrt{3}\times\sqrt{3}$ -Al <sub>2</sub> O <sub>3</sub> (0001) Surface: A First Principles Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 2863-2871.	1.5	20
8737	Are 4-Mercaptobenzoic Acid Self Assembled Monolayers on Au(111) a Suitable System to Test Atom Models?. <i>Journal of Physical Chemistry C</i> , 2012, 116, 25765-25771.	1.5	35
8738	Self-assembly mechanisms of short atomic chains on single-layer graphene and boron nitride. <i>Physical Review B</i> , 2012, 86, .	1.1	24
8739	Ligand effects on the stability of thiol-stabilized gold nanoclusters: Au <sub>25</sub> (SR) <sub>18</sub> <sup>-</sup> , Au <sub>38</sub> (SR) <sub>24</sub> , and Au <sub>102</sub> (SR) <sub>44</sub> . <i>Nanoscale</i> , 2012, 4, 4206.	2.8	103
8740	Microwave Magnetic Materials. <i>Handbook of Magnetic Materials</i> , 2012, 20, 1-63.	0.6	8
8741	Ab Initio Thermodynamics Examination of Sulfur Species Present on Rh, Ni, and Binary Rh-Ni Surfaces under Steam Reforming Reaction Conditions. <i>Langmuir</i> , 2012, 28, 5660-5668.	1.6	10
8742	An angular-dependent embedded atom method (A-EAM) interatomic potential to model thermodynamic and mechanical behavior of Al/Si composite materials. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2012, 20, 035007.	0.8	21
8743	The performance of density functional based methods in the description of selected biological systems and processes. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14943.	1.3	36
8744	First principles calculations of alloying element diffusion coefficients in Ni using the five-frequency model. <i>Chinese Physics B</i> , 2012, 21, 109102.	0.7	48



#	ARTICLE	IF	CITATIONS
8745	First-principles transport calculation method based on real-space finite-difference nonequilibrium Green's function scheme. <i>Physical Review B</i> , 2012, 86, .	1.1	20
8746	Molecular Metal Oxide Cluster-Surface Modified Titanium(IV) Dioxide Photocatalysts. <i>Australian Journal of Chemistry</i> , 2012, 65, 624.	0.5	36
8747	Stability and migration of large oxygen clusters in $\text{UO}_2$ : Density functional theory calculations. <i>Journal of Chemical Physics</i> , 2012, 136, 234702.	1.2	34
8748	Ignition-proof mechanism of magnesium alloy added with rare earth La from first-principle study. <i>Journal of Rare Earths</i> , 2012, 30, 573-578.	2.5	13
8749	First Principles Studies on the Electronics Structures of $(\text{Li}_{0.75}\text{Na}_{0.25})(\text{Fe}_{0.75}\text{Mn}_{0.25})\text{PO}_4$ Cathode Materials. <i>Rare Metal Materials and Engineering</i> , 2012, 41, 1323-1326.	0.8	3
8750	Charge-density distribution in potassium dihydrogen phosphoglycolate – a comparison of phosphate and phosphonate groups. <i>Acta Crystallographica Section B: Structural Science</i> , 2012, 68, 625-635.	1.8	7
8751	First-principles study of high-pressure elasticity of $\text{CF}_2\text{O}$ and $\text{CT}_2\text{O}$ structure $\text{MgAl}_2\text{O}_4$ . <i>Geophysical Research Letters</i> , 2012, 39, .	1.5	2
8752	Reversal of the negative natural aging effect in $\text{Al-Mg-Si}$ alloys. <i>Acta Materialia</i> , 2012, 60, 6091-6101.	3.8	72
8753	Double-atomic-wall-based dynamic precipitates of the early-stage S-phase in $\text{AlCuMg}$ alloys. <i>Acta Materialia</i> , 2012, 60, 6573-6580.	3.8	58
8754	Hybrid density functional study on $\text{SrTiO}_3$ for visible light photocatalysis. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 11611-11617.	3.8	67
8755	First principles study of various $\text{Zr-H}$ phases with low H concentrations. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 12393-12401.	3.8	26
8756	Selective and effective adsorption of methyl blue by barium phosphate nano-flake. <i>Journal of Colloid and Interface Science</i> , 2012, 386, 277-284.	5.0	72
8757	Theoretical investigation of pristine and functionalized $\text{AlN}$ and $\text{SiC}$ single walled nanotubes as an adsorption candidate for methane. <i>Applied Surface Science</i> , 2012, 263, 553-562.	3.1	28
8758	First-principle studies of properties of ternary layered $\text{M}_2\text{PbC}$ ( $\text{M}=\text{Ti}, \text{Zr}$ and $\text{Hf}$ ). <i>Computational Materials Science</i> , 2012, 65, 377-382.	1.4	12
8759	Ab initio investigations of structural, elastic and electronic properties of $\text{ZnSiP}_2$ : Pressure effect. <i>Computational Materials Science</i> , 2012, 65, 520-527.	1.4	29
8760	Ab initio calculations of structural, optical and thermoelectric properties for $\text{CoSb}_3$ and $\text{ACo}_4\text{Sb}_{12}$ ( $\text{A}=\text{La}, \text{Tl}$ and $\text{Y}$ ) compounds. <i>Computational Materials Science</i> , 2012, 65, 509-519.	1.4	95
8761	Density functional study of $\text{H}_2\text{S}$ binding on small cationic $(n+m\frac{1}{2})$ clusters. <i>Computational and Theoretical Chemistry</i> , 2012, 997, 70-76.	1.1	9
8762	Interaction of second-row dicarbides with molecular oxygen: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2012, 999, 184-189.	1.1	2

#	ARTICLE	IF	CITATIONS
8763	DFT study on stability and structure of bimetallic AumPdn (N=38, 55, 79, N=m+n, m/n=2:1 and 5:1) clusters. Computational and Theoretical Chemistry, 2012, 999, 246-250.	1.1	13
8764	2,4-Diazido-5-iodo-pyrimidine crystal under high pressure: A comparison of DFT and DFT-D studies. Computational and Theoretical Chemistry, 2012, 1000, 60-69.	1.1	10
8765	Density-functional investigation of the geometries, stabilities, electronic, and magnetic properties of gold cluster anions doped with aluminum: (1 <sup>-</sup> 2/8). Computational and Theoretical Chemistry, 2012, 1002, 31-36.	1.1	17
8766	Multiferroic and magnetoelectric nature of GaFeO <sub>3</sub> , AlFeO <sub>3</sub> and related oxides. Solid State Communications, 2012, 152, 1964-1968.	0.9	55
8767	Chemical trend of superconducting transition temperature in hole-doped delafossite of CuAlO <sub>2</sub> , AgAlO <sub>2</sub> and AuAlO <sub>2</sub> . Solid State Communications, 2012, 152, 2078-2081.	0.9	14
8768	Lattice distortion effect on electrical properties of GDC thin films: Experimental evidence and computational simulation. Solid State Ionics, 2012, 229, 45-53.	1.3	24
8769	Theoretical studies on the spectroscopic properties of a series of halide Zinc (II) complexes with pyridinylimine and pyridinylmethylamine derivatives. Synthetic Metals, 2012, 162, 2138-2148.	2.1	7
8770	The low velocity layer in subduction zone: Structure and elasticity of glaucophane at high pressures. Physics of the Earth and Planetary Interiors, 2012, 208-209, 50-58.	0.7	26
8771	Structure of Defects, their Interactions and Positron Characteristics in Fe <sub>3</sub> Al system. Physics Procedia, 2012, 35, 69-74.	1.2	4
8772	First-principles calculations of adhesion, bonding and magnetism of the Fe/HfC interface. Journal of Magnetism and Magnetic Materials, 2012, 324, 4155-4160.	1.0	13
8773	Microwave spectrum of arsenic triphosphide. Journal of Molecular Spectroscopy, 2012, 278, 68-71.	0.4	2
8774	Heterogeneous nucleation of Mg <sub>2</sub> Si on Sr <sub>11</sub> Sb <sub>10</sub> nucleus in Mg <sub>x</sub> (3.5, 5 wt.%)Si <sub>1</sub> Al alloys. Materials Chemistry and Physics, 2012, 135, 358-364.	2.0	27
8775	An intermediate fcc Zr state observed in the Cu-Zr-Ni system upon ion beam mixing. Materials Letters, 2012, 89, 90-92.	1.3	2
8776	First-Principles Modeling of the "Clean-Up" of Native Oxides during Atomic Layer Deposition onto III-V Substrates. Journal of Physical Chemistry C, 2012, 116, 643-654.	1.5	50
8777	Synthesis of Enantiomerically Pure anti-1,2-Diaryl and syn-1,2-Alkylaryl vic-Selenoamines. Journal of Organic Chemistry, 2012, 77, 1974-1982.	1.7	11
8778	The structure of Mn-doped tris(8-hydroxyquinoline)gallium by extended x-ray absorption fine structure spectroscopy and first principles calculations. Journal of Applied Physics, 2012, 112, 113519.	1.1	5
8779	Effects of strain, d-band filling, and oxidation state on the surface electronic structure and reactivity of 3d perovskite surfaces. Journal of Chemical Physics, 2012, 137, 084703.	1.2	67
8780	Global Minima of Protonated Water Clusters (H <sub>2</sub> O) <sub>20</sub> H <sup>+</sup> Revisited. Journal of Physical Chemistry A, 2012, 116, 10826-10835.	1.1	14

#	ARTICLE	IF	CITATIONS
8781	Synthesis of Pt@Pd Core-Shell Nanostructures by Atomic Layer Deposition: Application in Propane Oxidative Dehydrogenation to Propylene. <i>Chemistry of Materials</i> , 2012, 24, 3525-3533.	3.2	104
8782	DFT study of coverage-dependent adsorption of NH <sub>3</sub> on TiO <sub>2</sub> -B (100) surface. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 16618.	1.3	18
8783	Molecular Simulation for Gas Adsorption at NiO (100) Surface. <i>ACS Applied Materials &amp; Interfaces</i> , 2012, 4, 5691-5697.	4.0	64
8784	Extreme Poisson's ratios and their electronic origin in B2 CsCl-type AB intermetallic compounds. <i>Physical Review B</i> , 2012, 85, .	1.1	42
8785	Low-Spin versus High-Spin Ground State in Pseudo-Octahedral Iron Complexes. <i>Inorganic Chemistry</i> , 2012, 51, 6011-6019.	1.9	116
8786	Superatomic orbitals in sixteen-coordinate M@Li <sub>16</sub> bonded by metallic bonds. <i>Nanoscale</i> , 2012, 4, 2567.	2.8	12
8787	On the Structure of Î²-Molybdenum Dichloride. <i>Inorganic Chemistry</i> , 2012, 51, 4965-4971.	1.9	3
8788	CO <sub>2</sub> Reduction on Transition Metal (Fe, Co, Ni, and Cu) Surfaces: In Comparison with Homogeneous Catalysis. <i>Journal of Physical Chemistry C</i> , 2012, 116, 5681-5688.	1.5	247
8789	Insight into the Correlation between Net Topology and Ligand Coordination Mode in New Lanthanide MOFs Heterogeneous Catalysts: A Theoretical and Experimental Approach. <i>Crystal Growth and Design</i> , 2012, 12, 5535-5545.	1.4	45
8790	First-principles study of the oxygen adsorption and dissociation on graphene and nitrogen doped graphene for Li-air batteries. <i>Journal of Applied Physics</i> , 2012, 112, .	1.1	133
8792	Hydrogen Adsorption on PdGa(110): A DFT Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 17518-17524.	1.5	17
8793	Ce-Mn Oxides for High-Temperature Gasifier Effluent Desulfurization. <i>Energy &amp; Fuels</i> , 2012, 26, 6765-6776.	2.5	30
8794	Ruthenium-Arene Complexes of Curcumin: X-Ray and Density Functional Theory Structure, Synthesis, and Spectroscopic Characterization, in Vitro Antitumor Activity, and DNA Docking Studies of (<i>p</i>-Cymene)Ru(curcuminato)chloro. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 1072-1081.	2.9	202
8795	Linking 31P Magnetic Shielding Tensors to Crystal Structures: Experimental and Theoretical Studies on Metal(II) Aminotris(methylenephosphonates). <i>Inorganic Chemistry</i> , 2012, 51, 11466-11477.	1.9	19
8796	The delocalized nature of holes in (Ga, N) cluster-doped ZnO. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 415503.	0.7	4
8797	Surface lattice-engineered bimetallic nanoparticles and their catalytic properties. <i>Chemical Society Reviews</i> , 2012, 41, 8066.	18.7	258
8798	Nonadiabatic dynamics at metal surfaces: Independent electron surface hopping with phonon and electron thermostats. <i>Faraday Discussions</i> , 2012, 157, 325.	1.6	18
8799	Exploration of the formation of XLi <sub>3</sub> N <sub>2</sub> compounds (X=Sc-Zn) by means of density functional theory. <i>Physical Review B</i> , 2012, 85, .	1.1	7

#	ARTICLE	IF	CITATIONS
8800	Intrinsic Magnetism in Tin Dioxide. NATO Science for Peace and Security Series B: Physics and Biophysics, 2012, , 315-323.	0.2	0
8801	Strain relief and disorder in commensurate water layers formed on Pd(111). Journal of Physics Condensed Matter, 2012, 24, 124102.	0.7	14
8802	Effects of uniaxial strains on the magnetic properties and the electronic structures of Fe/graphene system: An ab initio study. Journal of Applied Physics, 2012, 111, 07C306.	1.1	4
8803	CO <sub>2</sub> Activation and Methanol Synthesis on Novel Au/TiC and Cu/TiC Catalysts. Journal of Physical Chemistry Letters, 2012, 3, 2275-2280.	2.1	129
8804	The effects of Mo doping on 0.3Li[Li <sub>0.33</sub> Mn <sub>0.67</sub> ]O <sub>2</sub> ·0.7Li[Ni <sub>0.5</sub> Co <sub>0.2</sub> Mn <sub>0.3</sub> ]O <sub>2</sub> cathode material. Dalton Transactions, 2012, 41, 3053.	1.6	76
8805	Role of Distant Al Atoms in Alkaline Earth Zeolites for Stabilization of Hydroxyl Groups. Journal of Physical Chemistry C, 2012, 116, 2399-2410.	1.5	10
8806	Mechanism for enhanced oxygen reduction kinetics at the (La,Sr)CoO <sub>3</sub> /(La,Sr)CoO <sub>4</sub> hetero-interface. Energy and Environmental Science, 2012, 5, 8598.	15.6	109
8807	FIRST-PRINCIPLES STUDY OF OXYGEN-VACANCY Cu <sub>2</sub> O (111) SURFACE. Journal of Theoretical and Computational Chemistry, 2012, 11, 1261-1280.	1.8	8
8808	The ionic conductivity in lithium-boron oxide materials and its relation to structural, electronic and defect properties: insights from theory. Journal of Physics Condensed Matter, 2012, 24, 203201.	0.7	22
8809	First-Principles Study of 8H-, 10H-, 12H-, and 18H-SiC Polytypes. Journal of the Physical Society of Japan, 2012, 81, 024714.	0.7	18
8810	Structural Stability and Electronic Properties of CdS Condensed Clusters. Journal of Physical Chemistry C, 2012, 116, 5981-5985.	1.5	12
8811	Fragmentation of the Fluorite Type in Fe <sub>8</sub> Al <sub>17.4</sub> Si <sub>7.6</sub> : Structural Complexity in Intermetallics Dictated by the 18 Electron Rule. Inorganic Chemistry, 2012, 51, 10341-10349.	1.9	21
8812	Stabilization of Silicon Islands in Silicoaluminophosphates by Proton Redistribution. Journal of Physical Chemistry C, 2012, 116, 7255-7259.	1.5	19
8813	Non-equilibrium alloy phase formation and transformation driven by ion beam mixing in the Fe-Hf-Nb multilayers. Science China Technological Sciences, 2012, 55, 640-645.	2.0	3
8814	Ab Initio Studies of the Unreconstructed Polar CdTe (111) Surface. Journal of Electronic Materials, 2012, 41, 2745-2753.	1.0	13
8815	Elastic Coefficients of Zn <sub>1-x</sub> Be <sub>x</sub> O Solid Solutions: a First-Principles Study. Journal of Electronic Materials, 2012, 41, 3007-3012.	1.0	6
8816	General formulation of spin-flip time-dependent density functional theory using non-collinear kernels: Theory, implementation, and benchmarks. Journal of Chemical Physics, 2012, 136, 204103.	1.2	188
8817	Band gap engineering in BiNbO <sub>4</sub> for visible-light photocatalysis. Applied Physics Letters, 2012, 100, 182102.	1.5	54

#	ARTICLE	IF	CITATIONS
8818	Electronic Structure of the CuCl <sub>2</sub> (100) Surface: A DFT First-Principle Study. Journal of Nanomaterials, 2012, 2012, 1-7.	1.5	5
8819	A comparative density functional study of the low pressure phases of solid ZnX, CdX, and HgX: Trends and relativistic effects. Journal of Chemical Physics, 2012, 136, 034504.	1.2	25
8820	Site preference and effect of alloying on elastic properties of ternary $B_2NiAl$ -based alloys. Physical Review B, 2012, 85, .	1.1	53
8821	Selected AB <sub>2</sub> (A = C, Si, Ge; B = Al, Ga, In) ions: a battle between covalency and aromaticity, and prediction of square planar Si in SiIn <sub>4</sub> . Physical Chemistry Chemical Physics, 2012, 14, 14815.	1.3	33
8822	Potential applications of two ultrathin Pd nanowires to the hydrogen economy. Journal of Materials Chemistry, 2012, 22, 20319.	6.7	12
8823	Ultrafast TRIR and DFT Studies of the Photochemical Dynamics of Co <sub>4</sub> (CO) <sub>12</sub> in Solution. Organometallics, 2012, 31, 4031-4038.	1.1	6
8824	Molecular Structure and Vibrational Spectra of Mixed MDyX <sub>4</sub> (M = Li, Na, K, Rb, Cs; X = F, Cl, Br, I). Inorganic Chemistry, 2012, 51, 543-556.	1.9	5
8825	Predicting Nuclear Resonance Vibrational Spectra of [Fe(OEP)(NO)]. Journal of Chemical Theory and Computation, 2012, 8, 214-223.	2.3	19
8826	Molecular structure and thermal behavior of N-Benzoyl-3,3-dinitroazetidine. Russian Journal of Physical Chemistry A, 2012, 86, 1962-1968.	0.1	14
8827	Analysis of Hydroxide Sorbents for CO <sub>2</sub> Capture from Warm Syngas. Industrial & Engineering Chemistry Research, 2012, 51, 13473-13481.	1.8	15
8828	Modification of Primary Mg <sub>2</sub> Si in Mg-4Si Alloys with Antimony. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2012, 43, 4926-4932.	1.1	20
8829	First-Principles Calculations on Stabilization of Iron Carbides (Fe <sub>3</sub> C, Fe <sub>5</sub> C <sub>2</sub> , and $\hat{I}$ -Fe <sub>2</sub> C) in Steels by Common Alloying Elements. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2012, 43, 4436-4444.	1.1	52
8830	A Hierarchy of Methods for the Energetically Accurate Modeling of Isomerism in Monosaccharides. Journal of Chemical Theory and Computation, 2012, 8, 2630-2645.	2.3	52
8831	Giant stability of substituent Co chains in ZnO:Co dilute magnetic oxides. AIP Advances, 2012, 2, 042155.	0.6	1
8832	Comparative theoretical studies of high pressure effect on polymorph I of 2,2,4,4,6,6-hexanitroazobenzene crystal. Structural Chemistry, 2012, 23, 1631-1642.	1.0	4
8833	Solubility and clustering of ruthenium fission products in uranium dioxide as determined by density functional theory. Physical Review B, 2012, 85, .	1.1	15
8834	Scalable properties of metal clusters: A comparative study of modern exchange-correlation functionals. Journal of Chemical Physics, 2012, 137, 034102.	1.2	20
8835	Ge adsorption on Ag(111): A density-functional theory investigation. Solid State Sciences, 2012, 14, 1480-1485.	1.5	2

#	ARTICLE	IF	CITATIONS
8836	Searching superhard cubic phases in ternary Ba-Ca-N phase diagram using first-principles calculations. <i>Diamond and Related Materials</i> , 2012, 27-28, 14-18.	1.8	2
8837	Communication: Improving the density functional theory+ <i>U</i> description of CeO <sub>2</sub> by including the contribution of the O 2 <i>p</i> electrons. <i>Journal of Chemical Physics</i> , 2012, 136, 041101.	1.2	62
8838	Adsorption of <i>l</i> -DOPA Intercalated in Hydrated Na-Saponite Clay: A Combined Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 26414-26421.	1.5	25
8839	Molecular Basis for Nanoscopic Membrane Curvature Generation from Quantum Mechanical Models and Synthetic Transporter Sequences. <i>Journal of the American Chemical Society</i> , 2012, 134, 19207-19216.	6.6	64
8840	Electronic Properties of Graphene Altered by Substrate Surface Chemistry and Externally Applied Electric Field. <i>Journal of Physical Chemistry C</i> , 2012, 116, 6259-6267.	1.5	28
8841	Multiorbital Kondo physics of Co in Cu hosts. <i>Physical Review B</i> , 2012, 85, .	1.1	50
8842	Reversal of atomic contrast in scanning probe microscopy on (111) metal surfaces. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 084003.	0.7	15
8843	Water Dissociation on Bimetallic Surfaces: General Trends. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10120-10128.	1.5	32
8844	First-Principles Study of CO Adsorption and Oxidation on Ru-Doped CeO <sub>2</sub> (111) Surface. <i>Journal of Physical Chemistry C</i> , 2012, 116, 6239-6246.	1.5	90
8845	Electron-mediated ferromagnetism in Fe-doped InP: Theory and experiment. <i>Chinese Physics B</i> , 2012, 21, 097502.	0.7	4
8846	Surface Charge Transfer Induced Ferromagnetism in Nanostructured ZnO/Al. <i>Journal of Physical Chemistry C</i> , 2012, 116, 8541-8547.	1.5	15
8847	On the Interaction of Phosphines with High Surface Area Mesoporous Silica. <i>Journal of Physical Chemistry C</i> , 2012, 116, 25919-25927.	1.5	15
8848	Tunable and sizable band gap in silicene by surface adsorption. <i>Scientific Reports</i> , 2012, 2, 853.	1.6	253
8849	Hydrogen storage of Mg <i>l</i> <i>M</i> <i>H</i> <i>Tj ETQq1 1,0,784314,rgBT /Ove</i>	0.7	35
8850	Complexes with a Single Metal-Metal Bond as a Sensitive Probe of Quality of Exchange-Correlation Functionals. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 908-914.	2.3	54
8851	Applying precipitate-host lattice coherency for compositional determination of precipitates in Al-Mg-Si-Cu alloys. <i>Philosophical Magazine</i> , 2012, 92, 3833-3856.	0.7	47
8852	Nucleation of Rh <sub><i>n</i></sub> ( <i>n</i> = 1-5) Clusters on $\beta$ -Al <sub>2</sub> O <sub>3</sub> Surfaces: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10623-10631.	1.5	45
8853	Single-crystal growth and electronic structure of $\text{Ti}_{3}\text{PbCl}_{5}$ , a prospective nonlinear optical material. , 2012, , .		0



#	ARTICLE	IF	CITATIONS
8854	Vibrational Analysis of Side Chain Model Compounds of Perfluorinated Alkyl Sulfonic Acid Ionomers. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10850-10863.	1.1	14
8855	Structures and stabilities of group 17 fluorides EF <sub>3</sub> (E = I, At, and element 117) with spin-orbit coupling. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 15816.	1.3	18
8856	First-principles study of hypothetical boron crystals: Bn (n = 13, 14, 15). <i>Solid State Sciences</i> , 2012, 14, 1636-1642.	1.5	14
8857	Structural Patterns Arising during Synthetic Growth of Fullerene-Like Sulfocarbide. <i>Journal of Physical Chemistry C</i> , 2012, 116, 21124-21131.	1.5	41
8858	Why Urease Is a Di-Nickel Enzyme whereas the CcrA <sup>12</sup> -Lactamase Is a Di-Zinc Enzyme. <i>Journal of Physical Chemistry B</i> , 2012, 116, 10649-10656.	1.2	27
8859	An embedded-atom-method model for alkali-metal vibrations. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 335401.	0.7	7
8860	Explicitly correlated benchmark calculations on C <sub>8</sub> H <sub>8</sub> isomer energy separations: how accurate are DFT, double-hybrid, and composite <i>ab initio</i> procedures?. <i>Molecular Physics</i> , 2012, 110, 2477-2491.	0.8	63
8861	Isobutene Protonation in H-FAU, H-MOR, H-ZSM-5, and H-ZSM-22. <i>Journal of Physical Chemistry C</i> , 2012, 116, 18236-18249.	1.5	44
8862	Strontium doping in mullite-type bismuth aluminate: a vacancy investigation using neutrons, photons and electrons. <i>Journal of Materials Chemistry</i> , 2012, 22, 18814.	6.7	20
8863	Electronic structure mechanism of martensitic phase transformation in binary titanium alloys. <i>Journal of Applied Physics</i> , 2012, 112, 123718.	1.1	23
8864	Ideal tensile and shear strength of a gum metal approximant: <i>Ab initio</i> density functional calculations. <i>Physical Review B</i> , 2012, 85, .	1.1	19
8865	First-Principles Study of Formaldehyde Adsorption on TiO <sub>2</sub> Rutile (110) and Anatase (001) Surfaces. <i>Journal of Physical Chemistry C</i> , 2012, 116, 8044-8053.	1.5	76
8866	Molecular Dynamics Simulations of Ion-Bombarded Graphene. <i>Journal of Physical Chemistry C</i> , 2012, 116, 4044-4049.	1.5	47
8867	Diffusion of hydrogen within idealized grains of bcc Fe: A kinetic Monte Carlo study. <i>Physical Review B</i> , 2012, 86, .	1.1	59
8868	Trends in Selective Hydrogen Peroxide Production on Transition Metal Surfaces from First Principles. <i>ACS Catalysis</i> , 2012, 2, 2664-2672.	5.5	137
8869	Theoretical prediction of mechanical stability of ferromagnetic fcc Fe-Cu alloys from first principles. <i>Journal of Applied Physics</i> , 2012, 111, 053517.	1.1	11
8870	Electronic Structure, Optical Properties, and Photocatalytic Activities of LaFeO <sub>3</sub> NaTaO <sub>3</sub> Solid Solution. <i>Journal of Physical Chemistry C</i> , 2012, 116, 22767-22773.	1.5	60
8871	Structural, electronic properties and heat of formation of Mg <sub>2</sub> FeH <sub>6</sub> complex hydride: an <i>ab initio</i> study. <i>Physica Scripta</i> , 2012, 86, 015701.	1.2	16



#	ARTICLE	IF	CITATIONS
8872	Conformational analysis of triphenylphosphine in square planar organometallic complexes: [(PPh <sub>3</sub> )(ML <sub>1</sub> L <sub>2</sub> L <sub>3</sub> )] and [M(acac)(L <sup>2</sup> )(PPh <sub>3</sub> )]. Dalton Transactions, 2012, 41, 10633.	1.6	15
8873	Probing the geometric, electronic and magnetic properties of bimetallic palladium-gold clusters (Au <sub>n</sub> Pd <sub>8-n</sub> ). Molecular Physics, 2012, 110, 2993-3000.	0.8	4
8874	Interplay between Magnetism and Magicness in Nanoclusters. Journal of Physical Chemistry C, 2012, 116, 20625-20632.	1.5	5
8875	Ab Initio Studies of the Electronic Structure of L-Cysteine Adsorbed on Ag(111). Langmuir, 2012, 28, 8084-8099.	1.6	25
8876	New Series of Intramolecularly Coordinated Diaryltellurium Compounds. Rational Synthesis of the Diarylhydroxytelluronium Triflate [(8-Me) <sub>2</sub> NC <sub>10</sub> H <sub>6</sub> ] <sub>2</sub> Te(OH)(O) <sub>3</sub> SCF <sub>3</sub> ]. Organometallics, 2012, 31, 238-245.	1.1	25
8877	Orbital selective coupling between Ni adatoms and graphene Dirac electrons. Physical Review B, 2012, 85, .	1.1	27
8878	Static surface temperature effects on the dissociation of H <sub>2</sub> and D <sub>2</sub> on Cu(111). Journal of Chemical Physics, 2012, 137, 054703.	1.2	27
8879	A comparative DFT study of the Schiff base formation from acetaldehyde and butylamine, glycine and phosphatidylethanolamine. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	13
8880	Tuning Fluorescent Molecules by Inclusion in a Metal-Organic Framework: An Experimental and Computational Study. ChemPlusChem, 2012, 77, 1112-1118.	1.3	66
8881	The magnetic coupling in manganese-based dinuclear superhalogens and their analogues. A theoretical characterization from a combined DFT and BS study. Physical Chemistry Chemical Physics, 2012, 14, 1121-1130.	1.3	56
8882	Polyoxometalates adsorbed on metallic surfaces: immediate reduction of [SiW <sub>12</sub> O <sub>40</sub> ] <sup>4-</sup> on Ag(100). Chemical Science, 2012, 3, 2020.	3.7	32
8883	Enhanced Oxidation Reactivity of WO <sub>3</sub> (001) Surface through the Formation of Oxygen Radical Centers. Journal of Physical Chemistry C, 2012, 116, 5067-5075.	1.5	27
8884	Mechanistic Insights on the Hydrogenation of $\alpha,\beta$ -Unsaturated Ketones and Aldehydes to Unsaturated Alcohols over Metal Catalysts. ACS Catalysis, 2012, 2, 671-683.	5.5	206
8885	Adsorption of NO <sub>2</sub> on Small Silver Clusters with Copper Impurity: A Density Functional Study. Journal of Cluster Science, 2012, 23, 1039-1048.	1.7	3
8886	Density functional study of water-gas shift reaction on M <sub>3</sub> O <sub>3</sub> /Cu(111). Physical Chemistry Chemical Physics, 2012, 14, 16626.	1.3	23
8887	Dominant Factors Governing the Rate Capability of a TiO <sub>2</sub> Nanotube Anode for High Power Lithium Ion Batteries. ACS Nano, 2012, 6, 8308-8315.	7.3	184
8888	Synthesis and evaluation of new guanidine-thiourea organocatalyst for the nitro-Michael reaction: Theoretical studies on mechanism and enantioselectivity. Beilstein Journal of Organic Chemistry, 2012, 8, 1485-1498.	1.3	36
8889	Experimental Study and Atomic Level Description of Adsorption Process of CO <sub>2</sub> on Doped Alkaline Earth Oxides. ISIJ International, 2012, 52, 1233-1240.	0.6	4

#	ARTICLE	IF	CITATIONS
8890	A theoretical rationalization of a total inelastic electron tunneling spectrum: The comparative cases of formate and benzoate on Cu(111). <i>Journal of Chemical Physics</i> , 2012, 136, 244507.	1.2	15
8891	Density functional theory studies on structures and absorption spectra of [Au(tpy)Cl] <sup>2+</sup> and its derivatives: Role of basis set, functional, solvent effect, and spin orbit effect. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1642-1653.	1.0	3
8892	Computational study of the catalytic effect of platinum on the decomposition of DNT. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1852-1858.	1.0	1
8893	Electronic structures of the Cu <sub>2</sub> S <sub>2</sub> core of the Cu <sub>A</sub> site in cytochrome <i>c</i> oxidase and nitrous oxide reductase. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 208-218.	1.0	7
8894	Ni <sub>2</sub> H and Ni <sub>2</sub> Cl homolytic bond dissociation energies and radical stabilization energies: An assessment of theoretical procedures through comparison with benchmark quality W2w data. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1862-1878.	1.0	46
8895	Combined XPS and first principle study of metastable Mg-Ti thin films. <i>Surface and Interface Analysis</i> , 2012, 44, 986-988.	0.8	6
8896	Nanospace charge polarization of monatomic layered platinum cluster disk constructed on silicon(111) surface. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 1193-1198.	0.7	18
8897	Density functional based prediction of a spin ordered open shell singlet in an unpassivated graphene nanofilm. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 283-291.	0.7	0
8898	CO adsorption on metal oxide surfaces doped with transition metal adatoms. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 1046-1057.	0.7	11
8899	Density functional theory study of ultrasmall diameter (2,2) boron nitride, silicon carbide, and carbon nanotubes. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 1027-1032.	0.7	24
8900	Synthesis and first principles calculations of the structural and electronic properties of type I clathrates Sr <sub>8</sub> Ga <sub>16</sub> Sn <sub>x</sub> Ge <sub>30-x</sub> . <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 1423-1430.	0.7	3
8901	Transition metal catalysis by density functional theory and density functional theory/molecular mechanics. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 375-385.	6.2	91
8902	Circular dichroism: electronic. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 150-166.	6.2	106
8903	Mechanical properties of L1 <sub>2</sub> type Al <sub>3</sub> X (X = Mg, Sc, Zr) from first principles study. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 1510-1516.	0.7	23
8904	Pressure dependent properties of a multifunctional material: Lithium platinum boride (LiPt <sub>3</sub> B). <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 1744-1755.	0.7	3
8905	The Importance of the DFT method on the computation of the second hyperpolarizability of semiconductor clusters of increasing size: A critical analysis on prolate aluminum phosphide clusters. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2115-2125.	1.0	17
8906	Adsorption of polyfunctional 5-fluorouracil and 2,4-dithio-5-fluorouracil on Au(111) surface: Structure, energy, and electronic transmission. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2287-2293.	1.0	2
8907	Exploring the surface reactivity of Ag nanoparticles with antimicrobial activity: A DFT study. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3033-3038.	1.0	5

#	ARTICLE	IF	CITATIONS
8908	Theoretical calculation of the zero-temperature isotherm and phase stability of silver up to 2 Gbar using the linear combinations of gaussian type orbitals method. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3822-3828.	1.0	4
8909	Oxidative addition of methyl iodide to [Rh(PhCOCHCOPh)(CO)(P(OCH <sub>2</sub> ) <sub>3</sub> CCH <sub>3</sub> )]: an experimental and computational study. <i>Open Chemistry</i> , 2012, 10, 256-266.	1.0	5
8910	The structural, elastic and thermodynamic properties of intermetallic compound CeGa <sub>2</sub> . <i>Open Physics</i> , 2012, 10, .	0.8	0
8911	High-pressure melting curve of platinum from <i>ab initio</i> Z method. <i>Physical Review B</i> , 2012, 85, .	1.1	50
8912	Observation of a Short-Lived Triplet Precursor in CpCo(CO)-Catalyzed Alkyne Cyclotrimerization. <i>Organometallics</i> , 2012, 31, 3582-3587.	1.1	20
8913	Geometries and stabilities of Ag <sub>n</sub> v (v = ±1, 0; n = 21-29) clusters. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	9
8914	Oxygen-Storage Materials BaYMn <sub>2</sub> O <sub>5</sub> from the Quantum-Chemical Point of View. <i>Chemistry of Materials</i> , 2012, 24, 1910-1916.	3.2	27
8915	Room temperature ferromagnetism in Teflon due to carbon dangling bonds. <i>Nature Communications</i> , 2012, 3, 727.	5.8	56
8916	DFT study on size-dependent geometries, stabilities, and electronic properties of Au <sub>n</sub> M <sub>2</sub> (M = Si, P; n =) Tj ETQq0 0.0 rgBT /Overlock 10	0.6	14
8917	Planar P <sub>6</sub> E <sub>6</sub> (E = Se, S) macrocycles incorporating P <sub>2</sub> N <sub>2</sub> scaffolds. <i>Chemical Communications</i> , 2012, 48, 6346.	2.2	43
8918	Coupled phonons, magnetic excitations, and ferroelectricity in AlFeO <sub>3</sub> : Raman and first-principles studies. <i>Physical Review B</i> , 2012, 85, .	1.1	31
8919	Theoretical and experimental investigation on the electronic properties of the shuttlecock shaped and the double-decker structured metal phthalocyanines, MPc and M(Pc) <sub>2</sub> (M = Sn and Pb). <i>Dalton Transactions</i> , 2012, 41, 7141.	1.6	14
8920	First-principles calculation of thermodynamic stability of acids and bases under <i>p</i> H environment: A microscopic <i>p</i> H theory. <i>Journal of Chemical Physics</i> , 2012, 136, 134112.	1.2	8
8921	Challenges for Density Functional Theory. <i>Chemical Reviews</i> , 2012, 112, 289-320.	23.0	1,869
8922	Hyper-generalized-gradient functionals constructed from the Lieb-Oxford bound: Implementation via local hybrids and thermochemical assessment. <i>Journal of Chemical Physics</i> , 2012, 136, 184102.	1.2	33
8923	Nature of Ag Islands and Nanoparticles on the CeO <sub>2</sub> (111) Surface. <i>Journal of Physical Chemistry C</i> , 2012, 116, 1122-1132.	1.5	92
8924	Stable, Single-Layer MX <sub>2</sub> Transition-Metal Oxides and Dichalcogenides in a Honeycomb-Like Structure. <i>Journal of Physical Chemistry C</i> , 2012, 116, 8983-8999.	1.5	1,196
8925	Observation of metal ion dependent packing structures and magnetic behaviors of metal-bis-1, 2-dithiolene complexes. <i>Dalton Transactions</i> , 2012, 41, 2667.	1.6	17

#	ARTICLE	IF	CITATIONS
8926	Transport properties of $\text{HfO}_2$ -based resistive-switching memories. Physical Review B, 2012, 85, .	1.1	51
8927	Encapsulation of small magnetic clusters in fullerene cages: A density functional theory investigation within van der Waals corrections. Physical Review B, 2012, 85, .	1.1	36
8928	Energetics and electronic properties of twisted single-walled carbon nanotubes. Physical Review B, 2012, 85, .	1.1	12
8929	Quantum size effects in the atomistic structure of armchair nanoribbons. Physical Review B, 2012, 85, .	1.1	17
8930	Effects of static charging and exfoliation of layered crystals. Physical Review B, 2012, 85, .	1.1	35
8931	Evolution of Structure and of Grafting Properties of $\gamma$ -Alumina with Pretreatment Temperature. Journal of Physical Chemistry C, 2012, 116, 834-843.	1.5	37
8932	Optical properties of PbTe and PbSe. Physical Review B, 2012, 85, .	1.1	72
8933	First-principles study of hydrogen ordering in lanthanum hydride and its effect on the metal-insulator transition. Physical Review B, 2012, 86, .	1.1	5
8934	Electronic Structure Engineering in Heterogeneous Catalysis: Identifying Novel Alloy Catalysts Based on Rapid Screening for Materials with Desired Electronic Properties. Topics in Catalysis, 2012, 55, 376-390.	1.3	80
8935	Benchmarking the performance of time-dependent density functional methods. Journal of Chemical Physics, 2012, 136, 104101.	1.2	295
8936	The DFT investigations of the electron injection in hydrazone-based sensitizers. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	49
8937	Electronic structure and thermodynamics of $\text{V}_2\text{O}_3$ polymorphs. Journal of Computational Chemistry, 2012, 33, 2102-2107.	1.5	18
8938	The role of the basis set and the level of quantum mechanical theory in the prediction of the structure and reactivity of cisplatin. Journal of Computational Chemistry, 2012, 33, 2292-2302.	1.5	39
8939	Vibrational frequency scale factors for density functional theory and the polarization consistent basis sets. Journal of Computational Chemistry, 2012, 33, 2380-2387.	1.5	186
8940	The effects of intramolecular and intermolecular coordination on $^{31}\text{P}$ nuclear shielding: phosphorylated azoles. Magnetic Resonance in Chemistry, 2012, 50, 120-127.	1.1	14
8941	Density functional theory study of nitrogen $^{14}\text{N}$ nuclear quadrupole coupling parameters of $\text{L-histidine}$ : hydrogen-bonded system. Magnetic Resonance in Chemistry, 2012, 50, 314-319.	1.1	2
8942	The Question of cis versus trans Configuration in Octahedral Metal Diketonates: An In-Depth Investigation on Diorganobis(4-acyl-5-pyrazolonato)tin(IV) Complexes. European Journal of Inorganic Chemistry, 2012, 2012, 1369-1379.	1.0	12
8943	Amide-Functionalized Bis(NHC) Systems: Anion Effect on Gold-Gold Interactions. European Journal of Inorganic Chemistry, 2012, 2012, 3892-3898.	1.0	23

#	ARTICLE	IF	CITATIONS
8944	Structure-Property Relationships in Pt <sup>II</sup> Diimine-Dithiolate Nonlinear Optical Chromophores Based on Arylethylene-1,2-dithiolate and 2-Thioxothiazoline-4,5-dithiolate. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 3577-3594.	1.0	21
8945	Initial oxidation structure of chlorinated Si(001). <i>Journal of the Korean Physical Society</i> , 2012, 60, 398-402.	0.3	0
8946	Theoretical Prediction of S-H Bond Rupture in Methanethiol upon Interaction with Gold. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7686-7693.	1.1	32
8947	Comparison of Reaction Pathways of Ethylene Glycol, Acetaldehyde, and Acetic Acid on Tungsten Carbide and Ni-Modified Tungsten Carbide Surfaces. <i>Journal of Physical Chemistry C</i> , 2012, 116, 5720-5729.	1.5	29
8948	2-Aminopyrimidine-silver(I) based organic semiconductors: Electronic structure and optical response. <i>Physical Review B</i> , 2012, 85, .	1.1	12
8949	Symmetry and Stability of the Rutile-Based TiO <sub>2</sub> Nanowires: Models and Comparative LCAO-Plane Wave DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 13395-13402.	1.5	21
8950	High-pressure-high-temperature equation of state of KCl and KBr. <i>Physical Review B</i> , 2012, 85, .	1.1	122
8951	An ab initio molecular dynamics study of ionic conductivity in hexagonal lithium lanthanum titanate oxide La <sub>0.5</sub> Li <sub>0.5</sub> TiO <sub>3</sub> . <i>Ionics</i> , 2012, 18, 371-377.	1.2	13
8952	Charge Transfer in Model Bioinspired Carotene-Porphyrin Dyads. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3926-3933.	1.1	9
8953	Electronic structure, equation of state, and lattice dynamics of low-pressure Ge polymorphs. <i>Physical Review B</i> , 2012, 86, .	1.1	36
8954	Thermoelectric transport properties of CaMg <sub>2</sub> Bi. <i>Physical Review B</i> , 2012, 86, .	1.1	75
8955	Preferential sites for adsorption of methanol and methoxy on Pt and Pt-alloy surfaces. <i>Physica Scripta</i> , 2012, 85, 015605.	1.2	5
8956	Emergence of giant magnetic anisotropy in freestanding Au/Co nanowires. <i>Applied Physics Letters</i> , 2012, 101, 043108.	1.5	21
8957	Triplet Exciton Confinement in Green Organic Light-Emitting Diodes Containing Luminescent Charge-Transfer Cu(I) Complexes. <i>Advanced Functional Materials</i> , 2012, 22, 2327-2336.	7.8	279
8958	Ionic transfer mechanism of COS reaction with CaO: Inert marker experiment and density functional theory (DFT) calculation. <i>AIChE Journal</i> , 2012, 58, 2617-2620.	1.8	7
8959	Molecular Understanding of Enyne Hydrogenation over Palladium and Copper Catalysts. <i>ChemCatChem</i> , 2012, 4, 1420-1427.	1.8	18
8960	The Surface Chemistry of Water on Fe(100): A Density Functional Theory Study. <i>ChemPhysChem</i> , 2012, 13, 1583-1590.	1.0	35
8961	A Density Functional Theory Study on the Effect of Zero-Point Energy Corrections on the Methanation Profile on Fe(100). <i>ChemPhysChem</i> , 2012, 13, 1591-1596.	1.0	50

#	ARTICLE	IF	CITATIONS
8962	Spinâ€“Spin Artificial DNA Intercalated with Silver Cations: Theoretical Prediction. ChemPhysChem, 2012, 13, 1332-1338.	1.0	8
8963	Photocatalytic Generation of Syngas Using Combustionâ€“Synthesized Silver Bismuth Tungstate. ChemPhysChem, 2012, 13, 2945-2955.	1.0	30
8964	Tuning Metalâ€“Organic Frameworks with Open-Metal Sites and Its Origin for Enhancing CO <sub>2</sub> Affinity by Metal Substitution. Journal of Physical Chemistry Letters, 2012, 3, 826-829.	2.1	116
8965	Near room-temperature synthesis of transfer-free graphene films. Nature Communications, 2012, 3, 645.	5.8	205
8966	Theoretical Calculations on the Oxidation of CO on Au <sub>55</sub> , Ag <sub>13</sub> Au <sub>42</sub> , Au <sub>13</sub> Ag <sub>42</sub> , and Ag <sub>55</sub> Clusters of Nanometer Size. Journal of Physical Chemistry C, 2012, 116, 13196-13201.	1.5	25
8967	Molecular Dynamics Simulation: From â€œAb Initioâ€“to â€œCoarse Grainedâ€“, 2012, , 195-238.		11
8968	Adsorption and Diffusion of Li on Pristine and Defective Graphene. ACS Applied Materials & Interfaces, 2012, 4, 2432-2438.	4.0	363
8969	Assessment of density functional theory to calculate the phase transition pressure of ice. Physical Chemistry Chemical Physics, 2012, 14, 11484.	1.3	22
8970	Terraces at ohmic contact in SiC electronics: Structure and electronic states. Journal of Applied Physics, 2012, 111, 113717.	1.1	10
8971	Electronic Structure of F-Doped Bulk Rutile, Anatase, and Brookite Polymorphs of TiO <sub>2</sub> . Journal of Physical Chemistry C, 2012, 116, 12738-12746.	1.5	68
8972	Graphene-Based Vibronic Devices. Journal of Physical Chemistry C, 2012, 116, 8409-8416.	1.5	15
8973	Giant magnetoresistance in silicene nanoribbons. Nanoscale, 2012, 4, 3111.	2.8	216
8974	Mechanical properties of bcc Fe-Cr alloys by first-principles simulations. Frontiers of Physics, 2012, 7, 360-365.	2.4	20
8975	Theoretical Study of Methanol Oxidation on the PtAu(111) Bimetallic Surface: CO Pathway vs Non-CO Pathway. Journal of Physical Chemistry C, 2012, 116, 2994-3000.	1.5	72
8976	Engineering the work function of armchair graphene nanoribbons using strain and functional species: a first principles study. Journal of Physics Condensed Matter, 2012, 24, 075501.	0.7	61
8977	Nature and Structure of Aluminum Surface Sites Grafted on Silica from a Combination of High-Field Aluminum-27 Solid-State NMR Spectroscopy and First-Principles Calculations. Journal of the American Chemical Society, 2012, 134, 6767-6775.	6.6	71
8978	Structural and electronic impact of SrTiO <sub>3</sub> substrate on TiO <sub>2</sub> thin films. Journal of Materials Science, 2012, 47, 5148-5157.	1.7	11
8979	First principles investigation of L-alanine in terahertz region. Journal of Biological Physics, 2012, 38, 405-413.	0.7	29



#	ARTICLE	IF	CITATIONS
8980	Density Functional Theory Studies on the Adsorption of NH <sub>2</sub> NO <sub>2</sub> on Al <sub>13</sub> Cluster. <i>Journal of Cluster Science</i> , 2012, 23, 395-410.	1.7	6
8981	Kinetics and mechanism of the oxidative addition of methyl iodide to [Rh(CH <sub>3</sub> COCHCOF <sub>3</sub> )(CO)(P(OCH <sub>2</sub> ) <sub>3</sub> CCH <sub>3</sub> )]: an experimental and computational study. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2012, 105, 233-247.	0.8	13
8982	First-principles study of the structure, mechanical properties, and phase stability of crystalline zirconia under high pressure. <i>Structural Chemistry</i> , 2012, 23, 601-611.	1.0	13
8983	A combined crystallographic, spectroscopic, antimicrobial, and computational study of novel dipicolinate copper(II) complex with 2-(2-hydroxyethyl)pyridine. <i>Structural Chemistry</i> , 2012, 23, 659-670.	1.0	45
8984	Adsorption of 2,4,6-trinitrotoluene on Al(111) ultrathin film: periodic DFT calculations. <i>Structural Chemistry</i> , 2012, 23, 921-930.	1.0	7
8985	Reactions of Propylene Oxide on Supported Silver Catalysts: Insights into Pathways Limiting Epoxidation Selectivity. <i>Topics in Catalysis</i> , 2012, 55, 3-12.	1.3	21
8986	Aqueous Phase Glycerol Reforming by PtMo Bimetallic Nano-Particle Catalyst: Product Selectivity and Structural Characterization. <i>Topics in Catalysis</i> , 2012, 55, 53-69.	1.3	62
8987	Aqueous N <sub>2</sub> O Reduction with H <sub>2</sub> Over Pd-Based Catalyst: Mechanistic Insights From Experiment and Simulation. <i>Topics in Catalysis</i> , 2012, 55, 300-312.	1.3	11
8988	Density Functional Theory Study of Selectivity Considerations for C–C Versus C–O Bond Scission in Glycerol Decomposition on Pt(111). <i>Topics in Catalysis</i> , 2012, 55, 280-289.	1.3	41
8989	Selectivity of Adsorption of Thiophene and its Derivatives on Titania Anatase Surfaces: A Density Functional Theory Study. <i>Topics in Catalysis</i> , 2012, 55, 229-242.	1.3	9
8990	Investigation of Ti Addition Effects on the Thickness of 55 Å Pt–Al–Zn–1.6 Å Pt–Si Coating by First-Principles Calculation. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2012, 43, 2012-2017.	1.1	11
8991	The calculation of active Raman modes of $\alpha$ -quartz crystal via density functional theory based on B3LYP Hamiltonian in 6-311+G(2d) basis set. <i>Pramana - Journal of Physics</i> , 2012, 78, 803-810.	0.9	5
8992	Coordinate reduction for exploring chemical reaction paths. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	7
8993	Adsorption of successive layers of H <sub>2</sub> molecules on a model copper surface: performances of second- to fifth-rung exchange-correlation functionals. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	3
8994	Role of step sites on water dissociation on stoichiometric ceria surfaces. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	30
8995	Ab initio parametrized polarizable force field for rutile-type SnO <sub>2</sub> . <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	9
8996	Crystal-structure properties and the molecular nature of hydrostatically compressed realgar. <i>Physics and Chemistry of Minerals</i> , 2012, 39, 399-412.	0.3	12
8997	Density functional theory study of the magnetic coupling interaction in a series of binuclear oxalate complexes. <i>Monatshefte für Chemie</i> , 2012, 143, 569-577.	0.9	5



#	ARTICLE	IF	CITATIONS
8998	A theoretical study on the hydrolysis mechanism of carbon disulfide. <i>Journal of Molecular Modeling</i> , 2012, 18, 1625-1632.	0.8	18
8999	Harmonic force field for nitro compounds. <i>Journal of Molecular Modeling</i> , 2012, 18, 2805-2811.	0.8	3
9000	Structural, electronic and magnetic effects of Al-doped niobium clusters: a density functional theory study. <i>Journal of Molecular Modeling</i> , 2012, 18, 2993-3001.	0.8	17
9001	Density functional study on size-dependent structures, stabilities, electronic and magnetic properties of Au <sub>n</sub> M (M = Al and Si, n = 1-9) clusters: comparison with pure gold clusters. <i>Journal of Molecular Modeling</i> , 2012, 18, 3061-3072.	0.8	27
9002	Large gallanes and the PSEPT theory: a theoretical study of Ga <sub>n</sub> H <sub>n+2</sub> clusters (n = 7-9). <i>Journal of Molecular Modeling</i> , 2012, 18, 3321-3328.	0.8	6
9003	The structure of long period stacking/order Mg-Zn-RE phases with extended non-stoichiometry ranges. <i>Acta Materialia</i> , 2012, 60, 166-178.	3.8	374
9004	No miscibility gap in Pt-Rh binary alloys: A first-principles study. <i>Acta Materialia</i> , 2012, 60, 1093-1098.	3.8	18
9005	Integrated operando X-ray absorption and DFT characterization of Cu-SSZ-13 exchange sites during the selective catalytic reduction of NO with NH <sub>3</sub> . <i>Catalysis Today</i> , 2012, 184, 129-144.	2.2	212
9006	Recent advances in computational modeling and simulations on the An(III)/Ln(III) separation process. <i>Coordination Chemistry Reviews</i> , 2012, 256, 1406-1417.	9.5	117
9007	Theoretical investigation of the hydrogen atom transfer in the hydrated A-T base pair. <i>Chemical Physics</i> , 2012, 394, 9-16.	0.9	17
9008	Ab initio calculation of chromium oxide containing Ti dopant. <i>Chemical Physics</i> , 2012, 393, 148-152.	0.9	30
9009	Theoretical investigation on pyrolysis mechanism of glycerol. <i>Fuel</i> , 2012, 93, 92-98.	3.4	37
9010	A first principle study of SO <sub>3</sub> decomposition on silver nano-clusters: Implications toward hydrogen production. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 3645-3651.	3.8	6
9011	Structural stability, mechanical property and elastic anisotropy of TiAl-H system. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 2676-2684.	3.8	27
9012	Band gap engineering by anion doping in the photocatalyst BiTaO <sub>4</sub> : First principle calculations. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 3014-3018.	3.8	29
9013	Effects of nonmetal element (B, C and Si) additives in Mg <sub>2</sub> Ni hydrogen storage alloy: A first-principles study. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 6700-6713.	3.8	19
9014	Hydrogenation of CO on molybdenum and cobalt molybdenum carbides. <i>Applied Catalysis A: General</i> , 2012, 423-424, 192-204.	2.2	43
9015	VASP on a GPU: Application to exact-exchange calculations of the stability of elemental boron. <i>Computer Physics Communications</i> , 2012, 183, 1422-1426.	3.0	115

#	ARTICLE	IF	CITATIONS
9016	DFT study of the M segregation on MAu alloys (M=Ni, Pd, Pt) in presence of adsorbed oxygen O and O <sub>2</sub> . Chemical Physics Letters, 2012, 521, 98-103.	1.2	47
9017	Theoretical study of intermolecular magnetic interaction of chromium(V) nitrido complex self-assembly with tetradentate Schiff base ligand. Chemical Physics Letters, 2012, 523, 65-68.	1.2	2
9018	Second-order optical response of single-walled zinc oxide nanotubes from first principles calculations. Chemical Physics Letters, 2012, 529, 49-53.	1.2	3
9019	Structural, electronic and magnetic properties of single transition-metal adsorbed BN sheet: A density functional study. Chemical Physics Letters, 2012, 532, 40-46.	1.2	42
9020	Tug of war between AO-hybridization and aromaticity in dictating structures of Li-doped alkali clusters. Chemical Physics Letters, 2012, 533, 1-5.	1.2	14
9021	THz spectroscopic investigation of chlorotoluron by solid-state density functional theory. Chemical Physics Letters, 2012, 534, 72-76.	1.2	10
9022	Structural and electronic properties of Ag-Pd bimetallic clusters on Al <sub>2</sub> O <sub>3</sub> substrates: A first principles study. Chemical Physics Letters, 2012, 537, 69-74.	1.2	6
9023	Mechanical and structural stability of zirconium dihydride. International Journal of Hydrogen Energy, 2012, 37, 9688-9695.	3.8	19
9024	A periodic hybrid DFT approach (including dispersion) to MgCl <sub>2</sub> -supported Ziegler-Natta catalysts 1: TiCl <sub>4</sub> adsorption on MgCl <sub>2</sub> crystal surfaces. Journal of Catalysis, 2012, 286, 103-110.	3.1	103
9025	Accurate coverage-dependence incorporated into first-principles kinetic models: Catalytic NO oxidation on Pt (111). Journal of Catalysis, 2012, 286, 88-94.	3.1	146
9026	Deoxygenation mechanisms on Ni-promoted MoS <sub>2</sub> bulk catalysts: A combined experimental and theoretical study. Journal of Catalysis, 2012, 286, 153-164.	3.1	107
9027	Unraveling the mechanism of the NO reduction by CO on gold based catalysts. Journal of Catalysis, 2012, 289, 11-20.	3.1	36
9028	Solvent effects in the hydrogenation of 2-butanone. Journal of Catalysis, 2012, 289, 30-41.	3.1	140
9029	The electric double layer on graphite. Electrochimica Acta, 2012, 71, 82-85.	2.6	53
9030	Modification of the adsorption properties of O and OH on Pt-Ni bimetallic surfaces by subsurface alloying. Electrochimica Acta, 2012, 76, 440-445.	2.6	25
9031	Investigation of substituted 6-aminohexanoates as skin penetration enhancers. Bioorganic and Medicinal Chemistry, 2012, 20, 86-95.	1.4	6
9032	Decomposition of methylamine on Mo(100) surface: A DFT study. Journal of Natural Gas Chemistry, 2012, 21, 132-137.	1.8	8
9033	Ni-Codoped Anatase TiO <sub>2</sub> Nanocrystals with Exposed {001} Facets Through Two-Step Hydrothermal Route. Journal of the American Ceramic Society, 2012, 95, 2951-2956.	1.9	35

#	ARTICLE	IF	CITATIONS
9034	Concerning the brittleness of iridium: An elastic and electronic view. <i>Materials Chemistry and Physics</i> , 2012, 133, 140-143.	2.0	10
9035	Comparison of DFT methods for molecular structure and vibration spectra of ofloxacin calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 85, 303-309.	2.0	13
9036	Synthesis, characterization and DFT study of methoxybenzylidene containing chromophores for DSSC materials. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 239-243.	2.0	46
9037	Theoretical and experimental study on the excited states of the X-, $\hat{1}\pm$ - and $\hat{1}^2$ -forms of lithium phthalocyanine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 118-125.	2.0	9
9038	Structural stability and generalized stacking fault energies in $\hat{1}^2$ Ti $\hat{1}$ -Nb alloys: Relation to dislocation properties. <i>Scripta Materialia</i> , 2012, 66, 682-685.	2.6	35
9039	Near-surface and bulk behavior of Ag in SiC. <i>Journal of Nuclear Materials</i> , 2012, 420, 123-130.	1.3	29
9040	Thermodynamics of the Zr $\hat{1}$ -H binary system related to nuclear fuel sheathing and pressure tube hydriding. <i>Journal of Nuclear Materials</i> , 2012, 423, 87-92.	1.3	27
9041	First-principles study of surface properties of PuO <sub>2</sub> : Effects of thickness and O-vacancy on surface stability and chemical activity. <i>Journal of Nuclear Materials</i> , 2012, 426, 139-147.	1.3	40
9042	A long-range U $\hat{1}$ -Nb potential for the calculation of some chemical and physical properties of the U $\hat{1}$ -Nb system. <i>Journal of Nuclear Materials</i> , 2012, 427, 239-244.	1.3	12
9043	Oxygen adsorption on the Ag/La $\hat{1}$ <sup>x</sup> Sr $\hat{1}$ MnO <sub>3</sub> (001) catalysts surfaces: A first-principles study. <i>Journal of Power Sources</i> , 2012, 209, 158-162.	4.0	15
9044	Solid L- $\hat{1}\pm$ -alanine: Spectroscopic properties and theoretical calculations. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2012, 113, 1266-1275.	1.1	14
9045	Structural and electronic properties of Sr $\hat{1}$ Ba $\hat{1}$ <sup>x</sup> SnO <sub>3</sub> from first principles calculations. <i>Journal of Solid State Chemistry</i> , 2012, 187, 186-194.	1.4	47
9046	The T <sub>2</sub> phase in the Nb $\hat{1}$ -Si $\hat{1}$ -B system studied by ab initio calculations and synchrotron X-ray diffraction. <i>Journal of Solid State Chemistry</i> , 2012, 190, 111-117.	1.4	11
9047	Decohesion of Ti <sub>3</sub> SiC <sub>2</sub> induced by He impurities. <i>Materials Letters</i> , 2012, 83, 23-26.	1.3	22
9048	A computational study on heteroatom distribution in zeotype materials. <i>Microporous and Mesoporous Materials</i> , 2012, 158, 175-179.	2.2	14
9049	Depression of pyrite in alkaline medium and its subsequent activation by copper. <i>Minerals Engineering</i> , 2012, 26, 64-69.	1.8	58
9050	First-principles study of the methyl formate pathway of methanol steam reforming on PdZn(111) with comparison to Cu(111). <i>Journal of Molecular Catalysis A</i> , 2012, 356, 165-170.	4.8	30
9051	Molecular structure, vibrational spectra, NBO analysis, first hyperpolarizability, and HOMO, LUMO studies of mesityl chloride by density functional methods. <i>Journal of Molecular Structure</i> , 2012, 1007, 136-145.	1.8	33

#	ARTICLE	IF	CITATIONS
9052	Comparison of the performance of different DFT methods in the calculations of the molecular structure and vibration spectra of serotonin (5-hydroxytryptamine, 5-HT). <i>Journal of Molecular Structure</i> , 2012, 1013, 111-118.	1.8	9
9053	Molecular design of new hydrazone dyes for dye-sensitized solar cells: Synthesis, characterization and DFT study. <i>Journal of Molecular Structure</i> , 2012, 1019, 130-134.	1.8	39
9054	Experimental and theoretical study of pure and doped crystals: Gd <sub>2</sub> O <sub>2</sub> S, Gd <sub>2</sub> O <sub>2</sub> S:Eu <sup>3+</sup> and Gd <sub>2</sub> O <sub>2</sub> S:Tb <sup>3+</sup> . <i>Journal of Molecular Structure</i> , 2012, 1020, 153-159.	1.8	21
9055	Structural, electronic, elastic, thermodynamic and vibration properties of TbN compound from first principles calculations. <i>Solid State Sciences</i> , 2012, 14, 401-408.	1.5	22
9056	First-principles calculations of Cd-doped ZnO thin films deposited by pulse laser deposition. <i>Solid State Sciences</i> , 2012, 14, 698-704.	1.5	34
9057	Possible approach to fabricate p-type ZnO through the Be-N codoping method: First-principles calculations. <i>Solid State Communications</i> , 2012, 152, 1-4.	0.9	19
9058	Ab initio study of V doping effects on electronic structure and magnetic properties in Co <sub>2</sub> Fe <sub>1-x</sub> V <sub>x</sub> Al. <i>Solid State Communications</i> , 2012, 152, 450-454.	0.9	3
9059	Electronic structure calculations of substitutional and interstitial hydrogen in Nb. <i>Solid State Communications</i> , 2012, 152, 788-790.	0.9	11
9060	Ab initio calculation of high pressure phases and electronic properties of CuInSe <sub>2</sub> . <i>Solid State Communications</i> , 2012, 152, 775-778.	0.9	13
9061	Proton transport mechanism and pathways in the superprotonic phase of CsHSO <sub>4</sub> from experiment and theory. <i>Solid State Ionics</i> , 2012, 213, 72-75.	1.3	9
9062	The adsorption of O on (001) and (111) CdTe surfaces: A first-principles study. <i>Thin Solid Films</i> , 2012, 520, 3960-3964.	0.8	6
9063	Quasiparticle optoelectronic properties of pure and doped indium oxide. <i>Optical Materials</i> , 2012, 34, 1406-1414.	1.7	12
9064	First principles study of pressure induced structural phase transition in hydrogen storage material MgH <sub>2</sub> . <i>Physica B: Condensed Matter</i> , 2012, 407, 54-59.	1.3	12
9065	A first-principle study of the structural, elastic, lattice dynamical and thermodynamic properties of PrX (X=P, As). <i>Physica B: Condensed Matter</i> , 2012, 407, 316-323.	1.3	8
9066	Optoelectronic properties of Li <sub>x</sub> A <sub>x</sub> NbO <sub>3</sub> (A=Na, K, Rb, Cs, Fr) crystals. <i>Physica B: Condensed Matter</i> , 2012, 407, 368-377.	1.3	16
9067	Ab-initio study of the coadsorption of Li and H on Pt(001), Pt(110) and Pt(111) surfaces. <i>Physica B: Condensed Matter</i> , 2012, 407, 698-704.	1.3	13
9068	Influence of Ni and N on generalized stacking-fault energies in Fe-Cr-Ni alloy: A first principle study. <i>Physica B: Condensed Matter</i> , 2012, 407, 891-895.	1.3	24
9069	Structural, electronic and vibrational properties of InN under high pressure. <i>Physica B: Condensed Matter</i> , 2012, 407, 1008-1013.	1.3	19

#	ARTICLE	IF	CITATIONS
9070	Structure, electronic and magnetic properties of Ca-doped chromium oxide studied by the DFT method. <i>Physica B: Condensed Matter</i> , 2012, 407, 1262-1267.	1.3	24
9071	Structural, elastic and mechanical properties of orthorhombic SrHfO <sub>3</sub> under pressure from first-principles calculations. <i>Physica B: Condensed Matter</i> , 2012, 407, 2009-2013.	1.3	13
9072	First-principles investigation of Fe-doped MgSiO <sub>3</sub> -ilmenite. <i>Physica B: Condensed Matter</i> , 2012, 407, 2037-2043.	1.3	5
9073	Structural relative stabilities and pressure-induced phase transitions for lanthanide trihydrides REH <sub>3</sub> (RE=Sm, Gd, Tb, Dy, Ho, Er, Tm, and Lu). <i>Physica B: Condensed Matter</i> , 2012, 407, 2050-2057.	1.3	16
9074	Orientation effect on the electronic transport properties of C <sub>24</sub> fullerene molecule. <i>Physica B: Condensed Matter</i> , 2012, 407, 2247-2253.	1.3	9
9075	Electronic band structure, stability, structural, and elastic properties of IrTi alloys. <i>Physica B: Condensed Matter</i> , 2012, 407, 2744-2748.	1.3	3
9076	Mechanical and electronic properties of monolayer MoS <sub>2</sub> under elastic strain. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012, 376, 1166-1170.	0.9	313
9077	First-principles studies of the hydrogenation effects in silicene sheets. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012, 376, 1230-1233.	0.9	119
9078	Hydrogenation of ethene catalyzed by Ir atom deposited on $\hat{\gamma}$ -Al <sub>2</sub> O <sub>3</sub> (001) surface: From ab initio calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012, 376, 1919-1923.	0.9	5
9079	DFT studies on the reaction of CO <sub>2</sub> with allyl-bridged dinuclear palladium(I) complexes. <i>Polyhedron</i> , 2012, 32, 35-40.	1.0	27
9080	Novel mixed-ligand palladium complexes [Pd <sub>2</sub> (acac) <sub>3</sub> NO <sub>3</sub> ] and [Pd(acac)NO <sub>3</sub> ] <sub>n</sub> involving O,O- and $\hat{\beta}$ -C-bonded acetylacetonate linkers. <i>Polyhedron</i> , 2012, 31, 272-277.	1.0	10
9081	A spectroscopic, electrochemical and DFT study of para-substituted ferrocene-containing chalcone derivatives: Structure of FcCOCHCH(p-tBuC <sub>6</sub> H <sub>4</sub> ). <i>Polyhedron</i> , 2012, 33, 257-266.	1.0	49
9082	Photophysical properties of [Cu(binap) <sub>2</sub> ] <sup>+</sup> and [Pd(binap) <sub>2</sub> ] complexes: A theoretical study. <i>Polyhedron</i> , 2012, 37, 54-59.	1.0	12
9083	Structural preferences and isomerism in nickel(II) and copper(II) complexes with 3-hydroxypicolinic acid. <i>Polyhedron</i> , 2012, 39, 66-75.	1.0	10
9084	A Kohn-Sham equation solver based on hexahedral finite elements. <i>Journal of Computational Physics</i> , 2012, 231, 3166-3180.	1.9	36
9085	<sup>1</sup> H, <sup>13</sup> C MAS NMR and DFT GIAO study of quercetin and its complex with Al(III) in solid state. <i>Journal of Inorganic Biochemistry</i> , 2012, 110, 27-35.	1.5	44
9086	Phase stability, mechanical property, and electronic structure of an Mg-Ca system. <i>Journal of the Mechanical Behavior of Biomedical Materials</i> , 2012, 8, 154-164.	1.5	42
9087	Magneto optical properties of $\hat{\gamma}$ <sup>2</sup> [110] and $\hat{\gamma}$ <sup>0</sup> [100] titanium nanowires. <i>Journal of Magnetism and Magnetic Materials</i> , 2012, 324, 418-423.	1.0	5

#	ARTICLE	IF	CITATIONS
9088	Electronic structure, magnetic and electrical properties of multiferroic PbFe <sub>1/2</sub> Ta <sub>1/2</sub> O <sub>3</sub> . Journal of Magnetism and Magnetic Materials, 2012, 324, 955-960.	1.0	6
9089	Co doping effects on structural, electronic and magnetic properties in Mn <sub>2</sub> VGa. Journal of Magnetism and Magnetic Materials, 2012, 324, 1463-1467.	1.0	13
9090	A first-principles investigation of the effect of relaxation on the alloy formation in the aluminum-3d-transition-metal system. Physics of Metals and Metallography, 2012, 113, 427-437.	0.3	1
9091	Interaction of scandium and titanium atoms with a carbon surface containing five- and seven-membered rings. Journal of Experimental and Theoretical Physics, 2012, 114, 80-84.	0.2	0
9092	Adhesion at the interfaces between BCC metals and $\sqrt{3}\times\sqrt{3}$ -Al <sub>2</sub> O <sub>3</sub> . Journal of Experimental and Theoretical Physics, 2012, 114, 305-313.	0.2	12
9093	Theoretical investigation on the structure and electronic properties of bimetallic gold-zinc cluster cations and their monocarbonyls. European Physical Journal D, 2012, 66, 1.	0.6	2
9094	Adsorption of Uranyl Species onto the Rutile (110) Surface: A Periodic DFT Study. Chemistry - A European Journal, 2012, 18, 1458-1466.	1.7	37
9095	Structure and properties of the aluminum borates Al(BO <sub>2</sub> ) <sub>n</sub> and Al(BO <sub>2</sub> ) <sub>n</sub> <sup>+</sup> , ( <i>n</i> = 1-4). Journal of Computational Chemistry, 2012, 33, 416-424.	1.5	47
9096	Electronic structure and thermochemical properties of silicon-doped lithium clusters Li <sub>n</sub> Si <sup>0/+</sup> , <i>n</i> = 1-8: New insights on their stability. Journal of Computational Chemistry, 2012, 33, 800-809.	1.5	14
9097	Structure and Electronic Properties and Phase Stabilities of the Cd <sub>1-x</sub> Zn <sub>x</sub> S Solid Solution in the Range of 0% <i>x</i> %1. ChemPhysChem, 2012, 13, 147-154.	1.0	21
9098	A first-principles study of site occupancy and interfacial energetics of an H-doped TiAl-Ti <sub>3</sub> Al alloy. Science China: Physics, Mechanics and Astronomy, 2012, 55, 228-234.	2.0	12
9099	Effects of 3d Transition Metal Elements in the B <sub>2</sub> -FeAl Structure. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2012, 43, 757-762.	1.1	4
9100	Microstructure and Thickness of 55 pct Al-Zn-1.6 pct Si-0.2 pct RE Hot-Dip Coatings: Experiment, Thermodynamic, and First-Principles Study. Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science, 2012, 43, 198-205.	1.0	16
9101	Chemical bonding descriptors based on electron density inhomogeneity measure: a comparison with ELI-D. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	17
9102	Low-lying electronic excitations and optical absorption spectra of the black dye sensitizer: a first-principles study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	9
9103	Quantum mechanical calculations of the vibrational spectra of quartz- and rutile-type GeO <sub>2</sub> . Physics and Chemistry of Minerals, 2012, 39, 47-55.	0.3	32
9104	Half-sandwich ruthenium(II) complexes with N- and N,(N,O)-donor ligands: molecular, electronic structures, and computational study. Structural Chemistry, 2012, 23, 461-472.	1.0	30
9105	Theoretical Studies of Species Related to Acrolein Hydrogenation. Catalysis Letters, 2012, 142, 287-293.	1.4	3



#	ARTICLE	IF	CITATIONS
9106	A DFT study on equilibrium geometries, stabilities, and electronic properties of small bimetallic Na-doped Au <sub>n</sub> (n = 1-9) clusters: comparison with pure gold clusters. <i>Journal of Molecular Modeling</i> , 2012, 18, 329-338.	0.8	8
9107	Chemisorptions effect of oxygen on the geometries, electronic and magnetic properties of small size Ni <sub>n</sub> (n = 1-6) clusters. <i>Journal of Molecular Modeling</i> , 2012, 18, 737-749.	0.8	28
9108	Noncovalent and covalent functionalization of a (5, 0) single-walled carbon nanotube with alanine and alanine radicals. <i>Journal of Molecular Modeling</i> , 2012, 18, 771-781.	0.8	19
9109	Mechanical and electronic properties of diborides of transition 3d-5d metals from first principles: Toward search of novel ultra-incompressible and superhard materials. <i>Progress in Materials Science</i> , 2012, 57, 184-228.	16.0	183
9110	Tribology of fluorinated diamond-like carbon coatings: first principles calculations and sliding experiments. <i>Lubrication Science</i> , 2013, 25, 111-121.	0.9	17
9111	Computational modeling of standard reduction potentials of B <sub>12</sub> cofactors. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 479-488.	1.0	12
9112	Crystal structures and thermodynamic investigations of NaSc(BH <sub>4</sub> ) <sub>4</sub> from first-principles calculations. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 119-124.	1.0	6
9113	The choice of the exchange-correlation functional for the determination of the jahn-teller parameters by the density functional theory. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 859-864.	1.0	11
9114	Thermodynamics of Sc-H and Sc-D Systems: Experimental and Theoretical Studies. <i>Journal of Fusion Energy</i> , 2013, 32, 254-257.	0.5	5
9115	A density functional theory analysis of trends in glycerol decomposition on close-packed transition metal surfaces. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6475.	1.3	72
9116	Reaction mechanism on the activation of ethane C-H and C-C bonds by a diplatinum cluster. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	10
9117	Parameterization of the prosthetic redox centers of the bacterial cytochrome bc <sub>1</sub> complex for atomistic molecular dynamics simulations. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	16
9118	Analysis of the origin of lateral interactions in the adsorption of small organic molecules on oxide surfaces. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	5
9119	An insight into evolution of electronic, magnetic, optical, and vibrational properties of ultrathin Pd nanowires. <i>Journal of Nanoparticle Research</i> , 2013, 15, 1.	0.8	4
9120	First-principle study on the electronic and optical properties of the anatase TiO <sub>2</sub> (101) surface. <i>Journal of Semiconductors</i> , 2013, 34, 073004.	2.0	9
9121	A B3LYP study on the C-H activation in propane by neutral and +1 charged low-energy platinum clusters with 2-6 atoms. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2013, 109, 315-333.	0.8	9
9122	DFT investigations for the reaction mechanism of dimethyl carbonate synthesis on Pd(ii)/ $\gamma$ -zeolites. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13116.	1.3	12
9123	SAM-like arrangement of thiolated graphene nanoribbons: decoupling the edge state from the metal substrate. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 3233.	1.3	2



#	ARTICLE	IF	CITATIONS
9124	DFT Study of the Adsorption of <i>d</i> -Cysteine on Flat and Chiral Stepped Gold Surfaces. <i>Langmuir</i> , 2013, 29, 8856-8864.	1.6	50
9125	DFT study on crystalline 1,1-diamino-2,2-dinitroethylene under high pressures. <i>Journal of Molecular Modeling</i> , 2013, 19, 4039-4047.	0.8	25
9126	Theoretical Design of $\pi$ -Conjugated Heteropolycyclic Compounds Containing a Tricoordinated Boron Center. <i>Journal of Physical Chemistry C</i> , 2013, 117, 14999-15008.	1.5	13
9127	On the connection between structural distortion and magnetism in graphene with a single vacancy. <i>Solid State Communications</i> , 2013, 175-176, 71-75.	0.9	25
9128	Reactivity of TEMPO toward 16- and 17-Electron Organometallic Reaction Intermediates: A Time-Resolved IR Study. <i>Journal of the American Chemical Society</i> , 2013, 135, 11266-11273.	6.6	23
9129	Bismuth alloying properties in GaAs nanowires. <i>Journal of Solid State Chemistry</i> , 2013, 205, 44-48.	1.4	8
9130	CO <sub>2</sub> /CH <sub>4</sub> Separation in Ion-Exchanged Zeolite-like Metal Organic Frameworks with Sodalite Topology ( <i>sod</i> -ZMOFs). <i>Journal of Physical Chemistry C</i> , 2013, 117, 15647-15658.	1.5	19
9131	Theoretical investigation of ytterbium trichelates compounds. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1447-1452.	1.0	0
9132	First-principles investigation of Li ion diffusion in Li <sub>2</sub> FeSiO <sub>4</sub> . <i>Solid State Ionics</i> , 2013, 247-248, 8-14.	1.3	25
9133	The shape of Au <sub>8</sub> : gold leaf or gold nugget?. <i>Nanoscale</i> , 2013, 5, 6445.	2.8	41
9134	Structural stability of higher-energy phases in Cu and Cu-Fe alloy revealed by ab initio calculations. <i>Computational Materials Science</i> , 2013, 79, 463-467.	1.4	8
9135	Determination of the Insulation Gap of Uranium Oxides by Spectroscopic Ellipsometry and Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2013, 117, 16540-16551.	1.5	57
9136	Optical properties of cubic and rhombohedral GeTe. <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	21
9137	Formation of CO <sub>2</sub> and Ethane from Propionyl over Platinum: A Density Functional Theory Study. <i>ACS Catalysis</i> , 2013, 3, 1730-1738.	5.5	5
9138	Atomic structure, mechanical quality, and thermodynamic property of TiH <sub>x</sub> phases. <i>Journal of Applied Physics</i> , 2013, 114, 043510.	1.1	32
9139	Strain induced variations in band offsets and built-in electric fields in InGaN/GaN multiple quantum wells. <i>Journal of Applied Physics</i> , 2013, 114, .	1.1	24
9140	A density functional theory study on the interaction mechanism between H <sub>2</sub> S and the $\hat{1}\pm$ -Fe <sub>2</sub> O <sub>3</sub> (0001) surface. <i>Fuel Processing Technology</i> , 2013, 115, 26-33.	3.7	58
9141	First principles investigations of structural, electronic, elastic, and dielectric properties of KMgF <sub>3</sub> . <i>Journal of Materials Science</i> , 2013, 48, 7635-7641.	1.7	19

#	ARTICLE	IF	CITATIONS
9142	Capture of H <sub>2</sub> S from binary gas mixture by imidazolium-based ionic liquids with nonfluorous anions: A theoretical study. <i>AIChE Journal</i> , 2013, 59, 3824-3833.	1.8	26
9143	Density Functional Theory-Computed Mechanisms of Ethylene and Diethyl Ether Formation from Ethanol on [Al <sub>2</sub> O <sub>3</sub> ](100). <i>ACS Catalysis</i> , 2013, 3, 1965-1975.	5.5	130
9144	Surface electronic bands of submonolayer Ge on Ag(111). <i>Physical Review B</i> , 2013, 88, .	1.1	36
9145	Orientation dependence of elastic constants and electronic properties of rhenium nitrides first-principle calculations. <i>Journal of Materials Science</i> , 2013, 48, 4284-4296.	1.7	6
9146	Nature of the Mixed-Oxide Interface in Ceria-Titania Catalysts: Clusters, Chains, and Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2013, 117, 14463-14471.	1.5	73
9147	Adsorption of formaldehyde and formyl intermediates on Pt, PtRu-, and PtRuMo-alloy surfaces: A density functional study. <i>Applied Surface Science</i> , 2013, 266, 405-409.	3.1	10
9148	New minima for the Pt <sub>8</sub> cluster. <i>Computational Materials Science</i> , 2013, 78, 9-11.	1.4	10
9149	Nanoscale Dielectric Capacitors Composed of Graphene and Boron Nitride Layers: A First-Principles Study of High Capacitance at Nanoscale. <i>Journal of Physical Chemistry C</i> , 2013, 117, 15327-15334.	1.5	45
9150	Benchmarking of classical force fields by ab initio calculations of atomic clusters: Ti and Ni-Ti case. <i>Computational and Theoretical Chemistry</i> , 2013, 1021, 101-108.	1.1	11
9151	Two-Dimensional Materials from Data Filtering and Ab Initio Calculations. <i>Physical Review X</i> , 2013, 3, .	2.8	180
9152	Stabilization mechanism for the polar ZnO(0001) surface. <i>Physical Review B</i> , 2013, 87, .	1.1	77
9153	How relevant is the choice of classical potentials in finding minimal energy cluster conformations?. <i>Computational and Theoretical Chemistry</i> , 2013, 1021, 155-163.	1.1	8
9154	Preparation-method-dependent morphological, band structural, microstructural, and photocatalytic properties of noble metal-GaNbO <sub>4</sub> nanocomposites. <i>RSC Advances</i> , 2013, 3, 16817.	1.7	10
9155	Tailored Formation of N-Doped Nanoarchitectures by Diffusion-Controlled on-Surface (Cyclo)Dehydrogenation of Heteroaromatics. <i>ACS Nano</i> , 2013, 7, 3676-3684.	7.3	52
9156	TiO <sub>2</sub> -Based Gas Sensor: A Possible Application to SO <sub>2</sub> . <i>ACS Applied Materials &amp; Interfaces</i> , 2013, 5, 8516-8522.	4.0	186
9157	A new family of hybrid density functionals. <i>Chemical Physics Letters</i> , 2013, 580, 166-171.	1.2	104
9158	Effects of trimethylaluminum and tetrakis(ethylmethylamino) hafnium in the early stages of the atomic-layer-deposition of aluminum oxide and hafnium oxide on hydroxylated GaN nanoclusters. <i>Journal of Molecular Modeling</i> , 2013, 19, 4419-4432.	0.8	2
9159	First principle study of electronic nanoscale structure of In <sub>x</sub> Ga <sub>1-x</sub> P with variable size, shape and alloying percentage. <i>Indian Journal of Physics</i> , 2013, 87, 1079-1085.	0.9	5

#	ARTICLE	IF	CITATIONS
9160	Time-dependent quantum transport theory from non-equilibrium Green's function approach. Journal of Computational Electronics, 2013, 12, 343-355.	1.3	12
9161	Strained coherent interface energy of the Guinier-Preston II phase in Al-Cu during stress aging. Journal of Materials Science, 2013, 48, 7927-7934.	1.7	9
9162	The Formation of Hydrogen-Bond Facilitated Salts with Tunable Optical Properties: An Experimental and Theoretical Study of 2,4,5-Triphenylimidazole. Crystal Growth and Design, 2013, 13, 333-340.	1.4	25
9163	Magnetic properties of transition-metal nanoalloys. , 2013, , 247-281.		1
9164	Copper(110) surface in thermodynamic equilibrium with water vapor studied from first principles. Surface Science, 2013, 612, 82-89.	0.8	14
9165	First-Principles Investigations of Metal (Cu, Ag, Au, Pt, Rh, Pd, Fe, Co, and Ir) Doped Hexagonal Boron Nitride Nanosheets: Stability and Catalysis of CO Oxidation. Journal of Physical Chemistry C, 2013, 117, 17319-17326.	1.5	300
9166	Atomic Oxygen Chemisorption on Carbon Nanotubes Revisited with Theory and Experiment. Journal of Physical Chemistry C, 2013, 117, 1948-1954.	1.5	8
9167	Electrochemistry and time dependent DFT study of a (vinylenedithio)-TTF derivative in different oxidation states. Electrochimica Acta, 2013, 100, 188-196.	2.6	5
9168	Vacancy-cluster mechanism of metal-atom diffusion in substoichiometric carbides. Physical Review B, 2013, 87, .	1.1	31
9169	Electronic structure of oxygen-functionalized armchair graphene nanoribbons. Physical Review B, 2013, 88, .	1.1	30
9170	Pressure dependence of the phonon spectrum in BaTiO <sub>3</sub> polytypes studied by <i>ab initio</i> calculations. Physical Review B, 2013, 88, .	1.1	31
9171	Chemisorption of uracil on gold surfaces via density functional theory. Surface Science, 2013, 614, 20-23.	0.8	13
9172	Highly efficient green organic light-emitting diodes containing luminescent tetrahedral copper complexes. Journal of Materials Chemistry C, 2013, 1, 542-551.	2.7	160
9173	Density functional study of Ag <sub>n</sub> Au and Ag <sub>n</sub> clusters interaction with a single S atom. Computational and Theoretical Chemistry, 2013, 1017, 188-193.	1.1	1
9174	<i>Ab initio</i> prediction of the critical thickness of a precipitate. Journal of Physics Condensed Matter, 2013, 25, 355005.	0.7	7
9175	CO Hydrogenation on Pd(111): Competition between Fischer-Tropsch and Oxygenate Synthesis Pathways. Journal of Physical Chemistry C, 2013, 117, 14667-14676.	1.5	30
9176	Probing the structural and electronic properties of bimetallic Group-III metal-doped gold clusters: AunM <sub>2</sub> (M = Na, Mg, Al; n = 1-8). European Physical Journal D, 2013, 67, 1.	0.6	12
9177	Electronic structure and band gap engineering of ZnO-based semiconductor alloy films. Molecular Simulation, 2013, 39, 1007-1012.	0.9	3

#	ARTICLE	IF	CITATIONS
9178	Adsorption and decomposition of NH <sub>3</sub> on Ir(111): A density functional theory study. <i>Surface Science</i> , 2013, 616, 29-35.	0.8	11
9179	A first-principles study of CO hydrogenation into methane on molybdenum carbides catalysts. <i>Surface Science</i> , 2013, 614, 53-63.	0.8	48
9180	Theoretical and experimental study of the interaction of CO on TiC surfaces: Regular versus low coordinated sites. <i>Surface Science</i> , 2013, 613, 63-73.	0.8	5
9181	Monolayer Doping via Phosphonic Acid Grafting on Silicon: Microscopic Insight from Infrared Spectroscopy and Density Functional Theory Calculations. <i>Advanced Functional Materials</i> , 2013, 23, 3471-3477.	7.8	64
9182	BaTiO <sub>3</sub> : Energy, geometrical and electronic structure, relationship between optical constant and density from first-principles calculations. <i>Optical Materials</i> , 2013, 35, 2629-2637.	1.7	69
9183	Fluoropropane sultone as an SEI-forming additive that outperforms vinylene carbonate. <i>Journal of Materials Chemistry A</i> , 2013, 1, 11975.	5.2	76
9184	<sup>15</sup> N NMR spectra and reactivity of 2,4,6-triazidopyridines, 2,4,6-triazidopyrimidine and 2,4,6-triazido-s-triazine. <i>Magnetic Resonance in Chemistry</i> , 2013, 51, 562-568.	1.1	14
9185	Effect of alloying elements on in-plane ordering and disordering of solute clusters in Mg-based long-period stacking ordered structures: A first-principles analysis. <i>Scripta Materialia</i> , 2013, 69, 594-597.	2.6	54
9186	Basis set effect on defect induced spin polarization of a carbon nanotube in density functional theory calculations. <i>Chemical Physics Letters</i> , 2013, 585, 107-111.	1.2	4
9187	Experimental and Theoretical Study of the Reactions between MO <sub>2</sub> (M = Fe, Co, Ni, Cu, and Zn) Cluster Anions and Hydrogen Sulfide. <i>Journal of Physical Chemistry A</i> , 2013, 117, 8377-8387.	1.1	16
9188	CO Oxidation on Supported Single Pt Atoms: Experimental and ab Initio Density Functional Studies of CO Interaction with Pt Atom on Ir <sub>2</sub> Al <sub>2</sub> O <sub>3</sub> (010) Surface. <i>Journal of the American Chemical Society</i> , 2013, 135, 12634-12645.	6.6	535
9189	Density Functional Investigation of the Adsorption of Ethanol-Water Mixture on the Pt(111) Surface. <i>Journal of Physical Chemistry C</i> , 2013, 117, 16942-16952.	1.5	25
9190	Catalytically favorable surface patterns in Pt-Au nanoclusters. <i>RSC Advances</i> , 2013, 3, 15350.	1.7	8
9191	X-ray photoelectron spectroscopy investigation of magnetron sputtered Mg-Ti-H thin films. <i>International Journal of Hydrogen Energy</i> , 2013, 38, 10704-10715.	3.8	21
9192	Structure Sensitivity Study of Waterborne Contaminant Hydrogenation Using Shape- and Size-Controlled Pd Nanoparticles. <i>ACS Catalysis</i> , 2013, 3, 453-463.	5.5	74
9193	Variable cell nudged elastic band method for studying solid-solid structural phase transitions. <i>Computer Physics Communications</i> , 2013, 184, 2111-2118.	3.0	71
9194	First-Principles Study on the Synergistic Mechanism of SnO <sub>2</sub> and Graphene As a Lithium Ion Battery Anode. <i>Journal of Physical Chemistry C</i> , 2013, 117, 23-27.	1.5	53
9195	NH <sub>3</sub> /Ir(100): Electronic structure and dehydrogenation. <i>International Journal of Hydrogen Energy</i> , 2013, 38, 2965-2972.	3.8	16

#	ARTICLE	IF	CITATIONS
9197	Proton-Induced Dysfunction Mechanism of Cathodes in an Aqueous Lithium Ion Battery. <i>Journal of Physical Chemistry C</i> , 2013, 117, 6929-6932.	1.5	21
9198	Effect of CO and H adsorption on the compositional structure of binary nanoalloys via DFT modeling. <i>European Physical Journal D</i> , 2013, 67, 1.	0.6	13
9199	Tuning the band gap of hematite $\alpha$ -Fe <sub>2</sub> O <sub>3</sub> by sulfur doping. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2013, 377, 1943-1947.	0.9	98
9200	Structural Properties of Azobenzene Self-Assembled Monolayers by Atomistic Simulations. <i>Langmuir</i> , 2013, 29, 10505-10512.	1.6	13
9201	Defect behavior in oxides: Insights from modern atomistic simulation methods. <i>Current Opinion in Solid State and Materials Science</i> , 2013, 17, 249-256.	5.6	18
9202	Calculation of arrangement of oxygen ions and vacancies in double perovskite GdBaCo <sub>2</sub> O <sub>5+<math>\delta</math></sub> by first-principles DFT with Monte Carlo simulations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10494.	1.3	18
9203	How Well Can DFT Reproduce Key Interactions in Ziegler-Natta Systems?. <i>Macromolecular Chemistry and Physics</i> , 2013, 214, 1980-1989.	1.1	40
9204	Layered Perovskite Sr <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub> for Visible Light Photocatalysis: A First Principles Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 5043-5050.	1.5	47
9205	Ca <sup>2+</sup> - and Mg <sup>2+</sup> -doped covalent organic frameworks exhibiting high hydrogen and acetylene storage. <i>Structural Chemistry</i> , 2013, 24, 691-703.	1.0	13
9206	Aqueous Phase Glycerol Reforming with Pt and PtMo Bimetallic Nanoparticle Catalysts: The Role of the Mo Promoter. <i>Topics in Catalysis</i> , 2013, 56, 1814-1828.	1.3	32
9207	Vapor Phase Ketonization of Acetic Acid on Ceria Based Metal Oxides. <i>Topics in Catalysis</i> , 2013, 56, 1782-1789.	1.3	33
9208	How Theoretical Simulations Can Address the Structure and Activity of Nanoparticles. <i>Topics in Catalysis</i> , 2013, 56, 1262-1272.	1.3	16
9209	Near Surface Phase Transition of Solute Derived Pt Monolayers. <i>Topics in Catalysis</i> , 2013, 56, 1065-1073.	1.3	8
9210	Spectroscopic Evidences of Charge Transfer Phenomena and Stabilization of Unusual Phases at Iron Oxide Monolayers Grown on Pt(111). <i>Topics in Catalysis</i> , 2013, 56, 1074-1081.	1.3	11
9211	Local structures and structural phase change in Ni-Zr-Nb glassy alloys composed of Ni <sub>5</sub> Zr <sub>5</sub> Nb <sub>3</sub> icosahedral clusters. <i>Journal of Applied Physics</i> , 2013, 114, 063501.	1.1	9
9212	The Role of Hydrogen Bonding and Proton Transfer in the Formation of Uracil Networks on the Gold (100) Surface: A Density Functional Theory Approach. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3949-3957.	1.5	31
9213	Tailoring structural and electronic properties of RuO <sub>2</sub> nanotubes: a many-body approach and electronic transport. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14715.	1.3	23
9214	First-principles investigations on polytypes of BaTiO <sub>3</sub> : Hybrid calculations and pressure dependences. <i>Journal of the Korean Physical Society</i> , 2013, 62, 1629-1635.	0.3	7

#	ARTICLE	IF	CITATIONS
9215	Ab initio calculations on the effect of Mn substitution in the $\delta$ -carbide Fe <sub>3</sub> AlC. Journal of the Korean Physical Society, 2013, 62, 481-485.	0.3	14
9216	DFT investigations on the interaction of oxygen reduction reaction intermediates with Au (100) and bimetallic Au/M (100) (M = Pt, Cu, and Fe) surfaces. International Journal of Industrial Chemistry, 2013, 4, 33.	3.1	7
9217	Investigation on structure and dynamic property of liquid Pd-Cu-Ni-P alloys using ab initio molecular dynamics simulation. Science China Technological Sciences, 2013, 56, 376-386.	2.0	3
9218	Bonding character and formation energy of point defects of He and vacancy on (001) surface of bcc iron by first principle calculations. Acta Metallurgica Sinica (English Letters), 2013, 26, 25-32.	1.5	4
9219	Performance of Density Functional Theory for Second Row ( <i>d</i> ) Transition Metal Thermochemistry. Journal of Chemical Theory and Computation, 2013, 9, 3939-3946.	2.3	74
9220	Ultrastable silver nanoparticles. Nature, 2013, 501, 399-402.	13.7	1,023
9221	Conductance of ferro- and antiferro-magnetic single-atom contacts: A first-principles study. Journal of Applied Physics, 2013, 114, 063711.	1.1	4
9222	Efficient red phosphor double-perovskite Ca <sub>3</sub> WO <sub>6</sub> with A-site substitution of Eu <sup>3+</sup> . Dalton Transactions, 2013, 42, 13502.	1.6	39
9223	Elastic properties of an Mg-Zn-Y alloy single crystal with a long-period stacking-ordered structure. Acta Materialia, 2013, 61, 6338-6351.	3.8	125
9224	Fragmentation Energetics of Clusters Relevant to Atmospheric New Particle Formation. Journal of the American Chemical Society, 2013, 135, 3276-3285.	6.6	42
9225	Theoretical Toolkits for Inorganic and Bioinorganic Complexes: Their Applications and Insights. , 2013, , 1-57.		1
9226	Computational Methods for Solids. , 2013, , 59-87.		2
9227	Mechanism of Acyl-Enzyme Complex Formation from the Henry-Michaelis Complex of Class C $\beta$ -Lactamases with $\beta$ -Lactam Antibiotics. Journal of the American Chemical Society, 2013, 135, 14679-14690.	6.6	40
9228	On the mobility of vacancy clusters in reduced activation steels: an atomistic study in the Fe-Cr-W model alloy. Journal of Physics Condensed Matter, 2013, 25, 315401.	0.7	25
9229	Formation and characterization of VUV photolytically-induced (NH <sub>2</sub> )(NH <sub>3</sub> ) <sub>n</sub> aggregates, 0 ≤ n ≤ 3. RSC Advances, 2013, 3, 10285.	1.7	6
9230	Quantum Degeneracy in Atomic Point Contacts Revealed by Chemical Force and Conductance. Physical Review Letters, 2013, 111, 106803.	2.9	23
9231	Oxygen subsurface adsorption on the Cu(110)-c( $\sqrt{3}\times\sqrt{3}$ ) surface. Surface Science, 2013, 615, 57-64.	0.8	15
9232	Spin-flip reactions of Zr + C <sub>2</sub> H <sub>6</sub> researched by relativistic density functional theory. Journal of Molecular Modeling, 2013, 19, 4003-4012.	0.8	2



#	ARTICLE	IF	CITATIONS
9233	Molecular modeling of the piezoelectric effect in the ferroelectric polymer poly(vinylidene fluoride) (PVDF). <i>Journal of Molecular Modeling</i> , 2013, 19, 3591-3602.	0.8	78
9234	Computational comparison of the kinetic stabilities of diamino- and diamidocarbenes in the 1,2-H shift reaction. <i>Journal of Molecular Modeling</i> , 2013, 19, 2935-2944.	0.8	3
9235	Density functional studies on photophysical properties and chemical reactivities of the triarylboranes: effect of the constraint of planarity. <i>Journal of Molecular Modeling</i> , 2013, 19, 3437-3446.	0.8	11
9236	Adsorption and decomposition mechanism of hexogen (RDX) on Al(111) surface by periodic DFT calculations. <i>Journal of Molecular Modeling</i> , 2013, 19, 2451-2458.	0.8	37
9237	Theoretical study of the thermodynamic and burning properties of oxygen-rich hydrazine derivatives – green and powerful oxidants for energetic materials. <i>Journal of Molecular Modeling</i> , 2013, 19, 2583-2591.	0.8	6
9238	Assessing the quantum mechanical level of theory for prediction of linear and nonlinear optical properties of push-pull organic molecules. <i>Journal of Molecular Modeling</i> , 2013, 19, 2079-2090.	0.8	18
9239	Exotic High Activity Surface Patterns in PtAu Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2013, 117, 9275-9280.	1.5	10
9240	Theoretical analysis of the structure and bonding in electron-rich edge-bridged octahedral tungsten chloride clusters. <i>Solid State Sciences</i> , 2013, 19, 150-155.	1.5	2
9241	Localized electronic states induced by oxygen vacancies on anatase TiO <sub>2</sub> (101) surface. <i>Surface Science</i> , 2013, 616, 115-119.	0.8	45
9242	A DFT study of adsorption and decomposition of hexahydro-1,3,5-trinitro-1,3,5-triazine on Mg(0001) surface. <i>Journal of Molecular Modeling</i> , 2013, 19, 4459-4465.	0.8	1
9243	Configurational, LFDFT and NBO analysis of chromium(III) complexes of edta-type ligands. <i>Polyhedron</i> , 2013, 55, 131-143.	1.0	15
9244	Examination of Oxygen Vacancy Formation in Mn-Doped CeO <sub>2</sub> (111) Using DFT+U and the Hybrid Functional HSE06. <i>Langmuir</i> , 2013, 29, 10120-10131.	1.6	53
9245	Effect of spin ordering on structure and structural transitions in the (MnS) <sub>6</sub> magic cluster. <i>Chemical Physics Letters</i> , 2013, 556, 207-210.	1.2	3
9246	The same in the bulk but different as clusters: X <sub>3</sub> Y <sub>3</sub> (X=B, Al, Ga; Y=P, As). <i>Chemical Physics Letters</i> , 2013, 588, 37-42.	1.2	5
9247	Preparation, characterization and electronic structures of Fe-doped TiO <sub>2</sub> nanostructured fibers. <i>Materials Research Bulletin</i> , 2013, 48, 2737-2745.	2.7	17
9248	First principles methods for elpasolite halide crystal structure prediction at finite temperatures. <i>Journal of Alloys and Compounds</i> , 2013, 577, 463-468.	2.8	9
9249	First principles study of $\hat{I}^{\pm 2}$ -Ti <sub>3</sub> Al(0001) surface and $\hat{I}^{\pm 3}$ -TiAl(111)/ $\hat{I}^{\pm 2}$ -Ti <sub>3</sub> Al(0001) interfaces. <i>Applied Surface Science</i> , 2013, 276, 198-202.	3.1	27
9250	A first-principles study of structure, orbital interactions and atomic oxygen and OH adsorption on Mo-, Sc- and Y-doped nickel bimetallic clusters. <i>Journal of Alloys and Compounds</i> , 2013, 580, 37-54.	2.8	9



#	ARTICLE	IF	CITATIONS
9251	Ab initio based interface modeling for fully coherent precipitates of arbitrary size in Al alloys. <i>Computational Materials Science</i> , 2013, 72, 146-157.	1.4	12
9252	Photoelectron spectroscopy and modeling of interface properties related to organic photovoltaic cells. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2013, 190, 33-41.	0.8	26
9253	Ab initio study of the effect of solute atoms Zn and Y on stacking faults in Mg solid solution. <i>Physica B: Condensed Matter</i> , 2013, 416, 39-44.	1.3	48
9254	The effect of doping Co on the electrochemical properties of LiFePO <sub>4</sub> /C nanoplates synthesized by solvothermal route. <i>Solid State Ionics</i> , 2013, 253, 39-46.	1.3	21
9255	CuSbS <sub>2</sub> and CuBiS <sub>2</sub> as potential absorber materials for thin-film solar cells. <i>Journal of Renewable and Sustainable Energy</i> , 2013, 5, .	0.8	63
9256	Direct Observation of a Bent Carbonyl Ligand in a 19-Electron Transition Metal Complex. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2317-2324.	1.1	8
9257	On the change of preferential growth orientation in chemical vapor deposition of titanium carbide by aromatic hydrocarbon precursors. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2013, 31, .	0.9	3
9258	Molecular dynamics simulations of an electrified water/Pt(111) interface using point charge dissociative water. <i>Electrochimica Acta</i> , 2013, 101, 308-325.	2.6	21
9259	Tunable band gap in few-layer graphene by surface adsorption. <i>Scientific Reports</i> , 2013, 3, .	1.6	55
9260	Nanometer size 3d <sup>4</sup> and 3d <sup>5</sup> substitutional clusters: Promising candidates for magnetic storage applications. <i>Journal of Magnetism and Magnetic Materials</i> , 2013, 334, 31-35.	1.0	9
9261	Reaction mechanism of ethanol decomposition on Mo <sub>2</sub> C(100) investigated by the first principles study. <i>Journal of Molecular Catalysis A</i> , 2013, 377, 180-189.	4.8	32
9262	First-principle insights into the catalytic role of indium oxide in methanol steam reforming. <i>Chinese Journal of Catalysis</i> , 2013, 34, 1855-1860.	6.9	11
9263	Electronic and optical performances of Si and Fe-codoped TiO <sub>2</sub> nanoparticles: A photocatalyst for the degradation of methylene blue. <i>Applied Catalysis B: Environmental</i> , 2013, 142-143, 38-44.	10.8	24
9264	Methane dissociation on Pt(111), Ir(111) and PtIr(111) surface: A density functional theory study. <i>Applied Surface Science</i> , 2013, 284, 784-791.	3.1	60
9265	Density functional theory study of neutral and oxidized thiophene oligomers. <i>Journal of Chemical Physics</i> , 2013, 139, 184905.	1.2	9
9266	Structure and stability of acrolein and allyl alcohol networks on Ag(111) from density functional theory based calculations with dispersion corrections. <i>Surface Science</i> , 2013, 617, 175-182.	0.8	6
9267	The initial stage of atmospheric corrosion on interstitial free steel investigated by in situ SPM. <i>Corrosion Science</i> , 2013, 70, 188-193.	3.0	24
9268	Ab initio prediction of the first and second pressure derivatives of isothermal bulk modulus for the high-pressure rocksalt phase of ZnO. <i>Chemical Physics Letters</i> , 2013, 559, 46-49.	1.2	3

#	ARTICLE	IF	CITATIONS
9269	Ab initio study of the structural, elastic, and thermodynamic properties of tungsten monocarbide at high pressure and high temperature. <i>Physica B: Condensed Matter</i> , 2013, 413, 109-115.	1.3	9
9270	Study of the Zn occupancy leading to the stability improvement for Cu <sub>6</sub> Sn <sub>5</sub> using a first-principles approach. <i>Materials Letters</i> , 2013, 93, 300-303.	1.3	19
9271	Depression effect of pseudo glycolylthiourea acid in flotation separation of copper–molybdenum. <i>Transactions of Nonferrous Metals Society of China</i> , 2013, 23, 824-831.	1.7	56
9272	Dinuclear gold(I) and gold(III) complexes involving di(N-heterocyclic carbene) ligands – Synthesis, characterization and DFT studies. <i>Journal of Organometallic Chemistry</i> , 2013, 745-746, 242-250.	0.8	20
9273	Vibrationally Resolved Photoelectron Imaging of Cu <sub>2</sub> H <sup>+</sup> and AgCuH <sup>+</sup> and Theoretical Calculations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1706-1711.	1.1	8
9274	A first-principles study of the diffusion of atomic oxygen in nickel. <i>Corrosion Science</i> , 2013, 75, 248-255.	3.0	21
9275	Poly(p-phenylenediamine) fluorescent nanosphere: A ultra-sensitive fluorescent probe for caffeine. <i>Synthetic Metals</i> , 2013, 181, 86-91.	2.1	38
9276	Theoretical Study of the Structures and Chemical Ordering of Palladium–Gold Nanoalloys Supported on MgO(100). <i>Journal of Physical Chemistry C</i> , 2013, 117, 293-301.	1.5	30
9277	First principles investigation on the stability, magnetic and electronic properties of the fully and partially hydrogenated BN nanoribbons in different conformers. <i>Journal of Materials Chemistry C</i> , 2013, 1, 6890.	2.7	17
9278	Stereoselectivity of A-ring contraction for 3-oxotriterpenoids. <i>RSC Advances</i> , 2013, 3, 19057.	1.7	6
9279	The Effect of Metal–Cation Vacancies on Vanadium Antimonate Surface Properties. A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 20548-20556.	1.5	4
9280	–Conjugated Molecules Containing Naphtho[2,3- <i>b</i> ]thiophene and Their Derivatives: Theoretical Design for Organic Semiconductors. <i>Journal of Physical Chemistry C</i> , 2013, 117, 10175-10184.	1.5	50
9281	Shock-induced plasticity in tantalum single crystals: Interatomic potentials and large-scale molecular-dynamics simulations. <i>Physical Review B</i> , 2013, 88, .	1.1	216
9282	How a single aluminum atom makes a difference to gallium: First-principles simulations of bimetallic cluster melting. <i>Journal of Chemical Physics</i> , 2013, 139, 094309.	1.2	9
9283	Water adsorption and dissociation on Ni surface: Effects of steps, dopants, coverage and self-aggregation. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17804.	1.3	28
9284	Predicting a new photocatalyst and its electronic properties by density functional theory. <i>Journal of Applied Physics</i> , 2013, 114, .	1.1	24
9285	Softening of hydroxyapatite by vacancies: A first principles investigation. <i>Materials Science and Engineering C</i> , 2013, 33, 1109-1115.	3.8	35
9286	Thermodynamic assessment of the Ga–X (X=B, Ca, Sr, Ba) systems supported by first-principles calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2013, 43, 52-60.	0.7	8

#	ARTICLE	IF	CITATIONS
9287	$\hat{\text{T}}\text{-Technetium Dichloride: Solid-State Modulated Structure, Electronic Structure, and Physical Properties. Journal of the American Chemical Society, 2013, 135, 15955-15962.}$	6.6	10
9288	Electronic Structure Assessment: Combined Density Functional Theory Calculations and Ru L <sub>2,3</sub> -Edge X-ray Absorption Near-Edge Spectroscopy of Water Oxidation Catalyst. Journal of Physical Chemistry C, 2013, 117, 18994-19001.	1.5	7
9289	Reactive high power impulse magnetron sputtering of CF <sub>x</sub> thin films in mixed Ar/CF <sub>4</sub> and Ar/C <sub>4</sub> F <sub>8</sub> discharges. Thin Solid Films, 2013, 542, 21-30.	0.8	17
9290	Study of $\text{H}_2$ physical adsorption in single-walled carbon nanotube array. AIP Advances, 2013, 3, .	0.6	20
9291	Quantum Chemical Free Energies: Structure Optimization and Vibrational Frequencies in Normal Modes. Journal of Chemical Theory and Computation, 2013, 9, 5038-5045.	2.3	53
9292	Structure and Stability of Zn, Cd, and Hg Atom Doped Golden Fullerene ( $\text{Au}_{32}$ ). Journal of Physical Chemistry C, 2013, 117, 18777-18788.	1.5	16
9293	Synthesis of Phosphorus Included Multiwalled Carbon Nanotubes by Pyrolysis of Sucrose. Journal of Physical Chemistry C, 2013, 117, 24554-24560.	1.5	3
9294	Deliquescence of NaBH <sub>4</sub> from Density Functional Theory and Experiments. Industrial & Engineering Chemistry Research, 2013, 52, 13849-13861.	1.8	4
9295	Improving Photocatalytic $\text{H}_2$ Evolution of TiO <sub>2</sub> via Formation of {001}–{010} Quasi-Heterojunctions. Journal of Physical Chemistry C, 2013, 117, 22894-22902.	1.5	38
9296	Incorporation of Lithium by MgH <sub>2</sub> : An Ab Initio Study. Journal of Physical Chemistry C, 2013, 117, 22467-22477.	1.5	23
9297	Peri-Substituted (Ace)Naphthylphosphinoboranes. (Frustrated) Lewis Pairs. Inorganic Chemistry, 2013, 52, 11881-11888.	1.9	48
9298	Anion-Doped NaTaO <sub>3</sub> for Visible Light Photocatalysis. Journal of Physical Chemistry C, 2013, 117, 22518-22524.	1.5	71
9299	Experimental and Computational Investigation of Effect of Sr on NO Oxidation and Oxygen Exchange for La <sub>1-x</sub> Sr <sub>x</sub> CoO <sub>3</sub> Perovskite Catalysts. ACS Catalysis, 2013, 3, 2719-2728.	5.5	74
9300	Water adsorption on a copper formate paddlewheel model of CuBTC: A comparative MP2 and DFT study. Chemical Physics Letters, 2013, 587, 7-13.	1.2	40
9301	Design of Nanosensors for Fissile Materials in Nuclear Waste Water. Journal of Physical Chemistry C, 2013, 117, 24033-24041.	1.5	22
9302	Atomic structure and edge magnetism in MoS <sub>2+x</sub> parallelogram shaped platelets. Physical Chemistry Chemical Physics, 2013, 15, 13077.	1.3	3
9303	Revision of the Li–Si Phase Diagram: Discovery and Single-Crystal X-ray Structure Determination of the High-Temperature Phase Li <sub>4.11</sub> Si. Chemistry of Materials, 2013, 25, 4623-4632.	3.2	51
9304	Electronic and magnetic properties of an organic multiferroic: (C <sub>2</sub> H <sub>5</sub> NH <sub>3</sub> ) <sub>2</sub> CuCl <sub>4</sub> . Journal of Magnetism and Magnetic Materials, 2013, 346, 91-95.	1.0	14

#	ARTICLE	IF	CITATIONS
9305	LiNb <sub>1-x</sub> Ta <sub>x</sub> O <sub>3</sub> Electronic Structure and Optical Response from First-Principles Calculations. <i>Ferroelectrics</i> , 2013, 447, 78-85.	0.3	6
9306	Interface energy determination for the fully coherent $\hat{2}\hat{3}$ phase in Al-Mg-Si: making a case for a first principles based hybrid atomistic modelling scheme. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2013, 21, 085018.	0.8	8
9307	Optical and Vibrational Studies of Partially Edge-Terminated Vertically Aligned Nanocrystalline MoS <sub>2</sub> Thin Films. <i>Journal of Physical Chemistry C</i> , 2013, 117, 26262-26268.	1.5	51
9308	Conformers of hydrogenated SiC honeycomb structure: A first principles study. <i>AIP Advances</i> , 2013, 3, 082136.	0.6	9
9309	Iron porphyrin molecules on Cu(001): Influence of adlayers and ligands on the magnetic properties. <i>Physical Review B</i> , 2013, 87, .	1.1	33
9310	First principles study of hydroxyapatite surface. <i>Journal of Chemical Physics</i> , 2013, 139, 044714.	1.2	40
9311	Quantum Monte Carlo studies of 13-atom simple metallic clusters. <i>Physical Review B</i> , 2013, 88, .	1.1	19
9312	A computational investigation of CO oxidation on ruthenium-embedded hexagonal boron nitride nanosheet. <i>Computational and Theoretical Chemistry</i> , 2013, 1011, 5-10.	1.1	107
9313	Electrical and Photoresponse Properties of Printed Thin-Film Transistors Based on Poly(9,9-dioctylfluorene-co-bithiophene) Sorted Large-Diameter Semiconducting Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2013, 117, 18243-18250.	1.5	76
9314	Activation energetics of actinide diffusion in UO <sub>2</sub> from first-principles calculations. <i>Journal of Nuclear Materials</i> , 2013, 433, 424-430.	1.3	9
9315	Acetate coverage effect on the reactivity of vinyl acetate synthesis on Pd/Au alloy surfaces. <i>Journal of Energy Chemistry</i> , 2013, 22, 671-679.	7.1	25
9316	Improvement in hydrogen storage characteristics of Mg-based metal hydrides by doping nonmetals with high electronegativity: A first-principle study. <i>Computational Materials Science</i> , 2013, 78, 83-90.	1.4	29
9317	Reactivity of metal oxide clusters with hydrogen peroxide and water – a DFT study evaluating the performance of different exchange-correlation functionals. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5539.	1.3	73
9318	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 355-363.	2.3	68
9319	First-principles DFT+U modeling of defect behaviors in anti-ferromagnetic uranium mononitride. <i>Journal of Applied Physics</i> , 2013, 114, .	1.1	21
9320	Study of geometry and electronic structure of molecules, cation-radicals, and anion-radicals of nitromethane, dimethylnitramine, and ethyl nitrate. <i>Russian Journal of General Chemistry</i> , 2013, 83, 1823-1839.	0.3	2
9321	Beyond standard local density approximation in the study of magnetoelectric effects in Fe/BaTiO <sub>3</sub> and Co/BaTiO <sub>3</sub> interfaces. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 066001.	0.7	14
9322	Calculation of Heats of Formation for Zn Complexes: Comparison of Density Functional Theory, Second Order Perturbation Theory, Coupled-Cluster and Complete Active Space Methods. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5277-5285.	2.3	23

#	ARTICLE	IF	CITATIONS
9323	Formation of TbCu <sub>7</sub> -type CeFe <sub>10</sub> Zr <sub>0.8</sub> by rapid solidification. Journal of Alloys and Compounds, 2013, 569, 6-8.	2.8	16
9324	An <i>in</i> -body potential for a Zr–Nb system based on the embedded-atom method. Journal of Physics Condensed Matter, 2013, 25, 105404.	0.7	23
9325	Quasiparticle semiconductor band structures including spin–orbit interactions. Journal of Physics Condensed Matter, 2013, 25, 105503.	0.7	55
9326	First-principles study on the structure, elastic properties, hardness and electronic structure of TM <sub>4</sub> (TM=Cr, Re, Ru and Os) compounds. Journal of Solid State Chemistry, 2013, 207, 29-34.	1.4	34
9327	Theoretical investigation of electronic and magnetic properties of HoRh layers. Journal of Magnetism and Magnetic Materials, 2013, 344, 220-223.	1.0	9
9328	Testing density functionals for structural phase transitions of solids under pressure: Si, SiO <sub>2</sub> , and Zr. Physical Review B, 2013, 88, .	1.1	87
9329	DFT model cluster studies of O <sub>2</sub> adsorption on hydrogenated titania sub-nanoparticles. Journal of Molecular Modeling, 2013, 19, 5063-5073.	0.8	14
9330	Self-stopping effects of lithium penetration into silicon nanowires. Nanoscale, 2013, 5, 12394.	2.8	3
9331	DFT study of iron impurity in ZrSiO <sub>4</sub> . Journal of Magnetism and Magnetic Materials, 2013, 344, 217-219.	1.0	2
9332	Adsorption of Carbon Dioxide on Al <sub>12</sub> X Clusters Studied by Density Functional Theory: Effect of Charge and Doping. Journal of Physical Chemistry A, 2013, 117, 12519-12528.	1.1	14
9333	Calculating Hyperfine Couplings in Large Ionic Crystals Containing Hundreds of QM Atoms: Subsystem DFT Is the Key. Journal of Physical Chemistry B, 2013, 117, 13967-13974.	1.2	15
9334	Effects of alloying and transmutation impurities on stability and mobility of helium in tungsten under a fusion environment. Nuclear Fusion, 2013, 53, 073049.	1.6	43
9335	Comparison of ReaxFF, DFTB, and DFT for Phenolic Pyrolysis. 2. Elementary Reaction Paths. Journal of Physical Chemistry A, 2013, 117, 11126-11135.	1.1	41
9336	Comparison of ReaxFF, DFTB, and DFT for Phenolic Pyrolysis. 1. Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2013, 117, 11115-11125.	1.1	88
9337	Nonstoichiometry and relative stabilities of Y <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub> polar surfaces: A density functional theory prediction. Acta Materialia, 2013, 61, 7260-7270.	3.8	27
9338	Synthetic Route to Metal Nitrides: High-Pressure Solid-State Metathesis Reaction. Inorganic Chemistry, 2013, 52, 13356-13362.	1.9	44
9339	The millimetre-wave spectrum of estragole. Chemical Physics Letters, 2013, 580, 37-42.	1.2	4
9340	Case study of Rb <sup>+</sup> (aq), quasi-chemical theory of ion hydration, and the no split occupancies rule. Annual Reports on the Progress of Chemistry Section C, 2013, 109, 266.	4.4	31

#	ARTICLE	IF	CITATIONS
9341	Electron tunneling characteristics of a cubic quantum dot, (PbS) <sub>32</sub> . Journal of Chemical Physics, 2013, 139, 244307.	1.2	13
9342	Efficient N <sub>2</sub> Formation on Ag(111) by Eley-Rideal Recombination of Hyperthermal Atoms. Journal of Physical Chemistry Letters, 2013, 4, 3704-3709.	2.1	32
9343	Face-Capping $\frac{1}{3}$ -BO in B <sub>6</sub> (BO) <sub>7</sub> : Boron Oxide Analogue of B <sub>6</sub> H <sub>7</sub> with Rhombic 4c <sup>2e</sup> Bonds. Journal of Physical Chemistry A, 2013, 117, 11587-11591.	1.1	12
9344	Shock-induced phase transformations in gallium single crystals by atomistic methods. Physical Review B, 2013, 88, .	1.1	15
9345	Energy stabilization of the $s$ -symmetry superatom molecular orbital by endohedral doping of C <sub>82</sub> fullerene with a lanthanum atom. Physical Review B, 2013, 88, .	1.1	13
9346	A density functional theory study on oxygen reduction reaction on nitrogen-doped graphene. Journal of Molecular Modeling, 2013, 19, 5515-5521.	0.8	42
9347	Structural and elastic properties of La <sub>2</sub> Mg <sub>17</sub> from first-principles calculations. Journal of Solid State Chemistry, 2013, 206, 272-276.	1.4	3
9348	7D Quantum Dynamics of H <sub>2</sub> Scattering from Cu(111): The Accuracy of the Phonon Sudden Approximation. Zeitschrift Fur Physikalische Chemie, 0, , 130617035227002.	1.4	17
9349	Lead oxide-modified TiO <sub>2</sub> photocatalyst: tuning light absorption and charge carrier separation by lead oxidation state. Catalysis Science and Technology, 2013, 3, 2000.	2.1	36
9350	Thermodynamic assessment of Sn-Cu-Ce system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2013, 43, 124-132.	0.7	8
9351	Electronic structure study of N, O related defects in GaP for photoelectrochemical applications. Journal of Materials Chemistry A, 2013, 1, 8425.	5.2	4
9352	Theoretical study of the structural phase transformation and elastic properties of the zirconium nitride under high pressure. Solid State Sciences, 2013, 17, 1-5.	1.5	12
9353	An Atomistic Study of Perfluoropolyether Lubricant Thermal Stability in Heat Assisted Magnetic Recording. IEEE Transactions on Magnetics, 2013, 49, 3748-3751.	1.2	3
9354	Can CO <sub>2</sub> molecule adsorb effectively on Al-doped boron nitride single walled nanotube?. Applied Surface Science, 2013, 285, 350-356.	3.1	47
9355	Electrochemical potentials of layered oxide and olivine phosphate with aluminum substitution: A first principles study. Bulletin of Materials Science, 2013, 36, 1331-1337.	0.8	3
9356	Optical response of stoichiometric and congruent lithium niobate from first-principles calculations. Physical Review B, 2013, 87, .	1.1	39
9357	Structural and electronic properties of $\frac{1}{2}$ -tin nanocrystals from first principles. Physical Review B, 2013, 87, .	1.1	29
9358	Effect of chemical and hydrostatic pressures on structural and magnetic properties of rare-earth orthoferrites: a first-principles study. Journal of Physics Condensed Matter, 2013, 25, 466002.	0.7	33



#	ARTICLE	IF	CITATIONS
9360	Theoretical investigation on helium incorporation in Ti <sub>3</sub> AlC <sub>2</sub> . Nuclear Instruments & Methods in Physics Research B, 2013, 304, 27-31.	0.6	26
9361	First-principles studies of the structural, elastic, electronic and thermal properties of $\hat{\Gamma}$ -Ni <sub>3</sub> Ti. Physica B: Condensed Matter, 2013, 412, 45-49.	1.3	20
9362	Mechanism of ammonia decomposition and oxidation on Ir(110): A first-principles study. Journal of Chemical Physics, 2013, 138, 144703.	1.2	10
9363	First-principles study of hydrogen vacancies in lithium amide doped with titanium and niobium. International Journal of Hydrogen Energy, 2013, 38, 11303-11312.	3.8	9
9364	Phase transition and thermodynamic properties of ThO <sub>2</sub> from first-principles calculations. Physica B: Condensed Matter, 2013, 423, 77-81.	1.3	5
9365	Disorder-Order Transformation and Significant Dislocation Motion Cooperating with a Surprisingly Large Hysteretic Magnetic Transition in a Nickel-Bisdithiolene Spin System. Inorganic Chemistry, 2013, 52, 3870-3877.	1.9	19
9366	High pressure induced structural, elastic and electronic properties of Calcium Chalcogenides CaX (X=S, Se and Te) via first-principles calculations. Computational Materials Science, 2013, 68, 325-334.	1.4	17
9367	Speciation of [Cp* <sub>2</sub> M <sub>2</sub> O <sub>5</sub> ] in Polar and Donor Solvents. Chemistry - A European Journal, 2013, 19, 3969-3985.	1.7	3
9368	Mechanical and electronic properties of Al <sup>x</sup> B <sub>x</sub> Hy (A and B=Ti, Zr, Hf) hydride alloys: A first-principles study. Journal of Alloys and Compounds, 2013, 581, 404-412.	2.8	5
9369	Pressure-induced phase transition for ScVO <sub>4</sub> : A first-principles study. Physica B: Condensed Matter, 2013, 426, 20-23.	1.3	3
9370	Edge-adsorption of potassium adatoms on graphene nanoribbon: A first principle study. Applied Surface Science, 2013, 280, 698-704.	3.1	19
9371	First-principles study of hydrogen storage on Li-decorated silicene. Journal of Nanoparticle Research, 2013, 15, 1.	0.8	23
9372	Effect of van der Waals interactions on H <sub>2</sub> dissociation on clean and defected Ru(0001) surface. European Physical Journal B, 2013, 86, 1.	0.6	6
9373	The structure of minimal magnetite cluster. Russian Journal of General Chemistry, 2013, 83, 1493-1500.	0.3	4
9374	Multiferroicity in vanadium-doped La <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub> : insights from first principles. European Physical Journal B, 2013, 86, 1.	0.6	12
9375	Magnetic interactions between native defects in ZnO: A first-principles study. Journal of the Korean Physical Society, 2013, 63, 2170-2174.	0.3	1
9376	A DFT study on CO oxidation on Pd <sub>4</sub> and Rh <sub>4</sub> clusters and adsorbed Pd and Rh atoms on CeO <sub>2</sub> and Ce <sub>0.75</sub> Zr <sub>0.25</sub> O <sub>2</sub> supports for TWC applications. Applied Surface Science, 2013, 285, 927-936.	3.1	19
9377	Mechanism and Enantioselectivity in Palladium-Catalyzed Conjugate Addition of Arylboronic Acids to $\hat{\Gamma}$ -Substituted Cyclic Enones: Insights from Computation and Experiment. Journal of the American Chemical Society, 2013, 135, 14996-15007.	6.6	131



#	ARTICLE	IF	CITATIONS
9378	Surface diffusion and coverage effect of Li atom on graphene as studied by several density functional theory methods. <i>Applied Surface Science</i> , 2013, 285, 846-852.	3.1	11
9379	Theoretical identification of carbonate geometry in zeolites from IR spectra. <i>Microporous and Mesoporous Materials</i> , 2013, 173, 15-21.	2.2	12
9380	One Site Is Enough: A Theoretical Investigation of Iron-Catalyzed Dehydrogenation of Formic Acid. <i>Chemistry - A European Journal</i> , 2013, 19, 11869-11873.	1.7	29
9381	First-principles study of H <sub>2</sub> adsorption on the pristine and oxidized (8,0) carbon nanotube. <i>International Journal of Hydrogen Energy</i> , 2013, 38, 13680-13686.	3.8	21
9382	Modern quantum chemical methods for calculating spin-spin coupling constants: theoretical basis and structural applications in chemistry. <i>Russian Chemical Reviews</i> , 2013, 82, 99-130.	2.5	107
9383	Characterization of small pure and Ni-doped titanium clusters: Ab initio versus classical approaches. <i>Computational Materials Science</i> , 2013, 76, 80-88.	1.4	17
9384	Investigation of boron antimonide as hot carrier absorber material. <i>Solar Energy Materials and Solar Cells</i> , 2013, 111, 123-126.	3.0	27
9385	DFT Studies on Doping Effect of Al <sub>12</sub> X: Adsorption and Dissociation of H <sub>2</sub> O on Al <sub>12</sub> X Clusters. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2213-2222.	1.1	21
9386	Significant role of surface activation on Pd enriched Pt nano catalysts in promoting the electrode kinetics of ethanol oxidation: Temperature effect, product analysis & theoretical computations. <i>International Journal of Hydrogen Energy</i> , 2013, 38, 7789-7800.	3.8	33
9387	Stacking Principle and Magic Sizes of Transition Metal Nanoclusters Based on Generalized Wulff Construction. <i>Physical Review Letters</i> , 2013, 111, 115501.	2.9	53
9388	Ordered bilayer ruthenium-platinum core-shell nanoparticles as carbon monoxide-tolerant fuel cell catalysts. <i>Nature Communications</i> , 2013, 4, 2466.	5.8	200
9389	On the thermal stability of late blooming phases in reactor pressure vessel steels: An atomistic study. <i>Journal of Nuclear Materials</i> , 2013, 442, 282-291.	1.3	83
9390	Electronic and magnetic properties of silicene nanoflakes by first-principles calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2013, 377, 2792-2795.	0.9	12
9391	Theory analysis and vestigial information of surface relaxation of natural chalcopyrite mineral crystal. <i>Transactions of Nonferrous Metals Society of China</i> , 2013, 23, 796-803.	1.7	14
9392	Non-Innocent Ligand Effects on Low-Oxidation State Indium Complexes. <i>Chemistry - A European Journal</i> , 2013, 19, 14470-14483.	1.7	25
9393	Effect of chemical pressure, misfit strain and hydrostatic pressure on structural and magnetic behaviors of rare-earth orthochromates. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 385604.	0.7	32
9394	Raman-scattering measurements and first-principles calculations of strain-induced phonon shifts in monolayer MoS <sub>2</sub> . <i>Physical Review B</i> , 2013, 87, .	1.1	495
9395	The high-capacity hydrogen storage abilities of the Ti atoms coated Si@Al <sub>12</sub> clusters. <i>Chemical Physics Letters</i> , 2013, 586, 116-120.	1.2	2

#	ARTICLE	IF	CITATIONS
9396	The investigation of NbO <sub>2</sub> and Nb <sub>2</sub> O <sub>5</sub> electronic structure by XPS, UPS and first principles methods. <i>Surface and Interface Analysis</i> , 2013, 45, 1206-1210.	0.8	112
9397	Crystal and electronic structures of tris[4,4,4-Trifluoro-1-(2-X)-1,3-butanedionato]iron(III) isomers (X=thienyl or furyl): An X-ray and computational study. <i>Journal of Molecular Structure</i> , 2013, 1053, 134-140.	1.8	21
9398	Giant photovoltaic effects driven by residual polar field within unit-cell-scale LaAlO <sub>3</sub> films on SrTiO <sub>3</sub> . <i>Scientific Reports</i> , 2013, 3, 1975.	1.6	44
9399	Double-shell C <sub>60</sub> /C <sub>240</sub> fullerenes with Stone-Wales defects for hydrogen storage: An <i>ab initio</i> study. <i>Journal of Applied Physics</i> , 2013, 114, .	1.1	5
9400	First-principles modeling of C <sub>60</sub> @Cr-graphene nanostructures for supporting metal clusters. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 19395.	1.3	7
9401	First-principles study of helium, carbon, and nitrogen in austenite, dilute austenitic iron alloys, and nickel. <i>Physical Review B</i> , 2013, 88, .	1.1	71
9402	Lithium Adsorption on Hexagonal Boron Nitride Nanosheet Using Dispersion-Corrected Density Functional Theory Calculations. <i>Japanese Journal of Applied Physics</i> , 2013, 52, 06GG08.	0.8	20
9403	Electronic and Structural Properties of Neutral, Anionic, and Cationic Rh <sub>x</sub> Cu <sub>4-x</sub> (x=0-4) Small Clusters: A DFT Study. <i>Journal of Cluster Science</i> , 2013, 24, 273-287.	1.7	25
9404	Comparative study on the performance of exchange and correlation in wide-gap semiconductors: the case of BeS, BeSe, and BeTe. <i>Journal of Materials Science</i> , 2013, 48, 5499-5508.	1.7	6
9405	Semiconducting layered technetium dichalcogenides: insights from first-principles. <i>Dalton Transactions</i> , 2013, 42, 15288.	1.6	23
9406	A multinuclear solid state NMR, density functional theory and X-Ray diffraction study of hydrogen bonding in Group I hydrogen dibenzoates. <i>CrystEngComm</i> , 2013, 15, 8823.	1.3	24
9407	Improved binding and stability in Si/CNT hybrid nanostructures via interfacial functionalization: a first-principles study. <i>RSC Advances</i> , 2013, 3, 8446.	1.7	12
9408	Water and ammonia on Cu{110}: comparative structure and bonding. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4785.	1.3	14
9409	Strain-induced Dirac cone-like electronic structures and semiconductor-semimetal transition in graphdiyne. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 8179.	1.3	81
9410	[Co(CN) <sub>2</sub> (CO) <sub>3</sub> ] <sup>-</sup> , a new discovery from an 80-year-old reaction. <i>Chemical Communications</i> , 2013, 49, 7382.	2.2	4
9411	First-principles melting of gallium clusters down to nine atoms: structural and electronic contributions to melting. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 15325.	1.3	37
9412	Bilayer silicene with an electrically-tunable wide band gap. <i>RSC Advances</i> , 2013, 3, 21943.	1.7	32
9413	Evolution of geometrical structures, stabilities and electronic properties of neutral and anionic LinCu <sub>l</sub> (n=0, 1, 9, l=0, 1) clusters: compare with pure lithium clusters. <i>Molecular Physics</i> , 2013, 111, 569-580.	0.8	7

#	ARTICLE	IF	CITATIONS
9414	Adsorption of hydrogen on the surface and sub-surface of Cu(111). <i>Journal of Chemical Physics</i> , 2013, 139, 044712.	1.2	38
9415	The Effect of Spin-Orbit Coupling on the Electronic Structures and Half-Metallicity of Heusler Compounds: $V_{1-x}Z_{2x}ReZ$ ( $Z=Al, Ga, In$ ). <i>Advanced Materials Research</i> , 0, 683, 211-217.	0.3	0
9416	Adsorption of Sulfur-Containing Species on $LaCrO_3$ (001) Surface: A First-Principles Study. <i>Fuel Cells</i> , 2013, 13, 1040-1047.	1.5	3
9417	Are trinuclear superhalogens promising candidates for building blocks of novel magnetic materials? A theoretical prospect from combined broken-symmetry density functional theory and ab initio study. <i>Journal of Chemical Physics</i> , 2013, 139, 054305.	1.2	39
9418	Fundamental Insight into the Substrate-Dependent Ripening of Monodisperse Clusters. <i>ChemCatChem</i> , 2013, 5, 3330-3341.	1.8	52
9419	Pressure effects on structural, electronic, absorption, and thermodynamic properties of crystalline 2,4,6-triamino-3,5-dinitropyridine-1-oxide: A DFT study. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 589-595.	0.9	6
9420	Density Functional Theory Methods for Electrocatalysis. <i>RSC Catalysis Series</i> , 2013, , 116-156.	0.1	5
9421	Effective band gap reduction of titanium oxide semiconductors by codoping from first-principles calculations. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2546-2553.	1.0	14
9422	The CO oxidation mechanism and reactivity on PdZn alloys. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 7768.	1.3	55
9423	Influence of natural adsorbates of magnesium oxide on its reactivity in basic catalysis. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 19870.	1.3	15
9424	Structure and stress of $Re(112\bar{1},1)$ ; chiral terraces at a racemic surface. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 20823.	1.3	2
9425	Investigation of work function and surface energy of aluminum: An ab-initio study. , 2013, , .		5
9426	Triisobutylaluminum: bulkier and yet more reactive towards silica surfaces than triethyl or trimethylaluminum. <i>Dalton Transactions</i> , 2013, 42, 12681.	1.6	35
9427	Regular assembly of 9-fluorenone-2,7-dicarboxylate within layered double hydroxide and its solid-state photoluminescence: a combined experiment and computational study. <i>RSC Advances</i> , 2013, 3, 4303.	1.7	26
9428	Theoretical study of water adsorption and dissociation on $Ta_3N_5(100)$ surfaces. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 16054.	1.3	28
9429	Investigation of the surface chemistry of phosphine-stabilized ruthenium nanoparticles – an advanced solid-state NMR study. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17383.	1.3	29
9430	Electron spin resonance parameters of cation vacancies in tin dioxide doped with fluorine and hydrogen. <i>Journal of Applied Physics</i> , 2013, 114, .	1.1	11
9431	Roughening of Pt nanoparticles induced by surface-oxide formation. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 2268.	1.3	21

#	ARTICLE	IF	CITATIONS
9432	The donor/acceptor edge-modification: an effective strategy to modulate the electronic and magnetic behaviors of zigzag silicon carbon nanoribbons. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18039.	1.3	23
9433	Towards efficient solar hydrogen production by intercalated carbon nitride photocatalyst. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18077.	1.3	309
9434	Influence of hydroxyl groups on the adsorption of HCHO on TiO <sub>2</sub> -B(100) surface by first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 3866.	1.3	7
9435	Computational investigation of defect segregation at the (001) surface of BaCeO <sub>3</sub> and BaZrO <sub>3</sub> : the role of metal-oxygen bond strength in controlling vacancy segregation. <i>Journal of Materials Chemistry A</i> , 2013, 1, 2840.	5.2	18
9436	Chemical and electrochemical oxidation of [Rh( $\eta^2$ -diketonato)(CO)(P(OCH <sub>2</sub> ) <sub>3</sub> CCH <sub>3</sub> )]: an experimental and DFT study. <i>Dalton Transactions</i> , 2013, 42, 8655.	1.6	18
9437	Mode selectivity in methane dissociative chemisorption on Ni(111). <i>Chemical Science</i> , 2013, 4, 3249.	3.7	115
9438	Layered Dinitrostilbene-Based Molecular Solids with Tunable Micro/Nanostructures and the Reversible Fluorescent Response to Explosives. <i>Crystal Growth and Design</i> , 2013, 13, 4495-4503.	1.4	13
9439	Mechanistic insights into iron catalyzed dehydrogenation of formic acid: $\eta^2$ -hydride elimination vs. direct hydride transfer. <i>Dalton Transactions</i> , 2013, 42, 11987.	1.6	58
9440	Diarylhalotelluronium(iv) cations [(8-Me <sub>2</sub> NC <sub>10</sub> H <sub>6</sub> ) <sub>2</sub> TeX] <sup>+</sup> (X = Cl, Br, I) stabilized by intramolecularly coordinating N-donor substituents. <i>Dalton Transactions</i> , 2013, 42, 12193.	1.6	20
9441	Single-crystal adsorption calorimetry and density functional theory of CO chemisorption on fcc Co{110}. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4059.	1.3	20
9442	Selective molecular adsorption in sub-nanometer cages of a Cu <sub>2</sub> O surface oxide. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10726.	1.3	22
9443	Methane storage capabilities of diamond analogues. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 20937.	1.3	10
9444	Ensemble and ligand effects on the acetylene adsorption on ordered Pd <sub>x</sub> Ag <sub>1-x</sub> /Pd(100) surface alloys investigated by periodic DFT study. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 20345.	1.3	18
9445	Six-dimensional quantum dynamics study for the dissociative adsorption of HCl on Au(111) surface. <i>Journal of Chemical Physics</i> , 2013, 139, 184705.	1.2	56
9446	First-principles study of CaFe <sub>2</sub> As <sub>2</sub> under pressure. <i>Physical Review B</i> , 2013, 88, .	1.1	15
9447	Development of the ReaxFF reactive force field for aluminum-molybdenum alloy. <i>Journal of Materials Research</i> , 2013, 28, 1155-1164.	1.2	10
9448	Study of band-structure, optical properties and native defects in A <sub>2</sub> B <sub>2</sub> O <sub>2</sub> (A = Cu or Tl, B = O or S). <i>Journal of Materials Chemistry C</i> , 2013, 1, 1065003.	1.0	49
9449	High Temperature Interconnect and Die Attach Technology: Au-Sn SLID Bonding. <i>IEEE Transactions on Components, Packaging and Manufacturing Technology</i> , 2013, 3, 904-914.	1.4	46

#	ARTICLE	IF	CITATIONS
9450	Crystal structure and phase stability of the $\hat{1}$ phase in the Al-Mg-Zn system. <i>Intermetallics</i> , 2013, 32, 259-273.	1.8	14
9451	Magnetic CrX and MnX (X=Si, Ge, and As) nanowires: Stability enhancement and linearization. <i>Journal of Alloys and Compounds</i> , 2013, 547, 138-146.	2.8	2
9452	Structure, electronic characteristic and thermodynamic properties of K <sub>2</sub> ZnH <sub>4</sub> hydride crystal: A first-principles study. <i>Journal of Alloys and Compounds</i> , 2013, 549, 30-37.	2.8	6
9453	Microkinetics of steam methane reforming on platinum and rhodium metal surfaces. <i>Journal of Catalysis</i> , 2013, 297, 227-235.	3.1	43
9454	Growth and structure of Si and Ge in vanadium oxide nanomesh on Pd(111) studied by STM and DFT. <i>Applied Surface Science</i> , 2013, 265, 291-295.	3.1	1
9455	Reaction mechanism for methanol oxidation on Au(111): A density functional theory study. <i>Applied Surface Science</i> , 2013, 265, 443-451.	3.1	29
9456	Insights into the preference of CH <sub>x</sub> (x=1-3) formation from CO hydrogenation on Cu(111) surface. <i>Applied Surface Science</i> , 2013, 265, 720-730.	3.1	51
9457	The adsorption of bisulfate and sulfate anions over a Pt(111) electrode: A first principle study of adsorption configurations, vibrational frequencies and linear sweep voltammogram simulations. <i>Catalysis Today</i> , 2013, 202, 20-35.	2.2	60
9458	Electronic structure of [Ni(II)S <sub>4</sub> ] complexes from S K-edge X-ray absorption spectroscopy. <i>Coordination Chemistry Reviews</i> , 2013, 257, 564-578.	9.5	33
9459	Structural and thermodynamic stability of Li <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> anode material for lithium-ion battery. <i>Journal of Power Sources</i> , 2013, 222, 448-454.	4.0	199
9460	Structural, elastic, and electronic properties of new 211 MAX phase Nb <sub>2</sub> GeC from first-principles calculations. <i>Physica B: Condensed Matter</i> , 2013, 410, 42-48.	1.3	28
9461	Graphene oxide as a chemically tunable 2-D material for visible-light photocatalyst applications. <i>Journal of Catalysis</i> , 2013, 299, 204-209.	3.1	115
9462	First principles study on the adsorption of CO <sub>2</sub> and H <sub>2</sub> O on the K <sub>2</sub> CO <sub>3</sub> (001) surface. <i>Surface Science</i> , 2013, 609, 140-146.	0.8	33
9463	Na-Si Clathrates Are High-Pressure Phases: A Melt-Based Route to Control Stoichiometry and Properties. <i>Crystal Growth and Design</i> , 2013, 13, 303-307.	1.4	75
9464	Electronic structure of A <sub>2</sub> CrSbO <sub>6</sub> [A=Sr, Ca]: Ab-initio study. <i>Journal of Physics and Chemistry of Solids</i> , 2013, 74, 250-254.	1.9	10
9465	Functionalization of multi-walled carbon nanotubes using water-assisted chemical vapor deposition. <i>Journal of Solid State Chemistry</i> , 2013, 197, 517-522.	1.4	37
9466	Ab-initio calculation of C and CO adsorption on the Co (110) surface. <i>Surface Science</i> , 2013, 608, 282-291.	0.8	3
9467	Current-Driven Spin Dynamics of Artificially Constructed Quantum Magnets. <i>Science</i> , 2013, 339, 55-59.	6.0	197

#	ARTICLE	IF	CITATIONS
9468	Copper coordination to the prion protein: Insights from theoretical studies. <i>Coordination Chemistry Reviews</i> , 2013, 257, 429-444.	9.5	32
9469	Effect of the Al Siting on the Structure of Co(II) and Cu(II) Cationic Sites in Ferrierite. A Periodic DFT Molecular Dynamics and FTIR Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3958-3968.	1.5	42
9470	Anion-radical oxygen centers in small (AgO) <sub>n</sub> clusters: Density functional theory predictions. <i>Chemical Physics Letters</i> , 2013, 560, 37-41.	1.2	12
9471	Density functional theory in materials science. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013, 3, 438-448.	6.2	102
9472	Theoretical Approach to the Study of Thiophene-Based Discotic Systems As Organic Semiconductors. <i>Journal of Physical Chemistry C</i> , 2013, 117, 15-22.	1.5	10
9473	Small Changes Have Consequences: Lessons from Tetrabenzyltitanium and Zirconium Surface Organometallic Chemistry. <i>Chemistry - A European Journal</i> , 2013, 19, 964-973.	1.7	24
9474	Mechanochemical synthesis of a fluorenone-based metal organic framework with polarized fluorescence: an experimental and computational study. <i>Journal of Materials Chemistry C</i> , 2013, 1, 997-1004.	2.7	59
9475	Impact of hydrogen and oxygen defects on the lattice parameter of chemical vapor deposited zinc sulfide. <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	19
9476	Theoretical Study of Sensitizer Candidates for Dye-Sensitized Solar Cells: Peripheral Substituted Dizinc Pyrazinoporphyrazine-Phthalocyanine Complexes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 430-438.	1.1	50
9477	Zinc Gallogermanate Solid Solution: A Novel Photocatalyst for Efficiently Converting CO <sub>2</sub> into Solar Fuels. <i>Advanced Functional Materials</i> , 2013, 23, 1839-1845.	7.8	89
9478	Compensation effect. A DFT study of the activation of N <sub>2</sub> O over M-CHA (M=Fe <sup>2+</sup> , Co <sup>2+</sup> , RuO <sub>2</sub> <sup>+</sup> , RuO <sup>+</sup> ). <i>Journal of Catalysis</i> , 2013, 298, 122-129.	3.1	9
9479	Structural variety of 5-fluoroarene-2-aminopyrimidine in comparison to 2-aminopyrimidine silver(i) coordination polymers: progress report and overview. <i>CrystEngComm</i> , 2013, 15, 4225.	1.3	13
9480	First Principles Study of O <sub>2</sub> Adsorption on Reduced Rutile TiO <sub>2</sub> -(110) Surface Under UV Illumination and Its Role on CO Oxidation. <i>Journal of Physical Chemistry C</i> , 2013, 117, 956-961.	1.5	29
9481	Electronic structure simulations of 2,6-dimethyl-2,5-heptadien-4-one by FTIR, FT-Raman, NMR, UV-vis, NBO and density functional theory. <i>Molecular Simulation</i> , 2013, 39, 185-198.	0.9	1
9482	Dibenzo[ <i>b,f</i> ]phosphepines: Novel Phosphane-Olefin Ligands for Transition Metals. <i>Organometallics</i> , 2013, 32, 363-373.	1.1	27
9483	First-principles studies on lattice constants and local lattice distortions in solid solution aluminum alloys. <i>Computational Materials Science</i> , 2013, 67, 1-10.	1.4	121
9484	Theoretical Approaches to Excited-State-Related Phenomena in Oxide Surfaces. <i>Chemical Reviews</i> , 2013, 113, 4456-4495.	23.0	80
9485	A new heterobimetallic manganese-rhodium carbonyl complex derived from partially alkylated s-indacene. <i>Inorganica Chimica Acta</i> , 2013, 394, 132-139.	1.2	14



#	ARTICLE	IF	CITATIONS
9486	Ab initio study of ZnCoO diluted magnetic semiconductor and its magnetic properties. Journal of Alloys and Compounds, 2013, 551, 306-311.	2.8	19
9487	New concepts and modeling strategies to design and evaluate photo-electro-catalysts based on transition metal oxides. Chemical Society Reviews, 2013, 42, 2401-2422.	18.7	225
9488	Contribution of high-energy conformations to NMR chemical shifts, a DFT-BOMD study. Physical Chemistry Chemical Physics, 2013, 15, 860-867.	1.3	13
9489	New type of possible high-pressure polymorphism in NiAs minerals in planetary cores. Physics and Chemistry of Minerals, 2013, 40, 183-193.	0.3	10
9490	Periodic density functional theory study of the high-pressure behavior of energetic crystalline 1,4-dinitrofurazano[3, 4-b]piperazine. Journal of Molecular Modeling, 2013, 19, 305-314.	0.8	7
9491	Density functional study of platinum polyene monomer, oligomer, and polymer: Ground state geometrical and electronic structures. International Journal of Quantum Chemistry, 2013, 113, 1650-1659.	1.0	8
9492	Structural and Bonding Analyses on a Homologous Metal-Host Series $M_{2@C_{50}X_{10}}$ (M = Zn, Cd, Hg; X = CH, N, B). European Journal of Inorganic Chemistry, 2013, 2013, 2220-2230.	1.0	5
9493	Tuning the Surface Chemistry of Pd by Atomic C and H: A Microscopic Picture. Chemistry - A European Journal, 2013, 19, 1335-1345.	1.7	28
9494	Relating the Composition of Pt <sub>x</sub> Ru <sub>100-x</sub> /C Nanoparticles to Their Structural Aspects and Electrocatalytic Activities in the Methanol Oxidation Reaction. Chemistry - A European Journal, 2013, 19, 905-915.	1.7	8
9495	[3,3] Sigmatropic Rearrangement Versus [2+2] Cycloaddition: A DFT Investigation of Formal S <sub>N</sub> 2 Substitution of Imido Metal Complexes with Allylic Electrophiles. Chemistry - A European Journal, 2013, 19, 1204-1208.	1.7	6
9496	Ketonic Decarboxylation Reaction Mechanism: A Combined Experimental and DFT Study. ChemSusChem, 2013, 6, 141-151.	3.6	121
9497	Adsorbed CO induced change of the adsorption site and charge of Au adatoms on FeO(111)/Ru(0001). Chinese Journal of Catalysis, 2013, 34, 1820-1825.	6.9	3
9498	Generalized planar fault energies and mechanical twinning in gamma TiAl alloys. Scripta Materialia, 2013, 68, 759-762.	2.6	32
9499	Interstitial hydrogen in ZnO and BeZnO. International Journal of Hydrogen Energy, 2013, 38, 5974-5982.	3.8	9
9500	Phase stability and elastic property of PdH and PdCuH phases. International Journal of Hydrogen Energy, 2013, 38, 16485-16494.	3.8	25
9501	Influence of oxygen and pH on the selective oxidation of ethanol on Pd catalysts. Journal of Catalysis, 2013, 299, 261-271.	3.1	63
9502	Thermodynamic assessment of the Cd-X (X= Sr, Ti, B, V) systems. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2013, 42, 6-12.	0.7	2
9503	Ideal strength of Mg <sub>2</sub> X (X=Si, Ge, Sn and Pb) from first-principles. Journal of Magnesium and Alloys, 2013, 1, 163-168.	5.5	23



#	ARTICLE	IF	CITATIONS
9504	Effect of non-metal elements (B, C, N, F, P, S) mono-doping as anions on electronic structure of SrTiO <sub>3</sub> . <i>Computational Materials Science</i> , 2013, 79, 69-74.	1.4	56
9505	The catalytic adsorption and dissociation of carbon dioxide on a double icosahedral Ru <sub>19</sub> nanocluster – A theoretical study. <i>Chemical Physics Letters</i> , 2013, 585, 149-152.	1.2	11
9506	Combined studies of DFT atomistic modelling and in situ FTIR spectroscopy on surface oxidants and CO oxidation at Ru electrodes. <i>Journal of Electroanalytical Chemistry</i> , 2013, 688, 216-223.	1.9	11
9507	Reactivity of adducts relevant to the deposition of hexagonal BN from first-principles calculations. <i>Chemical Physics Letters</i> , 2013, 583, 119-124.	1.2	40
9508	Structural stability and electronic structure study of YCu <sub>2</sub> Zn <sub>2</sub> Laves phases by first-principles calculations. <i>Computational Materials Science</i> , 2013, 77, 366-371.	1.4	9
9509	Adsorption of PTCDA on NaCl(100) and KCl(100). <i>Surface Science</i> , 2013, 617, 242-248.	0.8	29
9510	Catalytic behavior and surface species investigation over $\gamma$ -Al <sub>2</sub> O <sub>3</sub> in dimethyl ether hydrolysis. <i>Applied Catalysis A: General</i> , 2013, 460-461, 99-105.	2.2	13
9511	Prediction of elastic and electronic properties of cubic Al <sub>18</sub> Ti <sub>2</sub> Mg <sub>3</sub> phase coexisting with Al <sub>3</sub> Ti in Al–Ti–Mg system. <i>Physica B: Condensed Matter</i> , 2013, 408, 68-72.	1.3	14
9512	Novel titanocene derived from a partially alkylated s-indacene: Synthesis, characterization and comparative study with its zirconium analog. <i>Inorganica Chimica Acta</i> , 2013, 396, 35-39.	1.2	2
9513	Tetragonally compressed high-spin Mn(III) Schiff base complex: Synthesis, crystal structure, magnetic properties and theoretical calculations. <i>Polyhedron</i> , 2013, 52, 1199-1205.	1.0	22
9514	A first-principles study of the structure, electronic properties, and oxygen binding of FeO/Pt(111) and FeO <sub>2</sub> /Pt(111). <i>Chinese Journal of Catalysis</i> , 2013, 34, 973-978.	6.9	12
9515	Hydrogen diffusion on silicon surfaces. <i>Progress in Surface Science</i> , 2013, 88, 61-101.	3.8	38
9516	Thermodynamic modeling of the (U,Lu) <sub>2</sub> O <sub>7</sub> ±x solid solution phase. <i>Journal of Nuclear Materials</i> , 2013, 433, 227-232.	1.3	21
9517	An atomistic thermodynamics study of the structural evolution of the Pt <sub>3</sub> Ni(111) surface in an oxygen environment. <i>Chinese Journal of Catalysis</i> , 2013, 34, 1434-1442.	6.9	10
9518	Theoretical characterization on intrinsic ferrimagnetic phase in nanoscale laminated Cr <sub>2</sub> GeC. <i>Solid State Communications</i> , 2013, 174, 43-45.	0.9	14
9519	Highly efficient visible light photocatalytic activity of Cr–La codoped SrTiO <sub>3</sub> with surface alkalization: An insight from DFT calculation. <i>Computational Materials Science</i> , 2013, 79, 87-94.	1.4	19
9520	Characterization and oxidative addition reactions of rhodium(I) carbonyl cupferrate diphenyl-2-pyridylphosphine complexes. <i>Journal of Organometallic Chemistry</i> , 2013, 745-746, 439-453.	0.8	4
9521	Preparation of highly aligned arrays of conducting polymer nanowires using templated electropolymerization in supercritical fluids. <i>Electrochimica Acta</i> , 2013, 87, 409-415.	2.6	19

#	ARTICLE	IF	CITATIONS
9522	Theoretical study on the structure of ternary compounds AMn <sub>2</sub> X <sub>2</sub> (A=Ba, Ca and Y; X=Sn, Ge, and Si). Journal of Alloys and Compounds, 2013, 571, 69-74.	2.8	10
9523	M(C <sub>6</sub> X <sub>6</sub> Li <sub>6</sub> ) <sub>2</sub> (M=Cr, Mo, W; X=O, S): Transition-metal sandwich complexes with $\pi$ -aromatic C <sub>6</sub> X <sub>6</sub> Li <sub>6</sub> ligands. Computational and Theoretical Chemistry, 2013, 1018, 95-101.	1.1	6
9525	Theoretical study of the adsorption and dissociation mechanism for methylamine on Pd(111). Applied Surface Science, 2013, 271, 291-298.	3.1	16
9526	Ab-initio calculations of synergistic chromium-nitrogen codoping effects on the electronic and optical properties of anatase TiO <sub>2</sub> . Vacuum, 2013, 92, 32-38.	1.6	27
9527	Experimental and theoretical investigation on the interaction between palladium nanoparticles and functionalized carbon nanotubes for Heck synthesis. Catalysis Today, 2013, 212, 206-214.	2.2	42
9528	Prediction of the pressure-volume-temperature equation of state for zinc-blende ZnO from quasi-harmonic Debye model. Solid State Communications, 2013, 166, 27-31.	0.9	1
9529	Electronic structure and stability of hyperstoichiometric UO <sub>2+x</sub> under pressure. Physical Review B, 2013, 88, .	1.1	22
9530	Assembly of a Noncovalent DNA Junction on Graphene Sheets and Electron Transport Characteristics. Journal of Physical Chemistry C, 2013, 117, 26441-26453.	1.5	24
9531	Dependence of equilibrium stacking fault width in fcc metals on the $\gamma$ -surface. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 025015.	0.8	45
9532	Core-Shell Nanocatalyst Design by Combining High-Throughput Experiments and First-Principles Simulations. ChemCatChem, 2013, 5, 3712-3718.	1.8	8
9533	Conformational analysis of triphenylphosphine in square planar [Rh( $\eta^2$ -diketonato)(CO)(PPh <sub>3</sub> )] complexes. Crystal structure of [Rh(PhCOCHCO(CH <sub>2</sub> ) <sub>3</sub> CH <sub>3</sub> )(CO)(PPh <sub>3</sub> )]. Inorganica Chimica Acta, 2013, 395, 237-244.	1.2	9
9534	Ab Initio Prediction of Surface Stability of Fluorite Materials and Experimental Verification. Journal of Physical Chemistry C, 2013, 117, 6639-6650.	1.5	24
9535	Ab initio study of the cohesive properties, electronic structure and thermodynamic stability of the Ni-In and Ni-Sn intermetallics. Journal of Alloys and Compounds, 2013, 576, 302-316.	2.8	22
9536	Lithium transport investigation in Li <sub>x</sub> FeSiO <sub>4</sub> : A promising cathode material. Solid State Communications, 2013, 173, 9-13.	0.9	12
9537	The optical absorption and hydrogen production by water splitting of (Si,Fe)-codoped anatase TiO <sub>2</sub> photocatalyst. International Journal of Hydrogen Energy, 2013, 38, 5209-5214.	3.8	58
9538	Electronic band structure and influence of uniaxial stresses on the properties of K <sub>2</sub> SO <sub>4</sub> crystal: ab initio study. Computational Materials Science, 2013, 79, 442-447.	1.4	13
9539	An examination of nickel doping effect on the mechanical strength of a tungsten grain boundary. Computational Materials Science, 2013, 77, 131-138.	1.4	14
9540	Geometric and electronic structures of sulfur-edge-terminated zigzag edge graphene nanoribbons. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 49, 76-82.	1.3	3

#	ARTICLE	IF	CITATIONS
9541	Adsorption of a single Pt atom on polyaromatic hydrocarbons from first-principle calculations. <i>Chemical Physics Letters</i> , 2013, 575, 76-80.	1.2	8
9542	DFT and experimental study of the structure and vibrational spectra of 2-(benzylthio)-N-[pyridinylmethylidene]anilines. <i>Journal of Molecular Structure</i> , 2013, 1034, 29-37.	1.8	10
9543	Dissolution and diffusion behaviors of hydrogen in copper: A first-principles investigation. <i>Computational Materials Science</i> , 2013, 79, 923-928.	1.4	21
9544	Effects of spin-orbit coupling on various properties of hafnium dihydride. <i>Materials Chemistry and Physics</i> , 2013, 139, 139-146.	2.0	1
9545	Theoretical investigations of metal-free dyes for solar cells: Effects of electron donor and acceptor groups on sensitizers. <i>Journal of Power Sources</i> , 2013, 242, 464-471.	4.0	20
9546	Ordering and phonons in Ba <sub>3</sub> CaNb <sub>2</sub> O <sub>9</sub> complex perovskite. <i>Materials Research Bulletin</i> , 2013, 48, 3298-3303.	2.7	20
9547	Theoretical study on the electronic structures and magnetism of Fe <sub>3</sub> Si intermetallic compound. <i>Journal of Alloys and Compounds</i> , 2013, 552, 324-328.	2.8	20
9548	Oxygen adsorption on $\hat{1}^3$ -TiAl surfaces and the related surface phase diagrams: A density-functional theory study. <i>Acta Materialia</i> , 2013, 61, 1726-1738.	3.8	32
9549	Ground state of stoichiometric B <sub>2</sub> FeAl. <i>Solid State Communications</i> , 2013, 169, 57-61.	0.9	9
9550	Characterization of acetylacetonato carbonyl diphenyl-2-pyridylphosphine rhodium(I): Comparison with other carbonyl complexes. <i>Journal of Molecular Structure</i> , 2013, 1038, 220-229.	1.8	11
9551	Thermodynamic optimization of Co-Ge binary system. <i>Thermochimica Acta</i> , 2013, 572, 94-100.	1.2	6
9552	Mechanisms of dopants influence on hydrogen uptake in COF-108: A first principles study. <i>International Journal of Hydrogen Energy</i> , 2013, 38, 14668-14674.	3.8	9
9553	Electronic and optical properties of S/I-codoped anatase TiO <sub>2</sub> from ab initio calculations. <i>Solid State Communications</i> , 2013, 171, 17-21.	0.9	4
9554	Structural properties and energetics of GaAs nanowires. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2013, 52, 34-39.	1.3	12
9555	First-principles analysis of the effect of contact sites on electronic transport properties of diamino fluorene. <i>Physica B: Condensed Matter</i> , 2013, 417, 70-74.	1.3	7
9556	Influences of chemical structure and physical properties of coal macerals on coal liquefaction by quantum chemistry calculation. <i>Fuel Processing Technology</i> , 2013, 109, 19-26.	3.7	45
9557	Vacancies in ordered and disordered titanium monoxide: Mechanism of B1 structure stabilization. <i>Journal of Solid State Chemistry</i> , 2013, 204, 146-152.	1.4	32
9558	Effect of lattice anharmonicity in the structural phase transformation of Laves phase HfV <sub>2</sub> alloy: A first-principles investigation. <i>Acta Materialia</i> , 2013, 61, 7473-7480.	3.8	3

#	ARTICLE	IF	CITATIONS
9559	Influence of alloying elements on phase stability and elastic properties of aluminum and magnesium studied by first principles. <i>Computational Materials Science</i> , 2013, 74, 86-91.	1.4	8
9560	Adsorption of CO <sub>2</sub> on Cu <sub>2</sub> O (111) oxygen-vacancy surface: First-principles study. <i>Chemical Physics Letters</i> , 2013, 568-569, 84-89.	1.2	49
9561	First principles investigation of the electronic, elastic and vibrational properties of tungsten disilicide. <i>Journal of Alloys and Compounds</i> , 2013, 553, 93-98.	2.8	10
9562	Characterization of citrate capped gold nanoparticle-quercetin complex: Experimental and quantum chemical approach. <i>Journal of Molecular Structure</i> , 2013, 1046, 153-163.	1.8	48
9563	<sup>33</sup> S NMR spectroscopy. 4. Substituent effects on the <sup>33</sup> S nuclear quadrupole coupling constants and electric field gradient in 3- and 4-substituted benzenesulphonates studied by DFT calculations in vacuo and in aqueous solution. <i>Journal of Molecular Structure</i> , 2013, 1051, 115-123.	1.8	0
9564	Adhesion and fracture toughness at $\hat{1}\pm$ -Ti(0001)/TiC(111): A first-principles investigation. <i>Applied Surface Science</i> , 2013, 286, 240-248.	3.1	59
9565	First-principles thermodynamics of metal-oxide surfaces and interfaces: A case study review. <i>Transactions of Nonferrous Metals Society of China</i> , 2013, 23, 180-192.	1.7	19
9566	First-principles study of Sc-doping effect on the stability, electronic structure and photocatalytic properties of Sr <sub>2</sub> TiO <sub>4</sub> . <i>Thin Solid Films</i> , 2013, 542, 276-280.	0.8	9
9567	Methanol adsorption and decomposition on ZnO. <i>Journal of Molecular Structure</i> , 2013, 1051, 115-123.		
9568	Effect of site disorder on the electronic properties of Fe <sub>2</sub> VAl Heusler alloy. <i>Journal of Alloys and Compounds</i> , 2013, 577, 417-425.	2.8	24
9569	Theoretical investigations on phase stability, elastic constants and electronic structures of D0 <sub>22</sub> - and L1 <sub>2</sub> -Al <sub>3</sub> Ti under high pressure. <i>Journal of Alloys and Compounds</i> , 2013, 556, 214-220.	2.8	48
9570	Na adsorption on SrTiO <sub>3</sub> (0 0 1) surface and its interaction with water: A DFT calculation. <i>Applied Surface Science</i> , 2013, 270, 359-363.	3.1	6
9571	Structure-sensitivity of ethane hydrogenolysis over molybdenum carbides: A density functional theory study. <i>Applied Surface Science</i> , 2013, 276, 369-376.	3.1	12
9572	Structural, electronic and mechanical properties of W <sub>1-x</sub> Tc <sub>x</sub> B <sub>2</sub> alloys. <i>Solid State Communications</i> , 2013, 171, 1-4.	0.9	6
9573	P(OPh) <sub>3</sub> substitution at [Rh( $\hat{1}^2$ -diketonato)(cod)] complexes: The relationship between kinetics and frontier orbitals. <i>Inorganica Chimica Acta</i> , 2013, 406, 211-216.	1.2	5
9574	Density functional theory study on configurations and electronic properties of periodic nanoridges. <i>Computational Materials Science</i> , 2013, 77, 312-315.	1.4	1
9575	Density functional theory study of chlorine adsorption on the Pt(111) surface. <i>Surface Science</i> , 2013, 617, 233-236.	0.8	6
9576	The phase stability and elastic properties of MgZn <sub>2</sub> and Mg <sub>4</sub> Zn <sub>7</sub> in Mg $\hat{e}$ Zn alloys. <i>Scripta Materialia</i> , 2013, 68, 495-498.	2.6	69

#	ARTICLE	IF	CITATIONS
9577	Theoretical study of the Fluorine doped anatase surfaces. <i>Surface Science</i> , 2013, 618, 154-158.	0.8	25
9578	The effect of density functional and dispersion interaction on structure and bonding analysis of uranium(VI) nitride complex [NU{N(CH <sub>2</sub> CH <sub>2</sub> NSiMe <sub>3</sub> ) <sub>3</sub> }] : A theoretical study. <i>Inorganic Chemistry Communication</i> , 2013, 37, 4-6.	1.8	3
9579	Elastic and electronic properties of Ce <sub>2</sub> O <sub>3</sub> from first principles. <i>Journal of Alloys and Compounds</i> , 2013, 551, 672-676.	2.8	13
9580	Effects of Li and Na intercalation on electronic, bonding and thermoelectric transport properties of MX <sub>2</sub> (M=Ta; X=S or Se) dichalcogenides – Ab initio investigation. <i>Journal of Alloys and Compounds</i> , 2013, 581, 731-740.	2.8	19
9581	First-principles calculations of optical properties of Titanium nanochains. <i>Computational Materials Science</i> , 2013, 77, 224-229.	1.4	9
9582	Benchmark calculations of density functionals for organothiol adsorption on gold surfaces. <i>Computational and Theoretical Chemistry</i> , 2013, 1009, 60-69.	1.1	3
9583	Effect of carbon on helium trapping in tungsten: A first-principles investigation. <i>Journal of Nuclear Materials</i> , 2013, 440, 338-343.	1.3	16
9584	A theoretical study of the dielectric and magnetic responses of Fe-doped $\delta$ -MnO <sub>2</sub> based on quantum mechanical calculations. <i>Journal of Materials Chemistry C</i> , 2013, 1, 1990.	2.7	58
9585	Doped Graphene as a Material for Oxygen Reduction Reaction in Hydrogen Fuel Cells: A Computational Study. <i>ACS Catalysis</i> , 2013, 3, 159-165.	5.5	100
9586	Methane dehydrogenation on Au/Ni surface alloys – a first-principles study. <i>Catalysis Science and Technology</i> , 2013, 3, 1343.	2.1	36
9587	Decomposition and Oxidation of Methanol on Ir(111): A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 4574-4584.	1.5	23
9588	Manipulation of Microbial Extracellular Electron Transfer by Changing Molecular Structure of Phenazine-Type Redox Mediators. <i>Environmental Science &amp; Technology</i> , 2013, 47, 1033-1039.	4.6	39
9589	Phase transition and thermodynamic properties of BiFeO <sub>3</sub> from first-principles calculations. <i>Chinese Physics B</i> , 2013, 22, 037101.	0.7	24
9590	Driving Force of Phase Transition in Indium Nanowires on Si(111). <i>Physical Review Letters</i> , 2013, 110, 116801.	2.9	34
9591	Effect of halogen bonding interaction on supramolecular assembly of halogen-substituted phenylpyrazinamides. <i>CrystEngComm</i> , 2013, 15, 3222.	1.3	23
9592	Lactam derivatives as solid electrolyte interphase forming additives for a graphite anode of lithium-ion batteries. <i>Journal of Power Sources</i> , 2013, 244, 711-715.	4.0	16
9593	Enhanced Li adsorption and diffusion in silicon nanosheets based on first principles calculations. <i>RSC Advances</i> , 2013, 3, 4231.	1.7	61
9594	A DFT study of the reactivity of $\delta^2$ -diketonato-1,5-cyclo-octadieneiridium(II) complexes. <i>Polyhedron</i> , 2013, 51, 164-167.	1.0	7

#	ARTICLE	IF	CITATIONS
9595	Effects of the peripheral substituents ( $\text{NH}_2$ , $\text{OH}$ , $\text{CH}_3$ , $\text{H}$ , $\text{C}_6\text{H}_5$ , $\text{Cl}$ , $\text{CO}_2\text{H}$ and $\text{NO}_2$ ) on molecular properties of a Ni-Porphyrzine dimers family. <i>Polyhedron</i> , 2013, 50, 131-138.	1.0	8
9596	Electronic structure of the $S_{1/2}$ state in methylcobalamin: Insight from CASSCF/MCQDPT2, EOMCCSD, and TDFT calculations. <i>Journal of Computational Chemistry</i> , 2013, 34, 987-1004.	1.5	53
9597	First-principles calculations of H, O and OH adsorption on metallic layered supported thin films. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 175002.	0.7	6
9598	Stabilization of oxidovanadium(IV) by organic radicals. <i>Dalton Transactions</i> , 2013, 42, 4586.	1.6	22
9599	Surface-enhanced Raman scattering (SERS) from Au:Ag bimetallic nanoparticles: the effect of the molecular probe. <i>Chemical Science</i> , 2013, 4, 509-515.	3.7	183
9600	On the Mechanism of the Dehydroaromatization of Hexane to Benzene by an Iridium Pincer Catalyst. <i>Chemistry - A European Journal</i> , 2013, 19, 4069-4077.	1.7	20
9601	High-Pressure Electrical-Transport Properties of SnS: Experimental and Theoretical Approaches. <i>Journal of Physical Chemistry C</i> , 2013, 117, 6033-6038.	1.5	35
9602	The role of impurity oxygen in hydrogen bubble nucleation in tungsten. <i>Journal of Nuclear Materials</i> , 2013, 433, 357-363.	1.3	45
9603	A family of octahedral molybdenum cluster complexes $[\text{Mo}_6\text{Cl}_8(\text{H}_2\text{O})(\text{OH})_6]^{n-2}$ with $n=0-6$ as a pH-sensors: A theoretical study. <i>Chemical Physics Letters</i> , 2013, 567, 39-42.	1.2	11
9604	Defect-induced room temperature ferromagnetism in B-doped ZnO. <i>Ceramics International</i> , 2013, 39, 4609-4617.	2.3	30
9605	Theoretical investigation of hydrogen atom transfer in the hydrated C-G base pair. <i>Molecular Physics</i> , 2013, 111, 201-214.	0.8	11
9606	Influence of Halogen Bonding Interaction on Supramolecular Assembly of Coordination Compounds; Head-to-Tail N-H...X Synthons Repetitivity. <i>Inorganic Chemistry</i> , 2013, 52, 2891-2905.	1.9	63
9607	Composition- and Band-Gap-Tunable Synthesis of Wurtzite-Derived $\text{Cu}_2\text{ZnSn}(\text{S})_4\text{Se}_4$ Nanocrystals: Theoretical and Experimental Insights. <i>ACS Nano</i> , 2013, 7, 1454-1463.	7.3	89
9608	$\text{Cu}_3\text{BiS}_3$ as a potential photovoltaic absorber with high optical efficiency. <i>Applied Physics Letters</i> , 2013, 102, .	1.5	59
9609	Understanding the Second-Order Nonlinear Optical Properties of One-Dimensional Ruthenium(II) Ammine Complexes. <i>Journal of Physical Chemistry C</i> , 2013, 117, 1833-1848.	1.5	25
9610	Approaching chemical accuracy with density functional calculations: Diatomic energy corrections. <i>Physical Review B</i> , 2013, 87, .	1.1	75
9611	Quantum-chemical calculations of NMR chemical shifts of organic molecules: VII. Intramolecular coordination effect in the $^{29}\text{Si}$ NMR spectra of siletanes. <i>Russian Journal of Organic Chemistry</i> , 2013, 49, 34-41.	0.3	10
9612	Activated vibrational modes and Fermi resonance in tip-enhanced Raman spectroscopy. <i>Physical Review E</i> , 2013, 87, 020401.	0.8	78



#	ARTICLE	IF	CITATIONS
9613	Two-dimensional CdSe Nanosheets and their Interaction with Stabilizing Ligands. <i>Advanced Materials</i> , 2013, 25, 261-266.	11.1	39
9614	The Modulated Structure of $\text{Co}_3\text{Al}_4\text{Si}_2$ : Incommensurability and Co-Co Interactions in Search of Filled Octadecets. <i>Inorganic Chemistry</i> , 2013, 52, 3178-3189.	1.9	25
9615	DFT study on stability and H <sub>2</sub> adsorption activity of bimetallic Au <sub>79</sub> Pd (n = 1-55) clusters. <i>Chemical Physics</i> , 2013, 415, 179-185.	0.9	20
9616	High Surface Reactivity and Water Adsorption on $\text{NiFe}_2\text{O}_4$ (111) Surfaces. <i>Journal of Physical Chemistry C</i> , 2013, 117, 5678-5683.	1.5	52
9617	Formation of an oxygen vacancy-dinitrogen complex in nitrogen-doped hafnium oxide. <i>Journal of Analytical Atomic Spectrometry</i> , 2013, 28, 482.	1.6	8
9618	Oxygen reduction reaction on active sites of heteroatom-doped graphene. <i>RSC Advances</i> , 2013, 3, 5498.	1.7	59
9619	Assessment of density functional methods for thermochemistry of chromium oxo compounds and their application in a study of chromia-silica system. <i>Chemical Physics Letters</i> , 2013, 561-562, 87-91.	1.2	15
9621	Theory of variational calculation with a scaling correct moment functional to solve the electronic Schrödinger equation directly for ground state one-electron density and electronic energy. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1479-1492.	1.0	10
9622	Cation vacancies in the alloy compounds of $\text{Cu}_2\text{ZnSn}(\text{S}_1\text{Se})_4$ and $\text{CuIn}(\text{S}_1\text{Se})_2$ . <i>Thin Solid Films</i> , 2013, 535, 318-321.	0.8	15
9623	Theoretical studies on the spectroscopic properties of a series of palladium (II) complexes with 1-allyl-3-(2-pyridyl)thiourea. <i>Synthetic Metals</i> , 2013, 167, 51-63.	2.1	6
9624	The behaviour of oxygen at metal electrodes in HfO <sub>2</sub> based resistive switching devices. <i>Microelectronic Engineering</i> , 2013, 109, 346-350.	1.1	29
9625	Atomistic structures and phase transition of In <sub>2</sub> Se <sub>3</sub> nanowires studied by DFT calculations and synchrotron radiation X-ray diffraction. <i>Solid State Communications</i> , 2013, 162, 28-33.	0.9	4
9626	Synthesis and kinetics of electronically altered photochromic dithizonatophenylmercury(II) complexes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2013, 252, 159-166.	2.0	8
9627	An updated thermodynamic modeling of the Ga-Ti system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2013, 41, 140-149.	0.7	4
9628	Structure of Monomeric Chromium(VI) Oxide Species Supported on Silica: Periodic and Cluster DFT Studies. <i>Journal of Physical Chemistry C</i> , 2013, 117, 8138-8149.	1.5	63
9629	Phenothiazine Derivative-Accelerated Microbial Extracellular Electron Transfer in Bioelectrochemical System. <i>Scientific Reports</i> , 2013, 3, 1616.	1.6	30
9630	Catalytic Cycle for N≡CN Bond Cleavage by Molybdenum Silyl Catalyst: A DFT Study. <i>Organometallics</i> , 2013, 32, 2725-2735.	1.1	12
9631	Electrophilic monoiodination of terminal alkenes. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 2891.	1.5	6



#	ARTICLE	IF	CITATIONS
9632	The role of the Lewis acid–base properties in the supramolecular association of 1,2,5-chalcogenadiazoles. <i>Canadian Journal of Chemistry</i> , 2013, 91, 338-347.	0.6	35
9633	Computational simulations of solid state NMR spectra: a new era in structure determination of oxide glasses. <i>RSC Advances</i> , 2013, 3, 10550.	1.7	81
9634	First-principles study on the structural stability and electronic properties of AlN/GaN heterostructure nanoribbons. <i>Superlattices and Microstructures</i> , 2013, 57, 37-43.	1.4	2
9635	Enhanced Li Adsorption and Diffusion in Single-Walled Silicon Nanotubes: An ab Initio Study. <i>ChemPhysChem</i> , 2013, 14, 1161-1167.	1.0	21
9636	Dynamic Effect of Solvation on the Optical Properties of a CdTe Nanocrystal. <i>Advanced Optical Materials</i> , 2013, 1, 239-243.	3.6	2
9637	Configurational transitions in processes involving metal clusters. <i>Physics Reports</i> , 2013, 527, 205-250.	10.3	26
9638	Quantum-chemical calculations of NMR chemical shifts of organic molecules: VIII. Solvation effects on <sup>15</sup> N NMR chemical shifts of nitrogen-containing heterocycles. <i>Russian Journal of Organic Chemistry</i> , 2013, 49, 379-383.	0.3	15
9639	DFT study on the reaction of O <sub>2</sub> dissociation catalyzed by gold surfaces doped with transition metal atoms. <i>Applied Catalysis A: General</i> , 2013, 458, 90-102.	2.2	23
9640	Novel half-metal and spin gapless semiconductor properties in N-doped silicene nanoribbons. <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	37
9641	He, Kr and Xe diffusion in ZrN – An atomic scale study. <i>Journal of Nuclear Materials</i> , 2013, 438, 7-14.	1.3	12
9642	H <sub>3</sub> O <sub>2</sub> Bridging Ligand in a Metal–Organic Framework. Insight into the Aqua-Hydroxo–Hydroxyl Equilibrium: A Combined Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2013, 135, 5782-5792.	6.6	42
9643	Growth of carbon structured over Pd, Pt and Ni: A comparative DFT study. <i>Applied Surface Science</i> , 2013, 268, 11-15.	3.1	2
9644	A Systematic Investigation of <i>p</i> -Nitrophenol Reduction by Bimetallic Dendrimer Encapsulated Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2013, 117, 7598-7604.	1.5	349
9645	Initial-stage behaviors of tin and lead adsorption on vanadium surface oxide nanomesh on Pd(111). <i>Surface Science</i> , 2013, 613, 35-39.	0.8	0
9646	Bond energy decomposition analysis for subsystem density functional theory. <i>Journal of Chemical Physics</i> , 2013, 138, 094113.	1.2	14
9647	Surface structure and equilibrium particle shape of the LiMn <sub>2</sub> O <sub>4</sub> spinel from first-principles calculations. <i>Physical Review B</i> , 2013, 87, .	1.1	116
9648	Novel mercury selenidoantimonates with structures ranging from one-dimensional ribbon to three-dimensional open-framework. <i>Dalton Transactions</i> , 2013, 42, 5454.	1.6	17
9649	Interface phenomena between Li anode and lithium phosphate electrolyte for Li-ion battery. <i>Journal of Power Sources</i> , 2013, 244, 136-142.	4.0	25

#	ARTICLE	IF	CITATIONS
9650	Ring-opening polymerization of racemic Î²-butyrolactone promoted by rare earth trisborohydride complexes towards a PHB-diol: an experimental and DFT study. <i>Polymer Chemistry</i> , 2013, 4, 3077.	1.9	20
9651	Aqua(ethylenedisulfonato)europium(III) [Eu(O <sub>3</sub> SC <sub>2</sub> H <sub>4</sub> SO <sub>3</sub> )(H <sub>2</sub> O)] <sup>+</sup> Structure, spectroscopy and magnetic properties. <i>Polyhedron</i> , 2013, 50, 283-288.	1.0	3
9652	Quantum Transport Modeling From First Principles. <i>Proceedings of the IEEE</i> , 2013, 101, 518-530.	16.4	78
9653	First-principles study of layered antiferromagnetic CuCrX <sub>2</sub> (X = S, Se and Te). <i>Journal of Physics Condensed Matter</i> , 2013, 25, 105504.	0.7	15
9654	Comparative Investigation of Benzene Steam Reforming over Spinel Supported Rh and Ir Catalysts. <i>ACS Catalysis</i> , 2013, 3, 1133-1143.	5.5	39
9655	A comparison model between density functional and wave function theories by means of the LÃ¶wdin partitioning technique. <i>Journal of Chemical Physics</i> , 2013, 138, 174107.	1.2	5
9656	Selective Semihydrogenation of Alkynes on Shapeâ€Controlled Palladium Nanocrystals. <i>Chemistry - an Asian Journal</i> , 2013, 8, 919-925.	1.7	39
9657	Computational methods for contemporary carbene chemistry. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013, 3, 242-272.	6.2	29
9658	Theoretical study on the reactivity of the surface of pure oxides: The Influence of the support and oxygen vacancies. <i>Applied Surface Science</i> , 2013, 274, 1-6.	3.1	11
9659	Theoretical Study of Oxygen Reduction Reaction Catalysts: From Pt to Non-precious Metal Catalysts. <i>Lecture Notes in Energy</i> , 2013, , 339-373.	0.2	2
9660	On structure and bonding of lanthanoid trifluorides LnF <sub>3</sub> (Ln = La to Lu). <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 7839.	1.3	25
9661	Mechanism of Framework Oxygen Exchange in Feâ€Zeolites: A Combined DFT and Mass Spectrometry Study. <i>ChemPhysChem</i> , 2013, 14, 520-531.	1.0	10
9662	Accounting for van der Waals interactions between adsorbates and surfaces in density functional theory based calculations: selected examples. <i>RSC Advances</i> , 2013, 3, 13085.	1.7	138
9663	An experimental and first-principles study of the effect of B/N doping in TiO <sub>2</sub> thin films for visible light photo-catalysis. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2013, 254, 25-34.	2.0	27
9664	The Electronic Nature of Terminal Oxo Ligands in Transition-Metal Complexes: Ambiphilic Reactivity of Oxorhenium Species. <i>Journal of the American Chemical Society</i> , 2013, 135, 9433-9441.	6.6	46
9665	Solute effect on oxygen diffusion in Î±-titanium. <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	15
9666	Electronic structure of III-V zinc-blende semiconductors from first principles. <i>Physical Review B</i> , 2013, 87, .	1.1	47
9667	First principle study on structural, elastic and electronic properties of cubic BiFeO <sub>3</sub> . <i>Ceramics International</i> , 2013, 39, S283-S286.	2.3	33

#	ARTICLE	IF	CITATIONS
9668	Magnetic Heusler Compounds. Handbook of Magnetic Materials, 2013, , 1-75.	0.6	25
9669	Self-interstitial defects in hexagonal close packed metals revisited: Evidence for low-symmetry configurations in Ti, Zr, and Hf. Physical Review B, 2013, 87, .	1.1	66
9670	The role of secondary bonding on supramolecular assembly of coordination compounds: diversity of coordination modes and supramolecular structures. CrystEngComm, 2013, 15, 5799.	1.3	29
9671	Halogen bonding synthon crossover in conformational polymorphism. CrystEngComm, 2013, 15, 5813.	1.3	25
9672	Explicit Roles of Au and TiO <sub>2</sub> in a Bifunctional Au/TiO <sub>2</sub> Catalyst for the Water-Gas Shift Reaction: A DFT Study. ChemCatChem, 2013, 5, 2479-2488.	1.8	23
9673	Ab initio simulations of oxygen interaction with surfaces and interfaces in uranium mononitride. Journal of Nuclear Materials, 2013, 435, 102-106.	1.3	18
9674	Thermodynamics of oligomer formation: implications for secondary organic aerosol formation and reactivity. Physical Chemistry Chemical Physics, 2013, 15, 6935.	1.3	45
9675	Ultrasound-Assisted Construction of Halogen-Bonded Nanosized Cocrystals That Exhibit Thermosensitive Luminescence. Chemistry - A European Journal, 2013, 19, 8213-8219.	1.7	75
9676	Half-Metallic and Magnetic Silicon Nanowires Functionalized by Transition-Metal Atoms. Springer Series in Materials Science, 2013, , 149-169.	0.4	1
9677	Cation Size Mismatch and Charge Interactions Drive Dopant Segregation at the Surfaces of Manganite Perovskites. Journal of the American Chemical Society, 2013, 135, 7909-7925.	6.6	468
9678	Structural, electronic and optical properties of silver delafossite oxides: A first-principles study with hybrid functional. Physica B: Condensed Matter, 2013, 422, 20-27.	1.3	12
9679	Deposition of (WO <sub>3</sub> ) <sub>3</sub> nanoclusters on the MgO(001) surface: A possible way to identify the charge states of the defect centers. Journal of Chemical Physics, 2013, 138, 034711.	1.2	9
9680	Nickel promoter effect on hydrotreating catalysts structures by means of density functional theory (DFT). Fuel, 2013, 110, 212-218.	3.4	2
9681	Ethanol Photoreaction on RuO <sub>x</sub> /Ru-Modified TiO <sub>2</sub> (110). Journal of Physical Chemistry C, 2013, 117, 11149-11158.	1.5	34
9682	Computational Study of Surface Deposition and Gas Phase Powder Formation during Spinel Chemical Vapor Deposition Processes. Industrial & Engineering Chemistry Research, 2013, 52, 15270-15280.	1.8	7
9683	Understanding the Density Functional Dependence of DFT-Calculated Electronic Couplings in Organic Semiconductors. Journal of Physical Chemistry Letters, 2013, 4, 919-924.	2.1	79
9684	Theoretical study of structural, elastic, electronic properties, and dispersion of optical functions of hexagonal ZnTiO <sub>3</sub> . Physica Status Solidi (B): Basic Research, 2013, 250, 1810-1815.	0.7	14
9685	First principles assessment of perovskite dopants for proton conductors with chemical stability and high conductivity. RSC Advances, 2013, 3, 3333.	1.7	28

#	ARTICLE	IF	CITATIONS
9686	Nature of Mâ€“Ge Bonds in the Metallogermylene Complexes of Chromium, Molybdenum, and Tungsten [( $\eta^5$ -C <sub>5</sub> H <sub>5</sub> )(CO) <sub>3</sub> M{GeN(SiMe <sub>3</sub> )R}] and [( $\eta^5$ -C <sub>5</sub> H <sub>5</sub> )(CO) <sub>3</sub> M{GeN(Ph)R}] (R = Ph, Mesityl (Mes)): A Theoretical Study. <i>Organometallics</i> , 2013, 32, 3395-3403.	1.1	16
9687	Refining crystal structures with experimental <sup>13</sup> C NMR shift tensors and lattice-including electronic structure methods. <i>CrystEngComm</i> , 2013, 15, 8693.	1.3	49
9688	Reconstruction of Clean and Oxygen-Covered Pt(110) Surfaces. <i>Journal of Physical Chemistry C</i> , 2013, 117, 11251-11257.	1.5	24
9689	Chargeâ€“Transfer Interaction between Fewâ€“Layer MoS <sub>2</sub> and Tetrathiafulvalene. <i>Chemistry - an Asian Journal</i> , 2013, 8, 1780-1784.	1.7	61
9690	First-principles vdW-DF investigation on the interaction between the oxazepam molecule and C60 fullerene. <i>Journal of Molecular Modeling</i> , 2013, 19, 1929-1936.	0.8	17
9691	Enthalpies of formation of mono substituted nitrobenzenes: A quantum chemistry study. <i>Computational and Theoretical Chemistry</i> , 2013, 1011, 37-43.	1.1	13
9692	ReaxFF Reactive Force Field Study of the Dissociation of Water on Titania Surfaces. <i>Journal of Physical Chemistry C</i> , 2013, 117, 10558-10572.	1.5	109
9693	Electronic and optical properties of the triphenylamine-based organic dye sensitized TiO <sub>2</sub> semiconductor: insight from first principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13844.	1.3	32
9694	Novel hetero-layered materials with tunable direct band gaps by sandwiching different metal disulfides and diselenides. <i>Scientific Reports</i> , 2013, 3, 1549.	1.6	437
9695	Highly Congested Donorâ€“Acceptor Pâ€“B Compound: Synthesis and Properties of a BMes <sub>2</sub> - and a PPh <sub>2</sub> -Functionalized 1,8-Naphthalene. <i>Organometallics</i> , 2013, 32, 3063-3068.	1.1	37
9696	Element-specific quantitative determination of the local atomic order in CoPt alloy nanoparticles: Experiment and theory. <i>Physical Review B</i> , 2013, 87, .	1.1	33
9697	The effect of remote substitution on formation of preferential geometrical isomer of cobalt(III)â€“tetrazolato complexes formed via [2+3] cycloaddition. <i>Inorganic Chemistry Communication</i> , 2013, 34, 62-67.	1.8	10
9698	Insight into the Preference Mechanism of CH <sub>x</sub> ( $x = 1-3$ ) and Câ€“C Chain Formation Involved in C <sub>2</sub> Oxygenate Formation from Syngas on the Cu(110) Surface. <i>Journal of Physical Chemistry C</i> , 2013, 117, 6594-6606.	1.5	59
9699	Scanning Tunneling Microscopy and Density Functional Theory Studies of Adatom-Involved Adsorption of Methylnitrene on Copper(110) Surface. <i>Journal of Physical Chemistry C</i> , 2013, 117, 12111-12116.	1.5	5
9700	Periodic DFT study on mechanism of selective catalytic reduction of NO via NH <sub>3</sub> and O <sub>2</sub> over the V <sub>2</sub> O <sub>5</sub> (001) surface: Competitive sites and pathways. <i>Journal of Catalysis</i> , 2013, 305, 67-75.	3.1	33
9701	Coreâ€“shell and matryoshka structures in MgNi nanoalloys: a computational study. <i>RSC Advances</i> , 2013, 3, 9419.	1.7	12
9702	Size Dependence in the Stabilities and Electronic Properties of $\pm$ -Graphyne and Its Boron Nitride Analogue. <i>Journal of Physical Chemistry C</i> , 2013, 117, 2175-2182.	1.5	117
9703	Application of the Generalized Connectivity-Based Hierarchy to Biomonomers: Enthalpies of Formation of Cysteine and Methionine. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4973-4980.	1.1	27

#	ARTICLE	IF	CITATIONS
9704	A Theoretical Study of Water Adsorption and Decomposition on Low-Index Spinel ZnGa <sub>2</sub> O <sub>4</sub> Surfaces: Correlation between Surface Structure and Photocatalytic Properties. <i>Langmuir</i> , 2013, 29, 7025-7037.	1.6	22
9705	Dependence on the structure and surface polarity of ZnS photocatalytic activities of water splitting: first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 9531.	1.3	23
9706	Density functional theory investigation of the VIII B transition metal atoms deposited on (5,5) single-walled carbon nanotubes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2013, 49, 61-67.	1.3	33
9707	Periodic Trends in 3d Metal Mediated CO <sub>2</sub> Activation. <i>ACS Symposium Series</i> , 2013, , 67-88.	0.5	3
9708	Bulk modulus prediction of austenitic stainless steel using a hybrid GA-ANN as a data mining tools. <i>Computational Materials Science</i> , 2013, 77, 330-334.	1.4	16
9709	Density Functional Theory Study of Water-Gas-Shift Reaction on 3Cu/γ-Al <sub>2</sub> O <sub>3</sub> (0001) Surface. <i>Journal of Physical Chemistry C</i> , 2013, 117, 12045-12053.	1.5	10
9710	Oxidovanadium Catechol Complexes: Radical versus Non-Radical States and Redox Series. <i>Inorganic Chemistry</i> , 2013, 52, 7417-7430.	1.9	25
9711	Experimental and theoretical investigation into the elimination of organic pollutants from solution by layered double hydroxides. <i>Applied Catalysis B: Environmental</i> , 2013, 140-141, 241-248.	10.8	48
9712	Tunable Assembly of sp <sup>3</sup> Cross-Linked 3D Graphene Monoliths: A First-Principles Prediction. <i>Advanced Functional Materials</i> , 2013, 23, 5846-5853.	7.8	59
9713	Ab initio study of the fracture energy of LiFePO <sub>4</sub> /FePO <sub>4</sub> interfaces. <i>Journal of Power Sources</i> , 2013, 243, 706-714.	4.0	21
9714	Magnetism and structural distortions in uranium sulfide under pressure. <i>Physical Review B</i> , 2013, 87, .	1.1	11
9715	Surface Temperature Effects on Dissociative Chemisorption of H <sub>2</sub> on Cu(100). <i>Journal of Physical Chemistry C</i> , 2013, 117, 8851-8863.	1.5	33
9716	Four-component relativistic chemical shift calculations of halogenated organic compounds. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 679-687.	0.9	19
9717	Controlling Adsorption Structure of Eosin Y Dye on Nanocrystalline TiO <sub>2</sub> Films for Improved Photovoltaic Performances. <i>Journal of Physical Chemistry C</i> , 2013, 117, 14659-14666.	1.5	47
9718	Theoretical study on the molecular tautomerism of the 3-hydroxy-pyridin-4-one system. <i>Molecular Physics</i> , 2013, 111, 958-967.	0.8	8
9719	Ab-initio study of free standing TiO <sub>2</sub> clusters: Stability and magnetism. <i>Journal of Applied Physics</i> , 2013, 113, 17B526.	1.1	23
9720	Anion-Mediated Coupling in Layered Perovskite La <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub> for Visible Light Photocatalysis. <i>Journal of Physical Chemistry C</i> , 2013, 117, 13845-13852.	1.5	46
9721	Thermodynamic Modeling of the La-B and La-Bi Systems Supported by First-Principles Calculations. <i>Journal of Phase Equilibria and Diffusion</i> , 2013, 34, 297-306.	0.5	15

#	ARTICLE	IF	CITATIONS
9722	CHAPTER 6. Computational Approach to Chemical Reactivity of MOFs. RSC Catalysis Series, 0, , 209-234.	0.1	3
9723	Valley spin polarization by using the extraordinary Rashba effect on silicon. Nature Communications, 2013, 4, 2073.	5.8	71
9724	Benzene adsorption on PtCo(111): A DFT study. Applied Surface Science, 2013, 282, 17-24.	3.1	7
9725	Hybrid compounds based on fullerene and polycyclic aromatic hydrocarbons with absorption in the near infrared region. Computational and Theoretical Chemistry, 2013, 1018, 50-58.	1.1	1
9726	Preparation, configurational and DFTâ€NBO analysis of nickel(II) complexes with edta-type ligands containing six-membered backbone ring: crystal structure of [Ni(H <sub>2</sub> O) <sub>6</sub> ][Ni(1,3-pdta)] $\cdot$ 2H <sub>2</sub> O. Journal of Coordination Chemistry, 2013, 66, 1730-1745.	0.8	6
9727	Assigning EXAFS results for uranyl adsorption on minerals via formal charges of bonding oxygen centers. Surface Science, 2013, 615, 21-25.	0.8	9
9728	Benzene adsorption on binary Pt <sub>3</sub> M alloys and surface alloys: a DFT study. Physical Chemistry Chemical Physics, 2013, 15, 12197.	1.3	28
9729	Electron-pinned defect-dipoles for high-performance colossal permittivity materials. Nature Materials, 2013, 12, 821-826.	13.3	784
9730	Plasmon Absorption of Au-in-CoAl <sub>2</sub> O <sub>4</sub> Linear Nanopeapod Chains. Journal of Physical Chemistry C, 2013, 117, 14142-14148.	1.5	20
9731	Density functional theory study on adsorption of Pt nanoparticle on graphene. International Journal of Hydrogen Energy, 2013, 38, 6283-6287.	3.8	18
9732	Characterization of Metal Nanocatalyst State and Morphology during Simulated Single-Walled Carbon Nanotube Growth. Journal of Physical Chemistry C, 2013, 117, 12061-12070.	1.5	13
9733	Effect of interstitial carbon on the mechanical properties of electrodeposited bulk nanocrystalline Ni. Acta Materialia, 2013, 61, 3360-3369.	3.8	74
9734	Revision of the Geâ€Ti phase diagram and structural stability of the new phase Ge <sub>4</sub> Ti <sub>5</sub> . Journal of Alloys and Compounds, 2013, 577, 211-216.	2.8	13
9735	Density Scaling of Noninteracting Kinetic Energy Functionals. Journal of Chemical Theory and Computation, 2013, 9, 2250-2255.	2.3	29
9736	Novel electronic and magnetic properties in N or B doped silicene nanoribbons. Journal of Materials Chemistry C, 2013, 1, 2735.	2.7	73
9737	Vibrational, electronic and quantum chemical studies of 1,2,4-benzenetricarboxylic-1,2-anhydride. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 110, 141-150.	2.0	16
9738	Ab-initio study of phase stability, thermodynamic and elastic properties of beryllium sulfide under extreme condition. Journal of Alloys and Compounds, 2013, 554, 363-370.	2.8	7
9739	Boron diffusion induced symmetry reduction and scattering in CoFeB/MgO/CoFeB magnetic tunnel junctions. Physical Review B, 2013, 87, .	1.1	33



#	ARTICLE	IF	CITATIONS
9740	Pressure and Temperature Effects on the Formation of a Pd/C Surface Carbide: Insights into the Role of Pd/C as a Selective Catalytic State for the Partial Hydrogenation of Acetylene. <i>Journal of Physical Chemistry C</i> , 2013, 117, 11059-11065.	1.5	14
9741	Which density functional is close to CCSD accuracy to describe geometry and interaction energy of small noncovalent dimers? A benchmark study using Gaussian09. <i>Journal of Computational Chemistry</i> , 2013, 34, 1341-1353.	1.5	108
9742	Insight into the active phase of CO oxidation on Ni/Pt and NiO <sub>1-x</sub> /Pt model catalysts from a first principles investigation. <i>Surface Science</i> , 2013, 614, 30-37.	0.8	2
9743	Ab initio calculations for the tetragonal PbZr <sub>0.5</sub> Ti <sub>0.5</sub> O <sub>3</sub> . <i>Computational Materials Science</i> , 2013, 77, 399-402.	1.4	9
9744	Role of Van der Waals Forces in Graphene Adsorption over Pd, Pt, and Ni. <i>Brazilian Journal of Physics</i> , 2013, 43, 126-129.	0.7	5
9745	Hybrid Hartree-Fock density functional study of charged point defects in ferroelectric PbTiO <sub>3</sub> . <i>Physical Review B</i> , 2013, 87, .	1.1	63
9746	Spin switching and magnetization reversal in single-crystal NdFeO <sub>3</sub> . <i>Physical Review B</i> , 2013, 87, .	1.1	166
9747	A comparative DFT study of the mechanical and electronic properties of greigite Fe <sub>3</sub> S <sub>4</sub> and magnetite Fe <sub>3</sub> O <sub>4</sub> . <i>Journal of Chemical Physics</i> , 2013, 138, 204712.	1.2	75
9748	Site-different structures from dilithium hexaboride (Li <sub>2</sub> B <sub>6</sub> ) to dimagnesium hexaboride (Mg <sub>2</sub> B <sub>6</sub> ) by first-principles. <i>Journal of Alloys and Compounds</i> , 2013, 569, 118-125.	2.8	3
9749	Catalyst studies on the ring opening of tetrahydrofuran dimethanol to 1,2,6-hexanetriol. <i>Catalysis Today</i> , 2013, 210, 106-116.	2.2	67
9750	A DFT study of the NO dissociation on gold surfaces doped with transition metals. <i>Journal of Chemical Physics</i> , 2013, 138, 074701.	1.2	9
9751	Atomic and molecular adsorption on Ru(0001). <i>Surface Science</i> , 2013, 614, 64-74.	0.8	71
9752	A novel strategy for low-temperature synthesis of Ruddlesden-Popper type layered perovskite La <sub>3</sub> Mn <sub>2</sub> O <sub>7</sub> + $\delta$ for methane combustion. <i>Journal of Materials Chemistry A</i> , 2013, 1, 8411.	5.2	18
9753	First-Principles Study of the Electronic Properties of B/N Atom Doped Silicene Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2013, 117, 13620-13626.	1.5	49
9754	Single Crystal Growth and Thermodynamic Stability of Li <sub>17</sub> Si <sub>4</sub> . <i>Chemistry of Materials</i> , 2013, 25, 1960-1967.	3.2	50
9755	Ultrasensitive Fiber Enhanced UV Resonance Raman Sensing of Drugs. <i>Analytical Chemistry</i> , 2013, 85, 6264-6271.	3.2	75
9756	C/B codoping effect on band gap narrowing and optical performance of TiO <sub>2</sub> photocatalyst: a spin-polarized DFT study. <i>Journal of Materials Chemistry A</i> , 2013, 1, 4516.	5.2	42
9757	Theoretical structure and vibrational spectra of ciprofloxacin: Density functional theory study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 102, 134-141.	2.0	5



#	ARTICLE	IF	CITATIONS
9758	Substituents effect on the electronic structure and molecular properties of bis[organohydrazido(2 <sup>+</sup> )] molybdenum(VI) complexes. <i>Polyhedron</i> , 2013, 61, 27-32.	1.0	2
9759	DFT study on the sulfurization mechanism during the desulfurization of H <sub>2</sub> S on the ZnO desulfurizer. <i>Fuel Processing Technology</i> , 2013, 106, 222-230.	3.7	65
9760	Thermodynamic properties and lattice misfit of Ir-based superalloys. <i>Intermetallics</i> , 2013, 32, 429-436.	1.8	15
9761	A simulation study of the shape of $\delta$ precipitates in Mg-Y and Mg-Gd alloys. <i>Acta Materialia</i> , 2013, 61, 453-466.	3.8	150
9762	Ab initio LCAO study of the atomic, electronic and magnetic structures and the lattice dynamics of triclinic CuWO <sub>4</sub> . <i>Acta Materialia</i> , 2013, 61, 371-378.	3.8	49
9763	Elastic constants of austenitic stainless steel: Investigation by the first-principles calculations and the artificial neural network approach. <i>Computational Materials Science</i> , 2013, 67, 353-358.	1.4	37
9764	A DFT study of gas molecules adsorption on the anatase (001) nanotube arrays. <i>Computational Materials Science</i> , 2013, 67, 174-181.	1.4	39
9765	Synthesis, experimental and theoretical investigations of Zn <sub>1-x</sub> Cu <sub>x</sub> O nanopowders. <i>Journal of Magnetism and Magnetic Materials</i> , 2013, 325, 42-46.	1.0	24
9766	Coarse-graining Kohn-Sham Density Functional Theory. <i>Journal of the Mechanics and Physics of Solids</i> , 2013, 61, 38-60.	2.3	46
9767	LDA and GGA studies of Al-rich and bulk goethite ( $\alpha$ -FeOOH). <i>Materials Chemistry and Physics</i> , 2013, 137, 1012-1020.	2.0	14
9768	Accommodation at the interface of highly dissimilar GaN(0001)/Sc <sub>2</sub> O <sub>3</sub> (111) heteroepitaxial systems. <i>Scripta Materialia</i> , 2013, 68, 211-214.	2.6	2
9769	Effects of electrode orientation on the transport properties of pyridine-terminated dithienylethene light molecule switch under bias. <i>Solid State Communications</i> , 2013, 153, 1-7.	0.9	5
9770	Ab initio molecular dynamics study of H <sub>2</sub> adsorption on sulfur- and chlorine-covered Pd(100). <i>Surface Science</i> , 2013, 608, 249-254.	0.8	19
9771	Influence of Step Defects on Methanol Decomposition: Periodic Density Functional Studies on Pd(211) and Kinetic Monte Carlo Simulations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 451-459.	1.5	28
9772	First-Principles Studies on Hydrogen Desorption Mechanism of Mg <sub>2</sub> H ( $n = 3, 4$ ). <i>Journal of Physical Chemistry C</i> , 2013, 117, 8099-8104.	1.5	11
9773	Evaluation of Approximate Exchange-Correlation Functionals in Predicting One-Bond <sup>31</sup> P- <sup>1</sup> H NMR Indirect Spin-Spin Coupling Constants. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1443-1451.	2.3	13
9774	Structural Acid-Base Chemistry in the Metallic State: How $\frac{1}{4}$ -Neutralization Drives Interfaces and Helices in Ti <sub>21</sub> Mn <sub>25</sub> . <i>Inorganic Chemistry</i> , 2013, 52, 8349-8359.	1.9	9
9775	Effect of Transition Metal Dopants on Initial Mass Transport in the Dehydrogenation of NaAlH <sub>4</sub> : Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3-14.	1.5	19

#	ARTICLE	IF	CITATIONS
9776	Monoxide carbon frequency shift as a tool for the characterization of TiO <sub>2</sub> surfaces: Insights from first principles spectroscopy. <i>Journal of Chemical Physics</i> , 2013, 138, 124702.	1.2	17
9777	Structural Transformations and Absorption Properties of Crystalline 7-Amino-6-nitrobenzodifuroxan under High Pressures. <i>Journal of Physical Chemistry C</i> , 2013, 117, 16830-16839.	1.5	36
9778	Macroscopic scattering of cracks initiated at single impurity atoms. <i>Nature Communications</i> , 2013, 4, 2441.	5.8	42
9779	Revisiting the Dependence of the Optical and Mobility Gaps of Hydrogenated Amorphous Silicon on Hydrogen Concentration. <i>Journal of Physical Chemistry C</i> , 2013, 117, 23956-23963.	1.5	23
9780	Interaction of Titanium Oxide Nanostructures with Graphene and Functionalized Graphene Nanoribbons: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 25424-25432.	1.5	32
9781	The Effects of the Formation of Stone-Wales Defects on the Electronic and Magnetic Properties of Silicon Carbide Nanoribbons: A First-Principles Investigation. <i>ChemPhysChem</i> , 2013, 14, 2841-2852.	1.0	37
9782	d <sub>0</sub> magnetism and large magnetoelectric effect in BC <sub>4</sub> N nanoribbons. <i>Journal of Applied Physics</i> , 2013, 113, 133705.	1.1	3
9783	A Simple, Accurate Model for Alkyl Adsorption on Late Transition Metals. <i>Journal of Physical Chemistry C</i> , 2013, 117, 2835-2843.	1.5	12
9784	Computational Catalyst Screening. <i>RSC Catalysis Series</i> , 2013, , 1-58.	0.1	11
9785	Structural trends in [Rh(PhCOCHCO(CH <sub>2</sub> ) <sub>n</sub> CH <sub>3</sub> )(CO)(PPh <sub>3</sub> )] (n=3) and related complexes: crystal structure of [Rh(PhCOCHCO(CH <sub>2</sub> ) <sub>2</sub> CH <sub>3</sub> )(CO)(PPh <sub>3</sub> )]. <i>Transition Metal Chemistry</i> , 2013, 38, 429-440.	0.7	8
9786	The Effect of Chemical Composition and Heat Treatment Conditions on Stacking Fault Energy for Fe-Cr-Ni Austenitic Stainless Steel. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2013, 44, 5884-5896.	1.1	90
9787	Multiscale modeling of submonolayer growth for Fe/Mo (110). <i>European Physical Journal B</i> , 2013, 86, 1.	0.6	2
9788	Toward a Process-Based Molecular Model of SiC Membranes. 1. Development of a Reactive Force Field. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3308-3319.	1.5	39
9789	First-principles studies of phase stability and crystal structures in Li-Zn mixed-metal borohydrides. <i>Physical Review B</i> , 2013, 88, .	1.1	11
9790	Scattering of Nitrogen Atoms off Ag(111) Surfaces: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 9779-9790.	1.5	20
9791	Excess manganese as the origin of the low-temperature anomaly in NiMnSb. <i>Physical Review B</i> , 2013, 88, .	1.1	9
9792	Loading Effect in Copper(II) Oxide Cluster-Surface-Modified Titanium(IV) Oxide on Visible- and UV-Light Activities. <i>Journal of Physical Chemistry C</i> , 2013, 117, 23848-23857.	1.5	65
9793	Hybrid Ag@TiO <sub>2</sub> core-shell nanostructures with highly enhanced photocatalytic performance. <i>Nanotechnology</i> , 2013, 24, 415601.	1.3	57

#	ARTICLE	IF	CITATIONS
9794	Synthesis of a tung oil-rosin adduct via the diels-alder reaction: Its reaction mechanism and properties in an ultraviolet-curable adhesive. <i>Journal of Applied Polymer Science</i> , 2013, 130, 4201-4208.	1.3	8
9795	On the Track to Silica-Supported Tungsten Oxo Metathesis Catalysts: Input from <sup>17</sup> O Solid-State NMR. <i>Inorganic Chemistry</i> , 2013, 52, 10119-10130.	1.9	40
9796	Infrared Spectra of H <sub>2</sub> ThS and H <sub>2</sub> US in Noble Gas Matrixes: Enhanced H-An-S Covalent Bonding. <i>Inorganic Chemistry</i> , 2013, 52, 10275-10285.	1.9	25
9797	First-principles study of the structural transformation, electronic structure, and optical properties of crystalline 2,6-diamino-3,5-dinitropyrazine-1-oxide under high pressure. <i>Journal of Molecular Modeling</i> , 2013, 19, 5159-5170.	0.8	26
9798	Theoretical Study of H <sub>2</sub> O Adsorption on Zn <sub>2</sub> GeO <sub>4</sub> Surfaces: Effects of Surface State and Structure-Activity Relationships. <i>ACS Applied Materials &amp; Interfaces</i> , 2013, 5, 6893-6901.	4.0	11
9799	A DFT Study of the Amadori Rearrangement above a Phosphatidylethanolamine Surface: Comparison to Reactions in Aqueous Environment. <i>Journal of Physical Chemistry C</i> , 2013, 117, 8299-8309.	1.5	10
9800	Ferroelectric control of magnetic anisotropy of FePt/BaTiO <sub>3</sub> magnetoelectric heterojunction: A density functional theory study. <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	17
9801	Density functional theory studies on adsorption and decomposition mechanism of FOX-7 on Al <sub>13</sub> clusters. <i>Canadian Journal of Chemistry</i> , 2013, 91, 1207-1212.	0.6	8
9802	First-Principles Calculations of Hydrogen Monomers and Dimers Adsorbed in Graphene and Carbon Nanotubes. <i>Journal of the Physical Society of Japan</i> , 2013, 82, 044702.	0.7	7
9803	First principles study of magnetic anisotropy and magnetoelectric effect of FePd/MgO(001) ultrathin films. <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	8
9804	Origin of the Conformational Modulation of the <sup>13</sup> C NMR Chemical Shift of Methoxy Groups in Aromatic Natural Compounds. <i>Journal of Physical Chemistry A</i> , 2013, 117, 661-669.	1.1	19
9805	Mode and Bond Selectivities in Methane Dissociative Chemisorption: Quasi-Classical Trajectory Studies on Twelve-Dimensional Potential Energy Surface. <i>Journal of Physical Chemistry C</i> , 2013, 117, 16127-16135.	1.5	66
9806	Effect of Substituents on the Preferred Modes of One-Electron Reductive Cleavage of N-Cl and N-Br Bonds. <i>Journal of Physical Chemistry A</i> , 2013, 117, 460-472.	1.1	22
9807	Mixed Termination of Hematite (±-Fe <sub>2</sub> O <sub>3</sub> )(0001) Surface. <i>Journal of Physical Chemistry C</i> , 2013, 117, 24339-24344.	1.5	48
9808	Understanding the Site Selectivity in Small-Sized Neutral and Charged Al <sub>n</sub> (4 ≤ n ≤ 10) Clusters: A Study on Water Molecule Adsorption. <i>Journal of Physical Chemistry A</i> , 2013, 117, 8691-8702.	1.1	15
9809	Elementary Reaction Processes Involving Atomic and Molecular Oxygen on ZrB <sub>2</sub> (0001) Surface. <i>Journal of Physical Chemistry C</i> , 2013, 117, 5831-5839.	1.5	5
9810	High CO <sub>2</sub> Selectivity of ZnO Powder Catalysts for Methanol Steam Reforming. <i>Journal of Physical Chemistry C</i> , 2013, 117, 6493-6503.	1.5	27
9811	An ion-pair complex [TTF][Pd(mnt) <sub>2</sub> ]: synthesis, crystal structure, magnetic property, and electrical conductivity. <i>Journal of Coordination Chemistry</i> , 2013, 66, 2529-2540.	0.8	2

#	ARTICLE	IF	CITATIONS
9812	Computational study of the structural, electronic and optical properties of M <sub>2</sub> N <sub>2</sub> (NH): M=C, Si, Ge, Sn. Computational Materials Science, 2013, 79, 710-714.	1.4	9
9813	First-principle calculations on the electronic structures and magnetic properties of Heusler compounds V <sub>2</sub> ReZ (Z=B, Al, Ga, In, Si, Ge, Sn, Sb). Journal of Magnetism and Magnetic Materials, 2013, 343, 268-275.	1.0	10
9814	Ab initio studies of Mo-based alloys: Mechanical, elastic, and vibrational properties. Intermetallics, 2013, 38, 116-125.	1.8	36
9815	Chlorine adsorption on Mg, Ca, and MgCa surfaces. Materials Science and Engineering C, 2013, 33, 3826-3831.	3.8	6
9816	Pressure-induced half-metallicity in Co <sub>2</sub> MnGe <sub>0.75</sub> Ga <sub>0.25</sub> . Journal of Magnetism and Magnetic Materials, 2013, 346, 192-195.	1.0	1
9817	Tuning solid-state blue and red luminescence by the formation of solvate crystals. Physical Chemistry Chemical Physics, 2013, 15, 19845.	1.3	27
9818	The Importance of Electron Correlation on Stacking Interaction of Adenine-Thymine Base-Pair Step in B-DNA: A Quantum Monte Carlo Study. Journal of Chemical Theory and Computation, 2013, 9, 1081-1086.	2.3	27
9819	Modeling of configurational transitions in atomic systems. Physics-Uspexhi, 2013, 56, 973-998.	0.8	11
9820	Ab initio study of helium behavior in titanium tritides. Computational Materials Science, 2013, 69, 107-112.	1.4	19
9821	On the role of strong electron correlations in the surface properties and chemistry of uranium dioxide. Dalton Transactions, 2013, 42, 4570.	1.6	32
9822	Acoustic impedance and interface phonon scattering in Bi <sub>2</sub> Te <sub>3</sub> and other semiconducting materials. Physical Review B, 2013, 87, .	1.1	22
9823	Interface engineering through atomic dopants in HfO <sub>2</sub> -based gate stacks. Journal of Applied Physics, 2013, 114, .	1.1	14
9824	Computational Investigation of CO Adsorption and Oxidation on Mn/CeO <sub>2</sub> (111) Surface. Journal of Physical Chemistry C, 2013, 117, 433-441.	1.5	75
9825	Transport properties for liquid silicon-oxygen-iron mixtures at Earth's core conditions. Physical Review B, 2013, 87, .	1.1	131
9826	Pressure depended elastic, vibration and optical properties of NbIrSn from first principles calculations. Materials Science and Technology, 2013, 29, 925-930.	0.8	8
9827	Oxygen segregation at coherent grain boundaries of cubic boron nitride. Applied Physics Letters, 2013, 102, 091607.	1.5	4
9828	NiO-MgO and CoO-MgO Thin-Film Solid Oxide Solutions on a Mo(100) Support: Formation, Reduction, and Influence of the Support. Journal of Physical Chemistry C, 2013, 117, 280-287.	1.5	9
9829	Density functional study of bare gold clusters: the ten-vertex neutral system. Journal of Molecular Modeling, 2013, 19, 4585-4590.	0.8	4

#	ARTICLE	IF	CITATIONS
9830	Density Functional Theory and Reaction Kinetics Studies of the Water-Gas Shift Reaction on Pt-Re Catalysts. <i>ChemCatChem</i> , 2013, 5, 3690-3699.	1.8	28
9831	First principles study of the interface between silicone and undoped/doped BaTiO <sub>3</sub> . <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	5
9832	A Mechanistic Study of <i>Trichoderma reesei</i> Cel7B Catalyzed Glycosidic Bond Cleavage. <i>Journal of Physical Chemistry B</i> , 2013, 117, 8714-8722.	1.2	19
9833	Multi-Scale Characterization Studies of Aged Li-Ion Large Format Cells for Improved Performance: An Overview. <i>Journal of the Electrochemical Society</i> , 2013, 160, A2111-A2154.	1.3	50
9834	Transport Properties in the CeO <sub>2</sub> (111) Surface: From Charge Distribution to Ion-Electron Collaborative Migration. <i>Journal of Physical Chemistry C</i> , 2013, 117, 25497-25503.	1.5	41
9835	Interaction of Gold Acetylides with Gold(I) or Silver(I) Cations. <i>Organometallics</i> , 2013, 32, 7025-7033.	1.1	32
9836	The Influence of Water and Hydroxyl on a Bimetallic (Au <sub>3</sub> -Au <sub>3</sub> )R <sub>30</sub> Sn/Pt Surface Alloy. <i>Journal of Physical Chemistry C</i> , 2013, 117, 4032-4039.	1.5	11
9837	Site-Specific Scaling Relations for Hydrocarbon Adsorption on Hexagonal Transition Metal Surfaces. <i>Journal of Physical Chemistry C</i> , 2013, 117, 20078-20088.	1.5	36
9838	Formation of non-substitutional <sup>125</sup> Sn defects in Ge <sub>1-x</sub> Sn <sub>x</sub> alloys. <i>Journal of Applied Physics</i> , 2013, 114, 193508.	1.1	5
9839	First-Principles Investigations on the Na <sub>2</sub> MnPO <sub>4</sub> F as a Cathode Material for Na-Ion Batteries. <i>Journal of the Electrochemical Society</i> , 2013, 160, A927-A932.	1.3	34
9840	Synthesis of Zwitterionic Triphosphenium Transition Metal Complexes: A Boron Atom Makes The Difference. <i>Inorganic Chemistry</i> , 2013, 52, 11438-11449.	1.9	28
9841	Insights into H <sub>2</sub> formation in space from ab initio molecular dynamics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 6674-6677.	3.3	30
9842	Nonstoichiometry in Bixbyite-Type Vanadium Sesquioxide. <i>Journal of Physical Chemistry C</i> , 2013, 117, 20164-20170.	1.5	8
9843	The role of water in the adsorption of oxygenated aromatics on Pt and Pd. <i>Journal of Computational Chemistry</i> , 2013, 34, 60-66.	1.5	18
9844	Appropriate description of intermolecular interactions in the methane hydrates: An assessment of DFT methods. <i>Journal of Computational Chemistry</i> , 2013, 34, 121-131.	1.5	111
9845	Steering the Growth of Metal Adatoms via Interface Interactions Between a MgO Thin Film and a Mo Support. <i>Advanced Functional Materials</i> , 2013, 23, 75-80.	7.8	24
9846	Structure-Property Relations in All-Organic Dye-Sensitized Solar Cells. <i>Advanced Functional Materials</i> , 2013, 23, 424-429.	7.8	68
9847	An Ion-Exchange Phase Transformation to ZnGa <sub>2</sub> O <sub>4</sub> Nanocube Towards Efficient Solar Fuel Synthesis. <i>Advanced Functional Materials</i> , 2013, 23, 758-763.	7.8	72

#	ARTICLE	IF	CITATIONS
9848	Realization of the Switching Mechanism in Resistance Random Access Memory <sub>1,2</sub> Devices: Structural and Electronic Properties Affecting Electron Conductivity in a Hafnium Oxide <sub>1</sub> Electrode System Through First-Principles Calculations. <i>Journal of Electronic Materials</i> , 2013, 42, 143-150.	1.0	10
9849	Functionalization of Graphene Nanoribbons. <i>Nanoscience and Technology</i> , 2013, , 69-92.	1.5	1
9850	Electronic, optical, and charge transfer properties of donor <sub>1</sub> –bridge <sub>2</sub> –acceptor hydrazone sensitizers. <i>Structural Chemistry</i> , 2013, 24, 499-506.	1.0	32
9851	Sign-inverted response of aluminum work function to tangential strain. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 445012.	0.7	3
9852	Extended Czjzek model applied to NMR parameter distributions in sodium metaphosphate glass. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 255402.	0.7	15
9853	Adhesion of the iron <sub>1</sub> –chromium oxide interface from first-principles theory. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 495501.	0.7	10
9854	Charge localization on the hexa-interstitial cluster in MgO. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 065502.	0.7	2
9855	Hybridization between Cu <sub>1</sub> –O chain and Cu(110) surface states in the O(2 $\bar{1}$ –1)/Cu(110) surface from first principles. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 135003.	0.7	6
9856	Surface parameters of ferritic iron-rich Fe <sub>1</sub> –Cr alloy. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 305002.	0.7	8
9857	Optical absorption and emission of $\hat{1}$ –Sn nanocrystals from first principles. <i>Nanotechnology</i> , 2013, 24, 405702.	1.3	13
9858	Electron scattering from gas phase cis-diamminedichloroplatinum(II): Quantum analysis of resonance dynamics. <i>Journal of Chemical Physics</i> , 2013, 138, 204308.	1.2	2
9859	Origin of <i>c</i> - <i>i</i> axis ultraincompressibility of Zr <sub>2</sub> InC above 70 $\hat{1}$ –GPa via first-principles. <i>Journal of Applied Physics</i> , 2013, 114, .	1.1	24
9860	STM imagery and density functional calculations of C <sub>60</sub> fullerene adsorption on the 6H-SiC(0001)-3 $\bar{1}$ –3 surface. <i>Physical Review B</i> , 2013, 87, .	1.1	10
9861	Surface-termination-dependent Pd bonding and aggregation of nanoparticles on LaFeO <sub>3</sub> (001). <i>Journal of Chemical Physics</i> , 2013, 138, 144705.	1.2	10
9862	The structure of liquid GeSe revisited: A first principles molecular dynamics study. <i>Journal of Chemical Physics</i> , 2013, 138, 174505.	1.2	21
9863	Electronic and transport properties of zintl phase AeMg <sub>2</sub> Pn <sub>2</sub> , Ae <sub>1</sub> –Ca,Sr,Ba, Pn <sub>1</sub> –As,Sb,Bi in relation to Mg <sub>3</sub> Sb <sub>2</sub> . <i>Journal of Applied Physics</i> , 2013, 114, 143703.	1.1	45
9864	Oxidation of the two-phase Nb/Nb <sub>5</sub> Si <sub>3</sub> composite: The role of energetics, thermodynamics, segregation, and interfaces. <i>Journal of Chemical Physics</i> , 2013, 138, 014708.	1.2	17
9865	Validation of density functionals for transition metals and intermetallics using data from quantitative electron diffraction. <i>Journal of Chemical Physics</i> , 2013, 138, 084504.	1.2	6







#	ARTICLE	IF	CITATIONS
9884	Analytical Bond-order Potential for hcp-Y. Chinese Journal of Chemical Physics, 2013, 26, 526-532.	0.6	5
9885	Search for Barrier Materials for Cu Interconnects in Integrated Circuits. ECS Journal of Solid State Science and Technology, 2013, 2, P351-P356.	0.9	0
9886	Ab initio investigation of the structural and unusual electronic properties of $\text{I}\pm\text{-CuSe}$ (klockmannite). Chinese Physics B, 2013, 22, 127102.	0.7	5
9887	First-Principles Calculations of Elastic Properties of HoBi and ErBi. Advanced Materials Research, 2013, 664, 672-676.	0.3	0
9888	First-Principles Studies on Cd Doping in $\text{CuInSe}_2$ and Related Compounds during Chemical Bath Deposition of CdS Buffer Layer. Japanese Journal of Applied Physics, 2013, 52, 061201.	0.8	11
9889	Internal Geometric and Electronic Structures of Natural Bornite Crystal. Applied Mechanics and Materials, 2013, 368-370, 747-751.	0.2	1
9890	Optical fingerprints of Y2 ordering in III-V ternary semiconductor alloys. Semiconductor Science and Technology, 2013, 28, 065012.	1.0	2
9891	Theoretical prediction of ion conductivity in solid state $\text{HfO}_2$ . Chinese Physics B, 2013, 22, 016601.	0.7	8
9892	Electronic Structures in $\text{LaTiO}_3/\text{LaAlO}_3$ Multilayers. Advanced Materials Research, 2013, 771, 7-11.	0.3	2
9893	Photoelectric Properties of the Doped Silicon with Carbon Family Elements. Advanced Materials Research, 0, 873, 793-798.	0.3	3
9894	Design of Pt-Based Bimetallic Alloys for the Oxidation of $\text{H}_2\text{O}_2$ : A Combined Computational and Experimental Approach. ChemCatChem, 2013, 5, 1709-1712.	1.8	2
9895	Air-Promoted Adsorptive Desulfurization over $\text{Ti}_{0.9}\text{Ce}_{0.1}\text{O}_2$ Mixed Oxides from Diesel Fuel under Ambient Conditions. ChemCatChem, 2013, 5, 3582-3586.	1.8	17
9896	Electronic Structure Calculations in Molecules. Springer Tracts in Modern Physics, 2013, , 183-230.	0.1	0
9897	Influence of normal and shear strain on magnetic anisotropy energy of hcp cobalt: An ab initio study. Journal of Materials Research, 2013, 28, 1559-1566.	1.2	3
9898	The Development of Green Architectural Heritage Cave Civilization. Applied Mechanics and Materials, 0, 368-370, 115-118.	0.2	2
9899	Density Functional Study of the Structure, Stability and Oxygen Reduction Activity of Ultrathin Platinum Nanowires. Journal of the Electrochemical Society, 2013, 160, F548-F553.	1.3	7
9900	Density functional theory periodic slab calculations of adsorption and dissociation of $\text{H}_2\text{O}$ on the $\text{Cu}_2\text{O}(110)$ :CuO surface. Canadian Journal of Physics, 2013, 91, 1101-1106.	0.4	10
9901	Influence of on-site Coulomb interaction $U$ on properties of $\text{MnO}(001)2 \text{ \AA}^{-1}$ and $\text{NiO}(001)2 \text{ \AA}^{-1}$ surfaces. Journal of Physics Condensed Matter, 2013, 25, 094006.	0.7	11

#	ARTICLE	IF	CITATIONS
9902	Influence of H, C, N and O impurities on the stability of Mg and Al from first-principles calculations. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 055014.	0.8	4
9903	On the way to the highest coordination number in the planar metal-centred aromatic TaB <sub>10</sub> cluster: Evolution of the structures of TaB <sub>n</sub> (n = 3-8). Journal of Chemical Physics, 2013, 139, 104312.	1.2	61
9904	Atomic structure, energetics, and chemical bonding of Y doped $\lambda$ 13 grain boundaries in $\lambda$ -Al <sub>2</sub> O <sub>3</sub> . Philosophical Magazine, 2013, 93, 1158-1171.	0.7	10
9905	Double Ion Implantation and Pulsed Laser Melting Processes for Third Generation Solar Cells. International Journal of Photoenergy, 2013, 2013, 1-7.	1.4	5
9906	Vibrational Spectroscopic Studies of Tenofovir Using Density Functional Theory Method. Journal of Chemistry, 2013, 2013, 1-12.	0.9	8
9907	Electron density distribution in tetralithium hypodiphosphate hexahydrate, Li <sub>4</sub> P <sub>2</sub> O <sub>6</sub> ·6H <sub>2</sub> O. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2013, 69, 344-355.	0.5	12
9908	Ab initio elasticity workflow in the VLab science gateway. , 2013, , .		0
9909	Study of intrinsic defects in 3C-SiC using first-principles calculation with a hybrid functional. Journal of Chemical Physics, 2013, 139, 124707.	1.2	27
9910	Towards a specific reaction parameter density functional for reactive scattering of H <sub>2</sub> from Pd(111). Journal of Chemical Physics, 2013, 139, 244707.	1.2	14
9911	Bis(μ <sub>2</sub> -oxo and μ <sub>2</sub> -superoxo)dicopper complexes studied within (time-dependent) density-functional and many-body perturbation theory. Journal of Computational Chemistry, 2013, 34, 1035-1045.	1.5	29
9912	Koopmans' condition in self-interaction-corrected density-functional theory. Physical Review A, 2013, 88, .	1.0	41
9913	Density functional theory (DFT) investigation of the adsorption of the CH <sub>3</sub> OH/Au(100) system. Surface and Interface Analysis, 2013, 45, 1410-1418.	0.8	4
9914	Environment-dependent noncollinear magnetic orders and spin-wave spectra of Fe chains and stripes. Physical Review B, 2013, 87, .	1.1	9
9915	Gold-titania interface toughening and thermal conductance enhancement using an organophosphonate nanolayer. Applied Physics Letters, 2013, 102, 201605.	1.5	15
9916	First-principles study of stability and properties on $\lambda$ 2-SiC/TiC(111) interface. Journal of Applied Physics, 2013, 114, .	1.1	31
9917	Dissolving, trapping and detrapping mechanisms of hydrogen in bcc and fcc transition metals. AIP Advances, 2013, 3, .	0.6	82
9918	Chemistry at molecular junctions: Rotation and dissociation of O <sub>2</sub> on the Ag(110) surface induced by a scanning tunneling microscope. Journal of Chemical Physics, 2013, 139, 074702.	1.2	21
9919	Force mapping on a partially H-covered Si(111)-(7 $\times$ 7) surface. Physical Review B, 2013, 87, .	1.1	38

#	ARTICLE	IF	CITATIONS
9920	LARGE HOLE POLARONS IN Sc-DOPED TiO <sub>2</sub> CRYSTALS. Modern Physics Letters B, 2013, 27, 1350113.	1.0	16
9921	Reactive scattering of H <sub>2</sub> from Cu(100): Comparison of dynamics calculations based on the specific reaction parameter approach to density functional theory with experiment. Journal of Chemical Physics, 2013, 138, 044708.	1.2	73
9922	First-principles insights into the structure of the incipient magnesium oxide and its instability to decomposition: Oxygen chemisorption to Mg(0001) and thermodynamic stability. Physical Review B, 2013, 87, .	1.1	39
9923	Accuracy of exchange-correlation functionals and effect of solvation on the surface energy of copper. Physical Review B, 2013, 87, .	1.1	211
9924	Charge compensation by long-period reconstruction in strongly polar lithium niobate surfaces. Physical Review B, 2013, 88, .	1.1	23
9925	Quasiparticle spectra and excitons of organic molecules deposited on substrates: $G_{0.1}^{\text{MTO}}$ approach applied to benzene on graphene and metallic substrates. Physical Review B, 2013, 88, .		
9926	An ab initio study on compressibility of Al-containing MAX-phase carbides. Journal of Applied Physics, 2013, 114, 173709.	1.1	22
9927	Layered pnictide-oxide Na <sub>2</sub> Ti <sub>2</sub> Pn <sub>2</sub> O (Pn=As, Sb): a candidate for spin density waves. Journal of Physics Condensed Matter, 2013, 25, 365501.	0.7	22
9928	Applicability of carbon and boron nitride nanotubes as biosensors: Effect of biomolecular adsorption on the transport properties of carbon and boron nitride nanotubes. Applied Physics Letters, 2013, 102, .	1.5	10
9930	Methane dissociative chemisorption and detailed balance on Pt(111): Dynamical constraints and the modest influence of tunneling. Journal of Chemical Physics, 2013, 139, 214707.	1.2	13
9931	Change of the electronic conductivity of graphene nanoribbons and carbon nanotubes caused by a local deformation. , 2013, , .		0
9932	Multireference calculations for ring inversion and double bond shifting in cyclooctatetraene. Journal of Computational Chemistry, 2013, 34, 1393-1397.	1.5	22
9933	Mechanistic Role of Water on the Rate and Selectivity of Fischer-Tropsch Synthesis on Ruthenium Catalysts. Angewandte Chemie - International Edition, 2013, 52, 12273-12278.	7.2	138
9934	Influence of Dopants C on Dehydrogenating Properties of LiNH <sub>2</sub> . , 2013, , .		0
9935	Computational studies of catalyst-free single walled carbon nanotube growth. Journal of Chemical Physics, 2013, 139, 054308.	1.2	1
9936	Distortion of electronic structure in HfO <sub>2</sub> induced by the out-diffused As from GaAs substrate. Journal of Applied Physics, 2013, 113, 186101.	1.1	0
9937	Environment-dependent interfacial strength using first principles thermodynamics: The example of the Pt-HfO <sub>2</sub> interface. Journal of Applied Physics, 2013, 114, 163503.	1.1	6
9938	Theory and synthesis of bilayer graphene intercalated with ICl and IBr for low power device applications. Journal of Applied Physics, 2013, 114, .	1.1	7

#	ARTICLE	IF	CITATIONS
9939	Local and chemical environment dependence of the magnetic properties of CoRh core-shell nanoparticles. <i>Physical Review B</i> , 2013, 88, .	1.1	17
9940	Effects of Li doping on H-diffusion in MgH <sub>2</sub> : A first-principles study. <i>Journal of Applied Physics</i> , 2013, 114, .	1.1	12
9941	First principles investigation of Ti adsorption and migration on Si(100) surfaces. <i>Journal of Applied Physics</i> , 2013, 114, 243505.	1.1	3
9942	Development of a ReaxFF potential for Pd/O and application to palladium oxide formation. <i>Journal of Chemical Physics</i> , 2013, 139, 044109.	1.2	83
9943	Interfacial properties and electronic structure of $\hat{\Gamma}^2$ -SiC(111)/ $\hat{\Gamma}^2$ -Ti(0001): A first principle study. <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	28
9944	Adsorption of phosphorus molecules evaporated from an InP solid source on the Si(100) surface. <i>Physical Review B</i> , 2013, 87, .	1.1	5
9945	Geometrically induced melting variation in gallium clusters from first principles. <i>Physical Review B</i> , 2013, 88, .	1.1	17
9946	STRUCTURAL AND ELECTRONIC EVOLUTION FROM SiC SHEET TO SILICENE. <i>International Journal of Modern Physics B</i> , 2013, 27, 1350188.	1.0	2
9947	Superior Field Emission Properties of Layered WS <sub>2</sub> -RGO Nanocomposites. <i>Scientific Reports</i> , 2013, 3, 3282.	1.6	218
9948	Adsorption of methylamine on mackinawite (FES) surfaces: A density functional theory study. <i>Journal of Chemical Physics</i> , 2013, 139, 124708.	1.2	45
9949	A benchmark study of DFT methods on the electronic properties of lanthanofullerenes: a case study of Ce@C <sub>2v</sub> (9)-C <sub>82</sub> anion. <i>RSC Advances</i> , 2013, 3, 26252.	1.7	2
9950	Adsorption of NO on Pt(100) from first principles. <i>Physica Scripta</i> , 2013, 87, 055601.	1.2	8
9951	Structural, elastic, thermodynamic and lattice dynamic properties of PrX (X=As, Sb, Bi). <i>International Journal of Materials Research</i> , 2013, 104, 99-108.	0.1	3
9952	Towards understanding the carbon trapping mechanism in copper by investigating the carbon-vacancy interaction. <i>Chinese Physics B</i> , 2013, 22, 076104.	0.7	9
9953	IRON IMPURITY IN ZIRCON BY DFT COMPUTATIONS. <i>Modern Physics Letters B</i> , 2013, 27, 1350145.	1.0	6
9954	DENSITY FUNCTIONAL THEORY STUDY OF THE PHOTOELECTRON SPECTRA OF 5-METHYLTETRAZOLE. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1250096.	1.8	9
9955	ACHIEVING P-TYPE SEMICONDUCTING ZnO NANOWIRES VIA DONOR ADSORPTION. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1350014.	1.8	0
9956	FIRST-PRINCIPLES STUDY ON $\hat{\Gamma}^2$ -SiC/BNNT CORE/SHELL NANOCABLE. <i>Modern Physics Letters B</i> , 2013, 27, 1350169.	1.0	0

#	ARTICLE	IF	CITATIONS
9957	THERMODYNAMIC PROPERTIES OF MC (M = V, Nb, Ta): FIRST-PRINCIPLES CALCULATIONS. Modern Physics Letters B, 2013, 27, 1341035.	1.0	3
9958	THE STRUCTURE, MAGNETISM AND CONDUCTIVITY OF Li <sub>3</sub> V <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> : A THEORETICAL AND EXPERIMENTAL STUDY. Modern Physics Letters B, 2013, 27, 1350199.	1.0	5
9959	Pressure dependent stability and structure of carbon dioxide—A density functional study including long-range corrections. Journal of Chemical Physics, 2013, 139, 174501.	1.2	18
9960	Tensile properties of phase interfaces in Mg—Li alloy: A first principles study. Chinese Physics B, 2013, 22, 126802.	0.7	4
9961	A First-Principles Study of Electronic Structure of the Laves Phase MgZn <sub>2</sub> . Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 1963-1967.	0.6	8
9962	First-Principles Studies of the Electronic and Dielectric Properties of Si/SiO <sub>2</sub> /HfO <sub>2</sub> Interfaces. Japanese Journal of Applied Physics, 2013, 52, 041803.	0.8	7
9963	Quantifying stoichiometry-induced variations in structure and energy of a SrTiO <sub>3</sub> symmetric {110} grain boundary. Philosophical Magazine, 2013, 93, 1219-1229.	0.7	13
9964	Molecular distortion and charge transfer effects in ZnPc/Cu(111). Scientific Reports, 2013, 3, .	1.6	19
9965	Predicting Atomic Arrangement of Solute Clusters in Dilute Mg Alloys. Materials Research Letters, 2013, 1, 213-219.	4.1	44
9968	Magnetic and electronic structural properties of the GdGa <sub>7</sub> N <sub>8</sub> cluster. Proceedings of SPIE, 2013, , .	0.8	0
9969	Computational Study of Cage Like (ZnO) <sub>12</sub> Cluster Using Hybrid and Hybrid Meta Functionals. Journal of the Chinese Chemical Society, 2013, 60, 1082-1091.	0.8	6
9970	Quantum chemical study of conformational preferences of intermediates and transition states in the alkaline hydrolysis of dimethyl phosphate. Journal of Physics: Conference Series, 2013, 454, 012058.	0.3	0
9971	{111} dislocation core properties in L <sub>1</sub> <sub>2</sub> Al <sub>3</sub> Sc and Al <sub>3</sub> Mg based on the Peierls-Nabarro model. Physica Status Solidi (B): Basic Research, 2013, 250, 1825-1831.	0.7	1
9972	Bis(sulfonylimide)ruthenium(VI) Porphyrins: X-ray Crystal Structure and Mechanism of C-H Bond Amination by Density Functional Theory Calculations. Chemistry - A European Journal, 2013, 19, 11320-11331.	1.7	40
9973	First-principles study of structural and electronic properties of Laves phases structures YM <sub>2</sub> (M = Cu) Tj ETQqO 0 0 rgBT /Overlock 10 Tf 5	0.1	5
9974	Phase transition and elastic properties of beryllium sulfide semiconductor under high pressure. EPJ Applied Physics, 2013, 62, 20103.	0.3	4
9975	Preparation and study of the structural and electronic properties of the type-I clathrate phase Ba <sub>8</sub> Ga <sub>16</sub> Mg <sub>x</sub> Ge <sub>30-x</sub> . EPJ Applied Physics, 2013, 64, 30101.	0.3	2
9976	The interaction of hydrogen with the {010} surfaces of Mg and Fe olivine as models for interstellar dust grains: a density functional theory study. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2013, 371, 20110592.	1.6	17

#	ARTICLE	IF	CITATIONS
9977	Communication: In search of four-atom chiral metal clusters. <i>Journal of Chemical Physics</i> , 2013, 139, 111101.	1.2	8
9978	First-Principles Investigation on the Lithium Ion Insertion/Extraction in Trirutile $\text{Li}_x\text{FeF}_3$ . <i>Electrochemistry</i> , 2013, 81, 12-15.	0.6	8
9979	Enthalpies of Solution in Ti&ndash;X (X = Mo, Nb, V and W) Alloys from First-Principles Calculations. <i>Materials Transactions</i> , 2013, 54, 484-492.	0.4	36
9980	First-Principles Calculation of Grain Boundary Excess Volume and Free Volume in Nanocrystalline and Ultrafine-Grained Aluminum. <i>Materials Transactions</i> , 2013, 54, 1597-1604.	0.4	13
9981	Energetic Analysis of Deformation Twins and Twinning Dislocations in Magnesium. <i>Materials Transactions</i> , 2013, 54, 1524-1527.	0.4	12
9982	Collision dynamics of energetic carbon ions impinging on single-walled carbon nanotubes. <i>EPJ Applied Physics</i> , 2013, 64, 10401.	0.3	3
9983	Hydrodeoxygenation of Phenolic Compounds by Sulfided (Co)Mo/Al <sub>2</sub> O <sub>3</sub> Catalysts, a Combined Experimental and Theoretical Study. <i>Oil and Gas Science and Technology</i> , 2013, 68, 829-840.	1.4	37
9984	Promotion of Iron Oxide Reduction and Extracellular Electron Transfer in <i>Shewanella oneidensis</i> by DMSO. <i>PLoS ONE</i> , 2013, 8, e78466.	1.1	12
9985	Synthesis and Characterization of Novel Dendrons Bearing Amino-Nitro-Substituted Azobenzene Units and Oligo(ethylene glycol) Spacers: Thermal, Optical Properties, Langmuir Blodgett Films and Liquid-Crystalline Behaviour. <i>Molecules</i> , 2013, 18, 1502-1527.	1.7	9
9986	First-Principles Elucidation of the Surface Chemistry of the $\text{C}_2\text{H}_x$ ( $x = 0\text{--}6$ ) Adsorbate Series on Fe(100). <i>Molecules</i> , 2013, 18, 3806-3824.	1.7	22
9987	Benchmark Study on the Smallest Bimolecular Nucleophilic Substitution Reaction: $\text{H}^+ + \text{CH}_4 \rightarrow \text{CH}_5^+ + \text{H}^-$ . <i>Molecules</i> , 2013, 18, 7726-7738.	1.7	2
9988	Kinetics of Nitric Oxide and Oxygen Gases on Porous Y-Stabilized ZrO <sub>2</sub> -Based Sensors. <i>Molecules</i> , 2013, 18, 9901-9918.	1.7	10
9989	Scale Alpha and Beta of Quantitative Convergence and Chemical Reactivity Analysis in Dual Cholinesterase/Monoamine Oxidase Inhibitors for the Alzheimer Disease Treatment Using Density Functional Theory (DFT). <i>Journal of Theoretical Chemistry</i> , 2013, 2013, 1-13.	1.5	9
9990	Structures and Stabilities of Alkaline Earth Metal Oxide Nanoclusters: A DFT Study. <i>Journal of Theoretical Chemistry</i> , 2013, 2013, 1-14.	1.5	21
9991	Electronic Structure Calculations of $\text{A}_{2}\text{Ti}_{2}\text{O}_7$ (A = Dy, Ho, and Y). <i>Advances in Condensed Matter Physics</i> , 2013, 2013, 1-8.	0.4	6
9992	Effect of Intrinsic Point Defect on the Magnetic Properties of ZnO Nanowire. <i>Scientific World Journal</i> , The, 2013, 2013, 1-6.	0.8	5
9993	Theoretical Simulations of Reactive and Nonreactive Scattering of Light Diatomic Molecules from Metal Surfaces: Past, Present, and Future. <i>Advances in Chemistry</i> , 2014, 2014, 1-21.	1.1	0
9994	Preparation of Compensation Ions Codoped SrTiO <sub>3</sub> :Pr <sup>3+</sup> Red Phosphor with the Sol-Gel Method and Study of Its Luminescence Enhancement Mechanism. <i>Advances in OptoElectronics</i> , 2014, 2014, 1-9.	0.6	1



#	ARTICLE	IF	CITATIONS
9995	Topological Model on the Inductive Effect in Alkyl Halides Using Local Quantum Similarity and Reactivity Descriptors in the Density Functional Theory. <i>Journal of Quantum Chemistry</i> , 2014, 2014, 1-12.	0.6	9
9996	Recent Advances in Computational Materials Science. <i>Tetsu-To-Hagane/Journal of the Iron and Steel Institute of Japan</i> , 2014, 100, 1207-1219.	0.1	3
9997	The study on the geometry and electronic properties of (WO <sub>3</sub> ) <sub>x</sub> /(TiO <sub>2</sub> ) <sub>y</sub> heterostructure by using the layered structural model. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1450034.	1.8	1
9998	Ti <sub>2</sub> MnZ (Z = Si, Ge, Sn, Sb, Bi) compounds: A first-principles study of electronic structures and magnetism. <i>Journal of the Korean Physical Society</i> , 2014, 65, 2058-2065.	0.3	11
9999	Molecular dynamics study of the stability of a carbon nanotube atop a catalytic nanoparticle. <i>European Physical Journal D</i> , 2014, 68, 1.	0.6	23
10000	Adsorption of PTCDA on Terraces and at Steps Sites of the KCl(100) Surface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 29911-29918.	1.5	22
10001	Promoting alkali and alkaline-earth metals on MgO for enhancing CO <sub>2</sub> capture by first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24818-24823.	1.3	37
10002	Uniaxial strain-dependent magnetic and electronic properties of (Ga,Mn)As nanowires. <i>Chinese Physics B</i> , 2014, 23, 096103.	0.7	4
10003	Effects of C impurities on the elastic properties of NiAl intermetallics. <i>Progress in Natural Science: Materials International</i> , 2014, 24, 637-641.	1.8	9
10004	Luminescent centers in GaN codoped with Eu and Mg: Calculation on density functional theory. <i>Japanese Journal of Applied Physics</i> , 2014, 53, 061001.	0.8	8
10005	GEOMETRY OF DOPAMINE ADSORPTION ON RUTILE (110) SURFACE. <i>International Journal of Modern Physics B</i> , 2014, 28, 1450071.	1.0	4
10006	The hcp to fcc transformation path of scandium trihydride under high pressure. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 025405.	0.7	3
10007	DFT investigation on organic dyes with cross-conjugated cyano groups. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1450008.	1.8	0
10008	First-principles study of the stability of silicane and germanane under strain. <i>Modern Physics Letters B</i> , 2014, 28, 1450138.	1.0	4
10009	Spin and Orbital Magnetism in Free Nanoparticles. <i>Frontiers of Nanoscience</i> , 2014, 6, 33-84.	0.3	1
10010	Assessing the performance of commonly used DFT functionals in studying the chemistry of frustrated Lewis pairs. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1350074.	1.8	21
10011	Constraints on $\beta$ cellulose twist from DFT calculations of $^{13}\text{C}$ NMR chemical shifts. <i>Cellulose</i> , 2014, 21, 3979-3991.	2.4	14
10012	Effect of hydrostatic pressure on the thermoelectric properties of $\text{Bi}_2\text{Te}_3$ . <i>Physical Review B</i> , 2014, 90, ...	1.1	29



#	ARTICLE	IF	CITATIONS
10013	DFT calculation on relaxation and electronic structure of sulfide minerals surfaces in presence of H <sub>2</sub> O molecule. Journal of Central South University, 2014, 21, 3945-3954.	1.2	35
10014	First-principles theory on electronic structure and floatability of spodumene. Rare Metals, 2014, 33, 742-748.	3.6	31
10015	Influence of Ni on Cu precipitation in Fe-Cu-Ni ternary alloy by an atomic study. Chinese Physics B, 2014, 23, 063601.	0.7	14
10016	Polythiophene encapsulated inside (13, 0) CNT: A nano-hybrid system. Chinese Physics B, 2014, 23, 066201.	0.7	14
10017	Conditions for electronic reconstruction at stoichiometric polar/polar interfaces. Journal of Physics Condensed Matter, 2014, 26, 485010.	0.7	6
10018	Ab initio-based Er-He interatomic potential in hcp Er. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 065009.	0.8	3
10019	Structural stability and electrical properties of AlB <sub>2</sub> -type MnB <sub>2</sub> under high pressure. Chinese Physics B, 2014, 23, 016102.	0.7	8
10020	Use of surface plasmons for manipulation of organic molecule quasiparticles and optical properties. Journal of Physics Condensed Matter, 2014, 26, 485012.	0.7	2
10021	Defect formation energy in pyrochlore: the effect of crystal size. Materials Research Express, 2014, 1, 035501.	0.8	6
10022	Thermodynamic Properties of Copper in a Wide Range of Pressure and Temperature Within the Quasi-Harmonic Approximation. International Journal of Thermophysics, 2014, 35, 1501-1511.	1.0	7
10023	The Electronic Structure and Formation Energies of Ni-doped CuAlO <sub>2</sub> by Density Functional Theory Calculation. Chinese Physics Letters, 2014, 31, 037101.	1.3	4
10024	Reaction of Np atom with H <sub>2</sub> O in the gas phase: reaction mechanisms and ab initio molecular dynamics study. Journal of Molecular Modeling, 2014, 20, 2466.	0.8	3
10025	DFT study of pressure effects in molecular crystal 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazatetracyclo-[5.5.0.05,903,11]-dodecane. Canadian Journal of Chemistry, 2014, 92, 616-624.	0.6	9
10026	Density functional study of molecular nitrogen adsorption on gold-copper and gold-silver binary clusters. Journal of Molecular Modeling, 2014, 20, 2467.	0.8	4
10027	Density Functional Study of Benzoic Acid Derivatives Modified SnO <sub>2</sub> (110) Surface. Materials Research Society Symposia Proceedings, 2014, 1633, 69-74.	0.1	0
10028	First-principle study on thermodynamic property of superhard BC <sub>2</sub> N under extreme conditions. Journal of Materials Research, 2014, 29, 1326-1333.	1.2	0
10029	First-principles simulation on orientation dependence of piezoresistivity in graphene nanoribbon. , 2014, , .		1
10030	twins in the rolled Mg-Zn-Ca alloy with high formability. Journal of Materials Research, 2014, 29, 3024-3031.	1.2	14

#	ARTICLE	IF	CITATIONS
10031	Understanding the Behavior of Native Point Defects in $\text{ZrC}$ by First-Principles Calculations. <i>Journal of the American Ceramic Society</i> , 2014, 97, 4024-4030.	1.9	18
10032	Adsorption and activation of copper ions on chalcopyrite surfaces: A new viewpoint of self-activation. <i>Transactions of Nonferrous Metals Society of China</i> , 2014, 24, 3955-3963.	1.7	40
10033	In-Gap States in Electronic Structure of Nonpolar Surfaces of Insulating Metal Oxides. <i>Advanced Materials Interfaces</i> , 2014, 1, 1300131.	1.9	11
10034	Assessment of theoretical procedures for a diverse set of isomerization reactions involving double-bond migration in conjugated dienes. <i>Chemical Physics</i> , 2014, 441, 166-177.	0.9	49
10035	Structure, electronic and electrochemical properties of Li-rich metal phosphate by first-principles study. <i>Journal Physics D: Applied Physics</i> , 2014, 47, 025301.	1.3	2
10036	Identification of Active Sites in a Realistic Model of Strong Metal-Support Interaction Catalysts: The Case of Platinum-Supported Iron Oxide Film. <i>ChemCatChem</i> , 2014, 6, 185-190.	1.8	19
10037	Structural, elastic, electronic and optical properties of various mineral phases of $\text{TiO}_2$ from first-principles calculations. <i>Physica Scripta</i> , 2014, 89, 075703.	1.2	15
10038	Mechanistic Study of CO Titration on $\text{Cu}_2\text{O}/\text{Cu}(111)$ Surfaces. <i>ChemCatChem</i> , 2014, 6, 2364-2372.	1.8	31
10039	The $\text{R}_3\text{S}$ sulfur over layer on the iridium(111) surface: A DFT study. , 2014, , .		1
10040	Quantum size effect on dielectric function of ultrathin metal film: a first-principles study of $\text{Al}(111)$ . <i>Journal of Physics Condensed Matter</i> , 2014, 26, 505302.	0.7	16
10041	FIRST-PRINCIPLES INVESTIGATION ON BAND STRUCTURE AND ELECTRONIC TRANSPORT PROPERTY OF GALLIUM NITRIDE NANORIBBON. <i>Nano</i> , 2014, 09, 1450020.	0.5	14
10042	Density Functional Study of Bulk and Surface Properties of Rhodium Hydride. <i>Acta Physica Polonica A</i> , 2014, 125, 29-35.	0.2	6
10043	Quantum Chemical Investigation and Detonation Characterization of $\text{DNAN-HCl}$ . <i>Advanced Materials Research</i> , 2014, 997, 77-80.	0.3	0
10044	Grain Refinement Mechanism of Al-5Ti-1B Master Alloy by <i>Ab Initio</i> Calculations. <i>Materials Science Forum</i> , 0, 794-796, 746-751.	0.3	0
10045	The formation energy and bonding characteristics of small helium-vacancy clusters on the low-index surface of $\text{Fe}$ by first principles calculations. <i>Computational Materials Science</i> , 2014, 92, 387-394.	1.4	6
10046	Effects of density functionals and dispersion interactions on geometries, bond energies and harmonic frequencies of $\text{EUX}_3$ (E=N, P, CH; X=H, F, Cl). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 133, 846-855.	2.0	3
10047	Comparison of Grain Boundary Structure in Metals and Semiconductors as Probed by Positrons. <i>Acta Physica Polonica A</i> , 2014, 125, 722-725.	0.2	4
10048	Curie Temperature and Density of States at the Fermi Level for Al-Cu-Fe Phases: $\hat{I}^2$ -Solid State Solution-Approximants-Icosahedral Quasicrystals. <i>Acta Physica Polonica A</i> , 2014, 126, 572-576.	0.2	3

#	ARTICLE	IF	CITATIONS
10049	Characterization of Metallo-porphine Monolayer and Bilayer on Ag(111): Screening of Substrate Effects. <i>Applied Mechanics and Materials</i> , 2014, 618, 225-232.	0.2	0
10050	Deblocking effect of carbonates and hydrogen carbonates in the alkali form zeolites with narrow pores. <i>Microporous and Mesoporous Materials</i> , 2014, 200, 35-45.	2.2	8
10051	Effect of sulfur passivation on 6H-SiC surface stability. , 2014, , .		0
10052	Coordination-resolved local bond contraction and electron binding-energy entrapment of Si atomic clusters and solid skins. <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	7
10053	Atomic and electronic structure of the SrNbO <sub>3</sub> /SrNbO <sub>3.4</sub> interface. <i>Applied Physics Letters</i> , 2014, 105, .	1.5	18
10054	<i>Ab initio</i> study of electron-ion structure factors in binary liquids with different types of chemical bonding. <i>Journal of Chemical Physics</i> , 2014, 141, 214504.	1.2	4
10055	Implications of coverage-dependent O adsorption for catalytic NO oxidation on the late transition metals. <i>Catalysis Science and Technology</i> , 2014, 4, 4356-4365.	2.1	59
10056	DFT investigations of the adsorption and hydrodesulfurization mechanism of thiophene catalyzed by Pd(111) surface. <i>RSC Advances</i> , 2014, 4, 58315-58324.	1.7	9
10057	Pressure effects on the electronic structure and superconducting critical temperature of Li <sub>2</sub> B <sub>2</sub> . <i>Journal of Physics Condensed Matter</i> , 2014, 26, 115701.	0.7	8
10058	Validity of the site-averaging approximation for modeling the dissociative chemisorption of H <sub>2</sub> on Cu(111) surface: A quantum dynamics study on two potential energy surfaces. <i>Journal of Chemical Physics</i> , 2014, 141, 194302.	1.2	45
10059	Description of plasmon-like band in silver clusters: The importance of the long-range Hartree-Fock exchange in time-dependent density-functional theory simulations. <i>Journal of Chemical Physics</i> , 2014, 141, 144302.	1.2	28
10060	First-principles study of the effect of phosphorus on nickel grain boundary. <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	26
10061	First-principles study of HgTe/CdTe heterostructures under perturbations preserving time-reversal symmetry. <i>Physical Review B</i> , 2014, 90, .	1.1	14
10062	Alignment of the diamond nitrogen vacancy center by strain engineering. <i>Applied Physics Letters</i> , 2014, 105, .	1.5	22
10063	Tuning of noble metal work function with organophosphonate nanolayers. <i>Applied Physics Letters</i> , 2014, 105, .	1.5	10
10064	Influence of alloying elements Nb, Zr, Sn, and oxygen on structural stability and elastic properties of the Ti <sub>2448</sub> alloy. <i>Physical Review B</i> , 2014, 89, .	1.1	11
10065	Improved generalized gradient approximation for positron states in solids. <i>Physical Review B</i> , 2014, 89, .	1.1	51
10066	Rashba splitting and relativistic energy shifts in In/Si(111) nanowires. <i>Physical Review B</i> , 2014, 89, .	1.1	19

#	ARTICLE	IF	CITATIONS
10067	Initial and secondary oxidation products on the Si(111)-(7Å <sup>2</sup> ) surface identified by atomic force microscopy and first principles calculations. Applied Physics Letters, 2014, 104, 133107.	1.5	9
10069	Gedanken densities and exact constraints in density functional theory. Journal of Chemical Physics, 2014, 140, 18A533.	1.2	82
10070	Helium bubble nucleation and growth in $\alpha$ -Fe: insights from first-principles simulations. Journal of Physics Condensed Matter, 2014, 26, 255401.	0.7	14
10071	Recommending Hartree-Fock Theory with London-Dispersion and Basis-Set-Superposition Corrections for the Optimization or Quantum Refinement of Protein Structures. Journal of Physical Chemistry B, 2014, 118, 14612-14626.	1.2	53
10072	On-surface synthesis of a two-dimensional porous coordination network: Unraveling adsorbate interactions. Physical Review B, 2014, 90, .	1.1	61
10073	Dissociation and recombination of D2 on Cu(111): Ab initio molecular dynamics calculations and improved analysis of desorption experiments. Journal of Chemical Physics, 2014, 141, 124705.	1.2	35
10074	Electrode-Electrolyte Interface for Solid State Li-Ion Batteries: Point Defects and Mechanical Strain. Journal of the Electrochemical Society, 2014, 161, F3104-F3110.	1.3	28
10075	The PtAl <sup>+</sup> and PtAl <sup>2+</sup> anions: Theoretical and photoelectron spectroscopic characterization. Journal of Chemical Physics, 2014, 140, 164316.	1.2	12
10076	Analysis of vibrational spectra (FT-IR and VCD) and nonlinear optical properties of [Ru(L)3]2+ complexes. Journal of Coordination Chemistry, 2014, 67, 3288-3310.	0.8	17
10077	Anomalous magneto-structural behavior of MnBi explained: A path towards an improved permanent magnet. APL Materials, 2014, 2, .	2.2	35
10078	Effects of deformation on the crystal field parameter of the Nd ions in Nd2Fe14B. Journal of Applied Physics, 2014, 115, .	1.1	14
10079	Describing long-range charge-separation processes with subsystem density-functional theory. Journal of Chemical Physics, 2014, 140, 164103.	1.2	39
10080	TaON surface energetics and optical spectra. Physica Status Solidi - Rapid Research Letters, 2014, 8, 587-591.	1.2	10
10081	Structures and electronic properties of oxidized graphene from first-principles study. Europhysics Letters, 2014, 105, 37005.	0.7	8
10082	Boron deactivation in heavily boron-doped Czochralski silicon during rapid thermal anneal: Atomic level understanding. Applied Physics Letters, 2014, 104, 032102.	1.5	2
10083	Hydrogen activation, diffusion, and clustering on CeO2(111): A DFT+U study. Journal of Chemical Physics, 2014, 141, 014703.	1.2	109
10084	Local atomic structure inheritance in Ag50Sn50 melt. Journal of Applied Physics, 2014, 115, .	1.1	5
10085	Source and major species of CH <sub>x</sub> (x = 1-3) in acetic acid synthesis from methane syngas on Rh catalyst: a theoretical study. RSC Advances, 2014, 4, 58631-58642.	1.7	5

#	ARTICLE	IF	CITATIONS
10086	Strain tuning of Dirac states at the SnTe (001) surface. <i>Physical Review B</i> , 2014, 90, .	1.1	14
10087	Graphene on Crystalline Metal Surfaces. , 0, , 691-736.		0
10088	Prediction of Mode Specificity, Bond Selectivity, Normal Scaling, and Surface Lattice Effects in Water Dissociative Chemisorption on Several Metal Surfaces Using the Sudden Vector Projection Model. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26851-26858.	1.5	29
10089	Electronic and bonding analysis of hardness in pyrite-type transition-metal pernitrides. <i>Physical Review B</i> , 2014, 90, .	1.1	108
10090	Ethanol Synthesis from Syngas on the Stepped Rh(211) Surface: Effect of Surface Structure and Composition. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22691-22701.	1.5	46
10091	Ab initio investigation of tensile strengths of metal(111)/Al <sub>2</sub> O <sub>3</sub> interfaces. <i>Philosophical Magazine</i> , 2014, 94, 265-284.	0.7	13
10092	Experimental and Numerical Study of Submonolayer Sputter Deposition of Polystyrene Fragments on Silver for the Storing Matter Technique. <i>Analytical Chemistry</i> , 2014, 86, 11217-11225.	3.2	4
10093	Clustering of H and He, and their effects on vacancy evolution in tungsten in a fusion environment. <i>Nuclear Fusion</i> , 2014, 54, 103007.	1.6	69
10094	Probing Donor–Acceptor Interactions in peri-Substituted Diphenylphosphinoacenaphthyl–Element Dichlorides of Group 13 and 15 Elements. <i>Organometallics</i> , 2014, 33, 7247-7259.	1.1	56
10095	Quantum size effect of poly(o-phenylenediamine) quantum dots: From controllable fabrication to tunable photoluminescence properties. <i>Synthetic Metals</i> , 2014, 198, 142-149.	2.1	42
10096	Direct growth of porous crystalline NiCo <sub>2</sub> O <sub>4</sub> nanowire arrays on a conductive electrode for high-performance electrocatalytic water oxidation. <i>Journal of Materials Chemistry A</i> , 2014, 2, 20823-20831.	5.2	111
10097	Structural and Magnetic Properties of CoGe <sub>n</sub> ( <sup>n</sup> ) Clusters: Photoelectron Spectroscopy and Density Functional Calculations. <i>ChemPhysChem</i> , 2014, 15, 3987-3993.	1.0	57
10098	Structure and magnetism of Tm atoms and monolayers on W(110). <i>Physical Review B</i> , 2014, 90, .	1.1	11
10099	Theoretical calculation based synthesis of a poly(p-phenylenediamine)–Fe <sub>3</sub> O <sub>4</sub> composite: a magnetically recyclable photocatalyst with high selectivity for acid dyes. <i>RSC Advances</i> , 2014, 4, 54810-54818.	1.7	30
10100	Correlation between DFT calculated and X-ray structures from CSD, for Cu(II) and Cu(I) coordination spheres when coordinated to four acyclic amine ligands. A reconsideration of copper(II) planarity. <i>Journal of Coordination Chemistry</i> , 2014, 67, 3932-3939.	0.8	0
10101	The one-electron oxidation of a dithiolate molecule: The importance of chemical intuition. <i>Journal of Chemical Physics</i> , 2014, 140, 18A519.	1.2	8
10102	Method of increments for the halogen molecular crystals: Cl, Br, and I. <i>Journal of Chemical Physics</i> , 2014, 141, 124707.	1.2	13
10103	Optimizing the Electronic Properties of Photoactive Anticancer Oxypyridine-Bridged Dirhodium(II,II) Complexes. <i>Journal of the American Chemical Society</i> , 2014, 136, 17058-17070.	6.6	37

#	ARTICLE	IF	CITATIONS
10104	An ab initio approach to free-energy reconstruction using logarithmic mean force dynamics. Journal of Chemical Physics, 2014, 140, 184110.	1.2	5
10105	Enhanced osteoconductivity of sodium-substituted hydroxyapatite by system instability. Journal of Biomedical Materials Research - Part B Applied Biomaterials, 2014, 102, 1046-1062.	1.6	67
10106	Highly Active Nonpromoted Hydrotreating Catalysts through the Controlled Growth of a Supported Hexagonal WS <sub>2</sub> Phase. ACS Catalysis, 2014, 4, 4320-4331.	5.5	39
10107	Origin of High-Resolution IETS-STM Images of Organic Molecules with Functionalized Tips. Physical Review Letters, 2014, 113, 226101.	2.9	165
10108	Accurate density functional theory description of binding constants and NMR chemical shifts of weakly interacting complexes of C <sub>60</sub> with corannulene-based molecular bowls. Journal of Computational Chemistry, 2014, 35, 181-191.	1.5	16
10109	Electronic structure and stability of low symmetry Ta <sub>2</sub> O <sub>5</sub> polymorphs. Physica Status Solidi - Rapid Research Letters, 2014, 8, 560-565.	1.2	26
10110	Density functional theory study of the mechanism of Li diffusion in rutile RuO <sub>2</sub> . AIP Advances, 2014, 4, .	0.6	24
10111	Structural, mechanical, electronic and optical properties of layered ternary nitrides SrZrN <sub>2</sub> and SrHfN <sub>2</sub> : First-principles calculations. Computational Materials Science, 2014, 93, 249-254.	1.4	9
10112	Theoretical investigation of charge accumulation layer on the Bi-induced InAs(111)-(2×2) surface. Journal of Applied Physics, 2014, 115, 163702.	1.1	0
10113	First-Principles Screening of Complex Transition Metal Hydrides for High Temperature Applications. Inorganic Chemistry, 2014, 53, 11833-11848.	1.9	20
10114	Geometric Matching Principle for Adsorption Selectivity of Ionic Liquids: A Simple Method into the Fascinating World of Shape-Controlled Chemistry. Chemistry - A European Journal, 2014, 20, 9012-9017.	1.7	11
10115	A Stable Binary BeB <sub>2</sub> phase. Scientific Reports, 2014, 4, 6993.	1.6	25
10116	Thermodynamic and mechanical properties of TiC from <i>ab initio</i> calculation. Journal of Applied Physics, 2014, 116, .	1.1	29
10117	Activation Barriers in the Growth of Molecular Clusters Derived from Sulfuric Acid and Ammonia. Journal of Physical Chemistry A, 2014, 118, 11547-11554.	1.1	19
10118	Charge-density distribution in sodium bis(4-nitrophenyl)phosphate. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2014, 70, 723-731.	0.5	4
10119	(Sr,Ba)(Si,Ge) <sub>2</sub> for thin-film solar-cell applications: First-principles study. Journal of Applied Physics, 2014, 115, .	1.1	61
10120	Toward tailorable surfaces: A combined theoretical and experimental study of lanthanum niobate layered perovskites. Journal of Chemical Physics, 2014, 141, 024704.	1.2	7
10121	First principles studies of proton conduction in KTaO <sub>3</sub> . Journal of Chemical Physics, 2014, 141, 024707.	1.2	9



#	ARTICLE	IF	CITATIONS
10122	Phthalocyanine-Based Organometallic Nanocages: Properties and Gas Storage. <i>ChemPhysChem</i> , 2014, 15, 126-131.	1.0	9
10123	HOMO Stabilisation in Extended Dibenzotetrathiafulvalene Derivatives for Their Application in Organic Field-Effect Transistors. <i>Chemistry - A European Journal</i> , 2014, 20, 16672-16679.	1.7	14
10124	An experimental and theoretical study on the structure and photoactivity of $XFe_2O_4$ (X = Mn, Fe, Ni). <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf</i>	0.1	6
10125	First-principles calculation on $\hat{I}^2$ -SiC(111)/ $\hat{I}^{\pm}$ -WC(0001) interface. <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	39
10126	Geometrical and optical benchmarking of copper(II) guanidine-quinoline complexes: Insights from TD-DFT and many-body perturbation theory (part II). <i>Journal of Computational Chemistry</i> , 2014, 35, 2146-2161.	1.5	31
10127	Mechanical Properties, Electronic Structures, and Potential Applications in Lithium Ion Batteries: A First-Principles Study toward $SnSe_{2 \times 2}$ Nanotubes. <i>Journal of Physical Chemistry C</i> , 2014, 118, 28291-28298.	1.5	37
10128	The work functions of Au/Mg decorated Au(100), Mg(001), and AuMg alloy surfaces: A theoretical study. <i>Journal of Chemical Physics</i> , 2014, 141, 094705.	1.2	6
10129	Thermodynamic stability and structures of iron chloride surfaces: A first-principles investigation. <i>Journal of Chemical Physics</i> , 2014, 141, 054709.	1.2	9
10130	Ab initio studies of propene epoxidation on oxidized silver surfaces. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26546-26552.	1.3	17
10131	The structural and electronic properties of $Au_n$ clusters on the $\hat{I}^{\pm}$ -Al <sub>2</sub> O <sub>3</sub> (0001) surface: a first principles study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26561-26569.	1.3	14
10132	A first principles analysis of the effect of hydrogen concentration in hydrogenated amorphous silicon on the formation of strained Si-Si bonds and the optical and mobility gaps. <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	16
10133	Investigation of superconducting $Ba_2Ti_2O_7$ . <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26561-26569.	1.1	7
10134	Ab initio study of irradiation tolerance for different Mn+1AX <sub>n</sub> phases: Ti <sub>3</sub> SiC <sub>2</sub> and Ti <sub>3</sub> AlC <sub>2</sub> . <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	69
10135	Electronic Friction Dominates Hydrogen Hot-Atom Relaxation on Pd(100). <i>Physical Review Letters</i> , 2014, 112, 103203.	2.9	112
10136	Hydrogen-Bonding Interactions in Hard Segments of Shape Memory Polyurethane: Toluene Diisocyanates and 1,6-Hexamethylene Diisocyanate. A Theoretical and Comparative Study. <i>Journal of Physical Chemistry A</i> , 2014, 118, 12241-12255.	1.1	33
10137	Two-Dimensional Ordering of Solute Nanoclusters at a Close-Packed Stacking Fault: Modeling and Experimental Analysis. <i>Scientific Reports</i> , 2014, 4, 7318.	1.6	37
10138	Ab initio calculations of mechanical properties in $\hat{I}^2$ -MH <sub>2</sub> xHex (M = Er, Sc). <i>European Physical Journal B</i> , 2014, 87, 1.	0.6	2
10139	Effects of BaO codoping on the photocatalytic activities of Ta <sub>3</sub> N <sub>5</sub> photocatalyst: a DFT study. <i>RSC Advances</i> , 2014, 4, 55615-55621.	1.7	9



#	ARTICLE	IF	CITATIONS
10140	Ti <sub>2</sub> MnZ (<math>Z=Al, Ga, In</math>) compounds: Nearly spin gapless semiconductors. AIP Advances, 2014, 4, .	0.6	46
10141	Influence of shape anisotropy of self-interstitials on dislocation sink efficiencies in Zr: Multiscale modeling. Physical Review B, 2014, 90, .	1.1	16
10142	Vibronic structure of VO <sub>2</sub> probed by slow photoelectron velocity-map imaging spectroscopy. Journal of Chemical Physics, 2014, 140, 034307.	1.2	14
10143	Adsorption and STM imaging of tetracyanoethylene on Ag(001): An <math>ab initio</math> study. Physical Review B, 2014, 89, .	1.1	12
10144	Structural, thermodynamic, mechanical, and magnetic properties of FeW system. Journal of Applied Physics, 2014, 116, .	1.1	25
10145	Quantum confinement and band offsets in amorphous silicon quantum wells. Physical Review B, 2014, 90, .	1.1	6
10146	Combined experimental and theoretical study of fast atom diffraction on the GaAs(001) surface. Physical Review B, 2014, 90, .	1.1	4
10147	First-principles study of uniaxial strained and bent ZnO wires. Physical Review B, 2014, 89, .	1.1	22
10148	QSPR study on nematic transition temperatures of thermotropic liquid crystals based on DFT-calculated descriptors. Liquid Crystals, 2014, 41, 1575-1582.	0.9	9
10149	Relevance of Dispersion Interactions in the Germlyidyne and Stannilydyne Complexes of Manganese: Structure and Bonding-Energy Analysis. European Journal of Inorganic Chemistry, 2014, 2014, 2916-2923.	1.0	6
10150	First-principles investigation of the electronic and Li-ion diffusion properties of LiFePO <sub>4</sub> by sulfur surface modification. Journal of Applied Physics, 2014, 116, .	1.1	29
10151	Shape-Memory Transformations of NiTi: Minimum-Energy Pathways between Austenite, Martensites, and Kinetically Limited Intermediate States. Physical Review Letters, 2014, 113, 265701.	2.9	34
10152	Formation energies of carbon related defects in Cu<math>_{2}</math>ZnSnS<math>_{4}</math>, 2014, , .		0
10153	Possible origin of nonlinear magnetic anisotropy variation in electric field effect in a double interface system. Applied Physics Express, 2014, 7, 113005.	1.1	13
10154	Chain-like structures of gold supported by silicon substrate. Physica Status Solidi (B): Basic Research, 2014, 251, 924-932.	0.7	0
10155	Tuning nucleation density of metal island with charge doping of graphene substrate. Applied Physics Letters, 2014, 105, 071609.	1.5	8
10156	First-principles study of the formation and electronic structure of a conductive filament in ZnO-based resistive random access memory. Chinese Physics B, 2014, 23, 127301.	0.7	1
10157	A DFT study on structure, stabilities and electronic properties of double magnesium doped gold clusters. RSC Advances, 2014, 4, 56571-56581.	1.7	13

#	ARTICLE	IF	CITATIONS
10158	Impact of Functionalized Polystyrenes as the Electron Injection Layer on Gold and Aluminum Surfaces: A Combined Theoretical and Experimental Study. <i>Israel Journal of Chemistry</i> , 2014, 54, 779-788.	1.0	2
10159	Properties of the silver cyclic amide $\text{Ag}_2(\text{C}_4\text{H}_4\text{NO}_2)_2(\text{H}_2\text{O})$ crystal from the periodic DFT computations. <i>Journal of Structural Chemistry</i> , 2014, 55, 621-628.	0.3	0
10160	The interaction of oxygen with the $\text{TiO}_2$ -U(001) surface: an <i>ab initio</i> study. <i>Physica Scripta</i> , 2014, 89, 075701.	1.2	5
10161	Trapping Behavior of He in Ti Revisited by <i>ab initio</i> Calculations. <i>Chinese Physics Letters</i> , 2014, 31, 017102.	1.3	0
10162	Theoretical Chemical Investigation and Detonation Characterization of AAOF and ACOF. <i>Advanced Materials Research</i> , 0, 997, 85-88.	0.3	0
10163	Optical properties of Ni doped 3C-SiC with <i>ab initio</i> calculations. , 2014, , .		3
10164	X-ray emission and X-ray photoelectron study of the electronic structure of paramagnetic and diamagnetic derivatives of 3-imidazoline. <i>Journal of Structural Chemistry</i> , 2014, 55, 1044-1056.	0.3	3
10165	Effect of Ultrathin Inserted Ag Layer on Perpendicular Magnetic Anisotropy of CoFeB Thin Film. <i>IEEE Transactions on Magnetics</i> , 2014, 50, 1-4.	1.2	1
10166	The positions of inner hydroxide groups and aluminium ions in exfoliated kaolinite as indicators of the external chemical environment. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 25830-25839.	1.3	11
10167	Computational nano-materials design for circularly polarized luminescence in (Eu,Mg,O)-codoped GaN. <i>Applied Physics Express</i> , 2014, 7, 121002.	1.1	11
10168	Adsorption and diffusion of lithium on 1T-MoS <sub>2</sub> monolayer. <i>Computational Materials Science</i> , 2014, 93, 86-90.	1.4	62
10169	First principle calculations of hydrogen sulfide adsorption and dissociation on pure $\text{Pd}$ (111) and $\text{Au}$ (111), and alloy $\text{Pd}/\text{Au}$ (111) and $\text{Au}/\text{Pd}$ (111) surfaces. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1450065.	1.8	6
10170	The ground state and electronic structure of Gd@C <sub>82</sub> : A systematic theoretical investigation of first principle density functionals. <i>Journal of Chemical Physics</i> , 2014, 141, 244306.	1.2	22
10171	Comparative Study of Stability and Detonation Characterization of AMF and ACF. <i>Advanced Materials Research</i> , 0, 997, 97-100.	0.3	0
10172	Theoretical Investigations on Graphite Oxide Immersed in Water or Methanol. <i>Chinese Journal of Chemical Physics</i> , 2014, 27, 9-14.	0.6	4
10173	Structural and anisotropic elastic properties of Zintl $\text{M}_2\text{Pb}$ (M=Ca, Sr and Ba) compounds as a function of pressure. <i>Journal of Alloys and Compounds</i> , 2014, 614, 334-344.	2.8	23
10174	Double Columnar Structure with a Nanogradient Composite for Increased Oxygen Diffusivity and Reduction Activity. <i>Advanced Energy Materials</i> , 2014, 4, 1400783.	10.2	11
10175	First Principles Study Including Zero Point Energy on Hydrogen in Palladium for Hydrogen Membranes Applications. <i>Advanced Materials Research</i> , 0, 875-877, 635-641.	0.3	1

#	ARTICLE	IF	CITATIONS
10176	Dependence of Magnetic Anisotropy Energy on $c/a$ Ratio of $X_{2/3}Fe_{14/3}B$ ( $X = Y, Pr, Dy$ ). IEEE Transactions on Magnetics, 2014, 50, 1-4.	1.2	8
10177	Adsorption Mechanism of Carbon Monoxide on PtRu and PtRuMo Surfaces in the Density Functional Theory Perspective. Advanced Materials Research, 0, 896, 537-540.	0.3	4
10178	Terahertz absorption spectra of oxidized polyethylene and their analysis by quantum chemical calculations. Japanese Journal of Applied Physics, 2014, 53, 092402.	0.8	35
10179	Density Functional Theory Investigation and Detonation Characterization of DNP DNAZ. Advanced Materials Research, 2014, 997, 264-267.	0.3	0
10180	First-principles study on the synergistic effects of codoped anatase $TiO_2$ photocatalysts codoped with N/V or C/Cr. Journal of Semiconductors, 2014, 35, 102002.	2.0	7
10181	Detonation Characterization and Density Functional Theory Investigation of B DNAZ. Advanced Materials Research, 2014, 997, 81-84.	0.3	1
10182	Ti and Zr Transition Metals Effect in the D03 $Fe_3Al$ by $\alpha$ Ab Initio Study Approach. Materials Science Forum, 0, 783-786, 1640-1645.	0.3	0
10183	A Density Functional Theory Study of the Adsorption of Benzene on Hematite ( $\alpha$ - $Fe_2O_3$ ) Surfaces. Minerals (Basel, Switzerland), 2014, 4, 89-115.	0.8	105
10184	Dynamical stability of Pmn21 phase of $NH_3BH_3$ : a vdW density functional study. Philosophical Magazine Letters, 2014, 94, 278-287.	0.5	2
10185	DSSC anchoring groups: a surface dependent decision. Journal of Physics Condensed Matter, 2014, 26, 195302.	0.7	24
10186	Elastic properties, lattice dynamics and structural transitions in molybdenum at high pressures. Computational Materials Science, 2014, 81, 313-318.	1.4	23
10187	The mixed intermetallic silicide $Nb_{5-x}Ta_xSi_3$ ( $0 \leq x \leq 1/2$ ). Crystal and electronic structure. Journal of Alloys and Compounds, 2014, 584, 385-392.	2.8	9
10188	Multistep synthesis of the $SrFeO_2F$ perovskite oxyfluoride via the $SrFeO_2$ infinite-layer intermediate. Journal of Fluorine Chemistry, 2014, 159, 8-14.	0.9	30
10189	Migrations of oxygen vacancy in tungsten oxide ( $WO_3$ ): A density functional theory study. Computational Materials Science, 2014, 90, 171-176.	1.4	24
10190	Thermodynamic properties, detonation characterization and free radical of $N$ -2,4-dinitrophenyl-3,3-dinitroazetidine. Journal of Chemical Thermodynamics, 2014, 69, 152-156.	1.0	17
10191			

#	ARTICLE	IF	CITATIONS
10194	DFT study of mercury adsorption on $\alpha$ -Fe <sub>2</sub> O <sub>3</sub> surface: Role of oxygen. <i>Fuel</i> , 2014, 115, 179-185.	3.4	64
10195	Structural and mechanical properties of Laves phases YCu <sub>2</sub> and YZn <sub>2</sub> : First principles calculation analyzed with data mining approach. <i>Computational Materials Science</i> , 2014, 89, 176-181.	1.4	27
10196	Screening study of light-metal and transition-metal-doped NiTiH hydrides as Li-ion battery anode materials. <i>Solid State Ionics</i> , 2014, 258, 88-91.	1.3	9
10197	Influence of titanium and nickel dopants on the dehydrogenation properties of Mg(AlH <sub>4</sub> ) <sub>2</sub> : Electronic structure mechanisms. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 9276-9287.	3.8	8
10198	Effect of hydrogen concentration on various properties of gamma TiAl. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 1888-1896.	3.8	16
10199	Vacancy trapping behaviors of hydrogen in Ti <sub>3</sub> SiC <sub>2</sub> : A first-principles study. <i>Materials Letters</i> , 2014, 116, 322-327.	1.3	18
10200	Solution-based thermodynamic modeling of the Ni-Al-Mo system using first-principles calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014, 46, 124-133.	0.7	19
10201	First-principles study of the dislocation core structures on basal plane in magnesium. <i>European Journal of Mechanics, A/Solids</i> , 2014, 45, 1-7.	2.1	3
10202	Toward a microscopic understanding of the calcium-silicate hydrates/water interface. <i>Applied Surface Science</i> , 2014, 290, 207-214.	3.1	31
10203	First-principles investigation of the intrinsic defects in Ti <sub>3</sub> SiC <sub>2</sub> . <i>Journal of Physics and Chemistry of Solids</i> , 2014, 75, 384-390.	1.9	17
10204	Structural, electronic and magnetic properties of Fe, Co, Mn-doped GaN and ZnO diluted magnetic semiconductors. <i>Physica B: Condensed Matter</i> , 2014, 440, 1-9.	1.3	28
10205	Lithium-doped triazine-based graphitic C <sub>3</sub> N <sub>4</sub> sheet for hydrogen storage at ambient temperature. <i>Computational Materials Science</i> , 2014, 81, 275-279.	1.4	75
10206	Structural properties of a hypothetical H <sub>6</sub> -Boron with three-dimensional all sp <sup>2</sup> network. <i>Solid State Communications</i> , 2014, 177, 50-53.	0.9	1
10207	Interface structure of nanodiamond composite films: First-principles studies. <i>Journal of Alloys and Compounds</i> , 2014, 599, 183-187.	2.8	9
10208	An experimental and theoretical approach of spectroscopic and structural properties of a new chelidamate copper (II) complex. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 122, 758-766.	2.0	15
10209	Oxygen assisted H <sub>2</sub> O dissociation on the Pt{110}(1 $\times$ 2) surface from first principles. <i>Surface Science</i> , 2014, 627, 42-48.	0.8	13
10210	Pressure-induced phase transitions in LiBH <sub>4</sub> : Density functional theory calculations. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 9330-9338.	3.8	6
10211	Theoretical studies on hydrogen-bonding interactions in hard segments of shape memory polyurethane-III: Isophorone diisocyanate. <i>Journal of Molecular Structure</i> , 2014, 1072, 13-19.	1.8	19

#	ARTICLE	IF	CITATIONS
10212	Functionalization of hydrogenated graphene by polyolithiated species for efficient hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 2560-2566.	3.8	40
10213	Structural and electronic effects of helium interstitials in Y2Ti2O7: A first-principles study. <i>Journal of Nuclear Materials</i> , 2014, 452, 189-196.	1.3	20
10214	Structure and elasticity of phlogopite under compression: Geophysical implications. <i>Physics of the Earth and Planetary Interiors</i> , 2014, 233, 1-12.	0.7	36
10215	Obtaining half-metallic ferrimagnetism and antiferromagnetism by doping Mn and Fe for DO3-type Heusler compound Cr3Si. <i>Journal of Alloys and Compounds</i> , 2014, 597, 8-14.	2.8	13
10216	Density functional study of GaN(0001)/AlN(0001) high electron mobility transistor structures. <i>Journal of Crystal Growth</i> , 2014, 401, 30-32.	0.7	3
10217	A DFT study of adsorption and decomposition of nitroamine molecule on Mg(001) surface. <i>Structural Chemistry</i> , 2014, 25, 409-417.	1.0	8
10218	Electronic and Magnetic Theoretical Investigation of Antiferromagnetically ErRh Layers. <i>Journal of Superconductivity and Novel Magnetism</i> , 2014, 27, 235-238.	0.8	0
10219	Precipitation in $\alpha$ -Fe based Fe-Cu-Ni-Mn-alloys: behaviour of Ni and Mn modelled by ab initio and kinetic Monte Carlo simulations. <i>Applied Physics A: Materials Science and Processing</i> , 2014, 115, 679-687.	1.1	11
10220	Lattice-strain effect on oxygen vacancy formation in gadolinium-doped ceria. <i>Journal of Electroceramics</i> , 2014, 32, 72-77.	0.8	24
10221	Activation of propane C-H and C-C bonds by a diplatinum cluster: potential energy surfaces and reaction mechanisms. <i>Structural Chemistry</i> , 2014, 25, 471-481.	1.0	9
10222	Periodic DFT study of structural, electronic, absorption, and thermodynamic properties of crystalline $\alpha$ -RDX under hydrostatic compression. <i>Structural Chemistry</i> , 2014, 25, 451-461.	1.0	7
10223	The electric field screening and crossing point shift effects in coated carbon nanotubes. <i>Applied Physics A: Materials Science and Processing</i> , 2014, 116, 629-633.	1.1	3
10224	Experimental investigation and thermodynamic assessment of the Hf-Ge system. <i>Journal of Materials Science</i> , 2014, 49, 1306-1316.	1.7	0
10225	Properties of interfaces between iron-group metals (Fe, Co, Ni) and HfC via first-principles modeling. <i>Journal of Materials Science</i> , 2014, 49, 407-414.	1.7	8
10226	A DFT study of oxygen dissociation on platinum based nanoparticles. <i>Nanoscale</i> , 2014, 6, 1153-1165.	2.8	74
10227	Electronic structure, optical and thermoelectric transport properties of layered polyanionic hydrosulfate LiFeSO4OH: Electrode for Li-ion batteries. <i>Journal of Alloys and Compounds</i> , 2014, 591, 362-369.	2.8	11
10228	Structural, mechanical and electronic properties of OsTM and TMOs2 (TM=Ti, Zr and Hf): First-principles calculations. <i>Journal of Alloys and Compounds</i> , 2014, 589, 278-282.	2.8	22
10229	First-principles investigation of the structural, mechanical and electronic properties of the NbO-structured 3d, 4d and 5d transition metal nitrides. <i>Computational Materials Science</i> , 2014, 84, 365-373.	1.4	78

#	ARTICLE	IF	CITATIONS
10230	First-principles investigations on structural, electronic and elastic properties of BeSe under high pressure. <i>Solid State Sciences</i> , 2014, 28, 35-40.	1.5	13
10231	The inherent kinetic electrochemical reduction of oxygen into H <sub>2</sub> O on FeN <sub>4</sub> -carbon: A density functional theory study. <i>Journal of Power Sources</i> , 2014, 255, 65-69.	4.0	83
10232	Ab initio study of the structural, elastic, thermodynamic, electronic and vibration properties of TbMg intermetallic compound. <i>Superlattices and Microstructures</i> , 2014, 71, 46-61.	1.4	6
10233	First-principles investigation of the binary intermetallics in Mg-Al-Sr alloy: Stability, elastic properties and electronic structure. <i>Computational Materials Science</i> , 2014, 86, 24-29.	1.4	36
10234	First-principle calculations of structural, elastic and thermodynamic properties of Fe-B compounds. <i>Intermetallics</i> , 2014, 46, 211-221.	1.8	72
10235	Electronic and elastic properties of $\mu$ -phases Cr <sub>2-x</sub> V <sub>x</sub> N (x=0, 1, 2) from density-functional calculations. <i>Journal of Alloys and Compounds</i> , 2014, 583, 79-84.	2.8	21
10236	First-principle study of phase stability, electronic structure and thermodynamic properties of cadmium sulfide under high pressure. <i>Journal of Physics and Chemistry of Solids</i> , 2014, 75, 662-669.	1.9	12
10237	Pressure effect on the structural, elastic and electronic properties of Nb <sub>2</sub> AC (A=S and In) phases; ab initio study. <i>Computational Materials Science</i> , 2014, 81, 184-190.	1.4	19
10238	Hydrogen-bonded structure and mechanical chiral response of a silver nanoparticle superlattice. <i>Nature Materials</i> , 2014, 13, 807-811.	13.3	128
10239	Electronic and optical properties of SrTiO <sub>3</sub> under pressure effect: Ab initio study. <i>Solid State Communications</i> , 2014, 189, 32-37.	0.9	14
10240	Vacancy mechanism of oxygen diffusivity in bcc Fe: A first-principles study. <i>Corrosion Science</i> , 2014, 83, 94-102.	3.0	56
10241	Density functional theory in the solid state. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2014, 372, 20130270.	1.6	242
10242	Density functional study of CH <sub>3</sub> OH binding on small cationic Cu <sub>n</sub> Al <sub>m</sub> <sup>+</sup> (n+m=1/2) clusters. <i>Computational and Theoretical Chemistry</i> , 2014, 1037, 14-21.	1.1	7
10243	Iron-sulfur bond covalency from electronic structure calculations for classical iron-sulfur clusters. <i>Journal of Computational Chemistry</i> , 2014, 35, 540-552.	1.5	24
10244	First-principles studies concerning optimization of hydrogen storage in nanoporous reduced graphite oxide. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 4396-4403.	3.8	10
10245	High-capacity hydrogen storage in Li-decorated (AlN) <sub>n</sub> (n=12, 24, 36) nanocages. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 3780-3789.	3.8	39
10246	Geometrical and optical benchmarking of copper guanidine-quinoline complexes: Insights from TD-DFT and many-body perturbation theory. <i>Journal of Computational Chemistry</i> , 2014, 35, 1-17.	1.5	62
10247	Size-extensivity-corrected multireference configuration interaction schemes to accurately predict bond dissociation energies of oxygenated hydrocarbons. <i>Journal of Chemical Physics</i> , 2014, 140, 044317.	1.2	85

#	ARTICLE	IF	CITATIONS
10248	First-principles study of influence of Ti vacancy and Nb dopant on the bonding of TiAl/TiO <sub>2</sub> interface. <i>Intermetallics</i> , 2014, 49, 1-6.	1.8	39
10249	Interaction of third-row main group dicarbides, C <sub>2</sub> X (X=Kâ€“Br) with molecular oxygen: A density functional study. <i>Computational and Theoretical Chemistry</i> , 2014, 1032, 1-6.	1.1	7
10250	The Curious Case of the Allyl Ligand: A Study in Applying the 18-Electron Rule. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2014, 24, 87-94.	1.9	3
10251	The electronic properties of phosphorus-doped GaN nanowires from first-principle calculations. <i>Journal of Alloys and Compounds</i> , 2014, 596, 92-97.	2.8	30
10252	Centered Honeycomb NiSe <sub>2</sub> Nanoribbons: Structure and Electronic Properties. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3295-3304.	1.5	27
10253	The role of dipole moment in determining the nonlinear optical behavior of materials: ab initio studies on quaternary molybdenum tellurite crystals. <i>Journal of Materials Chemistry C</i> , 2014, 2, 530-537.	2.7	81
10254	Atomistic simulation of stacking faults in (001), (010), and (100) planes of cementite. <i>Physics of Metals and Metallography</i> , 2014, 115, 85-97.	0.3	13
10255	Direct visual evidence for chemical mechanism of SERRS of pyrazine adsorbed on Ag nanoparticle via charge transfer. <i>Vibrational Spectroscopy</i> , 2014, 70, 162-167.	1.2	5
10256	Tuning electrochemical potential of LiCoO <sub>2</sub> with cation substitution: first-principles predictions and electronic origin. <i>Ionics</i> , 2014, 20, 315-321.	1.2	9
10257	A periodic density functional theory study of tetrazole adsorption on anatase surfaces: potential application of tetrazole rings in dye-sensitized solar cells. <i>Journal of Molecular Modeling</i> , 2014, 20, 2086.	0.8	10
10258	Reaction mechanism of methylamine decomposition on Ru(0001): a density functional theory study. <i>Journal of Molecular Modeling</i> , 2014, 20, 2137.	0.8	5
10259	From Electronic Structure to Thermodynamics of Actinide-Based Alloys. <i>Jom</i> , 2014, 66, 375-388.	0.9	8
10260	First-principles study of molecular NO dissociation on Ir(100) surface. <i>European Physical Journal B</i> , 2014, 87, 1.	0.6	2
10261	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	37
10262	Dynamic Simulation of the Thermal Decomposition of Pyrite Under Vacuum. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2014, 45, 2445-2452.	1.1	20
10263	The infrared spectra of C <sub>96</sub> H <sub>25</sub> compared with that of C <sub>96</sub> H <sub>24</sub> . <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	3
10264	Theoretical studies of ground and excited states in a series of Zn(II) complexes, derived from thiourea and thiosemicarbazide. <i>European Physical Journal D</i> , 2014, 68, 1.	0.6	2
10265	First-principles study of electric field effects on the structure, decomposition mechanism, and stability of crystalline lead styphnate. <i>Journal of Molecular Modeling</i> , 2014, 20, 2072.	0.8	14



#	ARTICLE	IF	CITATIONS
10266	Half-metallicity and magnetism of the quaternary inverse full-Heusler alloy $Ti_{2-x}M_xCoAl$ ( $M = Nb, V$ ) from the first-principles calculations. <i>European Physical Journal B</i> , 2014, 87, 1.	0.6	14
10267	Effect of CVD diamond growth by doping with nitrogen. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	50
10268	Ions in solution: Density corrected density functional theory (DC-DFT). <i>Journal of Chemical Physics</i> , 2014, 140, 18A528.	1.2	87
10269	Intrinsic insulating ferromagnetism in manganese oxide thin films. <i>Physical Review B</i> , 2014, 89, .	1.1	47
10270	First-principles study on the structure, hardness and electronic structure of $TMB_{1.1}$ ( $TM=Rh, Ir$ and) $Tj$ $ETQq0$ $0$ $0$ $rgBT$ /Overlock 10 Tf 5	2.8	9
10271	Assessment of various density functionals for intermolecular $N\hat{a}^+Sn$ interactions: The test case of trimethyltin cyanide dimer. <i>Computational and Theoretical Chemistry</i> , 2014, 1036, 31-43.	1.1	7
10272	Structural, electronic properties and stability of $AlCMn_3$ (1 1 1) surfaces by first-principles calculations. <i>Applied Surface Science</i> , 2014, 289, 351-357.	3.1	7
10273	The segregation behavior of manganese and silicon at the coherent interfaces of copper precipitates in ferritic steels. <i>Journal of Nuclear Materials</i> , 2014, 445, 43-49.	1.3	12
10274	Experimental and DFT study on the catalytic asymmetric hydrogenation performance of (1 <i>S</i> ,2 <i>S</i> )-DPEN-Ru(TPP) <sub>2</sub> encapsulated in zeolite. <i>Journal of Molecular Catalysis A</i> , 2014, 385, 85-90.	4.8	5
10275	Generalized Brønsted-Evans-Polanyi relationships and descriptors for $O\hat{a}^+H$ bond cleavage of organic molecules on transition metal surfaces. <i>Journal of Catalysis</i> , 2014, 313, 24-33.	3.1	42
10276	Chlorodiethylaluminum supported on silica: A dinuclear aluminum surface species with bridging $\hat{I}^2-Cl$ -ligand as a highly efficient co-catalyst for the Ni-catalyzed dimerization of ethene. <i>Journal of Catalysis</i> , 2014, 313, 46-54.	3.1	43
10277	Quantum Anomalous Hall Effect in Graphene Proximity Coupled to an Antiferromagnetic Insulator. <i>Physical Review Letters</i> , 2014, 112, 116404.	2.9	361
10278	Formic acid decomposition on Au catalysts: DFT, microkinetic modeling, and reaction kinetics experiments. <i>AIChE Journal</i> , 2014, 60, 1303-1319.	1.8	87
10279	Phase transition and thermodynamic properties of beryllium from first-principles calculations. <i>Computational Materials Science</i> , 2014, 84, 139-144.	1.4	15
10280	Phase transition and elastic properties of TiN under pressure from first-principles calculations. <i>Computational Materials Science</i> , 2014, 86, 200-205.	1.4	14
10281	Thermodynamic and elastic properties of hexagonal ZnO under high temperature. <i>Journal of Alloys and Compounds</i> , 2014, 597, 50-57.	2.8	12
10282	Investigation of the adsorption of amino acids on Pd(111): A density functional theory study. <i>Applied Surface Science</i> , 2014, 301, 199-207.	3.1	13
10283	Heteronuclear NMR Spectroscopy as a Surface-Selective Technique: A Unique Look at the Hydroxyl Groups of $\hat{I}^3$ -Alumina.. <i>Chemistry - A European Journal</i> , 2014, 20, 4038-4046.	1.7	82

#	ARTICLE	IF	CITATIONS
10284	Recognition of carbon monoxide with SnO <sub>2</sub> /Ti thick-film sensor and its gas-sensing mechanism. <i>Sensors and Actuators B: Chemical</i> , 2014, 191, 1-8.	4.0	49
10285	Alkali metal adsorption on Ge(001)-c(2Å <sup>2</sup> ×4) surface: 0.25 monolayer of Na, K, Rb and Cs. <i>Applied Surface Science</i> , 2014, 301, 112-118.	3.1	0
10286	Influence of (Al, Fe, Mg) Impurities on Triclinic Ca <sub>3</sub> SiO <sub>5</sub> : Interpretations from DFT Calculations. <i>Crystal Growth and Design</i> , 2014, 14, 2158-2171.	1.4	29
10287	<i>Ab initio</i> -based thermal property predictions at a low cost: An error analysis. <i>Physical Review B</i> , 2014, 89, .	1.1	23
10288	Thermal and electrical conductivity of solid iron and iron-silicon mixtures at Earth's core conditions. <i>Earth and Planetary Science Letters</i> , 2014, 393, 159-164.	1.8	110
10289	Trapping helium in Y <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub> compared to in matrix iron: A first principles study. <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	42
10290	Sn <sub>1-x</sub> Ti <sub>x</sub> S <sub>2</sub> ternary alloys: A new visible optical material. <i>Acta Materialia</i> , 2014, 72, 223-228.	3.8	29
10291	Density functional theory studies of electronic properties of PdAg/Pd surface alloys. <i>Applied Surface Science</i> , 2014, 288, 69-75.	3.1	12
10292	First-principles study of 4d solute diffusion in nickel. <i>Journal of Materials Science</i> , 2014, 49, 4038-4044.	1.7	17
10293	Highly Crystalline Multimetallic Nanoframes with Three-Dimensional Electrocatalytic Surfaces. <i>Science</i> , 2014, 343, 1339-1343.	6.0	2,376
10294	Computational study of hydrogen induced lattice rearrangement and its influence on hydrogen permeance in Pd-Au alloys. <i>Journal of Alloys and Compounds</i> , 2014, 609, 244-252.	2.8	12
10295	Interaction of carbon-vacancy complex with minor alloying elements of ferritic steels. <i>Journal of Nuclear Materials</i> , 2014, 451, 82-87.	1.3	29
10296	A first principles investigation of Bi <sub>2</sub> O <sub>3</sub> -modified TiO <sub>2</sub> for visible light Activated photocatalysis: The role of TiO <sub>2</sub> crystal form and the Bi <sup>3+</sup> stereochemical lone pair. <i>Materials Science in Semiconductor Processing</i> , 2014, 25, 59-67.	1.9	26
10297	Intramolecularly Coordinated (6-(Diphenylphosphino)acenaphth-5-yl)stannanes. Repulsion vs Attraction of P- and Sn-Containing Substituents in the <i>peri</i> Positions. <i>Organometallics</i> , 2014, 33, 2409-2423.	1.1	29
10298	Vibrationally Promoted Dissociation of Water on Ni(111). <i>Science</i> , 2014, 344, 504-507.	6.0	175
10299	Optically Active Tetra- <i>tert</i> -butyl- $\Delta$ 5-deltacyclene Epimers: Preparation, Spectroscopy, Dynamic Equilibria, H/D Exchange, and Transition-Metal Complex Chemistry. <i>Chemistry - A European Journal</i> , 2014, 20, 5708-5720.	1.7	6
10300	First-principles studies on (001) surface electronic bonding and magnetic properties of ZnMn <sub>3</sub> and ZnNMn <sub>3</sub> intermetallic antiperovskites type compounds. <i>Journal of Alloys and Compounds</i> , 2014, 586, 230-238.	2.8	2
10301	Integrating computational modeling and first-principles calculations to predict stacking fault energy of dilute multicomponent Ni-base alloys. <i>Computational Materials Science</i> , 2014, 91, 50-55.	1.4	17

#	ARTICLE	IF	CITATIONS
10302	Longphyllinesides A and B: natural Diels-Alder adducts from <i>Daphniphyllum longeracemosum</i> ?. <i>Tetrahedron</i> , 2014, 70, 4017-4021.	1.0	14
10303	Construction of a parameter-free doubly hybrid density functional from adiabatic connection. <i>Journal of Chemical Physics</i> , 2014, 140, 18A512.	1.2	57
10304	The structure, electronic, and optical properties of (Sm,N)-codoped anatase TiO <sub>2</sub> photocatalyst: A density functional study. <i>Journal of Catalysis</i> , 2014, 309, 115-120.	3.1	21
10305	Acid strength and bifunctional catalytic behavior of alloys comprised of noble metals and oxophilic metal promoters. <i>Journal of Catalysis</i> , 2014, 315, 48-58.	3.1	39
10306	Ba <sub>2</sub> HgS <sub>5</sub> —A Molecular Trisulfide Salt with Dumbbell-like (HgS <sub>2</sub> ) <sup>2+</sup> Ions. <i>Inorganic Chemistry</i> , 2014, 53, 4698-4704.	1.9	30
10307	Selective hydrogenation of 1,3-butadiene on PdNi bimetallic catalyst: From model surfaces to supported catalysts. <i>Journal of Catalysis</i> , 2014, 316, 1-10.	3.1	55
10308	Magnifying the Morphology Change Induced by a Nickel Promoter in Tungsten(IV) Sulfide Industrial Hydrocracking Catalyst: A HAADF-STEM and DFT Study. <i>ChemCatChem</i> , 2014, 6, 1594-1598.	1.8	17
10309	A First-Principles Study of Carbon-Oxygen Bond Scission in Multiatomic Molecules on Flat and Stepped Metal Surfaces. <i>ChemCatChem</i> , 2014, 6, 1755-1762.	1.8	13
10310	Density functional theory studies of methanol adsorption and decomposition mechanism on Al <sub>13</sub> clusters. <i>Canadian Journal of Chemistry</i> , 2014, 92, 293-298.	0.6	2
10311	Assessment of density functionals and paucity of non-covalent interactions in aminoylyne complexes of molybdenum and tungsten [( $\eta$ -5-C <sub>5</sub> H <sub>5</sub> )(CO) <sub>2</sub> M(E)N(SiMe <sub>3</sub> )(R))] (E = Si, Ge, Sn, Pb): a dispersion-corrected DFT study. <i>Dalton Transactions</i> , 2014, 43, 9955-9967.	1.6	11
10312	Six-dimensional potential energy surface of the dissociative chemisorption of HCl on Au(111) using neural networks. <i>Science China Chemistry</i> , 2014, 57, 147-155.	4.2	50
10313	Enriching physisorption of H <sub>2</sub> S and NH <sub>3</sub> gases on a graphene sheet by doping with Li adatoms. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 8100-8105.	1.3	53
10314	First-principles studies on electronic transport properties of CdS nanoribbon based molecular device. <i>Ceramics International</i> , 2014, 40, 9211-9216.	2.3	15
10315	Six-dimensional quantum dynamics study for the dissociative adsorption of DCl on Au(111) surface. <i>Journal of Chemical Physics</i> , 2014, 140, 144701.	1.2	45
10316	Theoretical investigation of Cu-containing materials with different valence structure types: BaCu <sub>2</sub> S <sub>2</sub> , Li <sub>2</sub> CuSb, and LiCuS. <i>Journal of Physics and Chemistry of Solids</i> , 2014, 75, 927-930.	1.9	10
10317	Theoretical prediction of encapsulation and adsorption of platinum-anticancer drugs into single walled boron nitride and carbon nanotubes. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2014, 79, 443-457.	0.9	26
10318	Interaction of tetraethoxysilane with OH-terminated SiO <sub>2</sub> (001) surface: A first principles study. <i>Applied Surface Science</i> , 2014, 305, 247-251.	3.1	10
10319	Conformation analysis of triphenylphosphine in trans and cis triphenylphosphine-substituted Fischer carbene complexes. <i>Journal of Molecular Structure</i> , 2014, 1065-1066, 29-38.	1.8	17

#	ARTICLE	IF	CITATIONS
10320	Electronic structure of spinel-type LiNi <sub>1/2</sub> Ge <sub>3/2</sub> O <sub>4</sub> and LiNi <sub>1/2</sub> Mn <sub>3/2</sub> O <sub>4</sub> as positive electrodes for rechargeable Li-ion batteries studied by first-principles density functional theory. <i>Solid State Ionics</i> , 2014, 262, 74-76.	1.3	5
10321	Theoretical investigation of ethane and ethene monitoring using pristine and decorated aluminum nitride and silicon carbide nanotubes. <i>Sensors and Actuators B: Chemical</i> , 2014, 196, 555-566.	4.0	6
10322	Thermodynamic assessment of the Al–Dy, Dy–Zr and Al–Dy–Zr systems. <i>Science Bulletin</i> , 2014, 59, 1738-1746.	1.7	6
10323	Using Room Temperature Current Noise To Characterize Single Molecular Spectra. <i>ACS Nano</i> , 2014, 8, 2111-2117.	7.3	5
10324	Atomic and Molecular Adsorption on Re(0001). <i>Topics in Catalysis</i> , 2014, 57, 54-68.	1.3	28
10325	Density functional theory prediction for the second-order nonlinear optical responses of phenanthroline-fused phthalocyanine derivatives. <i>Journal of Porphyrins and Phthalocyanines</i> , 2014, 18, 58-66.	0.4	2
10326	The stability and diffusion properties of foreign impurity atoms on the surface and in the bulk of vanadium: A first-principles study. <i>Computational Materials Science</i> , 2014, 81, 191-198.	1.4	21
10327	Interactions of xanthate with pyrite and galena surfaces in the presence and absence of oxygen. <i>Journal of Industrial and Engineering Chemistry</i> , 2014, 20, 268-273.	2.9	35
10328	Width- and edge-dependent magnetic properties, electronic structures, and stability of SnSe <sub>2</sub> nanoribbons. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2014, 59, 102-106.	1.3	13
10329	Atomistic theory of hybrid improper ferroelectricity in perovskites. <i>Physical Review B</i> , 2014, 89, .	1.1	51
10330	All–Nitrogen Analogue of Ozone: Li <sub>3</sub> N <sub>3</sub> Species. <i>Chemistry - A European Journal</i> , 2014, 20, 6636-6640.	1.7	13
10331	First-principles study of the structural, elastic, and optical properties for Sr <sub>0.5</sub> Ca <sub>0.5</sub> TiO <sub>3</sub> . <i>Chinese Physics B</i> , 2014, 23, 026301.	0.7	5
10332	Hydroxylation of the surface of PbS nanocrystals passivated with oleic acid. <i>Science</i> , 2014, 344, 1380-1384.	6.0	404
10333	Density Functional Theory Study on the Metal–Support Interaction between Ru Cluster and Anatase TiO <sub>2</sub> (101) Surface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3514-3522.	1.5	59
10334	Photocatalytic Activity of NaTaO <sub>3</sub> Doped with N, Mo, and (N,Mo): A Hybrid Density Functional Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 10711-10719.	1.5	59
10335	Density functional theory study of propane steam reforming on Rh–Ni bimetallic surface: Sulfur tolerance and scaling/Brønsted–Evans–Polanyi relations. <i>Journal of Catalysis</i> , 2014, 309, 248-259.	3.1	28
10336	Study of Anion Order/Disorder in RTaN <sub>2</sub> O (R = La, Ce, Pr) Perovskite Nitride Oxides. <i>Crystal Growth and Design</i> , 2014, 14, 117-125.	1.4	42
10337	DFT study of benzene and CO co-adsorption on PtCo(111). <i>Applied Surface Science</i> , 2014, 289, 502-510.	3.1	8

#	ARTICLE	IF	CITATIONS
10338	Thermodynamic assessment of the Sr–In and Sr–Bi systems supported by first-principles calculations. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2014, 45, 49-54.	0.7	7
10339	On the Innocence of Bipyridine Ligands: How Well Do DFT Functionals Fare for These Challenging Spin Systems?. Journal of Chemical Theory and Computation, 2014, 10, 220-235.	2.3	34
10340	Study of lattice thermal conductivity of PbS. Journal of Alloys and Compounds, 2014, 584, 381-384.	2.8	9
10341	Can density functional theory methods be used to simulate the $\sqrt{2} \times \sqrt{2}$ phase of solid oxygen?. Chemical Physics Letters, 2014, 592, 170-174.	1.2	9
10342	Error Estimates for Solid-State Density-Functional Theory Predictions: An Overview by Means of the Ground-State Elemental Crystals. Critical Reviews in Solid State and Materials Sciences, 2014, 39, 1-24.	6.8	404
10343	Structural and electronic properties of armchair (7, 7) carbon nanotubes using DFT. Computational Materials Science, 2014, 82, 159-164.	1.4	29
10344	NH <sub>3</sub> adsorption on the Lewis and Bronsted acid sites of MoO <sub>3</sub> (010) surface: A cluster DFT study. Applied Surface Science, 2014, 288, 690-694.	3.1	38
10345	Magnetism, structure and chemical order in small CoPd clusters: A first-principles study. Journal of Magnetism and Magnetic Materials, 2014, 349, 109-115.	1.0	13
10346	25th Anniversary Article: Design of Polymethine Dyes for All-Optical Switching Applications: Guidance from Theoretical and Computational Studies. Advanced Materials, 2014, 26, 68-84.	11.1	97
10347	Interaction of minor alloying elements of high-Cr ferritic steels with lattice defects: An ab initio study. Journal of Nuclear Materials, 2014, 444, 237-246.	1.3	38
10348	First-principles study of hydrogen storage and diffusion in B2 FeTi alloy. Computational Materials Science, 2014, 81, 517-523.	1.4	23
10349	Improved plastic anisotropy of Mg–Zn–Ca alloys exhibiting high-stretch formability: A first-principles study. Acta Materialia, 2014, 65, 207-214.	3.8	90
10350	DFT study of chromium-doped SnO <sub>2</sub> materials. Journal of Materials Science, 2014, 49, 2904-2911.	1.7	33
10351	Formation and magnetic properties of metastable phases observed in the Fe <sub>50</sub> (Hf <sub>x</sub> Ta <sub>1-x</sub> ) <sub>50</sub> films by ion beam mixing. Applied Surface Science, 2014, 290, 495-498.	3.1	1
10352	First-principles study on electronic and magnetic properties of (Mn,Fe)-codoped ZnO. Journal of Magnetism and Magnetic Materials, 2014, 352, 66-71.	1.0	36
10353	Tuning photocatalytic performance of the near-infrared-driven photocatalyst Cu <sub>2</sub> (OH)PO <sub>4</sub> based on effective mass and dipole moment. Physical Chemistry Chemical Physics, 2014, 16, 3267.	1.3	69
10354	Anionogenic Mixed Valency in K <sub>x</sub> Ba <sub>1-x</sub> O <sub>2</sub> . Inorganic Chemistry, 2014, 53, 496-502.	1.9	4
10355	The density functional study of electronic structure, electronic charge density, linear and nonlinear optical properties of single crystal alpha-LiAlTe <sub>2</sub> . Journal of Alloys and Compounds, 2014, 592, 92-99.	2.8	30

#	ARTICLE	IF	CITATIONS
10356	Emergence of spin-filter states in Pt-Fe nanowires. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 8360-8366.	1.3	15
10357	A bibliometric study of highly cited reviews in the science citation index expanded. <i>Journal of the Association for Information Science and Technology</i> , 2014, 65, 372-385.	1.5	64
10358	A Bi-C-N hybrid porous sheet: an efficient metal-free visible-light absorption material. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4299.	1.3	13
10359	Dissociative adsorption of 2,3,7,8-TCDD on the surfaces of typical metal oxides: a first-principles density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 5553.	1.3	10
10360	Effect of pressure on elastic, mechanical and electronic properties of WSe <sub>2</sub> : A first-principles study. <i>Materials Research Bulletin</i> , 2014, 50, 503-508.	2.7	46
10361	On the mechanism of sulfur fast diffusion in 3-D transition metals. <i>Acta Materialia</i> , 2014, 67, 95-101.	3.8	16
10362	Theoretical Prediction and Experimental Confirmation of Unusual Ternary Ordered Semiconductor Compounds in Sr-Pb-S System. <i>Journal of the American Chemical Society</i> , 2014, 136, 1628-1635.	6.6	33
10363	Gupta potential for alkaline earth metals: Calcium and strontium. <i>Computational Materials Science</i> , 2014, 85, 142-146.	1.4	4
10364	Electronic structure and reactivity in water splitting of the iron oxide dimers and their hexacarbonyls: A density functional study. <i>Journal of Chemical Physics</i> , 2014, 140, 024303.	1.2	5
10365	Thermodynamic modeling of Fe-Ti-Bi system assisted with key experiments. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014, 46, 34-41.	0.7	5
10366	First-principles study of the high-pressure behavior of solid 1,7-diamino-1,7-dinitrimino-2,4,6-trinitro-2,4,6-triazaheptane. <i>Computational and Theoretical Chemistry</i> , 2014, 1030, 38-43.	1.1	4
10367	Magnetic and electronic properties of Cr- and Mn-doped SnO <sub>2</sub> : ab initio calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2014, 75, 701-709.	1.9	25
10368	Density-Dependent Exchange-Correlation Potentials Derived From highly Accurate Ab initio Calculations. <i>Advances in Quantum Chemistry</i> , 2014, 68, 125-151.	0.4	11
10369	Enhanced mechanical property of Fe-Al alloy due to Mn insertion: ab initio study. <i>Journal of Alloys and Compounds</i> , 2014, 583, 295-299.	2.8	19
10370	Adsorption of Pd, Pt, Cu, Ag, and Au Monomers on NiAl(110) Surface: A Comparative Study from DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5748-5755.	1.1	11
10371	H <sub>2</sub> dissociation on $\gamma$ -Al <sub>2</sub> O <sub>3</sub> supported Cu/Pd atoms: A DFT investigation. <i>Applied Surface Science</i> , 2014, 290, 154-160.	3.1	24
10372	Benchmark Assessment of Density Functional Methods on Group II-VI MX (M = Zn, Cd; X = S, Se, Te) Quantum Dots. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 76-89.	2.3	69
10373	Conformational Equilibria in Butane-1,4-diol: A Benchmark of a Prototypical System with Strong Intramolecular H-bonds. <i>Journal of Physical Chemistry A</i> , 2014, 118, 293-303.	1.1	53



#	ARTICLE	IF	CITATIONS
10374	New mono and bimetallic iron complexes derived from partially methylated s-indacene. Evidence of a trinuclear iron s-indacene complex. <i>Polyhedron</i> , 2014, 69, 15-24.	1.0	9
10375	Ab Initio Analysis of Silicon Nano-Clusters. <i>Journal of Physical Chemistry C</i> , 2014, 118, 1397-1406.	1.5	12
10376	Interatomic potential for accurate phonons and defects in UO <sub>2</sub> . <i>Journal of Nuclear Materials</i> , 2014, 446, 155-162.	1.3	10
10377	Amorphous Fe <sub>2</sub> O <sub>3</sub> as a high-capacity, high-rate and long-life anode material for lithium ion batteries. <i>Nano Energy</i> , 2014, 4, 23-30.	8.2	307
10378	A Combined Experimental and Theoretical Study of the Ti <sub>2</sub> + N <sub>2</sub> O Reaction. <i>Journal of Physical Chemistry A</i> , 2014, 118, 561-572.	1.1	6
10379	Mutual alloying of XAs (X=Ga, In, Al) materials: Tuning the optoelectronic and thermodynamic properties for solar energy applications. <i>Solar Energy</i> , 2014, 100, 1-8.	2.9	34
10380	Oxygen adsorption on single layer graphyne: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 974-980.	1.3	71
10381	First-principles study of the structural, electronic and elastic properties of ternary Zr <sub>2</sub> AN (A=Ga, In) <small>Tj ETQq1 1 0.784314 rgBT /Overlook</small>	1.4	7
10382	Modeling Water and Ammonia Adsorption in Hydrophobic Metal-Organic Frameworks: Single Components and Mixtures. <i>Journal of Physical Chemistry C</i> , 2014, 118, 1102-1110.	1.5	57
10383	First-principles phase stability, bonding, and electronic structure of actinide metals. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2014, 194, 2-7.	0.8	33
10384	Development of shape-engineered MnO <sub>2</sub> materials as bi-functional catalysts for oxygen evolution reaction and oxygen reduction reaction in alkaline medium. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 21024-21036.	3.8	112
10385	Assembly of Ruthenium-Based Complex into Metal-Organic Framework with Tunable Area-Selected Luminescence and Enhanced Photon-to-Electron Conversion Efficiency. <i>Journal of Physical Chemistry C</i> , 2014, 118, 25365-25373.	1.5	61
10386	Correlation matrix renormalization approximation for total-energy calculations of correlated electron systems. <i>Physical Review B</i> , 2014, 89, .	1.1	15
10387	Boron phosphide under pressure: In situ study by Raman scattering and X-ray diffraction. <i>Journal of Applied Physics</i> , 2014, 116, .	1.1	33
10388	The Role of Charge States in the Atomic Structure of Cu <sub>n</sub> and Pt <sub>n</sub> (n = 2-14 atoms) Clusters: A DFT Investigation. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10813-10821.	1.1	101
10389	Synthesis of One-Dimensional Copper Sulfide Nanorods as High-Performance Anode in Lithium Ion Batteries. <i>ChemSusChem</i> , 2014, 7, 3328-3333.	3.6	80
10390	A possible mechanism for the emergence of an additional band gap due to a Ti-O-C bond in the TiO <sub>2</sub> -graphene hybrid system for enhanced photodegradation of methylene blue under visible light. <i>RSC Advances</i> , 2014, 4, 59890-59901.	1.7	143
10391	Selenium adsorption at different coverages on Fe(1 0 0) and Fe(1 1 1): A DFT study. <i>Applied Surface Science</i> , 2014, 315, 252-260.	3.1	11



#	ARTICLE	IF	CITATIONS
10392	Creating multiferroics with large tunable electrical polarization from paraelectric rare-earth orthoferrites. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 472201.	0.7	39
10393	Trends in Formic Acid Decomposition on Model Transition Metal Surfaces: A Density Functional Theory study. <i>ACS Catalysis</i> , 2014, 4, 4434-4445.	5.5	190
10394	Tuning electronic and magnetic properties of SnSe <sub>2</sub> armchair nanoribbons via edge hydrogenation. <i>Journal of Materials Chemistry C</i> , 2014, 2, 10175-10183.	2.7	17
10395	First-principles studies of the structural, electronic and optical properties of dinitrides CN <sub>2</sub> , SiN <sub>2</sub> and GeN <sub>2</sub> . <i>Computational Materials Science</i> , 2014, 95, 706-711.	1.4	5
10396	First-Principles Prediction of New Complex Transition Metal Hydrides for High Temperature Applications. <i>Inorganic Chemistry</i> , 2014, 53, 11849-11860.	1.9	12
10397	Interactions between silver nanoparticles and polyvinyl alcohol nanofibers. <i>AIP Advances</i> , 2014, 4, .	0.6	28
10398	Dynamics of H <sub>2</sub> Eley-Rideal abstraction from W(110): Sensitivity to the representation of the molecule-surface potential. <i>Journal of Chemical Physics</i> , 2014, 141, 024701.	1.2	15
10399	First-principles calculations on the schottky barrier height of the NiGe/N-type Ge contact with dopant segregation. , 2014, , .		0
10400	Mechanism of Alkyne Alkoxy carbonylation at a Pd Catalyst with P,N Hemilabile Ligands: A Density Functional Study. <i>Chemistry - A European Journal</i> , 2014, 20, 13923-13926.	1.7	79
10401	Electronic, magnetic structure and water splitting reactivity of the iron-sulfur dimers and their hexacarbonyl complexes: A density functional study. <i>Journal of Chemical Physics</i> , 2014, 141, 044307.	1.2	7
10402	Propene epoxidation with O <sub>2</sub> or H <sub>2</sub> O mixtures over silver catalysts: theoretical insights into the role of the particle size. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26600-26612.	1.3	18
10403	Fe adsorption on hematite (α-Fe <sub>2</sub> O <sub>3</sub> ) (0001) and magnetite (Fe <sub>3</sub> O <sub>4</sub> ) (111) surfaces. <i>Journal of Chemical Physics</i> , 2014, 141, 134707.	1.2	14
10404	First-Principles Predictions and <i>in Situ</i> Experimental Validation of Alumina Atomic Layer Deposition on Metal Surfaces. <i>Chemistry of Materials</i> , 2014, 26, 6752-6761.	3.2	68
10405	Localization of metallicity and magnetic properties of graphene and of graphene nanoribbons doped with boron clusters. <i>Philosophical Magazine</i> , 2014, 94, 1841-1858.	0.7	8
10406	Thermodynamics and density functional theory study of potassium dichromate interaction with galena. <i>International Journal of Minerals, Metallurgy and Materials</i> , 2014, 21, 947-954.	2.4	6
10407	Status in Calculating Electronic Excited States in Transition Metal Oxides from First Principles. <i>Topics in Current Chemistry</i> , 2014, 347, 47-98.	4.0	15
10408	A first principle study of adsorption of two proximate nitrogen atoms on graphene. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1619-1629.	1.0	8
10409	Electronic structures and optical properties of SnSe <sub>2</sub> (1-x)O <sub>2x</sub> alloys. <i>Computational Materials Science</i> , 2014, 95, 712-717.	1.4	9

#	ARTICLE	IF	CITATIONS
10410	Insights into the Electronic Structure of Cu <sup>II</sup> Bound to an Imidazole Analogue of Westiellamide. <i>Inorganic Chemistry</i> , 2014, 53, 12323-12336.	1.9	14
10411	Methanol Oxidative Dehydrogenation on Oxide Catalysts: Molecular and Dissociative Routes and Hydrogen Addition Energies as Descriptors of Reactivity. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26115-26129.	1.5	39
10412	Work Function Changes of Azo-Derivatives Adsorbed on a Gold Surface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26033-26040.	1.5	9
10413	Theoretical studies on the penta-atomic planar coordinate carbon molecules [CGa <sub>3</sub> Sn] and [CGa <sub>3</sub> Sn] <sup>+</sup> . <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2014, 40, 594-597.	0.3	3
10414	Engineering the Work Function of Buckled Boron $\hat{\pm}$ -Sheet by Lithium Adsorption: A First-Principles Investigation. <i>ACS Applied Materials &amp; Interfaces</i> , 2014, 6, 19690-19701.	4.0	26
10415	Full Determination of Individual Reconstructed Atomic Columns in Intermixed Heterojunctions. <i>Nano Letters</i> , 2014, 14, 6584-6589.	4.5	1
10416	Efficient luminescent center by codoping (Eu,Mg,O) into GaN. <i>Applied Physics Express</i> , 2014, 7, 071005.	1.1	13
10417	The stabilities and electronic structures of single-layer bismuth oxyhalides for photocatalytic water splitting. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 25854-25861.	1.3	105
10418	Poisoning effect of adsorbed CO during CO <sub>2</sub> electroreduction on late transition metals. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20429-20435.	1.3	63
10419	Role of the nano amorphous interface in the crystallization of Sb <sub>2</sub> Te <sub>3</sub> towards non-volatile phase change memory: insights from first principles. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 10810.	1.3	24
10420	Improvements in DFT Calculations of Spin <sup>2</sup> Spin Coupling Constants. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4938-4949.	2.3	31
10421	Phase stability and mechanical properties of niobium dihydride. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 18989-18996.	3.8	12
10422	Band structure engineering and transport properties of aluminium phosphide nanoribbon – A first-principles study. <i>Superlattices and Microstructures</i> , 2014, 76, 135-148.	1.4	7
10423	Near-infrared photocatalytic activity induced by intrinsic defects in Bi <sub>2</sub> MO <sub>6</sub> (M = W, Mo). <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18596.	1.3	82
10424	Phase stability, hardness and bond characteristics of ruthenium borides from first-principles. <i>RSC Advances</i> , 2014, 4, 25093-25098.	1.7	9
10425	The adsorption and dissociation of methane on cobalt surfaces: thermochemistry and reaction barriers. <i>RSC Advances</i> , 2014, 4, 43004-43011.	1.7	25
10426	Structural skeleton of preferentially interpenetrated clusters and correlation with shear localization in Mg <sup>+</sup> Cu <sup>+</sup> Ni ternary metallic glasses. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19590.	1.3	19
10427	Analysis of sulfur modification mechanism for anatase and rutile TiO <sub>2</sub> by different doping modes based on GGA + U calculations. <i>RSC Advances</i> , 2014, 4, 32100.	1.7	22

#	ARTICLE	IF	CITATIONS
10428	Oxygen vacancies in self-assemblies of ceria nanoparticles. <i>Journal of Materials Chemistry A</i> , 2014, 2, 18329-18338.	5.2	33
10429	Gap openings in graphene regarding interfacial interaction from substrates. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 5600.	1.3	3
10430	Controlling Na diffusion by rational design of Si-based layered architectures. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4260.	1.3	75
10431	Irradiation induced non-equilibrium phase formation and structural transformation in the Fe/Ti/Nb multilayered films. <i>RSC Advances</i> , 2014, 4, 9098-9102.	1.7	1
10432	Direct vs. indirect pathway for nitrobenzene reduction reaction on a Ni catalyst surface: a density functional study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26365-26374.	1.3	103
10433	Well-Defined Supported Mononuclear Tungsten Oxo Species as Olefin Metathesis Pre-Catalysts. <i>ACS Catalysis</i> , 2014, 4, 4232-4241.	5.5	38
10434	Beyond the Corey Reaction II: Dimethylenation of Sterically Congested Ketones. <i>Journal of Organic Chemistry</i> , 2014, 79, 10669-10673.	1.7	9
10435	Improving photocatalytic properties of SrTiO <sub>3</sub> through (Sb, N) codoping: a hybrid density functional study. <i>RSC Advances</i> , 2014, 4, 45703-45709.	1.7	31
10436	Investigation of the electron structure of ZnO by the GGA and mBJ calculations associated with the characterization techniques AES and EELS. <i>International Journal of Modern Physics B</i> , 2014, 28, 1450078.	1.0	1
10437	Structural, electronic and optical properties of Cd <sub>x</sub> Zn <sub>1-x</sub> S alloys from first-principles calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2014, 378, 3382-3388.	0.9	6
10438	First-Principles Mechanistic Analysis of Dimethyl Ether Electro-Oxidation on Monometallic Single-Crystal Surfaces. <i>Journal of Physical Chemistry C</i> , 2014, 118, 24199-24211.	1.5	23
10439	A cluster DFT study of NH <sub>3</sub> and NO adsorption on the (MoO <sub>2</sub> ) <sub>2</sub> /HZSM-5 surface: Lewis versus Brønsted acid sites. <i>Applied Surface Science</i> , 2014, 321, 339-347.	3.1	21
10440	Cation Disorder Regulation by Microstate Configurational Entropy in Photovoltaic Absorber Materials Cu <sub>2</sub> ZnSn(S,Se) <sub>4</sub> . <i>Journal of Physical Chemistry C</i> , 2014, 118, 24884-24889.	1.5	18
10441	Thermodynamic study of benzene and hydrogen coadsorption on Pd(111). <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 23754-23768.	1.3	25
10442	Photoluminescence Quenching in Single-Layer MoS <sub>2</sub> via Oxygen Plasma Treatment. <i>Journal of Physical Chemistry C</i> , 2014, 118, 21258-21263.	1.5	228
10443	Nature of Tunable Optical Reflectivity of Rocksalt Hafnium Nitride Films. <i>Journal of Physical Chemistry C</i> , 2014, 118, 20511-20520.	1.5	23
10444	Effects of Mg and Al doping on the electronic structure and dehydrogenation of LiBH <sub>4</sub> -NH <sub>3</sub> . <i>International Journal of Hydrogen Energy</i> , 2014, 39, 17144-17152.	3.8	8
10445	Influence of ZrO <sub>2</sub> Structure and Copper Electronic State on Activity of Cu/ZrO <sub>2</sub> Catalysts in Methanol Synthesis from CO <sub>2</sub> . <i>ACS Catalysis</i> , 2014, 4, 3730-3741.	5.5	294

#	ARTICLE	IF	CITATIONS
10446	Tunability in electron transport of molybdenum chalcogenide nanowires by theoretical prediction. Chemical Physics Letters, 2014, 615, 99-104.	1.2	3
10447	Layered uranium( $\text{U}^{VI}$ ) hydroxides: structural and thermodynamic properties of dehydrated schoepite $\text{U}_2\text{O}_7(\text{OH})_2$ . Dalton Transactions, 2014, 43, 17191-17199.	1.6	35
10448	Twin-driven thermoelectric figure-of-merit enhancement of $\text{Bi}_2\text{Te}_3$ nanowires. Nanoscale, 2014, 6, 6158-6165.	2.8	60
10449	Pressure-induced hydrogen transfer and polymerization in crystalline furoxan. RSC Advances, 2014, 4, 15995-16004.	1.7	12
10450	Surface oxygen vacancies in gold based catalysts for CO oxidation. RSC Advances, 2014, 4, 13145-13152.	1.7	24
10451	Detecting gas molecules via atomic magnetization. Dalton Transactions, 2014, 43, 13070-13075.	1.6	5
10452	Investigation on spin-flip reaction of $\text{Re} + \text{CH}_3\text{CN}$ by relativistic density functional theory. Dalton Transactions, 2014, 43, 9508-9517.	1.6	3
10453	Theoretical study on optical and thermoelectric properties of the direct band gap $\text{In}_2\text{Ca}_2\text{CdAs}_2$ pnictide semiconductors. RSC Advances, 2014, 4, 46791-46799.	1.7	10
10454	DFT study on the effects of defect and metal-doping on the decomposition of $\text{H}_2\text{S}$ on the $\text{Fe}_2\text{O}_3(0001)$ surface. RSC Advances, 2014, 4, 22411-22418.	1.7	21
10455	Insights into the nature of $\text{M}^{\text{II}}\text{E}$ bonds in $[(\text{PMe}_3)_4\text{M}^{\text{II}}\text{E}(\text{Mes})]^+$ ( $\text{M} = \text{Mo}, \text{W}$ ) and $[(\text{PMe}_3)_5\text{W}^{\text{II}}\text{E}(\text{Mes})]^+$ : a dispersion-corrected DFT study. RSC Advances, 2014, 4, 13034.	1.7	4
10456	Influence of structure and atom sites on Sn-based anode materials for lithium ion batteries: a first-principle study. Science Bulletin, 2014, 59, 1459-1467.	1.7	1
10457	Molecular Binding in Post-Kohn-Sham Orbital-Free DFT. Journal of Chemical Theory and Computation, 2014, 10, 5338-5345.	2.3	19
10458	Strain-tunable extraordinary magnetocrystalline anisotropy in $\text{Sr}_2\text{CrReO}_6$ epitaxial films. Physical Review B, 2014, 90, .	1.1	14
10459	Quenching of the Photoisomerization of Azobenzene Self-Assembled Monolayers by the Metal Substrate. Journal of Physical Chemistry C, 2014, 118, 25906-25917.	1.5	14
10460	Oxidation kinetic mechanism study on the adsorption of O on $\text{Al}(110)$ surface. , 2014, , .		0
10461	Theoretical investigations on $\text{C}_2\text{H}_4\text{Nb}$ complex as a potential hydrogen storage system, using moller-plesset (MP2) and density functional theory. International Journal of Quantum Chemistry, 2014, 114, 449-457.	1.0	14
10462	Variational, Self-Consistent Implementation of the Perdew-Zunger Self-Interaction Correction with Complex Optimal Orbitals. Journal of Chemical Theory and Computation, 2014, 10, 5324-5337.	2.3	69
10463	Correlation between hardness and bond orientation of vanadium borides. RSC Advances, 2014, 4, 47377-47382.	1.7	22

#	ARTICLE	IF	CITATIONS
10464	Band gap engineering of NaTaO <sub>3</sub> using density functional theory: a charge compensated codoping strategy. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17116.	1.3	49
10465	The one-electron reduction of dithiolate and diselenolate ligands. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 10897.	1.3	11
10466	Effect of robust $\pi$ - $\pi$ stacking synthon on the formation of mercury coordination compounds; an unusual pseudo-square planar geometry. <i>Dalton Transactions</i> , 2014, 43, 5564-5573.	1.6	34
10467	Structural, mechanical properties and fracture mechanism of RuB1.1. <i>Dalton Transactions</i> , 2014, 43, 5168.	1.6	12
10468	Defect-induced semiconductor to metal transition in graphene monoxide. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 13477-13482.	1.3	12
10469	Several different charge transfer and Ce <sup>3+</sup> localization scenarios for Rh <sup>4+</sup> CeO <sub>2</sub> (111). <i>Journal of Materials Chemistry A</i> , 2014, 2, 2333-2345.	5.2	26
10470	The role of the CO adsorption on Pt monolayers supported on flat and stepped Au surfaces: a density functional investigation. <i>RSC Advances</i> , 2014, 4, 9247-9254.	1.7	18
10471	The surface chemistry of NO <sub>x</sub> on mackinawite (FeS) surfaces: a DFT-D2 study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 15444-15456.	1.3	40
10472	Structure and optical properties of (CdS <sub>x</sub> Se <sub>1-x</sub> ) <sub>42</sub> nanoclusters. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 13956.	1.3	3
10473	Theoretical investigation of the adsorption, IR, and electron injection of hydroxamate anchor at the TiO <sub>2</sub> anatase (1 0 1) surface. <i>RSC Advances</i> , 2014, 4, 19690-19693.	1.7	26
10474	Hydrogen-bonded intermediates and transition states during spontaneous and acid-catalyzed hydrolysis of the carcinogen (+)-anti-BPDE. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 12684.	1.3	1
10475	Insight into the general rule for the activation of the X-H bonds (X = C, N, O, S) induced by chemisorbed oxygen atoms. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 2621.	1.3	40
10476	Derivative discontinuities in density functional theory. <i>Molecular Physics</i> , 2014, 112, 2997-3013.	0.8	14
10477	The roles of surface structure, oxygen defects, and hydration in the adsorption of CO <sub>2</sub> on low-index ZnGa <sub>2</sub> O <sub>4</sub> surfaces: a first-principles investigation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 7538-7547.	1.3	19
10478	Modulated T carbon-like carbon allotropes: an ab initio study. <i>RSC Advances</i> , 2014, 4, 17364.	1.7	29
10479	Computational screening of structural and compositional factors for electrically conductive coordination polymers. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14463-14472.	1.3	23
10480	Phase stability and elastic properties of (W <sub>0.5</sub> Al <sub>0.5</sub> )C phase with a novel NiAs-type structure. <i>RSC Advances</i> , 2014, 4, 42585-42590.	1.7	0
10481	Reactivity of silica supported zirconium hydride towards N <sub>2</sub> O and CO <sub>2</sub> probe molecules: a computational point of view. <i>New Journal of Chemistry</i> , 2014, 38, 3717-3721.	1.4	7

#	ARTICLE	IF	CITATIONS
10482	Bilayers of transition metal dichalcogenides: Different stackings and heterostructures. <i>Journal of Materials Research</i> , 2014, 29, 373-382.	1.2	40
10483	Magnetically stabilized Fe <sub>8</sub> ( $\frac{1}{4}$ -S) <sub>6</sub> S <sub>8</sub> clusters in Ba <sub>6</sub> Fe <sub>25</sub> S <sub>27</sub> . <i>Dalton Transactions</i> , 2014, 43, 14612-14624.	1.6	9
10484	Coverage effect on reactivity can be more complicated than what you believe: H <sub>2</sub> dissociation on H-precovered Pd(111). <i>Journal of Chemical Physics</i> , 2014, 140, 244703.	1.2	1
10485	Ionic and Covalent Stabilization of Intermediates and Transition States in Catalysis by Solid Acids. <i>Journal of the American Chemical Society</i> , 2014, 136, 15229-15247.	6.6	43
10486	Magnetic and Ferroelectric Properties of BiCrO <sub>3</sub> from First-Principles Calculations. <i>Chinese Physics Letters</i> , 2014, 31, 107501.	1.3	3
10487	Theoretical study of small sodium-potassium alloy clusters through genetic algorithm and quantum chemical calculations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 8895-8904.	1.3	11
10488	Two novel metal borates with three-dimensional open-framework layers constructed from [M <sub>2</sub> B <sub>8</sub> O <sub>20</sub> (OH) <sub>2</sub> ] (M = Al, Ga) cluster units. <i>Dalton Transactions</i> , 2014, 43, 9427-9430.	1.6	20
10489	Recycling End-of-Life Polycarbonate in Steelmaking: Ab Initio Study of Carbon Dissolution in Molten Iron. <i>Industrial &amp; Engineering Chemistry Research</i> , 2014, 53, 3861-3864.	1.8	13
10490	Prediction on the Surface Phase Diagram and Growth Morphology of Nanocrystal Ruthenium Dioxide. <i>Journal of the American Ceramic Society</i> , 2014, 97, 3702-3709.	1.9	11
10491	A hybrid DFT based investigation of the photocatalytic activity of cation-anion codoped SrTiO <sub>3</sub> for water splitting under visible light. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24527-24535.	1.3	40
10492	CO <sub>2</sub> Adsorption Thermodynamics over N-Substituted/Grafted Graphanes: A DFT Study. <i>Langmuir</i> , 2014, 30, 1837-1844.	1.6	30
10493	The hydrogen adsorption on Zr-decorated LiB (001): A DFT study. <i>Vacuum</i> , 2014, 110, 62-68.	1.6	14
10494	Combination study of DFT calculation and experiment for photocatalytic properties of S-doped anatase TiO <sub>2</sub> . <i>Applied Surface Science</i> , 2014, 319, 50-59.	3.1	51
10495	Do Ni/Cu and Cu/Ni Alloys have Different Catalytic Performances towards Water-Gas Shift? A Density Functional Theory Investigation. <i>ChemPhysChem</i> , 2014, 15, 2490-2496.	1.0	17
10496	Structural, bonding and elastic properties of Mg(NH <sub>2</sub> BH <sub>3</sub> ) <sub>2</sub> , Ca(NH <sub>2</sub> BH <sub>3</sub> ) <sub>2</sub> and Sr(NH <sub>2</sub> BH <sub>3</sub> ) <sub>2</sub> . <i>Materials Chemistry and Physics</i> , 2014, 148, 364-370.	2.0	4
10497	Electronic Properties of Edge-Hydrogenated Phosphorene Nanoribbons: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22368-22372.	1.5	117
10498	DFT + U study of the CO + NO <sub>x</sub> reaction on a CeO <sub>2</sub> (110)-supported Au nanoparticle. <i>Chinese Journal of Catalysis</i> , 2014, 35, 1305-1317.	6.9	9
10499	Ferromagnetism in Nanostructured TiO <sub>2</sub> /Al System Due to Surface Charge Transfer. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3789-3794.	1.5	5



#	ARTICLE	IF	CITATIONS
10500	Shifting the Energy Landscape of Multicomponent Reactions Using Aziridine Aldehyde Dimers: A Mechanistic Study. <i>Journal of Organic Chemistry</i> , 2014, 79, 9465-9471.	1.7	22
10501	Graphene spintronics: Spin injection and proximity effects from first principles. <i>Physical Review B</i> , 2014, 90, .	1.1	43
10502	First-Principles Prediction of Ternary Interstitial Hydride Phase Stability in the Th-H System. <i>Journal of Chemical &amp; Engineering Data</i> , 2014, 59, 3232-3241.	1.0	3
10503	Spectroscopic Signatures for Interlayer Coupling in MoS <sub>2</sub> /WSe <sub>2</sub> van der Waals Stacking. <i>ACS Nano</i> , 2014, 8, 9649-9656.	7.3	288
10504	Ab initio study of the intermetallics in Nb-Si binary system. <i>Intermetallics</i> , 2014, 54, 125-132.	1.8	69
10505	Influence of the Ba <sup>2+</sup> /Sr <sup>2+</sup> content and oxygen vacancies on the stability of cubic Ba <sub>x</sub> Sr <sub>1-x</sub> Co <sub>0.75</sub> Fe <sub>0.25</sub> O <sub>3</sub> . <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 1333-1338.	1.3	7
10506	Prediction of Vapor-Liquid Coexistence Data for p-Cymene Using Equation of State Methods and Monte Carlo Simulations. <i>Journal of Chemical &amp; Engineering Data</i> , 2014, 59, 2987-2994.	1.0	6
10507	Ketonization of Carboxylic Acids in Biomass Conversion over TiO <sub>2</sub> and ZrO <sub>2</sub> Surfaces: A DFT Perspective. <i>ACS Catalysis</i> , 2014, 4, 2874-2888.	5.5	132
10508	Parametrization of the Stillinger-Weber potential for Si/N/H system and its application to simulations of silicon nitride film deposition with SiH <sub>4</sub> /NH <sub>3</sub> . <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	3
10509	Role of oxygen in Cu(1 1 0) surface restructuring in the vicinity of step edges. <i>Chemical Physics Letters</i> , 2014, 613, 64-69.	1.2	15
10510	Effects of chalcogen substitution on electronic properties and chemical bondings of delafossite CuAlO <sub>2</sub> . <i>Physica Status Solidi (B): Basic Research</i> , 2014, 251, 1630-1634.	0.7	11
10511	van der Waals effects at molecule-metal interfaces. <i>Physical Review B</i> , 2014, 90, .	1.1	22
10512	Thermodynamic phase diagram and electronic properties of Co <sub>2</sub> VO film: A first-principles study. <i>International Journal of Modern Physics B</i> , 2014, 28, 1450145.	1.0	9
10513	Catalytic propane reforming mechanism over Zr-doped CeO <sub>2</sub> (111). <i>Catalysis Science and Technology</i> , 2014, 4, 3278.	2.1	12
10514	Ultrafast Bulk Diffusion of AlH <sub>4</sub> in High-Entropy Dehydrogenation Intermediates of NaAlH <sub>4</sub> . <i>Journal of Physical Chemistry C</i> , 2014, 118, 18356-18361.	1.5	3
10515	High-resolution scanning tunneling microscopy imaging of Si(1 $\times$ 1)-7 $\times$ 7 structure and intrinsic molecular states. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 394001.	0.7	6
10516	Theoretical Insights on the C <sub>2</sub> H <sub>2</sub> Formation Mechanism During CH <sub>4</sub> Dissociation on Cu(100) Surface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 17662-17669.	1.5	3
10517	Bulk Iodoapatite Ceramic Densified by Spark Plasma Sintering with Exceptional Thermal Stability. <i>Journal of the American Ceramic Society</i> , 2014, 97, 2409-2412.	1.9	43



#	ARTICLE	IF	CITATIONS
10518	Investigations on the mechanisms of interactions between matrix metalloproteinase 9 and its flavonoid inhibitors using a combination of molecular docking, hybrid quantum mechanical/molecular mechanical calculations, and molecular dynamics simulations. Canadian Journal of Chemistry, 2014, 92, 821-830.	0.6	11
10519	Stability of the hcp Ruthenium at high pressures from first principles. Journal of Applied Physics, 2014, 116, .	1.1	15
10520	Interfacial defect complex at the MgO/SrTiO <sub>3</sub> heterojunction and its electronic impact. RSC Advances, 2014, 4, 51002-51007.	1.7	11
10521	The effect of remote substitution on the formation of preferential isomers of cobalt(III)-tetrazolate complexes by microwave assisted cycloaddition. Inorganic Chemistry Frontiers, 2014, 1, 599-610.	3.0	8
10522	On the nature of point defect and its effect on electronic structure of rocksalt hafnium nitride films. Acta Materialia, 2014, 81, 315-325.	3.8	31
10523	Solar Energy Storage in Phase Change Materials: First-Principles Thermodynamic Modeling of Magnesium Chloride Hydrates. Journal of Physical Chemistry C, 2014, 118, 4618-4625.	1.5	44
10524	Ab initio investigation of the structural and electronic properties of amorphous HgTe. Journal of Physics Condensed Matter, 2014, 26, 045503.	0.7	0
10525	Improvement of photocatalytic activity of NaTaO <sub>3</sub> under visible light by N and F doping. Chemical Physics Letters, 2014, 613, 54-58.	1.2	24
10526	An ab initio study on the electronic structures of the solid/liquid interface between TiB <sub>2</sub> (0 0 1) surface and Al melts. Journal of Alloys and Compounds, 2014, 615, 863-867.	2.8	14
10527	First-Principles Studies of Li Nucleation on Graphene. Journal of Physical Chemistry Letters, 2014, 5, 1225-1229.	2.1	82
10528	A theoretical study of the intermolecular interactions in the p-azoxyanisole liquid crystal. Journal of Molecular Liquids, 2014, 199, 530-537.	2.3	3
10529	First-principles calculations of structural phase transition and elastic properties of BeTe under high pressure. Philosophical Magazine Letters, 2014, 94, 103-111.	0.5	5
10530	Mono- and co-doped NaTaO <sub>3</sub> for visible light photocatalysis. Physical Chemistry Chemical Physics, 2014, 16, 16085-16094.	1.3	44
10531	Optical and magnetic properties of Ba <sub>5</sub> (BO <sub>3</sub> ) <sub>3</sub> F single crystals. Physical Chemistry Chemical Physics, 2014, 16, 24884-24891.	1.3	9
10532	Phosphorus vacancy cluster model for phosphorus diffusion gettering of metals in Si. Journal of Applied Physics, 2014, 115, 054906.	1.1	24
10533	Influence of Charge States on the π-π Interactions of Aromatic Side Chains with Surface of Graphene Sheet and Single-Walled Carbon Nanotubes in Bioelectrodes. Journal of Physical Chemistry C, 2014, 118, 20694-20701.	1.5	17
10534	Tweaking the magnetism of MoS <sub>2</sub> nanoribbon with hydrogen and carbon passivation. Nanotechnology, 2014, 25, 165703.	1.3	20
10535	Contribution of interstitial solute strengthening in aluminum. Philosophical Magazine Letters, 2014, 94, 63-71.	0.5	14

#	ARTICLE	IF	CITATIONS
10536	Formation and Growth of Molecular Clusters Containing Sulfuric Acid, Water, Ammonia, and Dimethylamine. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5464-5473.	1.1	67
10537	Validation of Classical Force Fields for the Description of Thermo-Mechanical Properties of Transition Metal Materials. <i>Journal of Physical Chemistry A</i> , 2014, 118, 8426-8436.	1.1	8
10538	Polymersâ€™ surface interactions with molten iron: A theoretical study. <i>Chemical Physics</i> , 2014, 443, 107-111.	0.9	11
10539	Reactivity trends of Fe phthalocyanines confined on graphite electrodes in terms of donorâ€™acceptor intermolecular hardness: Linear versus volcano correlations. <i>Chemical Physics Letters</i> , 2014, 614, 176-180.	1.2	12
10540	Communication: Self-interaction correction with unitary invariance in density functional theory. <i>Journal of Chemical Physics</i> , 2014, 140, 121103.	1.2	168
10541	Real Time Determination of the Electronic Structure of Unstable Reaction Intermediates during Au <sub>2</sub> O <sub>3</sub> Reduction. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 80-84.	2.1	30
10542	Synthesis, Structure, and Properties of the Electron-Poor IIâ€™V Semiconductor ZnAs. <i>Inorganic Chemistry</i> , 2014, 53, 8691-8699.	1.9	12
10543	First-principles investigations on vacancy formation and electronic structures of monolayer MoS <sub>2</sub> . <i>Materials Chemistry and Physics</i> , 2014, 148, 5-9.	2.0	49
10544	Density Differences in Embedding Theory with External Orbital Orthogonality. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9182-9200.	1.1	36
10545	Magnetic exchange in {Gd <sup>III</sup> â€™radical} complexes: method assessment, mechanism of coupling and magneto-structural correlations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14568-14577.	1.3	73
10546	Does the Preferred Mechanism of a Catalytic Transformation Depend on the Density Functional? Ethylene Hydrosilylation by a Metal Complex as a Case Study. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3004-3013.	1.1	6
10547	Internal (SiH) <sub>X</sub> groups, $X = 1-4$ , in microcrystalline hydrogenated silicon and their IR spectra on the basis of periodic DFT modelling. <i>Molecular Physics</i> , 2014, 112, 956-962.	0.8	4
10548	Elucidating Ionic Liquid Environments That Affect the Morphology of TiO <sub>2</sub> Nanocrystals: A DFT+D Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 23320-23327.	1.5	18
10549	Versatile Electronic and Magnetic Properties of SnSe <sub>2</sub> Nanostructures Induced by the Strain. <i>Journal of Physical Chemistry C</i> , 2014, 118, 9251-9260.	1.5	68
10550	An ab Initio Investigation of Proton Stability at BaZrO <sub>3</sub> Interfaces. <i>Chemistry of Materials</i> , 2014, 26, 4915-4924.	3.2	12
10551	How Surface Hydroxyls Enhance MgO Reactivity in Basic Catalysis: The Case of Methylbutynol Conversion. <i>ACS Catalysis</i> , 2014, 4, 4004-4014.	5.5	34
10552	Catalyst activation and the dimerization energy of alkylaluminium compounds. <i>Journal of Organometallic Chemistry</i> , 2014, 772-773, 161-171.	0.8	59
10553	Modeling Acid Oil Component Interactions with Carbonate Reservoirs: A First-Principles View on Low Salinity Recovery Mechanisms. <i>Journal of Physical Chemistry C</i> , 2014, 118, 19180-19187.	1.5	39

#	ARTICLE	IF	CITATIONS
10554	Molecular Dynamics Simulations of Proposed Intermediates in the CO <sub>2</sub> + Aqueous Amine Reaction. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1151-1156.	2.1	27
10555	Favored Composition Design and Atomic Structure Characterization for Ternary Al <sub>1-x</sub> Cu <sub>x</sub> Y Metallic Glasses via Proposed Interatomic Potential. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4442-4449.	1.2	16
10556	Formation of Hydroxyl Groups at Calcium-Silicate-Hydrate (C-S-H): Coexistence of Ca-OH and Si-OH on Wollastonite(001). <i>Journal of Physical Chemistry C</i> , 2014, 118, 8007-8013.	1.5	28
10557	Effect of vacancies on structural, electronic and optical properties of monolayer MoS <sub>2</sub> : A first-principles study. <i>Journal of Alloys and Compounds</i> , 2014, 613, 122-127.	2.8	89
10558	Structure Stability and Elastic Properties of $\beta$ Type Ti-X (X=Nb, Mo) Alloys from First-Principles Calculations. <i>Rare Metal Materials and Engineering</i> , 2014, 43, 553-558.	0.8	7
10559	Effect of vacancies (O, Ti) on the interfacial bonding strength and magnetoelectricity in Fe/BaTiO <sub>3</sub> : A first-principles study. <i>Computational Materials Science</i> , 2014, 93, 6-10.	1.4	0
10560	Interface properties in lamellar TiAl microstructures from density functional theory. <i>Intermetallics</i> , 2014, 54, 154-163.	1.8	39
10561	Slave mode expansion for obtaining <i>ab initio</i> interatomic potentials. <i>Physical Review B</i> , 2014, 90, .	1.1	15
10562	Surface Structural Reconstruction for Optical Response in Iodine-Modified TiO <sub>2</sub> Photocatalyst System. <i>Journal of Physical Chemistry C</i> , 2014, 118, 13726-13732.	1.5	19
10563	First-principles investigations on delithiation of Li <sub>4</sub> NiTeO <sub>6</sub> . <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16145.	1.3	14
10564	Thermodynamic re-assessment of the Al-Gd and Gd-Zr systems. <i>Thermochimica Acta</i> , 2014, 591, 51-56.	1.2	11
10565	The $\delta$ -Fe[N] and $\epsilon$ -Fe <sub>4</sub> N <sub>1-x</sub> phase boundaries in high-nitrogen steels: The cube cluster approximation and the effect of vibrational energy contributions. <i>Computational Materials Science</i> , 2014, 95, 8-12.	1.4	2
10566	The enhanced efficiency to 3.6% based on organic dye as donor and Si/TiO <sub>2</sub> acceptor bulk hetero-junction solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2014, 292, 1-9.	2.0	18
10567	The effect of hydrogen on the mechanical properties of FeTi for hydrogen storage applications. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 12667-12675.	3.8	24
10568	Comparison between cluster and slab model for Pt-group atom adsorption on gold and silver substrate. <i>Surface Science</i> , 2014, 630, 78-84.	0.8	4
10569	Shape-dependent catalytic activity of oxygen reduction reaction (ORR) on silver nanodecahedra and nanocubes. <i>Journal of Power Sources</i> , 2014, 269, 152-157.	4.0	89
10570	A study of the spin reorientation with <i>d</i> orbital hybridization in SmCrO <sub>3</sub> . <i>Solid State Communications</i> , 2014, 195, 21-25.	0.9	25
10571	Theoretical study of SO <sub>2</sub> adsorption on goethite (1 1 0) surface. <i>Applied Surface Science</i> , 2014, 314, 558-563.	3.1	14

#	ARTICLE	IF	CITATIONS
10572	Structural and mechanical properties of GaAs under pressure up to 200 GPa. Solid State Communications, 2014, 195, 26-30.	0.9	15
10573	Chain or Ring: Which One Is Favorable in Nitrogen-Rich Molecules $N_6XH_m$ , $N_8XH_m$ , and $N_{10}XH_m$ ( $X = B, Al, Ga$ , $m = 1$ and $X = C, Si, Ge$ )?. Journal of Physical Chemistry A, 2014, 118, 248-259.	1.1	3
10574	Computational Investigation of $NO_2$ Adsorption and Reduction on Ceria and M-Doped $CeO_2$ (111) (M = Mn, Fe) Surfaces. Journal of Physical Chemistry C, 2014, 118, 10043-10052.	1.5	20
10575	Theoretical Study on the Stability and Aromaticity of Metallasilapentalynes. Organometallics, 2014, 33, 1845-1850.	1.1	39
10576	Quantifying Environmental Effects on the Decay of Hole Transfer Couplings in Biosystems. Journal of Chemical Theory and Computation, 2014, 10, 2546-2556.	2.3	19
10577	Initial Stages of Oxygen Chemisorption on the Ge(001) Surface. Journal of Physical Chemistry C, 2014, 118, 15795-15803.	1.5	10
10578	Decomposition of Metal Alkylamides, Alkyls, and Halides at Reducible Oxide Surfaces: Mechanism of "Clean-up" During Atomic Layer Deposition of Dielectrics onto III-V Substrates. Chemistry of Materials, 2014, 26, 2427-2437.	3.2	16
10579	Trends in Electrochemical Stability of Transition Metal Carbides and Their Potential Use As Supports for Low-Cost Electrocatalysts. ACS Catalysis, 2014, 4, 1558-1562.	5.5	142
10580	First-principles investigation of elastic and thermodynamic properties of SiCN under pressure. Computational Materials Science, 2014, 95, 228-234.	1.4	5
10581	Theoretical study of the structural phase transition and elastic properties of HfN under high pressures. Journal of Physics and Chemistry of Solids, 2014, 75, 1295-1300.	1.9	4
10582	Tuning order-by-disorder multiferroicity in CuO by doping. Physical Review B, 2014, 90, .	1.1	17
10583	Quantum molecular dynamics simulation of shock-wave experiments in aluminum. Journal of Applied Physics, 2014, 115, .	1.1	68
10584	Density Functional Theory Study of Methanol Steam Reforming on Co(0001) and Co(111) Surfaces. Journal of Physical Chemistry C, 2014, 118, 15274-15285.	1.5	65
10585	Nature of the Resistive Switching Phenomena in $TiO_2$ and $SrTiO_3$ . Solid State Physics, 2014, , 353-559.	1.3	58
10586	Predicting and Comparing C-M and O-M Bond Strengths for Adsorption on Transition Metal Surfaces. Journal of Physical Chemistry C, 2014, 118, 2666-2672.	1.5	36
10587	Theoretical and experimental studies of the adsorption geometry and reaction pathways of furfural over FeNi bimetallic model surfaces and supported catalysts. Journal of Catalysis, 2014, 317, 253-262.	3.1	88
10588	Structure and reactivity of zero-, two- and three-dimensional Pd supported on $SrTiO_3(001)$ . Surface Science, 2014, 630, 46-63.	0.8	6
10589	Doping the transition metal atom Fe, Co, Ni into C <sub>48</sub> B <sub>12</sub> fullerene for enhancing H <sub>2</sub> capture: A theoretical study. International Journal of Hydrogen Energy, 2014, 39, 12741-12748.	3.8	24

#	ARTICLE	IF	CITATIONS
10590	Structural, electronic and elastic properties of noble metal sub-nitrides M <sub>2</sub> N (M=Ru, Rh, Pd). International Journal of Refractory Metals and Hard Materials, 2014, 47, 113-123.	1.7	3
10591	Disordered ZnO nanoparticles with extremely intense deep-level emission and enhanced photocatalytic activity. Applied Surface Science, 2014, 313, 888-895.	3.1	12
10592	Evaluating Pd-Ni layered catalysts for selective hydrogenation of 1,3-butadiene: A theoretical perspective. Journal of Molecular Catalysis A, 2014, 394, 151-161.	4.8	7
10593	Selective oxidation of vinyl chloride on Ag <sub>2</sub> O(100), Cu <sub>2</sub> O(100), and Au <sub>2</sub> O(100) surfaces: A density functional theory study. Surface Science, 2014, 630, 116-124.	0.8	4
10594	The performance of La <sub>0.6</sub> Sr <sub>1.4</sub> MnO <sub>4</sub> layered perovskite electrode material for intermediate temperature symmetrical solid oxide fuel cells. Journal of Power Sources, 2014, 270, 418-425.	4.0	68
10595	Benchmark Torsional Potentials of Building Blocks for Conjugated Materials: Bifuran, Bithiophene, and Biselenophene. Journal of Chemical Theory and Computation, 2014, 10, 3647-3655.	2.3	41
10596	The regeneration mechanisms of sulfurized $\gamma$ -Fe <sub>2</sub> O <sub>3</sub> surfaces under O <sub>2</sub> atmosphere: A density functional theory study. Fuel Processing Technology, 2014, 128, 238-250.	3.7	11
10597	Charge Transfer, Luminescence, and Phonon Bottleneck in TiO <sub>2</sub> Nanowires Computed by Eigenvectors of Liouville Superoperator. Journal of Chemical Theory and Computation, 2014, 10, 3996-4005.	2.3	26
10598	Influence of Structural Polymorphs on Tunable White Light Generation from Orange-Red-Emitting BiPO <sub>4</sub> :Eu <sup>3+</sup> Phosphor by Surface Modification. Journal of Physical Chemistry C, 2014, 118, 19308-19314.	1.5	7
10599	Relativistic and Electron-Correlation Effects on the Nuclear Magnetic Resonance Shieldings of Molecules Containing Tin and Lead Atoms. Journal of Physical Chemistry A, 2014, 118, 7863-7875.	1.1	34
10600	Surface Strain Improves Molecular Adsorption but Hampers Dissociation for $\text{N}_2$ on $\text{Cu}_2\text{O}$ Surfaces. Journal of Physical Chemistry C, 2014, 118, 19315-19324.	1.9	33
10601	Understanding the interaction of an antitumoral platinum(II) 7-azaindolate complex with proteins and DNA. BioMetals, 2014, 27, 1159-1177.	1.8	8
10602	Role of Gold(I) $\eta^2$ -Oxo Carbenes in the Oxidation Reactions of Alkynes Catalyzed by Gold(I) Complexes. Journal of the American Chemical Society, 2014, 136, 11513-11523.	6.6	80
10603	Effect of the alloying element titanium on the stability and trapping of hydrogen in pure vanadium: A first-principles study. International Journal of Modern Physics B, 2014, 28, 1450207.	1.0	16
10604	HAADF-STEM and DFT investigations of the Zn-containing $\eta^2$ phase in Al-Mg-Si alloys. Acta Materialia, 2014, 78, 245-253.	3.8	52
10605	Near-IR Two Photon Microscopy Imaging of Silica Nanoparticles Functionalized with Isolated Sensitized Yb(III) Centers. Chemistry of Materials, 2014, 26, 1062-1073.	3.2	61
10606	Role of Au in Graphene Growth on a Ni Surface. ACS Catalysis, 2014, 4, 892-902.	5.5	8
10607	Phase transformations of nano-sized cubic boron nitride to white graphene and white graphite. Applied Physics Letters, 2014, 104, 093104.	1.5	21

#	ARTICLE	IF	CITATIONS
10608	Roles of an oxygen Frenkel pair in the photoluminescence of Bi <sup>3+</sup> -doped Y <sub>2</sub> O <sub>3</sub> : computational predictions and experimental verifications. Journal of Materials Chemistry C, 2014, 2, 6017-6024.	2.7	25
10609	First-principles investigation on transport properties of NiO monowire-based molecular device. Molecular Physics, 2014, 112, 1954-1962.	0.8	20
10610	A first-principles study of CO oxidation by surface oxygen on Pt-incorporated perovskite catalyst (CaPt <sub>x</sub> Ti <sub>1-x</sub> O <sub>3</sub> ). RSC Advances, 2014, 4, 30530-30535.	1.7	5
10611	Intrinsic Oxygen Vacancy and Extrinsic Aluminum Dopant Interplay: A Route to the Restoration of Defective TiO <sub>2</sub> . Journal of Physical Chemistry C, 2014, 118, 7261-7271.	1.5	23
10612	Properties of the pressure-induced superconducting state in trihydrides ScH <sub>3</sub> and LaH <sub>3</sub> . Superconductor Science and Technology, 2014, 27, 115012.	1.8	25
10613	Surface magnetism of Mg doped AlN: a first principle study. Journal of Physics Condensed Matter, 2014, 26, 435801.	0.7	6
10614	Theoretical calculations on the adhesion, stability, electronic structure and bonding of SiC/W interface. Applied Surface Science, 2014, 314, 896-905.	3.1	25
10615	Facet development during platinum nanocube growth. Science, 2014, 345, 916-919.	6.0	429
10616	Remarks on the exact energy functional for fermions: an analysis using the L�wdin partitioning technique. Molecular Physics, 2014, 112, 809-817.	0.8	1
10617	Gapless $\text{MoS}_2$ possessing both massless Dirac and heavy fermions. Physical Review B, 2014, 89, .	1.0	109
10618	Nanostructures of C <sub>60</sub> ‐Metal‐Graphene (Metal = Ti, Cr, Mn, Fe, or Ni): A Spin-Polarized Density Functional Theory Study. Journal of Physical Chemistry C, 2014, 118, 21057-21065.	1.5	14
10619	Adsorption of phenol on Fe (110) and Pd (111) from first principles. Surface Science, 2014, 630, 244-253.	0.8	52
10620	Benchmarking of Density Functionals for the Accurate Description of Thiol‐Disulfide Exchange. Journal of Chemical Theory and Computation, 2014, 10, 4842-4856.	2.3	33
10621	Titanium Dioxide (Anatase and Rutile): Surface Chemistry, Liquid‐Solid Interface Chemistry, and Scientific Synthesis of Supported Catalysts. Chemical Reviews, 2014, 114, 9754-9823.	23.0	295
10622	Single-Hydrogen Dissociation Paths for Upright and Flat Acetophenone Adsorbates on the Si(001) Surface. Journal of Physical Chemistry C, 2014, 118, 23682-23689.	1.5	4
10623	Understanding the role of silicon oxide shell in oxide-assisted SiNWs growth. Materials Chemistry and Physics, 2014, 148, 1145-1148.	2.0	2
10624	Combined Experimental and Computational Approaches To Elucidate the Structures of Silver Clusters inside the ZSM-5 Cavity. Journal of Physical Chemistry C, 2014, 118, 23874-23887.	1.5	23
10625	Insights into the effect of coverage on CO adsorption and dissociation over Rh(1 0 0) surface: A theoretical study. Applied Surface Science, 2014, 320, 681-688.	3.1	11



#	ARTICLE	IF	CITATIONS
10626	Structures, Thermodynamics, and Li <sup>+</sup> Mobility of Li <sub>10</sub> GeP <sub>2</sub> S <sub>12</sub> : A First-Principles Analysis. Journal of Physical Chemistry C, 2014, 118, 10590-10595.	1.5	51
10627	Theoretical Study of a "Surface Explosion" Decomposition of Acetic Acid on Rh Surfaces. ACS Catalysis, 2014, 4, 944-953.	5.5	7
10628	Density functional plus dynamical mean-field theory of the metal-insulator transition in early transition-metal oxides. Physical Review B, 2014, 90, .	1.1	37
10629	A simple and efficient strategy for the synthesis of a chemically tailored g-C <sub>3</sub> N <sub>4</sub> material. Journal of Materials Chemistry A, 2014, 2, 17521-17529.	5.2	128
10630	Testing epitaxial Co <sub>1.5</sub> Fe <sub>1.5</sub> Ge(001) electrodes in MgO-based magnetic tunnel junctions. Applied Physics Letters, 2014, 104, 252412.	1.5	11
10631	Low-temperature carbon monoxide oxidation catalysed by regenerable atomically dispersed palladium on alumina. Nature Communications, 2014, 5, 4885.	5.8	498
10632	Fe doped TiO <sub>2</sub> " graphene nanostructures: synthesis, DFT modeling and photocatalysis. Nanotechnology, 2014, 25, 305601.	1.3	21
10633	Electronic Structure and Lattice Dynamics of BaCeO <sub>3</sub> Compound in Cubic Phase. Journal of Electronic Materials, 2014, 43, 4301-4307.	1.0	7
10634	Hydrogenation mechanism of carbon dioxide and carbon monoxide on Ru(0001) surface: a density functional theory study. RSC Advances, 2014, 4, 30241.	1.7	69
10635	Synthesis, characterization, microbiological evaluation, genotoxicity and synergism tests of new nano silver complexes with sulfamoxole. Journal of Inorganic Biochemistry, 2014, 141, 58-69.	1.5	31
10636	<i>Ab initio</i> study of TI on Si(111)-(3Å-1) surface. Physica Status Solidi (B): Basic Research, 2014, 251, 1570-1573.	0.7	4
10637	Adsorption and hydrogenation mechanism of crotonaldehyde on a Pd(111) surface by periodic DFT calculations. RSC Advances, 2014, 4, 27003-27012.	1.7	17
10638	Cl Species Transformation on CeO <sub>2</sub> (111) Surface and Its Effects on CVOCs Catalytic Abatement: A First-Principles Investigation. Journal of Physical Chemistry C, 2014, 118, 6758-6766.	1.5	35
10639	Comparative density functional theory based study of the reactivity of Cu, Ag, and Au nanoparticles and of (111) surfaces toward CO oxidation and NO <sub>2</sub> reduction. Journal of Molecular Modeling, 2014, 20, 2448.	0.8	12
10640	Diffusion in Metals and Alloys. , 2014, , 387-559.		27
10641	Structural and Electronic Properties of Bare and Capped Cd <sub>33</sub> Se <sub>33</sub> and Cd <sub>33</sub> Te <sub>33</sub> Quantum Dots. Journal of Physical Chemistry C, 2014, 118, 7094-7109.	1.5	32
10642	On the chemical behavior of C <sub>60</sub> hosting H <sub>2</sub> O and other isoelectronic neutral molecules. Journal of Molecular Modeling, 2014, 20, 2412.	0.8	21
10643	Understanding quantum confinement in nanowires: basics, applications and possible laws. Journal of Physics Condensed Matter, 2014, 26, 423202.	0.7	33



#	ARTICLE	IF	CITATIONS
10644	Density functional study of ethylene adsorption on small gold, palladium and gold-palladium binary clusters. <i>European Physical Journal D</i> , 2014, 68, 1.	0.6	7
10645	Role of Lewis and Brønsted Acid Sites in the Dehydration of Glycerol over Niobia. <i>ACS Catalysis</i> , 2014, 4, 3180-3192.	5.5	163
10646	Surface-Step-Induced Oscillatory Oxide Growth. <i>Physical Review Letters</i> , 2014, 113, 136104.	2.9	52
10647	Edge-Specific Au/Ag Functionalization-Induced Conductive Paths in Armchair MoS <sub>2</sub> Nanoribbons. <i>Chemistry of Materials</i> , 2014, 26, 5625-5631.	3.2	26
10648	Kinetic Barriers of the Phase Transition in the Oxygen Chemisorbed Cu(110)-(2 Å <sup>-1</sup> )-O as a Function of Oxygen Coverage. <i>Journal of Physical Chemistry C</i> , 2014, 118, 20858-20866.	1.5	24
10649	B-Doped Graphene as Catalyst To Improve Charge Rate of Lithium-Air Battery. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22412-22418.	1.5	81
10650	Elucidation of Aqueous Solvent-Mediated Hydrogen-Transfer Reactions by ab Initio Molecular Dynamics and Nudged Elastic-Band Studies of NaBH <sub>4</sub> Hydrolysis. <i>Journal of Physical Chemistry C</i> , 2014, 118, 21385-21399.	1.5	37
10651	Microwave and Conventional Hydro(solvo)thermal Syntheses of Three Co(II) Coordination Polymers: Supramolecular Isomerism and Structural Transformations Accompanied by Tunable Magnetic Properties. <i>Crystal Growth and Design</i> , 2014, 14, 4430-4438.	1.4	26
10652	Fractional Charge Behavior and Band Gap Predictions with the XYG3 Type of Doubly Hybrid Density Functionals. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9201-9211.	1.1	45
10653	Structure and IR Vibrational Spectra of Na <sub>8</sub> [AlSiO <sub>4</sub> ] <sub>6</sub> (BH <sub>4</sub> ) <sub>2</sub> : Comparison of Theory and Experiment. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7066-7073.	1.1	11
10654	Synthesis and Structure of Conjugated Molecules with the Benzofulvene Core. <i>Organic Letters</i> , 2014, 16, 3424-3427.	2.4	16
10655	Preparation, structural characterization, and decomposition studies of two new $\hat{3}$ -octamolybdates of 4-methylpyridine. <i>Monatshefte für Chemie</i> , 2014, 145, 921-929.	0.9	5
10656	DFT study of the mechanism of the reaction of aminoguanidine with methylglyoxal. <i>Journal of Molecular Modeling</i> , 2014, 20, 2202.	0.8	12
10657	Trends in Hydrodesulfurization Catalysis Based on Realistic Surface Models. <i>Catalysis Letters</i> , 2014, 144, 1425-1432.	1.4	32
10658	Replacing Platinum with Tungsten Carbide for Decalin Dehydrogenation. <i>Catalysis Letters</i> , 2014, 144, 1443-1449.	1.4	13
10659	Phase stabilization principle and precipitate-host lattice influences for Al-Mg-Cu alloy precipitates. <i>Journal of Materials Science</i> , 2014, 49, 6413-6426.	1.7	34
10660	First-Principles Investigation on Electronic Transport Properties of Tungsten Nitride Nanoribbon Based Molecular Device. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2014, 24, 737-744.	1.9	8
10661	DFT studies of oxygen dissociation on the 116-atom platinum truncated octahedron particle. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26539-26545.	1.3	23

#	ARTICLE	IF	CITATIONS
10662	First-principles studies of lithium storage in reduced graphite oxide. <i>Electrochimica Acta</i> , 2014, 140, 232-237.	2.6	20
10663	Temperature-dependent halogen-halogen synthon crossover in coordination compounds. <i>CrystEngComm</i> , 2014, 16, 8479-8485.	1.3	22
10664	<sup>17</sup> O NMR chemical shifts in oxometalates: from the simplest monometallic species to mixed-metal polyoxometalates. <i>Chemical Science</i> , 2014, 5, 2031.	3.7	44
10665	Using surface plasmonics to turn on fullerene's dark excitons. <i>Physical Review B</i> , 2014, 89, .	1.1	12
10666	Structural and elastic properties of TiN and AlN compounds: first-principles study. <i>Materials Science-Poland</i> , 2014, 32, 220-227.	0.4	9
10667	Electron quantum conductance of bimetallic Pt-Fe nanowires. <i>Bulletin of the Russian Academy of Sciences: Physics</i> , 2014, 78, 149-151.	0.1	1
10668	Effect of van der Waals interaction on the structural and cohesive properties of black phosphorus. <i>Journal of the Korean Physical Society</i> , 2014, 64, 547-553.	0.3	21
10669	Theoretical Prediction of Isotope Effects on Charge Transport in Organic Semiconductors. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2267-2273.	2.1	31
10670	Controllable low-bias negative differential resistance, switching, and rectifying behaviors of dipyrimidinyl-diphenyl induced by contact mode. <i>Physica B: Condensed Matter</i> , 2014, 434, 32-37.	1.3	18
10671	Graphene nucleation on a surface-molten copper catalyst: quantum chemical molecular dynamics simulations. <i>Chemical Science</i> , 2014, 5, 3493-3500.	3.7	40
10673	Atomic and molecular adsorption on Au(111). <i>Surface Science</i> , 2014, 627, 57-69.	0.8	78
10674	Theoretical Studies on Anatase and Less Common TiO <sub>2</sub> Phases: Bulk, Surfaces, and Nanomaterials. <i>Chemical Reviews</i> , 2014, 114, 9708-9753.	23.0	367
10675	Optical response of quantum-sized Ag and Au clusters - cage vs. compact structures and the remarkable insensitivity to compression. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 12495-12502.	1.3	17
10676	First principles study of the occurrence of gold in pyrite. <i>Computational Materials Science</i> , 2014, 88, 1-6.	1.4	33
10677	Edge-, width- and strain-dependent semiconductor-metal transition in SnSe nanoribbons. <i>RSC Advances</i> , 2014, 4, 6933.	1.7	23
10678	Density functional theory study of ethylene adsorption on clean anatase TiO <sub>2</sub> (001) surface. <i>Surface Science</i> , 2014, 619, 59-66.	0.8	18
10679	Structural, mechanical and electronic properties of 3d transition metal nitrides in cubic zincblende, rocksalt and cesium chloride structures: a first-principles investigation. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 025404.	0.7	86
10680	Ferromagnetism in Cr-based double perovskites: Effective model analysis and simulations. <i>Physical Review B</i> , 2014, 89, .	1.1	14

#	ARTICLE	IF	CITATIONS
10681	Effects of van der Waals density functional corrections on trends in furfural adsorption and hydrogenation on close-packed transition metal surfaces. <i>Surface Science</i> , 2014, 622, 51-59.	0.8	101
10682	The structure determination of Al <sub>20</sub> Cu <sub>2</sub> Mn <sub>3</sub> by near atomic resolution chemical mapping. <i>Journal of Alloys and Compounds</i> , 2014, 601, 25-30.	2.8	67
10683	Structural stability, electronic structure and mechanical properties of 4d transition metal nitrides TMN (TM=Ru, Rh, Pd). <i>Journal of Physics and Chemistry of Solids</i> , 2014, 75, 888-902.	1.9	11
10684	Ab initio calculations of mechanical stability of bcc Cu under pressure. <i>Solid State Communications</i> , 2014, 184, 25-28.	0.9	4
10685	Reassigning the most stable surface of hydroxyapatite to the water resistant hydroxyl terminated (010) surface. <i>Surface Science</i> , 2014, 623, 55-63.	0.8	21
10686	Structural, electronic, optical, elastic properties and Born effective charges of monoclinic HfO <sub>2</sub> from first-principles calculations. <i>Chinese Physics B</i> , 2014, 23, 047101.	0.7	41
10687	Making C-C Bonds with Gold Catalysts: A Theoretical Study of the Influence of Gold Particle Size on the Dissociation of the C-X Bond in Aryl Halides. <i>Journal of Physical Chemistry C</i> , 2014, 118, 9018-9029.	1.5	11
10688	First-principles study of intergranular embrittlement induced by Te in the Ni 5 grain boundary. <i>Computational Materials Science</i> , 2014, 88, 22-27.	1.4	40
10689	Experimental and Theoretical Scanning Tunneling Spectroscopy Analysis of an Ultrathin Titania Film and Adsorbed Au Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2014, 118, 14640-14646.	1.5	2
10690	Understanding the influence of grain boundary thickness variation on the mechanical strength of a nickel-doped tungsten grain boundary. <i>International Journal of Plasticity</i> , 2014, 53, 135-147.	4.1	14
10691	Catalytic Dissociation of Water on the (001), (011), and (111) Surfaces of Violarite, FeNi <sub>2</sub> S <sub>4</sub> : A DFT-D2 Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 1958-1967.	1.5	41
10692	Coinage-Metal Mediated Ring Opening of <i>cis</i> -1,2-Dimethoxycyclopropane: Trends from the Gold, Copper, and Silver Fischer Carbene Bond Strength. <i>Journal of the American Chemical Society</i> , 2014, 136, 9296-9307.	6.6	48
10693	First principles calculations of LiNH <sub>2</sub> BH <sub>3</sub> , LiNH <sub>3</sub> BH <sub>4</sub> , and NaNH <sub>2</sub> BH <sub>3</sub> . <i>Physica Status Solidi (B): Basic Research</i> , 2014, 251, 898-906.	0.7	5
10694	Deciphering aromaticity in porphyrinoids via adaptive natural density partitioning. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 6145-6150.	1.5	37
10695	Density functional theory study of the influence of Ti and V partitioning to cementite in ferritic steels. <i>Physica Status Solidi (B): Basic Research</i> , 2014, 251, 950-957.	0.7	9
10696	Theoretical Study of Hydrogen Permeation through Mixed Ni-MgO Films Supported on Mo(100): Role of the Oxide-Metal Interface. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5756-5761.	1.1	3
10697	Cooperative H <sub>2</sub> Activation at Ag Cluster/Al <sub>2</sub> O <sub>3</sub> (110) Dual Perimeter Sites: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 7996-8006.	1.5	31
10698	Tuning Ideal Tensile Strengths and Intrinsic Ductility of bcc Refractory Alloys. <i>Physical Review Letters</i> , 2014, 112, 115503.	2.9	139

#	ARTICLE	IF	CITATIONS
10699	Density functional theory: Foundations reviewed. <i>Physics Reports</i> , 2014, 544, 123-239.	10.3	91
10700	Coexistence of superconductivity and charge-density-wave domain in 1T-FexTa1-xSse. <i>Applied Physics Letters</i> , 2014, 104, 252601.	1.5	7
10701	A Stable, Magnetic, and Metallic Li3O4Compound as a Discharge Product in a Li-Air Battery. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2516-2521.	2.1	52
10702	Unveiling the structural and electronic properties of the neutral and anionic gallium sulfide clusters. <i>Structural Chemistry</i> , 2014, 25, 755-766.	1.0	6
10703	Computational design of intermolecularly stabilized cyclic compounds with low-valent phosphorus. <i>Structural Chemistry</i> , 2014, 25, 1133-1139.	1.0	2
10704	Influence of Se and Zn substitution on the electronic transport on a CdTe nanotube-based molecular device: a first-principles study. <i>Structural Chemistry</i> , 2014, 25, 1563-1572.	1.0	10
10705	Formation of the Face-Centered Cubic (FCC)-NdO x Phase at Nd/Nd-Fe-B Interface: A First-Principles Modeling. <i>Jom</i> , 2014, 66, 1133-1137.	0.9	10
10706	Strain-tunable electronic and transport properties of MoS2 nanotubes. <i>Nano Research</i> , 2014, 7, 518-527.	5.8	89
10707	Structural properties of Aluminum nitride compound. <i>Indian Journal of Physics</i> , 2014, 88, 1021-1029.	0.9	2
10708	Investigation on electronic transport property of cerium nitride nanoribbon-based molecular device: a first-principles study. <i>Journal of Nanostructure in Chemistry</i> , 2014, 4, 1.	5.3	2
10709	Density functional theory on the pentaatomic planar tetracoordinate carbon molecules CGa3Ge and [CGa3Ge]n. <i>Russian Journal of Physical Chemistry A</i> , 2014, 88, 823-826.	0.1	5
10710	The key role of carbon in hydrogen solubility in copper. <i>European Physical Journal B</i> , 2014, 87, 1.	0.6	2
10711	Site-selective substitutional doping with atomic precision on stepped Al (111) surface by single-atom manipulation. <i>Nanoscale Research Letters</i> , 2014, 9, 235.	3.1	2
10712	Optical properties of Eu2+/Eu3+ mixed valence, silicon nitride based materials. <i>Journal of Solid State Chemistry</i> , 2014, 213, 126-131.	1.4	9
10713	Design of I<sub>2</sub>-IV<sub>4</sub> Semiconductors through Element Substitution: The Thermodynamic Stability Limit and Chemical Trend. <i>Chemistry of Materials</i> , 2014, 26, 3411-3417.	3.2	128
10714	Properties of hydrofluorinated carbon- and boron nitride-based nanofilms: A first-principles study. <i>Physical Review B</i> , 2014, 89, .	1.1	9
10715	A charge optimized many-body (comb) potential for titanium and titania. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 315007.	0.7	21
10716	Stability of the D8m-Ti5Sn2Ga compound. Experimental determinations and first principle calculations. <i>Journal of Chemical Thermodynamics</i> , 2014, 78, 269-277.	1.0	2

#	ARTICLE	IF	CITATIONS
10717	Alkali cation specific adsorption onto fcc(111) transition metal electrodes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 13699-13707.	1.3	93
10718	Ab initio calculation of NbH phases with low H compositions. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 11798-11806.	3.8	5
10719	Development of a ReaxFF Reactive Force Field for Ammonium Nitrate and Application to Shock Compression and Thermal Decomposition. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1469-1478.	1.1	29
10720	Catalytic enhancement in dissociation of nitric oxide over rhodium and nickel small-size clusters: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 5393.	1.3	10
10721	Theoretical Foundation for the Presence of Oxacarbenium Ions in Chemical Glycoside Synthesis. <i>Journal of Organic Chemistry</i> , 2014, 79, 7889-7894.	1.7	60
10722	The role of F-dopants in adsorption of gases on anatase TiO <sub>2</sub> (001) surface: a first-principles study. <i>RSC Advances</i> , 2014, 4, 35928-35942.	1.7	6
10723	Adsorption Mechanism of Acetylene Hydrogenation. <i>Chinese Journal of Chemistry</i> , 2014, 32, 631-636.	2.6	8
10724	On the variation of dissolution rates at the orthoclase (0 0 1) surface with pH and temperature. <i>Geochimica Et Cosmochimica Acta</i> , 2014, 141, 598-611.	1.6	16
10725	Ground-state properties of rare-earth metals: an evaluation of density-functional theory. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 416001.	0.7	43
10726	Sm <sup>2+</sup> -Doped LaSi <sub>3</sub> N <sub>5</sub> : Synthesis, Computed Electronic Structure, and Band Gaps. <i>Journal of the American Ceramic Society</i> , 2014, 97, 2546-2551.	1.9	10
10727	Elastic, electronic and optical properties of baddeleyite TiO <sub>2</sub> by first-principles. <i>Materials Science in Semiconductor Processing</i> , 2014, 27, 958-965.	1.9	3
10728	Correlated Ab Initio and Density Functional Studies on H <sub>2</sub> Activation by FeO <sup>+</sup> . <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3807-3820.	2.3	95
10729	Achieving High-Quality Single-Atom Nitrogen Doping of Graphene/SiC(0001) by Ion Implantation and Subsequent Thermal Stabilization. <i>ACS Nano</i> , 2014, 8, 7318-7324.	7.3	81
10730	First-principles calculations of elastic and thermodynamic properties of the four main intermetallic phases in Al–Zn–Mg–Cu alloys. <i>Computational Materials Science</i> , 2014, 93, 210-220.	1.4	72
10731	Carbon Fluoride, CF <sub>x</sub> : Structural Diversity as Predicted by First Principles. <i>Journal of Physical Chemistry C</i> , 2014, 118, 6514-6521.	1.5	41
10732	Equation of state of lead from high-pressure neutron diffraction up to 8.9 GPa and its implication for the NaCl pressure scale. <i>Physical Review B</i> , 2014, 90, .	1.1	48
10733	Formation mechanism of methane during coal evolution: A density functional theory study. <i>Journal of Energy Chemistry</i> , 2014, 23, 669-678.	7.1	8
10734	Hierarchical Carbon–Nitrogen Architectures with Both Mesopores and Macrochannels as Excellent Cathodes for Rechargeable Li–O <sub>2</sub> Batteries. <i>Advanced Functional Materials</i> , 2014, 24, 6826-6833.	7.8	161

#	ARTICLE	IF	CITATIONS
10735	First-Principles Study on Doping Effects of Sodium in Kesterite Cu <sub>2</sub> ZnSnS <sub>4</sub> . Inorganic Chemistry, 2014, 53, 9235-9241.	1.9	30
10736	The $\frac{3}{4}X$ (X=O,N,C) Double Bond in Hypervalent Iodine Compounds: Is it Real?. Angewandte Chemie - International Edition, 2014, 53, 9617-9621.	7.2	57
10737	The covariance of the differences between experimental and theoretical chemical shifts as an aid for assigning two-dimensional heteronuclear correlation solid-state NMR spectra. Chemical Physics Letters, 2014, 608, 334-339.	1.2	20
10738	Probing the structural and electronic properties of small aluminum dideuteride clusters. Journal of Molecular Graphics and Modelling, 2014, 53, 168-178.	1.3	3
10739	Ab Initio Molecular Dynamics Calculations versus Quantum-State-Resolved Experiments on CHD <sub>3</sub> + Pt(111): New Insights into a Prototypical Gas-Surface Reaction. Journal of Physical Chemistry Letters, 2014, 5, 1294-1299.	2.1	120
10740	Ab initio Kinetic Monte Carlo simulations of dissolution at the NaCl-water interface. Physical Chemistry Chemical Physics, 2014, 16, 22545-22554.	1.3	30
10741	Strengthening N-H halogen bonding via nitrogen substitution in the aromatic framework of halogen-substituted arylpyrazinamides. CrystEngComm, 2014, 16, 4546-4553.	1.3	15
10742	Magic numbers in small iron clusters: A first-principles study. Chemical Physics Letters, 2014, 613, 59-63.	1.2	36
10743	Fullerene growth from encapsulated graphene flakes. Nanoscale, 2014, 6, 11213-11218.	2.8	7
10744	Predicting the Chiral Enrichment of Metallic SWCNTs on Ni-Cu Bimetallic Surfaces. Chemistry of Materials, 2014, 26, 4943-4950.	3.2	7
10745	Methane Activations by Lanthanum Oxide Clusters. Journal of Physical Chemistry C, 2014, 118, 7932-7945.	1.5	28
10746	Highly effective catalysis of the double-icosahedral Ru <sub>19</sub> cluster for dinitrogen dissociation - a first-principles investigation. Physical Chemistry Chemical Physics, 2014, 16, 7394.	1.3	4
10747	Role of Surface Hydroxyl Groups on Zinc Adsorption Characteristics on $\gamma$ -Al <sub>2</sub> O <sub>3</sub> (0001) Surfaces: First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 13578-13589.	1.5	33
10748	Optical and electronic properties of nanosized BiTaO <sub>4</sub> and BiNbO <sub>4</sub> photocatalysts: Experiment and theory. Physica Status Solidi (B): Basic Research, 2014, 251, 1034-1039.	0.7	11
10749	Correlation between structure, phonon spectra, thermal expansion, and thermomechanics of single-layer MoS <sub>2</sub> . Physical Review B, 2014, 90, .	1.1	138
10750	The effects of Si substitution on the glass forming ability of Ni-P system, a DFT study on crystalline related clusters. Journal of Non-Crystalline Solids, 2014, 387, 117-123.	1.5	6
10751	Interface configuration stability and interfacial energy for the $\gamma$ phase in Al-Mg-Si as examined with a first principles based hierarchical multi-scale scheme. Journal of Alloys and Compounds, 2014, 591, 329-336.	2.8	7
10752	Engineering by Mn embedment and adsorption in defective boron nitrogen sheet. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 56, 24-31.	1.3	3



#	ARTICLE	IF	CITATIONS
10753	Negatively curved cubic carbon crystals with octahedral symmetry. <i>Carbon</i> , 2014, 76, 266-274.	5.4	48
10754	Ab initio interface configuration determination for $\text{Li}_2\text{Si}$ in $\text{Al-Mg-Si}$ : Beyond the constraint of a preserved precipitate stoichiometry. <i>Computational Materials Science</i> , 2014, 81, 617-629.	1.4	24
10755	Carbon dioxide adsorption on doped boron nitride nanotubes. <i>RSC Advances</i> , 2014, 4, 28249-28258.	1.7	34
10756	A ReaxFF Investigation of Hydride Formation in Palladium Nanoclusters via Monte Carlo and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 4967-4981.	1.5	53
10757	Effects of a Carbon Surface Environment on the Decomposition Properties of Nanoparticle $\text{LiBH}_4$ : A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 8852-8858.	1.5	17
10758	A systematic first-principles study of surface energies, surface relaxation and Friedel oscillation of magnesium surfaces. <i>Journal Physics D: Applied Physics</i> , 2014, 47, 115305.	1.3	39
10759	Synthesis and Systematic Trends in Structure and Electrical Properties of $[(\text{SnSe})_{1.15}\text{m}(\text{VSe}_2)_1]$ , $m = 1, 2, 3$ , and 4. <i>Chemistry of Materials</i> , 2014, 26, 2862-2872.	3.2	33
10760	Theoretical Design of n-Type Organic Semiconducting Materials Containing Thiazole and Oxazole Frameworks. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3335-3343.	1.1	32
10761	Investigation of Acrylic Acid at High Pressure Using Neutron Diffraction. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4044-4051.	1.2	14
10762	Anisotropic thermal expansion in molecular solids: Theory and experiment on $\text{LiBH}_4$ . <i>Physical Review B</i> , 2014, 89, .	1.1	11
10763	Density functional study of hydrogen adsorption and diffusion on Ni-loaded graphene and graphene oxide. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 879-884.	1.0	8
10764	Interaction of atmospheric gases with ETS-10: A DFT study. <i>Microporous and Mesoporous Materials</i> , 2014, 190, 38-45.	2.2	10
10765	DFT-GGA errors in NO chemisorption energies on (111) transition metal surfaces. <i>Surface Science</i> , 2014, 621, 23-30.	0.8	20
10766	First-principle study of adhesion, wetting and bonding on $\text{Al}/\text{Al}_3\text{V}(001)$ interface. <i>Surface Science</i> , 2014, 624, 1-7.	0.8	19
10767	Combined experimental and theoretical studies on the X-ray crystal structure, FT-IR, $^1\text{H}$ NMR, $^{13}\text{C}$ NMR, UV-Vis spectra, NLO behavior and antimicrobial activity of 2-hydroxyacetophenone benzoylhydrazone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 124, 548-555.	2.0	33
10768	Tailoring the formation of metastable Mg through interfacial engineering: A phase stability analysis. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014, 45, 145-150.	0.7	15
10769	Generalized stacking fault energy, ideal strength and twinnability of dilute Mg-based alloys: A first-principles study of shear deformation. <i>Acta Materialia</i> , 2014, 67, 168-180.	3.8	193
10770	Theoretical confirmation of Ga-stabilized anti-ferromagnetism in plutonium metal. <i>Journal of Nuclear Materials</i> , 2014, 448, 310-314.	1.3	13



#	ARTICLE	IF	CITATIONS
10771	Ab initio study of V <sub>2</sub> CuAl as a new ternary Heusler alloy. <i>Journal of Alloys and Compounds</i> , 2014, 603, 180-182.	2.8	6
10772	On the composition of bimetallic near-surface alloys in the presence of oxygen and carbon monoxide. <i>Catalysis Communications</i> , 2014, 52, 65-71.	1.6	26
10773	The highly effective catalytic behavior of a metal nanocluster Ru <sub>79</sub> on the dissociation of a N <sub>2</sub> molecule—A quantum-chemical calculation. <i>Catalysis Communications</i> , 2014, 52, 5-9.	1.6	3
10774	Effects of oxygen doping on optical band gap and band edge positions of Ta <sub>3</sub> N <sub>5</sub> photocatalyst: A GGA+U calculation. <i>Journal of Catalysis</i> , 2014, 309, 291-299.	3.1	67
10775	Influences of alloying elements and oxygen on the stability and elastic properties of Mg <sub>17</sub> Al <sub>12</sub> . <i>Journal of Alloys and Compounds</i> , 2014, 595, 142-147.	2.8	14
10776	Electronic effects of isolated halogen atoms on the Ge(001) surface. <i>Surface Science</i> , 2014, 627, 49-56.	0.8	5
10777	Theoretical investigation of conformational stabilities and <sup>13</sup> C NMR chemical shifts of a seven-membered ring thiosugar, (3R,4R,5R,7S)-7-(hydroxymethyl)thiepane-3,4,5-triol. <i>Journal of Molecular Structure</i> , 2014, 1068, 84-93.	1.8	3
10778	Modeling H <sub>2</sub> transport through a Pd or Pd/Ag membrane, and its inhibition by co-adsorbates, from first principles. <i>Journal of Membrane Science</i> , 2014, 466, 58-69.	4.1	49
10779	The photo-catalytic activities of MP (M=Ba, Ca, Cu, Sr, Ag; P=PO <sub>4</sub> <sup>3-</sup> , HPO <sub>4</sub> <sup>2-</sup> ) microparticles. <i>Applied Surface Science</i> , 2014, 292, 570-575.	3.1	9
10780	Dispersion interactions with density functional theory: Bonding description of V≡NS bond in vanadium≡thionitrosyl complex [(nacnac)(OAr)V(NS)]. <i>Computational and Theoretical Chemistry</i> , 2014, 1028, 1-6.	1.1	2
10781	First-principles investigation of structural stability, mechanical properties and electronic structure of Ru <sub>1-x</sub> RexB <sub>2</sub> and Re <sub>1-x</sub> RuxB <sub>2</sub> borides. <i>Computational Materials Science</i> , 2014, 89, 19-23.	1.4	11
10782	First principle investigations on Boron doped Fe <sub>2</sub> VAl Heusler alloy. <i>Physica B: Condensed Matter</i> , 2014, 448, 237-243.	1.3	5
10783	Magneto-elastic effects and thermodynamic properties of ferromagnetic hcp Co. <i>Physica B: Condensed Matter</i> , 2014, 441, 72-79.	1.3	6
10784	Shared electron versus donor≡acceptor bonding description of Fe≡ER bonds in [( $\eta$ -5-C <sub>5</sub> H <sub>5</sub> )(L) <sub>2</sub> Fe(ER)] (L $\hat{=}$ ACO, PMe <sub>3</sub> ; E $\hat{=}$ ASi, Ge, Sn, Pb; R $\hat{=}$ A $\hat{=}$ Ph, Me). <i>Journal of Organometallic Chemistry</i> , 2014, 761, 134-141.	0.8	8
10785	Electronic structure and magnetic properties of transition-metal (Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag and Tl) $\eta$ -5-C <sub>5</sub> H <sub>5</sub> complexes. <i>Journal of Organometallic Chemistry</i> , 2014, 761, 142-151.	1.4	16
10786	Theoretical investigation on homoleptic Yttrium tri-guanidines. <i>Arabian Journal of Chemistry</i> , 2014, 7, 1124-1130.	2.3	1
10787	First-principles study of O <sub>2</sub> adsorption on the $\eta$ -U(001) surface. <i>Journal of Physics and Chemistry of Solids</i> , 2014, 75, 130-135.	1.9	14
10788	First-principles investigations on the electronic properties and stabilities of low-index surfaces of L <sub>12</sub> -Al <sub>3</sub> Sc intermetallic. <i>Applied Surface Science</i> , 2014, 288, 609-618.	3.1	45

#	ARTICLE	IF	CITATIONS
10789	Effect of spin-orbit coupling on the ground state structure of mercury. <i>Solid State Communications</i> , 2014, 186, 38-41.	0.9	5
10790	Effect of carbon vacancies on thermodynamic properties of Ti-ZrC mixed carbides. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014, 46, 87-91.	0.7	28
10791	Ab initio thermodynamics of zirconium hydrides and deuterides. <i>Computational Materials Science</i> , 2014, 86, 211-222.	1.4	64
10792	Compressive strain as the main origin of enhanced oxygen reduction reaction activity for Pt electrocatalysts on chromium-doped titania support. <i>Applied Catalysis B: Environmental</i> , 2014, 158-159, 112-118.	10.8	50
10793	CF <sub>3</sub> CF <sub>2</sub> NS(F)CF <sub>3</sub> : Vibrational spectra and conformational properties. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 125, 1-6.	2.0	3
10794	Cerium-doped LaSi <sub>3</sub> N <sub>5</sub> : Computed electronic structure and band gaps. <i>Journal of the European Ceramic Society</i> , 2014, 34, 2705-2712.	2.8	11
10795	Fundamental mechanism of tetragonal transitions in titanium hydride. <i>Materials Letters</i> , 2014, 115, 252-255.	1.3	19
10796	DFT investigations of the reaction mechanism of diethyl carbonate synthesis catalyzed by Cu(I)/Pd(II) zeolites. <i>Applied Surface Science</i> , 2014, 308, 237-246.	3.1	7
10797	Influence of Cr/Zr doping on the electronic structure and hydrogen storage properties of the Mg <sub>2</sub> Ni (010) surface: A first principles study. <i>Journal of Alloys and Compounds</i> , 2014, 601, 280-288.	2.8	7
10798	Crystal structures of La <sub>1-x</sub> F <sub>x</sub> BiS <sub>2</sub> (x=0.23, 0.46): Effect of F doping on distortion of Bi-S plane. <i>Journal of Solid State Chemistry</i> , 2014, 212, 213-217.	1.4	58
10799	Theoretical investigations of the structures and electronic spectra of Zn(II) and Ni(II) complexes with cyclohexylamine-N-dithiocarbamate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 122, 283-287.	2.0	10
10800	Quantum chemical characterization of zwitterionic structures: Supramolecular complexes for modifying the wettability of oil-water-limestone system. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 51, 128-136.	1.3	15
10801	Synergetic effects of Mn and Si in the interaction with point defects in bcc Fe. <i>Journal of Nuclear Materials</i> , 2014, 455, 5-9.	1.3	16
10802	Oxygen chemisorption-induced surface phase transitions on Cu(110). <i>Surface Science</i> , 2014, 627, 75-84.	0.8	40
10803	When reconstruction comes around: Ni, Cu, and Au adatoms on $\sqrt{3}\times\sqrt{3}$ -MoC(001). <i>Surface Science</i> , 2014, 624, 32-36.	0.8	5
10804	Investigation on band structure and electronic transport properties of indium nitride nanoribbon - A first-principles study. <i>Superlattices and Microstructures</i> , 2014, 65, 22-34.	1.4	24
10805	Structural and mechanical properties of H <sub>6</sub> -carbon. <i>Computational Materials Science</i> , 2014, 82, 540-543.	1.4	9
10806	Quantitative computational screening of Pd-based intermetallic membranes for hydrogen separation. <i>Journal of Membrane Science</i> , 2014, 453, 516-524.	4.1	15

#	ARTICLE	IF	CITATIONS
10807	Functional electrospun polymeric nanofibers incorporating geraniol $\alpha$ -cyclodextrin inclusion complexes: High thermal stability and enhanced durability of geraniol. <i>Food Research International</i> , 2014, 62, 424-431.	2.9	131
10808	Comparative study of metal atom adsorption on free-standing h-BN and h-BN/Ni (111) surfaces. <i>Applied Surface Science</i> , 2014, 299, 29-34.	3.1	36
10809	Quantum chemical and spectroscopic investigations of 3-methyladenine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 128, 653-664.	2.0	39
10810	Self diffusion anomaly in ferromagnetic metals: A density-functional-theory investigation of magnetically ordered and disordered Fe and Co. <i>Acta Materialia</i> , 2014, 70, 130-136.	3.8	39
10811	Effect of liquid-phase O <sub>3</sub> oxidation of activated carbon on the adsorption of thiophene. <i>Chemical Engineering Journal</i> , 2014, 242, 211-219.	6.6	56
10812	Structural and electrochemical properties of aluminium doped LiMn <sub>2</sub> O <sub>4</sub> cathode materials for Li battery: Experimental and ab initio calculations. <i>Sustainable Energy Technologies and Assessments</i> , 2014, 5, 44-49.	1.7	38
10813	Doping effect on electronic structures and band gap of inverse Heusler compound: Ti <sub>2</sub> CrSn. <i>Journal of Magnetism and Magnetic Materials</i> , 2014, 367, 33-39.	1.0	30
10814	Local structure, magnetic and electronic properties of N-doped $\hat{\Gamma}$ -Cr <sub>2</sub> O <sub>3</sub> from the first-principles. <i>Computational Materials Science</i> , 2014, 81, 353-357.	1.4	12
10815	Structural and electronic properties of wurtzite GaX (X=N, P, As, Sb, Bi) under in-plane biaxial strains. <i>Superlattices and Microstructures</i> , 2014, 67, 25-32.	1.4	8
10816	First-principles study of the hydrogen adsorption and diffusion on ordered Ni <sub>3</sub> Fe(111) surface and in the bulk. <i>Intermetallics</i> , 2014, 44, 64-72.	1.8	5
10817	First principles thermodynamic studies for recycling spent nuclear fuels using electrorefining with a molten salt electrolyte. <i>Energy</i> , 2014, 68, 751-755.	4.5	14
10818	Density Functional Theory Study of the Water Dissociation on Platinum Surfaces: General Trends. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5832-5840.	1.1	106
10819	Role of the main adsorption modes in the interaction of the dye [COOH $\alpha$ -TPP-Zn(ii)] on a periodic TiO <sub>2</sub> slab exposing a rutile (110) surface in a dye-sensitized solar cell. <i>RSC Advances</i> , 2014, 4, 9639.	1.7	12
10820	Effect of Anharmonicity on Adsorption Thermodynamics. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2479-2487.	2.3	101
10821	Experimental and Computational Studies of the Neutral and Reduced States of Indeno[1,2- <i>b</i> ]fluorene. <i>Journal of the American Chemical Society</i> , 2014, 136, 9181-9189.	6.6	41
10822	Visualized method of chemical enhancement mechanism on SERS and TERS. <i>Journal of Raman Spectroscopy</i> , 2014, 45, 533-540.	1.2	107
10823	What Factors Influence the Metal $\alpha$ -Proton Spin $\alpha$ -Spin Coupling Constants in Mercury- and Cadmium-Substituted Rubredoxin?. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4471-4479.	1.1	10
10824	Synthesis of $\hat{\Gamma}$ <sup>2</sup> -Mg <sub>2</sub> C <sub>3</sub> : A Monoclinic High-Pressure Polymorph of Magnesium Sesquicarbide. <i>Inorganic Chemistry</i> , 2014, 53, 7020-7027.	1.9	40

#	ARTICLE	IF	CITATIONS
10825	Vapor Pressure of Water Nanodroplets. <i>Journal of the American Chemical Society</i> , 2014, 136, 4508-4514.	6.6	75
10826	Perspectives on point defect thermodynamics. <i>Physica Status Solidi (B): Basic Research</i> , 2014, 251, 97-129.	0.7	58
10827	Zinc inclusion to heterogeneous nickel catalysts reduces oligomerization during the semi-hydrogenation of acetylene. <i>Journal of Catalysis</i> , 2014, 316, 164-173.	3.1	82
10828	Surface Dipoles and Electron Transfer at the Metal Oxide-Metal Interface: A 2PPE Study of Size-Selected Metal Oxide Clusters Supported on Cu(111). <i>Journal of Physical Chemistry C</i> , 2014, 118, 13697-13706.	1.5	30
10829	Structural and elastic properties of a hypothetical high density $sp^2$ -rich amorphous carbon phase. <i>Journal of Chemical Physics</i> , 2014, 140, .	1.2	5
10830	$^{13}C$ NMR Analysis of 3,6-Dihydro-2H-pyrans: Assignment of Remote Stereochemistry Using Axial Shielding Effects. <i>Journal of Organic Chemistry</i> , 2014, 79, 5521-5532.	1.7	11
10831	Adsorption of hydrogen and hydrocarbon molecules on SiC(001). <i>Surface Science Reports</i> , 2014, 69, 55-104.	3.8	13
10832	First principles study of helium trapping by solute elements in tungsten. <i>Journal of Nuclear Materials</i> , 2014, 455, 151-156.	1.3	24
10833	Fragment Hamiltonian model potential for nickel: metallic character and defects in crystalline lattices. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2014, 22, 045013.	0.8	4
10834	The embedded atom method ansatz: validation and violation. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2014, 22, 025025.	0.8	3
10835	Shape-Dependent Electronic Excitations in Metallic Chains. <i>Journal of Physical Chemistry C</i> , 2014, 118, 13059-13069.	1.5	10
10836	Dimethylamine formation from N-nitrosodimethylamine adsorbed on the Ni{111} surface from first principles. <i>Journal of Molecular Catalysis A</i> , 2014, 392, 157-163.	4.8	6
10837	Highly active and stable MgAl <sub>2</sub> O <sub>4</sub> -supported Rh and Ir catalysts for methane steam reforming: A combined experimental and theoretical study. <i>Journal of Catalysis</i> , 2014, 316, 11-23.	3.1	104
10838	CO oxidation on Ag(111): The catalytic role of H <sub>2</sub> O. <i>Surface Science</i> , 2014, 628, 104-110.	0.8	10
10839	3D modelling of $\delta$ -Fe <sub>2</sub> in Al-Mg-Si: Towards an atomistic level ab initio based examination of a full precipitate enclosed in a host lattice. <i>Computational Materials Science</i> , 2014, 91, 200-210.	1.4	16
10840	Investigation of the reactions of U, U <sup>+</sup> and U <sup>2+</sup> with ammonia: mechanisms and topological analysis. <i>RSC Advances</i> , 2014, 4, 29806.	1.7	20
10841	Interplay between Electronic Properties and Interatomic Spacing in Artificial Gold Chains on NiAl(110). <i>Journal of Physical Chemistry C</i> , 2014, 118, 29001-29006.	1.5	4
10842	Understanding the Interplay of Dopants, Interfaces, and Anionic Conductivity in Doped Ceria/Zirconia Heteroepitaxial Structures. <i>Chemistry of Materials</i> , 2014, 26, 3385-3390.	3.2	16

#	ARTICLE	IF	CITATIONS
10843	Many-body central force potentials for tungsten. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 053001.	0.8	72
10844	Compositional evolution of Q-phase precipitates in an aluminum alloy. Acta Materialia, 2014, 75, 322-336.	3.8	83
10845	Prediction and fabrication of Ti-Zr-Co ternary metallic glasses based on effective atomic radius in Ti solid solution from first-principles calculations. Journal of Non-Crystalline Solids, 2014, 400, 67-71.	1.5	9
10846	Effect of transition metal (M) and M-C slabs on equilibrium properties of Al-containing MAX carbides: An ab initio study. Computational Materials Science, 2014, 91, 28-37.	1.4	24
10847	Crystal structure, disorder and composition of the 2/1 approximant in the Al-Mg-Zn system revisited. Intermetallics, 2014, 53, 67-84.	1.8	10
10848	Theoretical investigation on the electronic and charge transport characteristics of push-pull molecules for organic photovoltaic cells. Synthetic Metals, 2014, 194, 118-125.	2.1	12
10849	An ab initio computational study of pure Zn <sub>3</sub> N <sub>2</sub> and its native point defects and dopants Cu, Ag and Au. Thin Solid Films, 2014, 564, 331-338.	0.8	29
10850	A new mixed-ligand copper(II) complex of (E)-N <sup>2</sup> -(2-hydroxybenzylidene) acetohydrazide: Synthesis, characterization, NLO behavior, DFT calculation and biological activities. Journal of Molecular Structure, 2014, 1072, 267-276.	1.8	47
10851	Isolation, characterization, spectroscopic properties and quantum chemical computations of an important phytoalexin resveratrol as antioxidant component from Vitis labrusca L. and their chemical compositions. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 133, 378-395.	2.0	24
10852	First-principles studies of oxygen chemisorption on Co(0001). Surface Science, 2014, 619, 90-97.	0.8	22
10853	Density-functional study of luminescence in polypyridine ruthenium complexes. Journal of Photochemistry and Photobiology A: Chemistry, 2014, 276, 8-15.	2.0	16
10854	Redox reaction characteristics of riboflavin: A fluorescence spectroelectrochemical analysis and density functional theory calculation. Bioelectrochemistry, 2014, 98, 103-108.	2.4	34
10855	Accurate theoretical description of the M-PNR <sub>2</sub> bonds in phosphinidene complexes of manganese and rhenium [(CO) <sub>5</sub> M-PNR <sub>2</sub> ]+ (R=Me, iPr, tBu) and [(PMe <sub>3</sub> )(CO) <sub>4</sub> M-PNiPr <sub>2</sub> ]+: A DFT-D3 study. Journal of Organometallic Chemistry, 2014, 751, 781-787.	0.8	1
10856	Elements doping to expand the light response of SrTiO <sub>3</sub> . Journal of Photochemistry and Photobiology A: Chemistry, 2014, 275, 65-71.	2.0	72
10857	Enhanced bioactivity and osteoconductivity of hydroxyapatite through chloride substitution. Journal of Biomedical Materials Research - Part A, 2014, 102, 455-469.	2.1	45
10858	The theoretical study on electronic structure and electromagnetic properties of $\pm$ -MnO <sub>2</sub> based on crystal defects. EPJ Applied Physics, 2014, 68, 30901.	0.3	3
10859	The effect of the exchange-correlation functional on H <sub>2</sub> dissociation on Ru(0001). Journal of Chemical Physics, 2014, 140, 084702.	1.2	57
10860	Interface electronic structures of reversible double-docking self-assembled monolayers on an Au(111) surface. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130018.	1.6	8

#	ARTICLE	IF	CITATIONS
10861	Theoretical Study on the Relationship between the Geometric Change and the s-p Hybridization Formation of LiAl <sub>n</sub> Clusters ( $n = 3-13$ ). Bulletin of the Chemical Society of Japan, 2014, 87, 1391-1401.	2.0	3
10862	Lambda transitions in materials science: Recent advances in CALPHAD and first-principles modelling. Physica Status Solidi (B): Basic Research, 2014, 251, 53-80.	0.7	75
10863	An Effect of the Supercell Calculation on Muon Positions and Local Deformations of Crystal Structure in La <sub>2</sub> CuO <sub>4</sub> . Journal of Physics: Conference Series, 2014, 551, 012051.	0.3	11
10864	Insights into the Mechanism of Polymer Coating Self-Healing Using Raman Spectroscopy. Applied Spectroscopy, 2014, 68, 541-548.	1.2	20
10865	Computational materials design: Realization of the switching mechanism in RRAM. , 2014, , .		0
10866	Mitigation of Surface Aggregation in Modified Phthalocyanines as Potential Photo Sensitizers. Materials Research Society Symposia Proceedings, 2015, 1784, 1.	0.1	0
10867	Synthesis of Peptidomimetics Through the Disrupted Ugi Reaction with Aziridine Aldehyde Dimers. Topics in Heterocyclic Chemistry, 2015, , 127-158.	0.2	0
10868	Spin polarization in diamagnetic tris(8-hydroxyquinoline) cobalt induced by nonmagnetic metal Al. Computational and Theoretical Chemistry, 2015, 1069, 36-39.	1.1	1
10869	A model study of hydrothermal reactions of trigonal bipyramidal Zn <sub>5</sub> cluster with two water molecules. Computational and Theoretical Chemistry, 2015, 1070, 126-131.	1.1	3
10870	Structure and bonding analysis of germanones [(Eind) <sub>2</sub> GeO], [(Tbt)(Tip)GeO] and [R <sub>2</sub> GeO] (R = Me, Et). Journal of Computational Chemistry, 2015, 36, 20-26.	1.1	4
10871	The AFLOW standard for high-throughput materials science calculations. Computational Materials Science, 2015, 108, 233-238.	1.4	244
10872	First-principles calculations on atomic and electronic properties of Si(111)/6H-SiC(0001) heterojunction. Modern Physics Letters B, 2015, 29, 1550182.	1.0	6
10873	Ferromagnetism of wide-bandgap semiconductor surfaces: Mg-doped AlN. Japanese Journal of Applied Physics, 2015, 54, 110302.	0.8	2
10874	Virtual Crystal Approximation of Pd-Ru-Zr System. Rare Metal Materials and Engineering, 2015, 44, 2976-2981.	0.8	7
10875	Elastic properties of solids at high pressure. Physics-Usppekhi, 2015, 58, 1106-1114.	0.8	8
10876	Effect of Subsurface Oxygen on Selective Catalytic Reduction of NO by H <sub>2</sub> on Pt(100): A First-Principles Study. Journal of Physical Chemistry C, 2015, 119, 24819-24826.	1.5	14
10877	Red-light emission induced by Mn-doped magnesium fluorogermanate. Journal Physics D: Applied Physics, 2015, 48, 475101.	1.3	1
10878	Simulation Evidence of Hexagonal to Tetragonal ZnSe Structure Transition: A Monolayer Material with a Wide Range Tunable Direct Bandgap. Advanced Science, 2015, 2, 1500290.	5.6	44



#	ARTICLE	IF	CITATIONS
10879	Importance of coordination number and bond length in titanium revealed by electronic structure investigations. <i>Physica Status Solidi (B): Basic Research</i> , 2015, 252, 1907-1924.	0.7	27
10880	Hybrid functional study on the ferroelectricity of domain walls with O-vacancies in $\text{PbTiO}_3$ . <i>Mechanical Engineering Journal</i> , 2015, 2, 15-00037-15-00037.	0.2	3
10881	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. <i>Scientific Reports</i> , 2015, 5, 15433.	1.6	71
10883	Electronic and magnetic structures of the ferroelectric compound $\text{PbBaFe}_2\text{O}_5$ . <i>Physical Review B</i> , 2015, 91, .	1.1	11
10884	Thermodynamic stability of transition metals on the Mg-terminated $\text{MgB}_2$ surface and their effects on hydrogen dissociation and diffusion. <i>Physical Review B</i> , 2015, 91, .	1.1	11
10885	Influence of isolated and clustered defects on electronic and dielectric properties of $\text{w}\sqrt{14}$ stite. <i>Physical Review B</i> , 2015, 91, .	1.1	7
10886	Initial growth of Ba on $\text{Ge}$ . An STM and DFT study. <i>Physical Review B</i> , 2015, 91, .	1.1	11
10887	Transition metal solute interactions with point defects in fcc iron from first principles. <i>Physical Review B</i> , 2015, 92, .	1.1	28
10888	Effect of structure on the magnetic anisotropy of $\text{L}_2\text{O}$ nanoparticles. <i>Physical Review B</i> , 2015, 92, .	1.1	11
10889	Sound velocity in shock compressed molybdenum obtained by ab initio molecular dynamics. <i>Physical Review B</i> , 2015, 92, .	1.1	9
10890	Pressure-induced transition in the multiferroic $\text{CoC}_2\text{O}_7$ . <i>Physical Review B</i> , 2015, 92, .	1.1	35
10891	X-ray absorption spectra of graphene and graphene oxide by full-potential multiple scattering calculations with self-consistent charge density. <i>Physical Review B</i> , 2015, 92, .	1.1	24
10892	Dispersion effects in $\text{SiO}_2$ . An ab initio study. <i>Physical Review B</i> , 2015, 92, .	1.1	11
10893	First-principles study of the adsorption of $\text{MgO}$ molecules on a clean $\text{Fe}(001)$ surface. <i>Physical Review B</i> , 2015, 92, .	1.1	11
10894	Magnetic moment formation in metal-organic monolayers. <i>Physical Review B</i> , 2015, 92, .	1.1	11
10895	Mechanism for nuclear and electron spin excitation by radio frequency current. <i>Physical Review B</i> , 2015, 92, .	1.1	8
10896	Electrochemical phase diagrams for Ti oxides from density functional calculations. <i>Physical Review B</i> , 2015, 92, .	1.1	35
10897	Origin of Spinel Nanocheckerboards via First Principles. <i>Physical Review Letters</i> , 2015, 114, 226102.	2.9	3



#	ARTICLE	IF	CITATIONS
10898	Strongly Constrained and Appropriately Normed Semilocal Density Functional. Physical Review Letters, 2015, 115, 036402.	2.9	2,273
10899	Charge Redistribution and Transport in Molecular Contacts. Physical Review Letters, 2015, 115, 136101.	2.9	22
10900	Structure of Self-Assembled Mn Atom Chains on Si(001). Physical Review Letters, 2015, 115, 256104.	2.9	9
10901	Electron-Injection-Assisted Generation of Oxygen Vacancies in Monoclinic $\text{HfO}_2$ . Physical Review Applied, 2015, 4, .	1.5	67
10902	Topological orbital magnetization and emergent Hall effect of an atomic-scale spin lattice at a surface. Physical Review B, 2015, 92, .	1.1	41
10903	Giant voltage modulation of magnetic anisotropy in strained heavy metal/magnet/insulator heterostructures. Physical Review B, 2015, 92, .	1.1	79
10904	Ferromagnetic instability of interlayer floating electrons in the quasi-two-dimensional electride $\text{Y}_2\text{C}$ . Physical Review B, 2015, 92, .	1.1	40
10905	NEUTRAL Na IN COMETARY TAILS AS A REMNANT OF EARLY AQUEOUS ALTERATION. Astrophysical Journal Letters, 2015, 801, L30.	3.0	9
10906	First-principles simulation on wire diameter dependence of piezoresistivity in zinc oxide nanowires. Japanese Journal of Applied Physics, 2015, 54, 06FJ11.	0.8	2
10907	Atomistic Design of Favored Compositions for Synthesizing the Al-Ni-Y Metallic Glasses. Scientific Reports, 2015, 5, 16218.	1.6	6
10908	Anisotropic electronic conduction in stacked two-dimensional titanium carbide. Scientific Reports, 2015, 5, 16329.	1.6	107
10909	Surface and bulk properties of chromium oxide: Implications for reduction by methane. AIP Conference Proceedings, 2015, , .	0.3	1
10910	Designing field-controllable graphene-dot-graphene single molecule switches: A quantum-theoretical proof-of-concept under realistic operating conditions. Journal of Chemical Physics, 2015, 143, 244704.	1.2	1
10911	Crystal structure optimisation using an auxiliary equation of state. Journal of Chemical Physics, 2015, 143, 184101.	1.2	21
10912	Proton disorder in cubic ice: Effect on the electronic and optical properties. Journal of Chemical Physics, 2015, 143, 084507.	1.2	7
10913	A density functional for core-valence correlation energy. Journal of Chemical Physics, 2015, 143, 214111.	1.2	9
10914	Pressure-induced dissociation of water molecules in ice VII. Scientific Reports, 2015, 5, 12551.	1.6	9
10915	Complete mineralization of perfluorooctanoic acid (PFOA) by $\text{H}^3$ -irradiation in aqueous solution. Scientific Reports, 2014, 4, 7418.	1.6	96

#	ARTICLE	IF	CITATIONS
10916	Influences of carbon concentration on crystal structures and ideal strengths of B <sub>2</sub> C <sub>x</sub> O compounds in the B-C-O system. <i>Scientific Reports</i> , 2015, 5, 15481.	1.6	23
10917	The strain induced band gap modulation from narrow gap semiconductor to half-metal on Ti <sub>2</sub> CrGe: A first principles study. <i>AIP Advances</i> , 2015, 5, 117225.	0.6	4
10918	Towards a new class of heavy ion doped magnetic semiconductors for room temperature applications. <i>Scientific Reports</i> , 2015, 5, 17053.	1.6	19
10919	Study of structural and electronic properties of ScN and ScAs in rocksalt and zincblende structure: A DFT approach. <i>AIP Conference Proceedings</i> , 2015, , .	0.3	0
10920	Assessment of TD-DFT and LF-DFT for study of <i>d</i> → <i>d</i> transitions in first row transition metal hexaaqua complexes. <i>Journal of Chemical Physics</i> , 2015, 142, 214111.	1.2	32
10921	Intriguing structures and magic sizes of heavy noble metal nanoclusters around size 55 governed by relativistic effect and covalent bonding. <i>Journal of Chemical Physics</i> , 2015, 143, 174302.	1.2	4
10922	Optical properties of armchair (7, 7) single walled carbon nanotubes. <i>AIP Advances</i> , 2015, 5, .	0.6	26
10923	Strain effect on electronic structure and thermoelectric properties of orthorhombic SnSe: A first principles study. <i>AIP Advances</i> , 2015, 5, .	0.6	35
10924	N <sub>2</sub> dissociation on W(110): An <i>ab initio</i> molecular dynamics study on the effect of phonons. <i>Journal of Chemical Physics</i> , 2015, 142, 104702.	1.2	22
10925	Discovery of carbon-vacancy ordering in Nb <sub>4</sub> AlC <sub>3</sub> under the guidance of first-principles calculations. <i>Scientific Reports</i> , 2015, 5, 14192.	1.6	37
10926	Adhesion at TiNi interfaces with Ta, Mo and Si. <i>MATEC Web of Conferences</i> , 2015, 33, 03006.	0.1	1
10927	Lattice Distortion in In <sub>3</sub> SbTe <sub>2</sub> Phase Change Material with Substitutional Bi. <i>Scientific Reports</i> , 2015, 5, 12867.	1.6	17
10928	Probing the structural and dynamical properties of liquid water with models including non-local electron correlation. <i>Journal of Chemical Physics</i> , 2015, 143, 054506.	1.2	89
10929	Excitation energies from frozen-density embedding with accurate embedding potentials. <i>Journal of Chemical Physics</i> , 2015, 142, 234101.	1.2	23
10930	Effects of the local structure dependence of evaporation fields on field evaporation behavior. <i>Applied Physics Letters</i> , 2015, 107, .	1.5	18
10931	On the accuracy of commonly used density functional approximations in determining the elastic constants of insulators and semiconductors. <i>Journal of Chemical Physics</i> , 2015, 143, 144104.	1.2	52
10932	Rotational states of the interstitial molecular hydrogen in silicon: A theoretical study. <i>Journal of Chemical Physics</i> , 2015, 143, 164305.	1.2	5
10933	Liquid iron-hydrogen alloys at outer core conditions by first-principles calculations. <i>Geophysical Research Letters</i> , 2015, 42, 7513-7520.	1.5	64

#	ARTICLE	IF	CITATIONS
10934	Charge-transfer potentials for ionic crystals: Cauchy violation, LO-TO splitting, and the necessity of an ionic reference state. <i>Journal of Chemical Physics</i> , 2015, 143, 224101.	1.2	2
10935	Self-assembled biomimetic nanoreactors II: Noble metal active centers. <i>Chemical Physics Letters</i> , 2015, 636, 221-227.	1.2	3
10936	First-Principles Study on Structural and Electronic Properties in Fe/MgO Double Interface. , 2015, , .		0
10937	Structures and bonding of homoleptic bis(2,3-dihydro-1,3-diborole) complexes of nickel and platinum. <i>Journal of Organometallic Chemistry</i> , 2015, 798, 146-151.	0.8	2
10938	Magnetization dynamics of mixed Coâ€“Au chains on Cu(110) substrate: Combined <i>ab initio</i> and kinetic Monte Carlo study. <i>Chinese Physics B</i> , 2015, 24, 097302.	0.7	21
10939	Electron density analysis of large (molecular and periodic) systems: A parallel implementation. <i>Journal of Computational Chemistry</i> , 2015, 36, n/a-n/a.	1.5	30
10940	Mechanistic insights into the structureâ€“dependent selectivity of catalytic furfural conversion on platinum catalysts. <i>AIChE Journal</i> , 2015, 61, 3812-3824.	1.8	53
10941	Direct Detection of <sup>17</sup> O in [Gd(DOTA)] <sup>â€“</sup> by NMR Spectroscopy. <i>Chemistry - A European Journal</i> , 2015, 21, 1955-1960.	1.7	8
10942	Realistic molecular cluster models for exfoliated kaolinite. <i>Clay Minerals</i> , 2015, 50, 307-327.	0.2	7
10943	Quantum mechanical <i>ab initio</i> calculations of the structural, electronic and optical properties of bulk gold nitrides. <i>European Physical Journal B</i> , 2015, 88, 1.	0.6	3
10945	Timeâ€“and Energyâ€“Efficient Solution Combustion Synthesis of Binary Metal Tungstate Nanoparticles with Enhanced Photocatalytic Activity. <i>ChemSusChem</i> , 2015, 8, 1652-1663.	3.6	44
10946	Combined Experimental and Computational Studies of a Na <sub>2</sub> Ni <sub>1-x</sub> Cu <sub>x</sub> Fe(CN) <sub>6</sub> Cathode with Tunable Potential for Aqueous Rechargeable Sodiumâ€“ion Batteries. <i>Chemistry - A European Journal</i> , 2015, 21, 15686-15691.	1.7	19
10947	Hydrogen Storage Materials for Mobile and Stationary Applications: Current State of the Art. <i>ChemSusChem</i> , 2015, 8, 2789-2825.	3.6	302
10948	Adsorption of nitrogenâ€“and sulfurâ€“containing compounds on NiMoS for hydrotreating reactions: A DFT and vdWâ€“corrected study. <i>AIChE Journal</i> , 2015, 61, 4036-4050.	1.8	39
10949	Lattice dynamics of Alâ€“containing MAXâ€“phase carbides: a firstâ€“principle study. <i>Journal of Raman Spectroscopy</i> , 2015, 46, 784-794.	1.2	21
10950	First-principles study of oxygen adsorption and diffusion on the UN(001) surface. <i>Physica Scripta</i> , 2015, 90, 125801.	1.2	3
10951	Carbonates in zeolites: Formation, properties, reactivity. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1709-1717.	1.0	10
10952	A Comprehensive Study of Formic Acid Oxidation on Palladium Nanocrystals with Different Types of Facets and Twin Defects. <i>ChemCatChem</i> , 2015, 7, 2077-2084.	1.8	111

#	ARTICLE	IF	CITATIONS
10953	The First Introduction of Graphene to Rechargeable Li <sup>+</sup> CO <sub>2</sub> Batteries. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 6550-6553.	7.2	305
10954	Enhanced CO Oxidation on the Oxide/Metal Interface: From Ultra-High Vacuum to Near-Atmospheric Pressures. <i>ChemCatChem</i> , 2015, 7, 2620-2627.	1.8	47
10955	Mononuclear Iron(II) Dicarbonyls Derived from NNS Ligands - Structural Models Related to a Pre-Acyl-Active Site of Mono-Iron (Hmd) Hydrogenase. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 1675-1691.	1.0	16
10956	Synergy between Palladium and Potassium Species for Efficient Activation of Carbon Monoxide in the Synthesis of Dimethyl Carbonate. <i>ChemCatChem</i> , 2015, 7, 2460-2466.	1.8	15
10957	Potassium-Induced Effect on the Structure and Chemical Activity of the Cu <sub>x</sub> O/Cu(1-x) Surface: A Combined Scanning Tunneling Microscopy and Density Functional Theory Study. <i>ChemCatChem</i> , 2015, 7, 3865-3872.	1.8	38
10958	DFT-Aided Vibrational Circular Dichroism Spectroscopy Study of (S)-Nicotine. <i>ChemPhysChem</i> , 2015, 16, 1416-1427.	1.0	8
10959	Localization of Au Nanoclusters on Layered Double Hydroxides Nanosheets: Confinement-Induced Emission Enhancement and Temperature-Responsive Luminescence. <i>Advanced Functional Materials</i> , 2015, 25, 5006-5015.	7.8	167
10960	The Cu <sub>2</sub> O <sub>2</sub> torture track for a real-life system: [Cu <sub>2</sub> (btmgp) <sub>2</sub> O <sub>2</sub> ] <sub>2</sub> oxo and peroxo species in density functional calculations. <i>Journal of Computational Chemistry</i> , 2015, 36, 1672-1685.	1.5	33
10961	Solid-state reaction as a mechanism of 1 <sup>+</sup> → 2 <sup>+</sup> transformation in M <sub>2</sub> S <sub>2</sub> monolayers. <i>Journal of Computational Chemistry</i> , 2015, 36, 2131-2134.	1.5	12
10962	Theoretical calculations on the structural, electronic, and optical properties of bulk silver nitrides. <i>Physica Status Solidi (B): Basic Research</i> , 2015, 252, 2840-2852.	0.7	10
10963	A Theoretical Study of the Binding of [Re <sub>6</sub> Se <sub>8</sub> (OH) <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub> ] Rhenium Clusters to DNA Purine Base Guanine. <i>Materials</i> , 2015, 8, 3938-3944.	1.3	21
10964	Structure Determination of Au on Pt(111) Surface: LEED, STM and DFT Study. <i>Materials</i> , 2015, 8, 2935-2952.	1.3	45
10965	T <sub>cn</sub> and T <sub>cn</sub> @C <sub>70</sub> Endohedral Metalofullerenes: ab initio Spin-density-functional Calculations. <i>Chinese Journal of Chemical Physics</i> , 2015, 28, 481-488.	0.6	0
10966	Structural and thermoelectric properties of FeSb <sub>3</sub> skutterudite thin films. <i>Physical Review B</i> , 2015, 91, .	1.1	11
10967	Hydrogen influence on diffusion in nickel from first-principles calculations. <i>Physical Review B</i> , 2015, 91, .	1.1	19
10968	Effect of solute atoms on dislocation motion in Mg: An electronic structure perspective. <i>Scientific Reports</i> , 2015, 5, 8793.	1.6	69
10969	Facet-dependent photocatalytic and antibacterial properties of Ag <sub>2</sub> WO <sub>4</sub> crystals: combining experimental data and theoretical insights. <i>Catalysis Science and Technology</i> , 2015, 5, 4091-4107.	2.1	123
10970	Synthesis and characterization of a new mid-infrared transparent compound: acentric Ba <sub>5</sub> In <sub>4</sub> Te <sub>4</sub> S <sub>7</sub> . <i>Dalton Transactions</i> , 2015, 44, 7673-7678.	1.6	14

#	ARTICLE	IF	CITATIONS
10971	On how differently the quasi-harmonic approximation works for two isostructural crystals: Thermal properties of periclase and lime. <i>Journal of Chemical Physics</i> , 2015, 142, 044114.	1.2	72
10972	Impact of branching on the supramolecular assembly of thioethers on Au(111). <i>Journal of Chemical Physics</i> , 2015, 142, 101915.	1.2	10
10973	Origin of the smaller conductances of Rh, Pb, and Co atomic junctions in hydrogen environment. <i>Journal of Applied Physics</i> , 2015, 117, 064310.	1.1	1
10974	Structure Sensitivity of NO Adsorptionâ€“Dissociation on Pd <sub>n</sub> (<math>n = 8, 13, 19, 25</math>) Clusters. <i>Journal of Physical Chemistry C</i> , 2015, 119, 12941-12948.	1.5	23
10975	M <sub>4</sub> Ag <sub>44</sub> (p-MBA) <sub>30</sub> Molecular Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2015, 119, 11238-11249.	1.5	37
10976	Direct Momentum-Resolved Observation of One-Dimensional Confinement of Externally Doped Electrons within a Single Subnanometer-Scale Wire. <i>Nano Letters</i> , 2015, 15, 281-288.	4.5	20
10977	Capacity retention behavior and morphology evolution of Si <sub>x</sub> Ge <sub>1-x</sub> nanoparticles as lithium-ion battery anode. <i>Nanotechnology</i> , 2015, 26, 255702.	1.3	13
10978	Influence of borate structure on the thermal stability of boron-containing phenolic resins: A DFT study. <i>Polymer Degradation and Stability</i> , 2015, 119, 190-197.	2.7	24
10979	Evaluation of magneto-optic properties of LaXPO(X=Mn, Fe, Ni) new superconductors by DFT. <i>Computational Materials Science</i> , 2015, 106, 5-14.	1.4	4
10980	Experimental (X-ray, <sup>13</sup> C CP/MAS NMR, IR, RS, INS, THz) and Solid-State DFT Study on (1:1) Co-Crystal of Bromanilic Acid and 2,6-Dimethylpyrazine. <i>Journal of Physical Chemistry B</i> , 2015, 119, 6852-6872.	1.2	18
10981	Calculation of Half-Metal, Debye and Curie Temperatures of Co <sub>2</sub> VAI Compound: First Principles Study*. <i>Communications in Theoretical Physics</i> , 2015, 63, 641-647.	1.1	42
10982	Density Functional Theory (DFT) study on the pyrolysis of cellulose: The pyran ring breaking mechanism. <i>Computational and Theoretical Chemistry</i> , 2015, 1067, 13-23.	1.1	52
10983	W <sup>6+</sup> & Br <sup>+</sup> codoped Li <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> anode with super rate performance for Li-ion batteries. <i>Journal of Materials Chemistry A</i> , 2015, 3, 13706-13716.	5.2	73
10984	Charge Trapping Memory Characteristics of Amorphous-Indiumâ€“Galliumâ€“Zinc Oxide Thin-Film Transistors With Defect-Engineered Alumina Dielectric. <i>IEEE Transactions on Electron Devices</i> , 2015, 62, 1184-1188.	1.6	27
10985	Enhanced electrochemical performance of LiNi <sub>0.6</sub> Co <sub>0.2</sub> Mn <sub>0.2</sub> O <sub>2</sub> cathode materials by ultrasonic-assisted co-precipitation method. <i>Journal of Alloys and Compounds</i> , 2015, 644, 607-614.	2.8	35
10986	Investigation on the Electronic Structure and Optical Properties of ZnO Nanofilms. <i>Applied Mechanics and Materials</i> , 0, 713-715, 2731-2736.	0.2	0
10987	Poly-(2,6-diaminopyridine) nanoparticles enhanced fluorescent system: An â€œoffâ€“fluorescent switch triggered by fluorescent sensing platform. <i>Synthetic Metals</i> , 2015, 205, 32-41.	2.1	12
10988	Positional isomers of cyanostilbene: two-component molecular assembly and multiple-stimuli responsive luminescence. <i>Scientific Reports</i> , 2014, 4, 4933.	1.6	92

#	ARTICLE	IF	CITATIONS
10989	Mechanism of Oxygen Atom Transfer from Fe <sup>V</sup> (O) to Olefins at Room Temperature. <i>Inorganic Chemistry</i> , 2015, 54, 6112-6121.	1.9	45
10990	<i>Ab initio</i> atomistic thermodynamics study on the oxidation mechanism of binary and ternary alloy surfaces. <i>Journal of Chemical Physics</i> , 2015, 142, 064705.	1.2	18
10991	First-principles study on the effect of alloying elements on the elastic deformation response in $\beta$ -titanium alloys. <i>Journal of Applied Physics</i> , 2015, 117, .	1.1	14
10992	A computational analysis of the apparent nido vs. hypho conflict: are we dealing with six- or eight-vertex open-face diheteroboranes?. <i>Dalton Transactions</i> , 2015, 44, 11819-11826.	1.6	7
10993	Adsorption of Normal-Alkanes on Fe(110), FeO(110), and Fe <sub>2</sub> O <sub>3</sub> (001): Influence of Iron Oxide Surfaces. <i>Journal of Physical Chemistry C</i> , 2015, 119, 12999-13010.	1.5	49
10994	Defect Engineering and Phase Junction Architecture of Wide-Bandgap ZnS for Conflicting Visible Light Activity in Photocatalytic H <sub>2</sub> Evolution. <i>ACS Applied Materials &amp; Interfaces</i> , 2015, 7, 13915-13924.	4.0	193
10995	Improvement in dehydrogenation performance of Mg(BH <sub>4</sub> ) <sub>2</sub> ·2NH <sub>3</sub> doped with transition metal: First-principles investigation. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 8721-8731.	3.8	15
10996	Synthesis, molecular structure, FT-IR, FT-Raman and XRD spectroscopic investigations of (E)-1-(5-((4-bromophenyl)diazenyl)-2-hydroxyphenyl)ethanone: A comparative DFT study. <i>Journal of Molecular Structure</i> , 2015, 1098, 84-91.	1.8	3
10997	Structural investigation of trifluoromethyl substituted bis( $\beta$ -diketonato)-dichlorotitanium(IV) complexes displaying a mono-dinuclear equilibrium hydrolysis reaction. <i>Journal of Molecular Structure</i> , 2015, 1098, 267-276.	1.8	4
10998	Surface structure effect on the magnetic anisotropy of Co/Pd (001) thin film: A first principles study. <i>Thin Solid Films</i> , 2015, 589, 252-257.	0.8	2
10999	On the interaction between gold and silver metal atoms and DNA/RNA nucleobases – a comprehensive computational study of ground state properties. <i>Nanotechnology Reviews</i> , 2015, 4, 173-191.	2.6	23
11000	A combined theoretical and experimental investigation of uranium dioxide under high static pressure. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 265401.	0.7	9
11001	Electrospun nylon 6,6 nanofibers functionalized with cyclodextrins for removal of toluene vapor. <i>Journal of Applied Polymer Science</i> , 2015, 132, .	1.3	24
11002	Solution vs. gas phase relative stability of the choline/acetylcholine cavitated complexes. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4448-4457.	1.3	9
11003	The effect of cation order on the elasticity of omphacite from atomistic calculations. <i>Physics and Chemistry of Minerals</i> , 2015, 42, 677-691.	0.3	9
11004	Interaction between PH <sub>3</sub> and small water clusters: Understanding the electronic and spectroscopic properties. <i>Computational and Theoretical Chemistry</i> , 2015, 1059, 35-44.	1.1	21
11005	Kaolinite: Defect defined material properties – A soft X-ray and first principles study of the band gap. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2015, 202, 11-15.	0.8	10
11006	Methane, formaldehyde and methanol formation pathways from carbon monoxide and hydrogen on the (0 0 1) surface of the iron carbide $\beta$ -Fe <sub>5</sub> C <sub>2</sub> . <i>Journal of Catalysis</i> , 2015, 325, 9-18.	3.1	44



#	ARTICLE	IF	CITATIONS
11007	Structural, electronic and magnetic properties of 8-hydroxyquinoline-based small molecules TMQx (TM=Cr, Mn, Fe, Co, Ni, Cu, Zn, and x=2 or 3). <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2015, 70, 77-83.	1.3	5
11008	Electronic State and Piezoresistivity Analysis of Zinc Oxide Nanowires for Force Sensing Devices. <i>Key Engineering Materials</i> , 0, 644, 16-21.	0.4	3
11009	The origins and mechanism of phase transformation in bulk $\text{Li}_2\text{MnO}_3$ : first-principles calculations and experimental studies. <i>Journal of Materials Chemistry A</i> , 2015, 3, 7066-7076.	5.2	91
11010	Evolution of boron clusters in iron tetraborides under high pressure: semiconducting and ferromagnetic superhard materials. <i>RSC Advances</i> , 2015, 5, 48012-48023.	1.7	11
11011	Structure and bonding of water molecules in zeolite hosts: Benchmarking plane-wave DFT against crystal structure data. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2015, 230, 325-336.	0.4	33
11012	Atomistic modeling of the self-diffusion in $\hat{1}^3\text{-U}$ and $\hat{1}^3\text{-U-Mo}$ . <i>Physics of Metals and Metallography</i> , 2015, 116, 445-455.	0.3	31
11013	First-principle investigation of the d <sup>0</sup> half-metallic properties in full-Heusler compounds CsAX <sub>2</sub> (A =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.3	8
11014	Elucidating the real-time Ag nanoparticle growth on $\hat{1}^{\pm}\text{-Ag}_2\text{WO}_4$ during electron beam irradiation: experimental evidence and theoretical insights. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 5352-5359.	1.3	54
11015	Structural, Electronic and Optical Properties of S-Doped Anatase $\text{TiO}_2$ . <i>Applied Mechanics and Materials</i> , 0, 727-728, 79-82.	0.2	2
11016	Ab initio-based fracture toughness estimates and transgranular traction-separation modelling of zirconium hydrides. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2015, 23, 045015.	0.8	10
11017	Subsystem-DFT potential-energy curves for weakly interacting systems. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14323-14341.	1.3	33
11018	Capture and Release of $\text{CO}_2$ in Monoethanolamine Aqueous Solutions: New Insights from First-Principles Reaction Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3189-3198.	2.3	55
11019	Insight into the mechanism and possibility of ethanol formation from syngas on Cu(100) surface. <i>Journal of Molecular Catalysis A</i> , 2015, 404-405, 115-130.	4.8	46
11020	The infrared spectra of nonplanar polycyclic aromatic hydrocarbons with five- or seven-membered rings. <i>Chemical Physics</i> , 2015, 448, 43-52.	0.9	10
11021	Theoretical Modeling of Tunneling Barriers in Carbon-Based Molecular Electronic Junctions. <i>Journal of Physical Chemistry C</i> , 2015, 119, 11286-11295.	1.5	13
11022	Optimizing the Volmer Step by Single-Layer Nickel Hydroxide Nanosheets in Hydrogen Evolution Reaction of Platinum. <i>ACS Catalysis</i> , 2015, 5, 3801-3806.	5.5	142
11023	Effects of vanadium impurity on $\text{TiO}_2$ properties. <i>International Journal of Modern Physics B</i> , 2015, 29, 1550094.	1.0	5
11024	Fischer-Tropsch Synthesis on Multicomponent Catalysts: What Can We Learn from Computer Simulations?. <i>Catalysts</i> , 2015, 5, 3-17.	1.6	20



#	ARTICLE	IF	CITATIONS
11025	A systematic study of chloride ion solvation in water using van der Waals inclusive hybrid density functional theory. <i>Molecular Physics</i> , 2015, 113, 2842-2854.	0.8	47
11026	Fundamental properties of GaN(0001) films grown directly on Gd <sub>2</sub> O <sub>3</sub> (0001) platforms: Ab initio structural simulations. , 2015, , .		0
11027	The Structure and Magnetic Moment Study of Fe <sup>2+</sup> Al by First-Principles Calculation. <i>IEEE Transactions on Magnetics</i> , 2015, 51, 1-4.	1.2	2
11028	Exploring the Role of La Codoping beyond Charge Compensation for Enhanced Hydrogen Evolution by Rh <sup>3+</sup> /SrTiO <sub>3</sub> . <i>Journal of Physical Chemistry B</i> , 2015, 119, 11089-11098.	1.2	54
11029	The influence of the composition of eight-atom Pt <sup>2+</sup> Ir clusters on the magnetic properties. <i>Molecular Physics</i> , 2015, 113, 3628-3636.	0.8	5
11030	Electronic properties of the SnSe <sup>2</sup> -metal contacts: First-principles study. <i>Chinese Physics B</i> , 2015, 24, 117308.	0.7	7
11031	Structural and electronic properties of Diisopropylammonium bromide molecular ferroelectric crystal. <i>IOP Conference Series: Materials Science and Engineering</i> , 2015, 92, 012017.	0.3	4
11032	On the relaxation dynamics in active pharmaceutical ingredients: solid-state 1H NMR, quasi-elastic neutron scattering and periodic DFT study of acebutolol hydrochloride. <i>RSC Advances</i> , 2015, 5, 57502-57514.	1.7	4
11033	First-Principle Study on the Structural Phase Transition, and Electronic Structures of Cobalt under Pressure. <i>Applied Mechanics and Materials</i> , 0, 729, 15-20.	0.2	0
11034	Covalency-Dependent Vibrational Dynamics in Two-Dimensional Titanium Carbides. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12977-12984.	1.1	34
11035	An Adsorption Study of CH <sub>4</sub> on ZSM-5, MOR, and ZSM-12 Zeolites. <i>Journal of Physical Chemistry C</i> , 2015, 119, 28970-28978.	1.5	32
11036	Probing the structural and electronic properties of doped gallium oxide and sulfide, M(GaX <sub>2</sub> ) <sub>2</sub> where M = alkali or coinage metal; X = O, S. <i>RSC Advances</i> , 2015, 5, 106141-106150.	1.7	0
11037	Effects of oxygen impurities and nitrogen vacancies on the surface properties of the Ta <sub>3</sub> N <sub>5</sub> photocatalyst: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 23265-23272.	1.3	19
11038	Vibrational Spectroscopy and Phonon-Related Properties of the <i>l</i> -Aspartic Acid Anhydrous Monoclinic Crystal. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11791-11803.	1.1	22
11039	Structural and electronic properties of alkali metal peroxides at high pressures. <i>RSC Advances</i> , 2015, 5, 104337-104342.	1.7	12
11040	Computational Chemistry Analysis of Hydrodesulfurization Reactions Catalyzed by Molybdenum Disulfide Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2015, 119, 29157-29170.	1.5	21
11041	On the Structure Sensitivity of Dimethyl Ether Electro-oxidation on Eight FCC Metals: A First-Principles Study. <i>Topics in Catalysis</i> , 2015, 58, 1159-1173.	1.3	13
11042	Piezoelectricity in two-dimensional group-III monochalcogenides. <i>Nano Research</i> , 2015, 8, 3796-3802.	5.8	219

#	ARTICLE	IF	CITATIONS
11043	Identifying and rationalizing the morphological, structural, and optical properties of $\text{Ag}_2\text{MoO}_4$ microcrystals, and the formation process of Ag nanoparticles on their surfaces: combining experimental data and first-principles calculations. <i>Science and Technology of Advanced Materials</i> , 2015, 16, 065002.	2.8	61
11044	Charge density distribution and theoretical analysis of low and high energy phosphate esters. <i>RSC Advances</i> , 2015, 5, 96623-96638.	1.7	1
11045	Calculation of electronic structure and mechanical properties of $\text{DO}_3$ $\text{Fe}_{75-x}\text{Si}_{25-x}\text{Ni}_x$ intermetallic compounds by first principles. <i>International Journal of Modern Physics B</i> , 2015, 29, 1550087.	1.0	1
11046	First-principles study of oxygen and hydrogen adsorption on Pt(111) and PtML/Pd(111) surfaces. <i>Modern Physics Letters B</i> , 2015, 29, 1550199.	1.0	2
11047	Electronic Structure and Photocatalytic Water-Splitting Properties of $\text{Ag}_2\text{ZnSn(S)}_4$ . <i>Journal of Physical Chemistry C</i> , 2015, 119, 27900-27908.	1.5	68
11048	Tolerance of Intrinsic Defects in PbS Quantum Dots. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4711-4716.	2.1	44
11049	Comparative study of the lanthanide (Ln) and actinide (An) triflate complexes $\text{M}(\text{OTf})_n$ . <i>Journal of Structural Chemistry</i> , 2015, 56, 1495-1504.	0.3	1
11050	Products of ozone oxidation of some saturated cyclic hydrocarbons. <i>Russian Journal of Organic Chemistry</i> , 2015, 51, 1710-1716.	0.3	3
11051	Structure formation in diindenoperylene thin films on copper(111). <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8776-8783.	1.3	10
11052	First-principles study on the electronic and bonding properties of $\text{PbTiO}_3$ (110) polar terminations. <i>Chemical Research in Chinese Universities</i> , 2015, 31, 825-829.	1.3	1
11053	An alternative methodology to assess the quality of empirical potentials for small gold clusters. <i>Computational and Theoretical Chemistry</i> , 2015, 1067, 24-32.	1.1	4
11054	Charge Transfer Stabilization of Late Transition Metal Oxide Nanoparticles on a Layered Niobate Support. <i>Journal of the American Chemical Society</i> , 2015, 137, 16216-16224.	6.6	60
11055	Tungsten adsorption on $\text{La}_2\text{O}_3$ (001) surfaces. <i>Materials Letters</i> , 2015, 161, 313-316.	1.3	6
11056	Singlet-Triplet Gaps of Cobalt Nitrosyls: Insights from Tropocoronand Complexes. <i>Inorganic Chemistry</i> , 2015, 54, 7362-7367.	1.9	13
11057	Defect stability in thorium monocarbide: An ab initio study. <i>Chinese Physics B</i> , 2015, 24, 097101.	0.7	4
11058	Investigating the Energetic Ordering of Stable and Metastable $\text{TiO}_2$ Polymorphs Using $\text{DFT}+\text{U}$ and Hybrid Functionals. <i>Journal of Physical Chemistry C</i> , 2015, 119, 21060-21071.	1.5	81
11059	The electronic configurations of $\text{LnX}$ ( $\text{Ln}=\text{La-Eu}$ , $\text{X}=\text{O, S, Se, Te}$ ): A FON-DFT investigation. <i>Computational and Theoretical Chemistry</i> , 2015, 1068, 81-87.	1.1	11
11060	Highly-spin-polarized interface in $\text{CoTiSb/Fe(Mn)/CoTiSb}$ superlattice. <i>Superlattices and Microstructures</i> , 2015, 86, 493-500.	1.4	1

#	ARTICLE	IF	CITATIONS
11061	Electronic and chemical structures of pyrite and arsenopyrite. <i>Mineralogical Magazine</i> , 2015, 79, 1779-1789.	0.6	20
11062	First principles study of structural, electronic and optical properties of BiFeO <sub>3</sub> in ferroelectric and paraelectric phases. <i>Materials Research Innovations</i> , 2015, 19, S5-684-S5-688.	1.0	15
11063	Pressure-Induced Insulator to Metal Transition and Superconductivity of the Inert Gases. <i>Journal of Superconductivity and Novel Magnetism</i> , 2015, 28, 3525-3533.	0.8	3
11064	Adsorption and Diffusion Behavior of Cl <sup>-</sup> on Sputtering Fe <sup>20</sup> Cr Nanocrystalline Thin Film in Acid Solution (pH=2). <i>Journal of Materials Science and Technology</i> , 2015, 31, 1198-1206.	5.6	5
11065	Influence of the ab-initio calculation parameters on prediction of energy of point defects in silicon. <i>Modern Electronic Materials</i> , 2015, 1, 103-108.	0.2	5
11066	Assessing density functionals for the prediction of thermochemistry of Ti-O-Cl species. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550055.	1.8	2
11067	A DFT study of STO adsorption on GaN (0 0 0 1) surface. <i>Chemical Physics Letters</i> , 2015, 640, 119-123.	1.2	1
11068	The Hubbard dimer: a density functional case study of a many-body problem. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 393001.	0.7	83
11069	Band structure and transport studies on impurity substituted InSe nanosheet – A first-principles investigation. <i>Superlattices and Microstructures</i> , 2015, 79, 135-147.	1.4	12
11070	Structural stability, electronic structure and mechanical properties of ZnN and CdN: A first principles study. <i>Computational Materials Science</i> , 2015, 99, 117-124.	1.4	9
11071	Ab initio investigation of the intermetallics in the Nb-Sn binary system. <i>Acta Materialia</i> , 2015, 86, 23-33.	3.8	39
11072	Phonon and electronic properties of Ti <sub>2</sub> SiC from first-principles calculations. <i>Solid State Communications</i> , 2015, 204, 37-40.	0.9	18
11073	Fe <sub>3</sub> W <sub>3</sub> C/WC/Graphitic Carbon Ternary Nanojunction Hybrids for Dye-Sensitized Solar Cells. <i>ChemSusChem</i> , 2015, 8, 726-733.	3.6	16
11074	DFT investigations on the structure and properties of MBP dimers and crystal with strong hydrogen-bonding interactions. <i>Structural Chemistry</i> , 2015, 26, 845-858.	1.0	4
11075	Interaction of H <sub>2</sub> with gold-palladium binary clusters: Molecular and dissociative adsorption. <i>Computational and Theoretical Chemistry</i> , 2015, 1055, 1-7.	1.1	9
11076	Hg oxidation reaction mechanism on Fe <sub>2</sub> O <sub>3</sub> with H <sub>2</sub> S: Comparison between theory and experiments. <i>Proceedings of the Combustion Institute</i> , 2015, 35, 2867-2874.	2.4	27
11077	Cs <sub>2</sub> Hg <sub>3</sub> S <sub>4</sub> : A Low-Dimensional Direct Bandgap Semiconductor. <i>Chemistry of Materials</i> , 2015, 27, 370-378.	3.2	26
11078	Experimental and Theoretical Approaches for the Surface Interaction between Copper and Activated Sludge Microorganisms at Molecular Scale. <i>Scientific Reports</i> , 2014, 4, 7078.	1.6	21

#	ARTICLE	IF	CITATIONS
11079	Adsorption of Bitumen Model Compounds on Kaolinite in Liquid and Supercritical Carbon Dioxide Solvents: A Study by Periodic Density Functional Theory and Molecular Theory of Solvation. <i>Energy &amp; Fuels</i> , 2015, 29, 2853-2863.	2.5	12
11080	Structures, stabilities and electronic properties of $Cu_nNa$ ( $n=1-8$ ) clusters. <i>Computational and Theoretical Chemistry</i> , 2015, 1055, 51-60.	1.1	5
11081	Doping properties of MoS <sub>2</sub> /ZnO (0001) heterojunction ruled by interfacial micro-structure: From first principles. <i>Solid State Communications</i> , 2015, 204, 67-71.	0.9	23
11082	New Insight into Structural Evolution in Layered NaCrO <sub>2</sub> during Electrochemical Sodium Extraction. <i>Journal of Physical Chemistry C</i> , 2015, 119, 166-175.	1.5	152
11083	Structural stability of ternary $D_8m\text{-}Ti_5Sb_2X$ ( $X=Al, Ga, In, Si, Ge, Sn$ ) compounds. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015, 49, 8-18.	0.7	2
11084	Ultra-small rhenium clusters supported on graphene. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7898-7906.	1.3	21
11085	Density functional theory studies on the corrosion inhibition of benzoin, benzil, benzoin-(4-phenylthiosemicarbazone) and benzil-(4-phenylthiosemicarbazone) of mild steel in hydrochloric acid. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2015, 51, 143-154.	0.3	10
11086	Phase transitions and mechanical stability of TiO <sub>2</sub> polymorphs under high pressure. <i>Journal of Alloys and Compounds</i> , 2015, 631, 192-201.	2.8	70
11087	Surface effects on the Frenkel pair defects stability in the vicinity of the Si(001) surface. <i>Materials Science in Semiconductor Processing</i> , 2015, 32, 179-187.	1.9	1
11088	Work function and cohesion properties of $W\text{-}Fe$ interfaces. <i>Materials Letters</i> , 2015, 145, 205-208.	1.3	21
11089	5V-class high-voltage batteries with over-lithiated oxide and a multi-functional additive. <i>Journal of Materials Chemistry A</i> , 2015, 3, 6157-6167.	5.2	51
11090	Electron Transfer of Squaraine-Derived Dyes Adsorbed on TiO <sub>2</sub> Clusters in Dye-Sensitized Solar Cells: A Density Functional Theory Investigation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 4431-4443.	1.5	43
11091	A Series of Noncentrosymmetric Antimony Sulfides $Ln_8Sb_2S_{15}$ ( $Ln = Tm, Er, Yb, Lu$ ). <i>Inorganic Chemistry</i> , 2015, 54, 964-968.	1.0	17
11092	Carotenoids and Light-Harvesting: From DFT/MRCI to the Tamm-Dancoff Approximation. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 655-666.	2.3	44
11093	Solvation of Actinide Salts in Water Using a Polarizable Continuum Model. <i>Journal of Physical Chemistry A</i> , 2015, 119, 689-703.	1.1	11
11094	Ultrafast and Directional Diffusion of Lithium in Phosphorene for High-Performance Lithium-Ion Battery. <i>Nano Letters</i> , 2015, 15, 1691-1697.	4.5	628
11095	A first-principles modeling of glycerol and ammonia interactions on the cation-deficient VSbO <sub>4</sub> (110) surface. <i>Catalysis Today</i> , 2015, 254, 53-61.	2.2	2
11096	A DFT study of the carboxymethyl-phosphatidylethanolamine formation from glyoxal and phosphatidylethanolamine surface. Comparison with the formation of N( $\mu$ )-(carboxymethyl)lysine from glyoxal and l-lysine. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8210-8222.	1.3	4

#	ARTICLE	IF	CITATIONS
11097	Theoretical study on the stability of double-decker type metal phthalocyanines, $M(\text{Pc})_2$ and $M(\text{Pc})_2^+$ ( $M = \text{Ti}, \text{Sn}$ and $\text{Sc}$ ): a critical assessment on the performance of density functionals. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6478-6483.	1.3	9
11098	$\text{PbGa}_2\text{MSe}_6$ ( $M = \text{Si}, \text{Ge}$ ): Two Exceptional Infrared Nonlinear Optical Crystals. <i>Chemistry of Materials</i> , 2015, 27, 914-922.	3.2	110
11099	Vacancy formation energies in metals: A comparison of MetaGGA with LDA and GGA exchange-correlation functionals. <i>Computational Materials Science</i> , 2015, 101, 96-107.	1.4	69
11100	Electrochemical performance of Zr-doped $\text{Li}_3\text{V}_2(\text{PO}_4)_3/\text{C}$ composite cathode materials for lithium ion batteries. <i>Journal of Applied Electrochemistry</i> , 2015, 45, 123-130.	1.5	28
11101	The fundamental flaw of the HSAB principle is revealed by a complete speciation analysis of the $[\text{PtCl}_6]^{n-}$ ( $n = 0-6$ ) system. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 5712-5724.	1.3	2
11102	2D covalent triazine framework: a new class of organic photocatalyst for water splitting. <i>Journal of Materials Chemistry A</i> , 2015, 3, 7750-7758.	5.2	229
11103	Lithiation Behavior of High Capacity $\text{SiCO}$ Anode Material for Lithium-ion Battery: A First Principle Study. <i>Electrochimica Acta</i> , 2015, 156, 115-120.	2.6	11
11104	Can B3LYP be improved by optimization of the proportions of exchange and correlation functionals?. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 502-509.	1.0	21
11105	Exploring the activity of a novel $\text{Au}/\text{TiC}(001)$ model catalyst towards $\text{CO}$ and $\text{CO}_2$ hydrogenation. <i>Surface Science</i> , 2015, 640, 141-149.	0.8	17
11106	Binding of $\text{SO}_3$ to fly ash components: $\text{CaO}$ , $\text{MgO}$ , $\text{Na}_2\text{O}$ and $\text{K}_2\text{O}$ . <i>Fuel</i> , 2015, 145, 79-83.	3.4	35
11107	Magnetism of hexagonal close-packed nickel calculated by full-potential linearized augmented plane wave method. <i>Journal of Magnetism and Magnetic Materials</i> , 2015, 384, 49-51.	1.0	1
11108	First principle calculations of nitric oxide on metallic $\text{Pt}(111)$ and $\text{Pt}(100)$ , and bimetallic $\text{Au}/\text{Pt}(111)$ and $\text{Au}/\text{Pt}(100)$ surfaces. <i>Applied Surface Science</i> , 2015, 328, 591-595.	3.1	9
11109	$\text{Air}^{\ominus}$ -promoted adsorptive desulfurization of diesel fuel over $\text{T}^{\ominus}\text{C}^{\ominus}$ mixed metal oxides. <i>AIChE Journal</i> , 2015, 61, 631-639.	1.8	53
11110	Separation of the attractive and repulsive contributions to the adsorbate-adsorbate interactions of polar adsorbates on $\text{Si}(100)$ . <i>Surface Science</i> , 2015, 641, 282-288.	0.8	7
11111	Atomic study on the ordered structure in Al melts induced by liquid/substrate interface with Ti solute. <i>Applied Physics Letters</i> , 2015, 106, .	1.5	16
11112	Impact of sulfur-, tantalum-, or co-doping on the electronic structure of anatase titanium dioxide: A systematic density functional theory investigation. <i>Materials Science in Semiconductor Processing</i> , 2015, 33, 94-102.	1.9	10
11113	A dislocation core in titanium dioxide and its electronic structure. <i>RSC Advances</i> , 2015, 5, 18506-18510.	1.7	23
11114	Density Functional Theory and Hydrogen Bonds: Are We There Yet?. <i>ChemPhysChem</i> , 2015, 16, 978-985.	1.0	129

#	ARTICLE	IF	CITATIONS
11115	Formation and Spectroscopy of Dicyanotriacetylene (NC <sub>8</sub> N) in Solid Kr. Journal of Physical Chemistry A, 2015, 119, 2701-2708.	1.1	7
11116	Structural Stability, Electronic Structure and Mechanical Properties of Li-N-H System. Acta Metallurgica Sinica (English Letters), 2015, 28, 550-558.	1.5	2
11117	Scandium Carbene Complexes: Synthesis of Mixed Alkyl, Amido, and Phosphido Derivatives. Organometallics, 2015, 34, 63-72.	1.1	22
11118	Mono and digallium selenide clusters as potential superhalogens. Journal of Molecular Modeling, 2015, 21, 42.	0.8	7
11119	Mechanistic Insights into CO <sub>2</sub> Activation via Reverse Water-Gas Shift on Metal Surfaces. Journal of Physical Chemistry C, 2015, 119, 4959-4966.	1.5	144
11120	Ultrathin Gold Nanowires: Soft-Templating versus Liquid Phase Synthesis, a Quantitative Study. Journal of Physical Chemistry C, 2015, 119, 4422-4430.	1.5	40
11121	Adsorption of Benzene on Cu(100) and on Cu(100) Covered with an Ultrathin NaCl Film: Molecule-Substrate Interaction and Decoupling. Journal of Physical Chemistry C, 2015, 119, 4062-4071.	1.5	20
11122	Propylene Adsorption On a Nonstoichiometric VSbO <sub>4</sub> (110) Surface. Journal of Physical Chemistry C, 2015, 119, 4967-4975.	1.5	2
11123	Possibility of Morphological Control To Improve the Activity of Oxygen Carriers for Chemical Looping Combustion. Energy & Fuels, 2015, 29, 1210-1218.	2.5	19
11124	Diarylethene Molecules on a Ag(111) Surface: Stability and Electron-Induced Switching. Journal of Physical Chemistry C, 2015, 119, 4874-4883.	1.5	30
11125	Hydrogen-Tunneling in Biologically Relevant Small Molecules: The Rotamerizations of $\alpha$ -Ketocarboxylic Acids. Journal of Physical Chemistry B, 2015, 119, 693-703.	1.2	38
11126	Trends in the Hydrogen Activation and Storage by Adsorbed 3d Transition Metal Atoms onto Graphene and Nanotube Surfaces: A DFT Study and Molecular Orbital Analysis. Journal of Physical Chemistry C, 2015, 119, 5506-5522.	1.5	59
11127	Effects of different concentration S-doping on the structural stability and electronic structures of delafossite CuAlO <sub>2</sub> . Computational Materials Science, 2015, 101, 152-155.	1.4	14
11128	NiAl(110) Surface as a Template for Growing Transition Metal Linear Atomic Chains: A DFT Investigation. Journal of Physical Chemistry C, 2015, 119, 2456-2461.	1.5	5
11129	Interface-level thermodynamic stability diagram for in situ internal oxidation of Ag(SnO <sub>2</sub> ) <sub>p</sub> composites. Journal of Materials Science, 2015, 50, 1646-1654.	1.7	14
11130	Single-point kinetic energy density functionals: A pointwise kinetic energy density analysis and numerical convergence investigation. Physical Review B, 2015, 91, .	1.1	46
11131	Cu-Decorated Ru Catalysts Supported on Layered Double Hydroxides for Selective Benzene Hydrogenation to Cyclohexene. ChemCatChem, 2015, 7, 846-855.	1.8	26
11132	Isocyanate (NCO) evidence in the CO+NO reaction over palladium. Applied Catalysis A: General, 2015, 494, 48-56.	2.2	12



#	ARTICLE	IF	CITATIONS
11133	First-principle and molecular dynamics calculations for physical properties of Ni–Sn alloy system. <i>Computational Materials Science</i> , 2015, 99, 274-284.	1.4	21
11134	Theoretical limits on the stability of single-phase kesterite-Cu <sub>2</sub> ZnSnS <sub>4</sub> . <i>Journal of Applied Physics</i> , 2015, 117, .	1.1	22
11135	First principles investigations of vinazene molecule and molecular crystal: a prospective candidate for organic photovoltaic applications. <i>Journal of Molecular Modeling</i> , 2015, 21, 27.	0.8	12
11136	DFT-driven multi-site microkinetic modeling of ethanol conversion to ethylene and diethyl ether on $\beta$ -Al <sub>2</sub> O <sub>3</sub> (1 1 1). <i>Journal of Catalysis</i> , 2015, 323, 121-131.	3.1	54
11137	Investigation on the electronic transport properties of MgS nanotube based molecular devices – a first-principles study. <i>Molecular Physics</i> , 2015, 113, 535-543.	0.8	2
11138	Quantum Size Effects in the Size–Temperature Phase Diagram of Gallium: Structural Characterization of Shape-Shifting Clusters. <i>Chemistry - A European Journal</i> , 2015, 21, 2862-2869.	1.7	16
11139	Amido Analogues of Nonbent Lanthanide (II) and Calcium Metallocenes. Heterolytic Cleavage of C–Bond Ln–Carbazoyl Ligand Promoted by Lewis Base Coordination. <i>Organometallics</i> , 2015, 34, 555-562.	1.1	16
11140	Photoelectron Spectroscopy and Density Functional Calculations of VGe <sub>n</sub> <sup>+</sup> ( <i>n</i> = 3–12) Clusters. <i>Journal of Physical Chemistry C</i> , 2015, 119, 11048-11055.	1.5	63
11141	Investigations on Radiation Tolerance of M <sub>n+1</sub> AX <sub>n</sub> Phases: Study of Ti <sub>3</sub> SiC <sub>2</sub> , Ti <sub>3</sub> AlC <sub>2</sub> , Cr <sub>2</sub> AlC, Cr <sub>2</sub> GeC, Ti <sub>2</sub> AlC, and Ti <sub>2</sub> AlN. <i>Journal of the American Ceramic Society</i> , 2015, 98, 1323-1331.	1.9	83
11142	Stereospecificity in vanadium Schiff base complexes: Formation, crystallization and epimerization processes. <i>Journal of Inorganic Biochemistry</i> , 2015, 147, 65-70.	1.5	9
11143	Theoretical investigation for adsorption of CO <sub>2</sub> and CO on MIL-101 compounds with unsaturated metal sites. <i>Computational and Theoretical Chemistry</i> , 2015, 1055, 8-14.	1.1	15
11144	Identification of a potential superhard compound ReCN. <i>Journal of Alloys and Compounds</i> , 2015, 631, 321-327.	2.8	9
11145	Effect of defects on the electronic properties of WS <sub>2</sub> armchair nanoribbon. <i>Journal of Semiconductors</i> , 2015, 36, 013003.	2.0	3
11146	Uncovering the Mechanism of Homogeneous Methyl Methacrylate Formation with P,N Chelating Ligands and Palladium: Favored Reaction Channels and Selectivities. <i>Organometallics</i> , 2015, 34, 438-449.	1.1	57
11147	First principles simulations of elastic properties of radiopaque NiTiPt. <i>Journal of Alloys and Compounds</i> , 2015, 630, 54-59.	2.8	13
11148	New insights into the nitroaromatics-detection mechanism of the luminescent metal–organic framework sensor. <i>Dalton Transactions</i> , 2015, 44, 2897-2906.	1.6	50
11149	Al <sub>20</sub> <sup>+</sup> does melt, albeit above the bulk melting temperature of aluminium. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 3741-3748.	1.3	10
11150	First-principles study of lithium insertion into Si <sub>10</sub> H <sub>16</sub> cluster. <i>Computational and Theoretical Chemistry</i> , 2015, 1056, 56-60.	1.1	9



#	ARTICLE	IF	CITATIONS
11151	6-Diphenylphosphinoacenaphth-5-yl-mercurials as Ligands for $d^{10}$ Metals. Observation of Closed-Shell Interactions of the Type $Hg(II) \cdot \cdot \cdot M$ ; $M = Hg(II), Ag(I), Au(I)$ . <i>Inorganic Chemistry</i> , 2015, 54, 1847-1859.	1.9	43
11152	Few-quintuple $Bi_2Te_3$ nanofilms as potential thermoelectric materials. <i>Scientific Reports</i> , 2015, 5, 8099.	1.6	56
11153	Surface $ReO_x$ Sites on $Al_2O_3$ and Their Molecular Structure-Reactivity Relationships for Olefin Metathesis. <i>ACS Catalysis</i> , 2015, 5, 1432-1444.	5.5	64
11154	Conversion of $CO_2$ and $C_2H_6$ to Propanoic Acid on an Iridium-Modified Graphene Oxide Surface: Quantum-Chemical Investigation. <i>Industrial &amp; Engineering Chemistry Research</i> , 2015, 54, 1539-1546.	1.8	5
11155	Strain effects on the electronic structure of $ZnSnP_2$ via modified Becke-Johnson exchange potential. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2015, 379, 427-430.	0.9	9
11156	Density functional theory calculations of atomic, electronic and thermodynamic properties of cubic $LaCoO_3$ and $La_{1-x}Sr_xCoO_3$ surfaces. <i>RSC Advances</i> , 2015, 5, 760-769.	1.7	43
11157	Square-Antiprismatic Eight-Coordinate Complexes of Divalent First-Row Transition Metal Cations: A Density Functional Theory Exploration of the Electronic-Structural Landscape. <i>Inorganic Chemistry</i> , 2015, 54, 1375-1383.	1.9	7
11158	Energy band structure of $LiNH_4SO_4$ crystals. <i>Physics of the Solid State</i> , 2015, 57, 53-58.	0.2	11
11159	Recent progress in theoretical and computational investigations of Li-ion battery materials and electrolytes. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4799-4844.	1.3	237
11160	First-principles study on band structure and transport property of GaP nanoribbon. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2015, 194, 55-61.	1.7	3
11161	Reaction pathways for pyridine adsorption on silicon ( $O_2$ ). <i>Journal of Physics Condensed Matter</i> , 2015, 27, 054001.	0.7	3
11162	The Dynamics of Molecular Interactions and Chemical Reactions at Metal Surfaces: Testing the Foundations of Theory. <i>Annual Review of Physical Chemistry</i> , 2015, 66, 399-425.	4.8	99
11163	Semilocal density functional obeying a strongly tightened bound for exchange. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 685-689.	3.3	119
11164	Pressure Modulation of Backbone Conformation and Intermolecular Distance of Conjugated Polymers Toward Understanding the Dynamism of $\pi$ - $\pi$ Stacking of their Conjugated System. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7219-7230.	1.2	22
11165	First-principles study of electronic structure of $CuSbS_2$ and $CuSbSe_2$ photovoltaic semiconductors. <i>Thin Solid Films</i> , 2015, 582, 401-407.	0.8	44
11166	Ab initio study on the adsorption of oxygen on $Co(111)$ and its subsurface incorporation. <i>European Physical Journal B</i> , 2015, 88, 1.	0.6	4
11167	$O_2$ Dissociation on $M@Pt$ Core-Shell Particles for 3d, 4d, and 5d Transition Metals. <i>Journal of Physical Chemistry C</i> , 2015, 119, 11031-11041.	1.5	37
11168	Tuning the Reactivity of $Fe^V(O)$ toward C-H Bonds at Room Temperature: Effect of Water. <i>Inorganic Chemistry</i> , 2015, 54, 1535-1542.	1.9	24

#	ARTICLE	IF	CITATIONS
11169	Structural and theoretical studies of a new CuI-CuI complex bearing bulky unsymmetrical benzamidinate Ligand. <i>Chemical Research in Chinese Universities</i> , 2015, 31, 112-116.	1.3	2
11170	Ionic bonding of lanthanides, as influenced by d- and f-atomic orbitals, by core-shells and by relativity. <i>Journal of Computational Chemistry</i> , 2015, 36, 449-458.	1.5	19
11171	Density functional theory calculations of Rh- $\eta^2$ -diketonato complexes. <i>Dalton Transactions</i> , 2015, 44, 1503-1515.	1.6	44
11172	Theoretical study on the effects of the magnesium hydride doping with cobalt and nickel on the hydrogen release. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 5319-5325.	3.8	16
11173	Design of novel tetra-hetero[8]circulenes: a theoretical study of electronic structure and charge transport characteristics. <i>RSC Advances</i> , 2015, 5, 24167-24174.	1.7	13
11174	Hydroxyapatite: Vibrational spectra and monoclinic to hexagonal phase transition. <i>Journal of Applied Physics</i> , 2015, 117, 074701.	1.1	15
11175	Intrinsic interfacial phenomena in manganite heterostructures. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 123001.	0.7	25
11176	Hydrogen diffusion behavior and vacancy interaction behavior in OsO <sub>2</sub> and RuO <sub>2</sub> by ab initio calculations. <i>Computational Materials Science</i> , 2015, 102, 14-20.	1.4	2
11177	Evidence of a graphene-like Sn-sheet on a Au(111) substrate: electronic structure and transport properties from first principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6705-6712.	1.3	33
11178	Structural, conformational and vibrational properties of 1,1,1-Trifluoro-N-(1,1,2,2,2-pentafluoroethyl) methanesulfinimidoyl chloride, CF <sub>3</sub> CF <sub>2</sub> N(S(Cl)CF <sub>3</sub> ). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 145, 139-144.	2.0	0
11179	Electronic structures and mechanical properties of Al(111)/ZrB <sub>2</sub> (0001) heterojunctions from first-principles calculation. <i>Molecular Physics</i> , 2015, 113, 1794-1801.	0.8	21
11180	Adsorption and decomposition of methylamine on a Pt(100) surface: a density functional theory study. <i>RSC Advances</i> , 2015, 5, 20208-20217.	1.7	9
11181	Influence of Cl substitution on the electronic structure and catalytic activity of ceria. <i>Science China Chemistry</i> , 2015, 58, 601-606.	4.2	8
11182	Total energy equation leading to exchange-correlation functional. <i>Science China: Physics, Mechanics and Astronomy</i> , 2015, 58, 1-6.	2.0	0
11183	Structural relaxation effects on the lowest $4f-5d$ transition of $\text{Ce}^{3+}$ in garnets. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	12
11184	The Study on the Medium-Sized Carbon Islands on Ru(0001) Surface. <i>Journal of Cluster Science</i> , 2015, 26, 347-360.	1.7	10
11185	Rutile Band-Gap States Induced by Doping with Manganese in Various Oxidation States. <i>Journal of Physical Chemistry C</i> , 2015, 119, 5534-5541.	1.5	16
11186	Dynamics and stability of icosahedral FePt nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28096-28102.	1.3	6

#	ARTICLE	IF	CITATIONS
11187	Phase transitions of NbH (1ÅxÅ2) from first principles calculation. International Journal of Hydrogen Energy, 2015, 40, 4579-4584.	3.8	1
11188	Chemical tuning of band alignments for Cu/HfO2 interfaces. Physica Status Solidi (B): Basic Research, 2015, 252, 298-304.	0.7	3
11189	Energetic stability of solute-carbon-vacancy complexes in bcc iron. Nuclear Instruments & Methods in Physics Research B, 2015, 352, 47-50.	0.6	7
11190	Microscopic structure and properties of discrete water layer in Na-exchanged montmorillonite. Journal of Colloid and Interface Science, 2015, 448, 24-31.	5.0	28
11191	Structural characterization of 2,3,5,6-tetramethyl-p-phenylenediamine radical cation and its dimer in molecular crystals. Journal of Molecular Structure, 2015, 1083, 260-267.	1.8	6
11192	Establishing the most favorable metal-carbon bond strength for carbon nanotube catalysts. Journal of Materials Chemistry C, 2015, 3, 3422-3427.	2.7	36
11193	Experimental and first-principles DFT studies of electronic, optical and magnetic properties of cerium-manganese codoped zinc oxide nanostructures. Materials Science in Semiconductor Processing, 2015, 34, 27-38.	1.9	36
11194	First-principles insights on tuning band structure and transport property of GaN nanotube. Structural Chemistry, 2015, 26, 375-382.	1.0	10
11195	Constrained density functional for noncollinear magnetism. Physical Review B, 2015, 91, .	1.1	68
11196	Carbon-Carbon Bond Formation by Activation of CH <sub>3</sub> F on Alumina. Journal of Physical Chemistry C, 2015, 119, 7156-7163.	1.5	28
11197	First-principles Study of Structural Properties of Mg <sub>x</sub> Zn <sub>1-x</sub> O ternary alloys. Journal of Physics: Conference Series, 2015, 574, 012169.	0.3	1
11198	ZnO-dotted porous ZnS cluster microspheres for high efficient, Pt-free photocatalytic hydrogen evolution. Scientific Reports, 2015, 5, 8858.	1.6	34
11200	Identification and thermodynamic mechanism of the phase transition in hafnium nitride films. Acta Materialia, 2015, 90, 59-68.	3.8	31
11201	Interaction of carbon, nitrogen and oxygen with vacancies and solutes in tungsten. RSC Advances, 2015, 5, 23261-23270.	1.7	21
11202	Novel Evolution Process of Zn-Induced Nanoclusters on Si(111)-(7Å-7) Surface. Nano-Micro Letters, 2015, 7, 194-202.	14.4	2
11203	Accurate Adsorption Thermodynamics of Small Alkanes in Zeolites. Ab initio Theory and Experiment for H-Chabazite. Journal of Physical Chemistry C, 2015, 119, 6128-6137.	1.5	120
11204	Active Sites on Ti-Ce Mixed Metal Oxides for Reactive Adsorption of Thiophene and Its Derivatives: A DFT Study. Journal of Physical Chemistry C, 2015, 119, 5903-5913.	1.5	15
11205	Synthesis and Characterization of a Cu <sub>14</sub> Hydride Cluster Supported by Neutral Donor Ligands. Chemistry - A European Journal, 2015, 21, 5341-5344.	1.7	60

#	ARTICLE	IF	CITATIONS
11206	Understanding the $\hat{\mu}$ and $\hat{\eta}$ High-Pressure Solid Phases of Oxygen. Systematic Periodic Density Functional Theory Studies Using Localized Atomic Basis. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1195-1205.	2.3	15
11207	Tailoring the optical properties of lanthanide phosphors: prediction and characterization of the luminescence of Pr <sup>3+</sup> -doped LiYF <sub>4</sub> . <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9116-9125.	1.3	18
11208	Influence of the van der Waals interaction in the dissociation dynamics of N <sub>2</sub> on W(110) from first principles. <i>Journal of Chemical Physics</i> , 2015, 142, 074704.	1.2	23
11209	Magnetic domain wall induced ferroelectricity in double perovskites. <i>Applied Physics Letters</i> , 2015, 106, 152901.	1.5	18
11210	Coexistence pressure for a martensitic transformation from theory and experiment: Revisiting the bcc-hcp transition of iron under pressure. <i>Physical Review B</i> , 2015, 91, .	1.1	30
11211	Trends of Oxygen Reduction Reaction on Platinum Alloys: A Computational and Experimental Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 15224-15231.	1.5	52
11212	Roles of Mass, Structure, and Bond Strength in the Phonon Properties and Lattice Anharmonicity of Single-Layer Mo and W Dichalcogenides. <i>Journal of Physical Chemistry C</i> , 2015, 119, 18779-18789.	1.5	67
11213	Reaction barrier heights for cycloreversion of heterocyclic rings: An Achilles' heel for DFT and standard ab initio procedures. <i>Chemical Physics</i> , 2015, 458, 1-8.	0.9	68
11214	Part and whole in wavefunction/DFT embedding. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	30
11215	Study of Poly (3,4-ethylenedioxythiophene)/MnO <sub>2</sub> as Composite Cathode Materials for Aluminum-Air Battery. <i>Electrochimica Acta</i> , 2015, 176, 1324-1331.	2.6	23
11216	Understanding Polyol Decomposition on Bimetallic Pt-Mo Catalysts: A DFT Study of Glycerol. <i>ACS Catalysis</i> , 2015, 5, 4942-4950.	5.5	25
11217	A comparative ab initio study to investigate the rich structural variety and electronic properties of GamTen (m = 1, 2 and n = 1-4) with analogous oxides, sulfides and selenides. <i>RSC Advances</i> , 2015, 5, 68076-68084.	1.7	1
11218	Site preference and alloying effect of Re atoms in the edge dislocation cores in Ni <sub>3</sub> Al. <i>Philosophical Magazine Letters</i> , 2015, 95, 253-259.	0.5	5
11219	Trends in the Reactivity of Molecular O <sub>2</sub> with Copper Clusters: Influence of Size and Shape. <i>Journal of Physical Chemistry C</i> , 2015, 119, 19832-19846.	1.5	63
11220	Promoting ethylene epoxidation on gold nanoclusters: self and CO induced O <sub>2</sub> activation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22336-22341.	1.3	13
11221	First principles study of the structural, mechanical, phonon, optical, and thermodynamic properties of half-Heusler (HH) compound NbFeSb. <i>Physica Scripta</i> , 2015, 90, 095701.	1.2	17
11222	The role of density functional theory methods in the prediction of nanostructured gas-adsorbent materials. <i>Coordination Chemistry Reviews</i> , 2015, 300, 142-163.	9.5	36
11223	Electronic structures, magnetic properties and half-metallicity in Heusler alloys Zr <sub>2</sub> IrZ (Z=Al, Ga, In). <i>Current Applied Physics</i> , 2015, 15, 1117-1123.	1.1	17

#	ARTICLE	IF	CITATIONS
11224	Model form uncertainty versus intrinsic atomic variability in amorphous silicon oxides and nitrides. <i>Computational Materials Science</i> , 2015, 109, 124-128.	1.4	1
11225	Investigation of Geminally Diaurated Arene Complexes in the Gas Phase. <i>Organometallics</i> , 2015, 34, 3979-3987.	1.1	14
11226	Grafting of lanthanide complexes on silica surfaces dehydroxylated at 200 Å°C: a theoretical investigation. <i>New Journal of Chemistry</i> , 2015, 39, 7703-7715.	1.4	15
11227	A Comparative Study of Methanol Adsorption and Dissociation over WO <sub>3</sub> (001) and ReO <sub>3</sub> (001). <i>Topics in Catalysis</i> , 2015, 58, 655-664.	1.3	6
11228	Self-Interaction Corrections Within the Fermi-Orbital-Based Formalism. <i>Advances in Atomic, Molecular and Optical Physics</i> , 2015, 64, 153-180.	2.3	42
11229	Stable structures of LnSi <sub>6</sub> <sup>+</sup> and LnSi <sub>6</sub> clusters (Ln=Pr, Eu, Gd, Tb, Yb), C <sub>2v</sub> or C <sub>5v</sub> ? Explanation of photoelectron spectra. <i>Computational and Theoretical Chemistry</i> , 2015, 1070, 1-8.	1.1	9
11230	Density functional perturbation theory calculations of vibrational and thermodynamic properties of Zn <sub>1-x</sub> Be <sub>x</sub> O alloys. <i>Materials Science in Semiconductor Processing</i> , 2015, 40, 209-217.	1.9	4
11231	Scattering of H(D) from LiF(100) under fast grazing incidence conditions: To what extent is classical dynamics a useful tool?. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2015, 354, 9-15.	0.6	9
11232	High pressure stability of the monosilicides of cobalt and the platinum group elements. <i>Journal of Alloys and Compounds</i> , 2015, 626, 375-380.	2.8	16
11233	Recovering near-band-edge ultraviolet responses in a wide-bandgap oxide with dipole-forbidden bandgap transition. <i>Journal of Alloys and Compounds</i> , 2015, 649, 625-629.	2.8	6
11234	Low thermal conductivity of Lu <sub>4</sub> Si <sub>2</sub> O <sub>7</sub> N <sub>2</sub> : Theoretical and experimental studies. <i>Journal of the European Ceramic Society</i> , 2015, 35, 3237-3247.	2.8	5
11235	Rapid thermal processing induced vacancy-oxygen complexes in Czochralski-grown Si <sub>1-x</sub> Gex. <i>Journal of Materials Science: Materials in Electronics</i> , 2015, 26, 7666-7672.	1.1	0
11236	Water adsorbate influence on the Cu(110) surface optical response. <i>Surface Science</i> , 2015, 641, 231-236.	0.8	9
11237	2,2-Diisilylazobenzenes featuring double intramolecular nitrogen-silicon coordination: a photoisomerizable fluorophore. <i>Dalton Transactions</i> , 2015, 44, 16256-16265.	1.6	12
11238	Fischer aminocarbene conformers containing a 2-thienyl or 2-furyl ring: a crystallographic, NMR, and DFT study. <i>Journal of Coordination Chemistry</i> , 2015, 68, 2388-2408.	0.8	13
11239	Raman scattering efficiency in $\text{LiTaO}_3$ and $\text{LiNbO}_3$ . <i>Physical Review B</i> , 2015, 91, ...		14
11240	Relative stability and reducibility of CeO <sub>2</sub> and Rh/CeO <sub>2</sub> species on the surface and in the cavities of $\gamma$ -Al <sub>2</sub> O <sub>3</sub> : a periodic DFT study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22389-22401.	1.3	6
11241	Examining the Critical Roles of Protons in Facilitating Oxidation of Chloride Ions by Permanganates: A Cluster Model Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6244-6251.	1.1	3

#	ARTICLE	IF	CITATIONS
11242	Fluorescence Enhancement/Quenching Based on Metal Orbital Control: Computational Studies of a 6-Thienylmazine-Based Mercury Sensor. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8106-8116.	1.1	49
11243	Nanopatterning on H-Terminated Si(111) Explained as Dynamic Equilibrium of the Chemical Reaction with Methanol. <i>Journal of Physical Chemistry C</i> , 2015, 119, 16947-16953.	1.5	10
11244	New Insight into CO Formation during HCOOH Oxidation on Pt(111): Intermolecular Dehydration of HCOOH Dimers. <i>Journal of Physical Chemistry C</i> , 2015, 119, 19287-19296.	1.5	7
11245	Sterically Congested 5-Diphenylphosphinoacenaphth-6-yl-silanes and -silanols. <i>Organometallics</i> , 2015, 34, 3873-3887.	1.1	21
11246	Chemical structure imaging of a single molecule by atomic force microscopy at room temperature. <i>Nature Communications</i> , 2015, 6, 7766.	5.8	81
11247	Alkane reforming on partially sulfided CeO <sub>2</sub> (1 1 1) surfaces. <i>Journal of Catalysis</i> , 2015, 330, 167-176.	3.1	17
11248	Mechanistic Insight into the Facet-Dependent Adsorption of Methanol on a Pt <sub>3</sub> Ni Nanocatalyst. <i>Journal of Physical Chemistry C</i> , 2015, 119, 18352-18363.	1.5	19
11249	Towards an Optimal Gradient-dependent Energy Functional of the PZ-SIC Form. <i>Procedia Computer Science</i> , 2015, 51, 1858-1864.	1.2	12
11250	Electronic and Chemical Properties of Donor, Acceptor Centers in Graphene. <i>ACS Nano</i> , 2015, 9, 9180-9187.	7.3	36
11251	A density functional theory study of adsorption and dissociation of isopropyl nitrate on an Al(111) surface. <i>Canadian Journal of Chemistry</i> , 2015, 93, 362-367.	0.6	12
11252	Effects of intrinsic defects and extrinsic doping on the electronic and photocatalytic properties of Ta <sub>3</sub> N <sub>5</sub> . <i>RSC Advances</i> , 2015, 5, 59390-59397.	1.7	33
11253	Nature of Acid Sites in Silica-Supported Zirconium Oxide: A Combined Experimental and Periodic DFT Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 15150-15159.	1.5	22
11254	Structural evolution, mechanical properties, and electronic structure of Al-Mg-Si compounds from first principles. <i>Journal of Materials Science</i> , 2015, 50, 6498-6509.	1.7	19
11255	First-principles study of B or Al-doping effect on the structural, electronic structure and magnetic properties of I <sup>3</sup> -graphyne. <i>Computational Materials Science</i> , 2015, 108, 147-152.	1.4	20
11256	Elastic properties of rhombohedral, cubic, and monoclinic phases of LaNiO <sub>3</sub> by first principles calculations. <i>Computational Materials Science</i> , 2015, 108, 153-159.	1.4	22
11257	Characterization of the Dielectric Constant in the <i>Trichoderma reesei</i> Cel7B Active Site. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1369-1376.	2.5	5
11258	Periodically Modulated Size-Dependent Elastic Properties of Armchair Graphene Nanoribbons. <i>Nano Letters</i> , 2015, 15, 4883-4888.	4.5	10
11259	Quantum Chemical Simulation of Carbon Nanotube Nucleation on Al <sub>2</sub> O <sub>3</sub> Catalysts via CH <sub>4</sub> Chemical Vapor Deposition. <i>Journal of the American Chemical Society</i> , 2015, 137, 9281-9288.	6.6	25



#	ARTICLE	IF	CITATIONS
11260	Optical conductivity enhancement and band gap opening with silicon doped graphene. Carbon, 2015, 94, 1021-1027.	5.4	84
11261	First-principles study of the bonding characteristics of TiAl(111)/Al <sub>2</sub> O <sub>3</sub> (0001) interface. Intermetallics, 2015, 60, 58-65.	1.8	42
11262	First-principles study of B doping effect on the electronic structure and magnetic properties of $\beta$ -graphyne. Thin Solid Films, 2015, 589, 662-668.	0.8	11
11263	Pb <sub>2</sub> Ba <sub>3</sub> (BO <sub>3</sub> ) <sub>3</sub> Cl: A Material with Large SHG Enhancement Activated by Pb-Chelated BO <sub>3</sub> Groups. Journal of the American Chemical Society, 2015, 137, 9417-9422.	6.6	255
11264	Hydrogen-bonding-mediated structural stability and electrochemical performance of iron fluoride cathode materials. Journal of Materials Chemistry A, 2015, 3, 16222-16228.	5.2	34
11265	Real-space formulation of orbital-free density functional theory using finite-element discretization: The case for Al, Mg, and Al-Mg intermetallics. Physical Review B, 2015, 92, .	1.1	21
11266	Theoretical and experimental analysis of the oxidation of CO on Pt catalysts supported on modified TiO <sub>2</sub> (101). Journal of Molecular Catalysis A, 2015, 407, 102-112.	4.8	14
11267	Gas-phase ammonia activation by Th, Th <sup>+</sup> , and Th <sup>2+</sup> : Reaction mechanisms, bonding analysis, and rate constant calculations. International Journal of Quantum Chemistry, 2015, 115, 6-18.	1.0	15
11268	First principles study on d <sup>0</sup> half-metallic properties of full-Heusler compounds RbCa <sub>2</sub> X <sub>2</sub> (X = C, N, and O). Chinese Physics B, 2015, 24, 067102.	0.7	11
11269	Transition metal Ti coated porous fullerene C <sub>24</sub> B <sub>24</sub> : Potential material for hydrogen storage. International Journal of Hydrogen Energy, 2015, 40, 16271-16277.	3.8	51
11270	Exploring the Adsorption and the Potential Energy Surface of Acrylonitrile on Cu(100) and Cu(100) Coated with NaCl Layers. Journal of Physical Chemistry C, 2015, 119, 15125-15136.	1.5	6
11271	The dynamics of adsorption and dissociation of N <sub>2</sub> in a monolayer of iron on W(110). Physical Chemistry Chemical Physics, 2015, 17, 19432-19445.	1.3	7
11272	A cuboctahedral platinum (Pt <sub>79</sub> ) nanocluster enclosed by well defined facets favours di-sigma adsorption and improves the reaction kinetics for methanol fuel cells. Nanoscale, 2015, 7, 13438-13451.	2.8	17
11273	Highly crystalline, small sized, monodisperse $\beta$ -NiS nanocrystal ink as an efficient counter electrode for dye-sensitized solar cells. Journal of Materials Chemistry A, 2015, 3, 15905-15912.	5.2	69
11274	The solubility of cerium in La <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub> by DFT+ $\Delta$ calculations. Journal of Alloys and Compounds, 2015, 648, 609-614.	2.8	6
11275	Influence of Cluster-Support Interactions on Reactivity of Size-Selected Nb <sub>x</sub> O <sub>y</sub> Clusters. Journal of Physical Chemistry C, 2015, 119, 14756-14768.	1.5	29
11276	A first-principles study of oxygen vacancy induced changes in structural, electronic and magnetic properties of La <sub>2/3</sub> Sr <sub>1/3</sub> MnO <sub>3</sub> . Journal of Alloys and Compounds, 2015, 649, 973-980.	2.8	13
11277	Electronic structure, magnetic and optical properties of the Ba <sub>7</sub> (BO <sub>3</sub> ) <sub>4</sub> F <sub>2+3</sub> crystal. Journal of Solid State Chemistry, 2015, 229, 358-365.	1.4	7



#	ARTICLE	IF	CITATIONS
11278	Reactivity of Perovskites with Water: Role of Hydroxylation in Wetting and Implications for Oxygen Electrocatalysis. <i>Journal of Physical Chemistry C</i> , 2015, 119, 18504-18512.	1.5	88
11279	A first-principles investigation of various gas (CO, H <sub>2</sub> , O, NO, and O <sub>2</sub> ) absorptions on a WS <sub>2</sub> monolayer: stability and electronic properties. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 305005.	0.7	80
11280	A theoretical view of 1,3-butadiene selective hydrogenation toward cis-2-butene on PdNi layered catalyst. <i>Applied Surface Science</i> , 2015, 353, 820-828.	3.1	12
11281	A density functional theory study of methanol dehydrogenation on the PtPd 3 (111) surface. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 9656-9669.	3.8	10
11282	Magnetic properties of 2D nickel nanostrips: structure dependent magnetism and Stoner criterion. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 316002.	0.7	1
11283	First principle calculations of elastic and thermodynamic properties of Ir <sub>3</sub> Nb and Ir <sub>3</sub> V with L12 structure under high pressure. <i>Intermetallics</i> , 2015, 66, 103-110.	1.8	11
11284	New interatomic potentials for studying the behavior of noble gas atoms in tungsten. <i>Journal of Nuclear Materials</i> , 2015, 467, 398-405.	1.3	16
11285	First principles calculations of structural, elastic, electronic properties of Ir <sub>3</sub> Zr with L12 structure under high pressure. <i>Materials Chemistry and Physics</i> , 2015, 162, 807-812.	2.0	12
11286	Chemical State Analysis of Phosphorus Performed by X-ray Emission Spectroscopy. <i>Analytical Chemistry</i> , 2015, 87, 5632-5639.	3.2	22
11287	Theoretical study of the fluorination effect on charge transport properties in fused thiophene derivatives. <i>RSC Advances</i> , 2015, 5, 65192-65202.	1.7	10
11288	Performance of Frozen Density Embedding for Modeling Hole Transfer Reactions. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7541-7557.	1.2	46
11289	Ab initio study of La <sub>10-x</sub> Sr <sub>x</sub> (Si,Ge) <sub>6</sub> O <sub>27-0.5x</sub> apatite for SOFC electrolyte. <i>Computational Materials Science</i> , 2015, 109, 25-33.	1.4	4
11290	Is It Possible To Obtain Coupled Cluster Quality Energies at near Density Functional Theory Cost? Domain-Based Local Pair Natural Orbital Coupled Cluster vs Modern Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4054-4063.	2.3	248
11291	Mechanistic Study of Carbon Monoxide Methanation over Pure and Rhodium- or Ruthenium-Doped Nickel Catalysts. <i>Journal of Physical Chemistry C</i> , 2015, 119, 16537-16551.	1.5	44
11292	Atomic-Scale View of VO <sub>x</sub> WO <sub>x</sub> Coreduction on the $\sqrt{3}\times\sqrt{3}$ O <sub>3</sub> (0001) Surface. <i>Journal of Physical Chemistry C</i> , 2015, 119, 16179-16187.	1.5	9
11293	The atomic structure of liquid Fe-C alloys. <i>Journal of Alloys and Compounds</i> , 2015, 648, 178-183.	2.8	18
11294	Electronic structures and magnetism in the Li <sub>2</sub> AgSb-type Heusler alloys, Zr <sub>2</sub> CoZ (Z=Al, Ga, In, Si, Ge, Sn). <i>Journal of Applied Physics</i> , 2015, 118, 043705.	1.0	54
11295	Ab initio molecular dynamics simulation of the surface composition of Co <sub>54</sub> Ta <sub>11</sub> B <sub>35</sub> metallic glasses. <i>Journal of Non-Crystalline Solids</i> , 2015, 425, 199-206.	1.5	4

#	ARTICLE	IF	CITATIONS
11296	Reaction path analysis for 1-butanol dehydration in H-ZSM-5 zeolite: Ab initio and microkinetic modeling. <i>Journal of Catalysis</i> , 2015, 330, 28-45.	3.1	65
11297	Phase stability and mechanical properties of hafnium borides: A first-principles study. <i>Computational Materials Science</i> , 2015, 109, 1-6.	1.4	26
11298	Relationship between crystal structure and thermo-mechanical properties of kaolinite clay: beyond standard density functional theory. <i>Dalton Transactions</i> , 2015, 44, 12550-12560.	1.6	40
11299	Development of a tight-binding model for Cu and its application to a Cu-heat-sink under irradiation. <i>Journal of Materials Science</i> , 2015, 50, 5684-5693.	1.7	17
11300	Heusler Compounds: Applications in Spintronics. , 2015, , 1-24.		2
11301	Density Functional Theory Study on the Carbon-Adhering Reaction on Fe <sub>3</sub> O <sub>4</sub> (111) Surface. <i>Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science</i> , 2015, 46, 2288-2295.	1.0	17
11302	Effects of stacking sequence and short-range ordering of solute atoms on elastic properties of Mg-Zn-Y alloys with long-period stacking ordered structures. <i>Acta Materialia</i> , 2015, 96, 170-188.	3.8	42
11303	Octahedral and trigonal-prismatic coordination preferences in Nb-, Mo-, Ta-, and W-based ABX <sub>2</sub> layered oxides, oxynitrides, and nitrides. <i>Journal of Solid State Chemistry</i> , 2015, 229, 272-277.	1.4	17
11304	Reaction pathways of model compounds of biomass-derived oxygenates on Fe/Ni bimetallic surfaces. <i>Surface Science</i> , 2015, 640, 159-164.	0.8	10
11305	Preferential Adsorption of TiO <sub>2</sub> Nanostructures on Functionalized Single-Walled Carbon Nanotubes: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 15085-15093.	1.5	18
11306	CO Oxidation over Strained Pt(100) Surface: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 15500-15505.	1.5	48
11307	The Role of Valence Electron Concentration in Tuning the Structure, Stability, and Electronic Properties of Mo <sub>6</sub> S <sub>9</sub> Nanowires. <i>Journal of Physical Chemistry C</i> , 2015, 119, 13979-13985.	1.5	8
11308	Origin of enhanced visible light driven water splitting by (Rh, Sb)-SrTiO <sub>3</sub> . <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 15274-15283.	1.3	40
11309	The synergistic effect between effective mass and built-in electric field for the transfer of carriers in nonlinear optical materials. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 17710-17717.	1.3	17
11310	Thermodynamics of technetium: reconciling theory and experiment using density functional perturbation analysis. <i>Dalton Transactions</i> , 2015, 44, 12735-12742.	1.6	11
11311	Ten-fold coordinated polymorph and metallization of TiO <sub>2</sub> under high pressure. <i>RSC Advances</i> , 2015, 5, 54253-54257.	1.7	16
11312	Octa-Coordination and the Aqueous Ba <sup>2+</sup> Ion. <i>Journal of Physical Chemistry B</i> , 2015, 119, 8746-8753.	1.2	34
11313	Detection of concealed targets using spintronic microwave sensor. , 2015, , .		0

#	ARTICLE	IF	CITATIONS
11314	Catalytic reduction of NO <sub>x</sub> by CO over a Ni-Ga based oxide catalyst. Journal of Materials Chemistry A, 2015, 3, 15133-15140.	5.2	6
11315	Unstrained C-C bond activation and directed fluorination through photocatalytically-generated radical cations. Chemical Science, 2015, 6, 5225-5229.	3.7	49
11316	Raman scattering investigation of large positive magnetoresistance material WTe <sub>2</sub> . Applied Physics Letters, 2015, 106, 081906.	1.5	66
11317	Phase stability and elastic properties of CuGaSe <sub>2</sub> under high pressure. Solid State Communications, 2015, 218, 1-5.	0.9	12
11318	The First Principles Study of Hydrogen Adsorption on Ni-Decorated LiB (001) Surface. Chinese Physics Letters, 2015, 32, 057302.	1.3	3
11319	The Composition of the Protosolar Disk and the Formation Conditions for Comets. Space Science Reviews, 2015, 197, 151-190.	3.7	46
11320	Phase Transitions and Mineralogy of the Lower Mantle. , 2015, , 33-60.		26
11321	Giant magnetization canting due to symmetry breaking in zigzag Co chains on Ir(001). New Journal of Physics, 2015, 17, 023014.	1.2	19
11322	First-principles study of NO oxidation on Pt/CaTiO <sub>3</sub> interface. Computational and Theoretical Chemistry, 2015, 1066, 88-93.	1.1	1
11323	Dynamics of Water Dissociative Chemisorption on Ni(111): Effects of Impact Sites and Incident Angles. Physical Review Letters, 2015, 114, 166101.	2.9	90
11324	Electron-phonon superconductivity in BaSn <sub>5</sub> . Philosophical Magazine, 2015, 95, 1728-1737.	0.7	5
11325	A Density Functional Theory Study on Mechanism of Electrochemical Oxygen Reduction on FeN <sub>4</sub> -Graphene. Journal of the Electrochemical Society, 2015, 162, F796-F801.	1.3	33
11326	Reactivity and reaction intermediates for acetic acid adsorbed on CeO <sub>2</sub> (1 1 1). Catalysis Today, 2015, 253, 65-76.	2.2	43
11327	Al Atom Activation of C-S Bonds: Characterization of the Aluminathietane Formed in the Reaction of Al Atoms with 1,2-Butylene Sulfide. Organometallics, 2015, 34, 1264-1271.	1.1	2
11328	Electric-Field-Induced Structural and Electronic Changes and Decomposition of Crystalline Lead Azide: A Computational Study. Journal of Physical Chemistry C, 2015, 119, 8431-8437.	1.5	14
11329	Density Functional Theory of MH-MOH Solid Solubility (M = Alkali) and Experiments in NaH-NaOH. Journal of Physical Chemistry C, 2015, 119, 8062-8069.	1.5	1
11330	Electrocatalytic Oxidation of Ammonia on Transition-Metal Surfaces: A First-Principles Study. Journal of Physical Chemistry C, 2015, 119, 14692-14701.	1.5	137
11331	Self-Assembled Patterns and Young's Modulus of Single-Layer Naphthalocyanine Molecules on Ag(111). Journal of Physical Chemistry C, 2015, 119, 8208-8212.	1.5	18

#	ARTICLE	IF	CITATIONS
11332	Insight into structural, elastic, phonon, and thermodynamic properties of $\hat{1}\pm$ -sulfur and energy-related sulfides: a comprehensive first-principles study. <i>Journal of Materials Chemistry A</i> , 2015, 3, 8002-8014.	5.2	33
11333	Effect of double aluminium doping on the structure, stability and electronic properties of small gold clusters. <i>Journal of Materials Science</i> , 2015, 50, 4586-4599.	1.7	7
11334	Density Functional Theory Calculations for the Quantum Capacitance Performance of Graphene-Based Electrode Material. <i>Journal of Physical Chemistry C</i> , 2015, 119, 6464-6470.	1.5	166
11335	Synthesis and characterization of ZnS with controlled amount of S vacancies for photocatalytic H <sub>2</sub> production under visible light. <i>Scientific Reports</i> , 2015, 5, 8544.	1.6	171
11336	d0 half-metallicity of DO3-type XN <sub>3</sub> (X=Na, K and Rb): A first-principle study. <i>Computational Materials Science</i> , 2015, 104, 1-9.	1.4	20
11337	DFT study and crystal structure analysis of a new nano-structure five coordinated Hg(II) complex involving C $\hat{a}$ $\hat{e}$ $\hat{r}$ H $\hat{a}$ $\hat{c}$ O, N $\hat{a}$ $\hat{c}$ O and I $\hat{e}$ $\hat{a}$ $\hat{r}$ I interactions in a supra-molecular structure. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 147, 139-150.	2.0	16
11338	Ab initio study of the electronic structure and band gaps of Eu-doped LaSi <sub>3</sub> N <sub>5</sub> phosphors: A role of oxygen atom. <i>Journal of the European Ceramic Society</i> , 2015, 35, 3249-3253.	2.8	2
11339	The process of dissociation of Cl <sub>2</sub> molecule on the Ge(001)-p(1 $\hat{A}$ –2) surface. <i>Applied Surface Science</i> , 2015, 335, 198-207.	3.1	1
11340	Electronic structure and energy level schemes of RE <sub>3+</sub> :LaSi <sub>3</sub> N <sub>5</sub> and RE <sub>2+</sub> :LaSi <sub>3</sub> N <sub>5</sub> $\hat{a}$ $\hat{r}$ xO <sub>x</sub> phosphors (RE=Ce, Pr, ND, Pm, Sm, Eu) from first principles. <i>Journal of Luminescence</i> , 2015, 164, 131-137.	1.5	21
11341	First-Principles Study about the Effect of Coverage on H <sub>2</sub> Adsorption and Dissociation over a Rh(100) Surface. <i>Journal of Physical Chemistry C</i> , 2015, 119, 10355-10364.	1.5	17
11342	Quantum Mechanical Studies of Large Metal, Metal Oxide, and Metal Chalcogenide Nanoparticles and Clusters. <i>Chemical Reviews</i> , 2015, 115, 6112-6216.	23.0	329
11343	Spin $\hat{a}$ $\hat{r}$ bit coupling in the band structure of monolayer WSe <sub>2</sub> . <i>Journal of Physics Condensed Matter</i> , 2015, 27, 182201.	0.7	67
11344	Half-metallic ferromagnetism in TM-doped MgH <sub>2</sub> hydride. <i>Applied Physics A: Materials Science and Processing</i> , 2015, 119, 1587-1593.	1.1	3
11345	Unexpected dimerization of 1,3 $\hat{a}$ $\hat{r}$ dimethyl $\hat{e}$ $\hat{5}$ $\hat{a}$ $\hat{r}$ methylenebarbituric acid revealed by a combined experimental and computational study. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 354-357.	0.9	2
11346	First-principles study of structural, electronic and magnetic properties of double perovskite oxides Ba <sub>2</sub> CoMO <sub>6</sub> (M=Mo and W). <i>Materials Science in Semiconductor Processing</i> , 2015, 34, 281-290.	1.9	4
11347	E versus Z isomers of Fischer aminocarbene complex [Mo(CO) <sub>4</sub> (PPh <sub>3</sub> ){C(NHCy)(2-furyl)}]: NH $\hat{a}$ $\hat{c}$ O versus CH $\hat{a}$ $\hat{c}$ O intramolecular hydrogen bonds. <i>Journal of Molecular Structure</i> , 2015, 1094, 36-45.	1.8	3
11348	Effects of rare-earth on the cohesion of Ni $\hat{1}\hat{5}$ (0 1 2) grain boundary from first-principles calculations. <i>Computational Materials Science</i> , 2015, 96, 374-378.	1.4	23
11349	Single PTCDA molecules on planar and stepped KCl and NaCl(100) surfaces. <i>Surface Science</i> , 2015, 641, 278-281.	0.8	12

#	Association of the $1/3\text{Å}^{-1}$	IF	CITATIONS
11350	Experimental study and thermodynamic assessment of the Zr-Al-Gd system. Thermochemica Acta, 2015, 609, 36-48.	3.8	5
11351	Experimental study and thermodynamic assessment of the Zr-Al-Gd system. Thermochemica Acta, 2015, 609, 36-48.	1.2	1
11352	Mechanical properties and electronic structures of the Hf-Si system: First-principles calculations. Solid State Communications, 2015, 205, 39-45.	0.9	14
11353	First-principles investigation of site preference and diffusion behaviors of carbon in copper. Nuclear Instruments & Methods in Physics Research B, 2015, 352, 72-76.	0.6	4
11354	Spectroscopic and Computational Study of Cr Oxide Structures and Their Anchoring Sites on ZSM-5 Zeolites. ACS Catalysis, 2015, 5, 3078-3092.	5.5	68
11355	Relationship between unbranched alkane dimer interaction energies using different theoretical methods and correlations with thermodynamic properties. Chemical Physics Letters, 2015, 625, 20-25.	1.2	5
11356	Decomposition mechanisms of Cu-based oxygen carriers for chemical looping with oxygen uncoupling based on density functional theory calculations. Combustion and Flame, 2015, 162, 1265-1274.	2.8	58
11357	Adsorption and transformation mechanism of NO <sub>2</sub> on NaCl(100) surface: A density functional theory study. Science of the Total Environment, 2015, 524-525, 195-200.	3.9	2
11358	Quantum-Chemical Characterization of the Properties and Reactivities of Metal-Organic Frameworks. Chemical Reviews, 2015, 115, 6051-6111.	23.0	241
11359	Pristine and defect-containing phosphorene as promising anode materials for rechargeable Li batteries. Journal of Materials Chemistry A, 2015, 3, 11246-11252.	5.2	136
11360	Exploring d <sub>0</sub> magnetism in doped SnO <sub>2</sub> – a first principles DFT study. Journal of Magnetism and Magnetic Materials, 2015, 385, 207-216.	1.0	20
11361	Facile production of stable silicon nanoparticles: laser chemistry coupled to in situ stabilization via room temperature hydrosilylation. Nanoscale, 2015, 7, 8566-8573.	2.8	10
11362	Interaction of cesium adatoms with free-standing graphene and graphene-veiled SiO <sub>2</sub> surfaces. RSC Advances, 2015, 5, 38623-38629.	1.7	2
11363	Complexation of Sm <sup>3+</sup> and pamidronate: A DFT study. Journal of Rare Earths, 2015, 33, 310-319.	2.5	2
11364	Structures, stabilities, and electronic properties of the neutral and anionic Si <sub>n</sub> Sm <sup>+</sup> (n=9, 10, 11) clusters: comparison with pure silicon clusters. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	17
11365	Scavenger mechanism of methylglyoxal by metformin. A DFT study. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	11
11366	New semi-empirical computational analysis of catalytic reactions for automobile. Research on Chemical Intermediates, 2015, 41, 9475-9484.	1.3	0
11367	Selection of Surface Coatings for High H <sub>2</sub> Permeability Group 5 Metal Membranes Using First-Principles Calculations. Journal of Physical Chemistry C, 2015, 119, 7848-7855.	1.5	9

#	ARTICLE	IF	CITATIONS
11368	First principles study of thermodynamic and mechanical properties of Pd <sub>50</sub> Cu <sub>50</sub> . Journal of Alloys and Compounds, 2015, 639, 635-641.	2.8	16
11369	Intrinsic defects and Na doping in Cu <sub>2</sub> ZnSnS <sub>4</sub> : A density-functional theory study. Solar Energy, 2015, 116, 125-132.	2.9	49
11370	Insight into the role of Li <sub>2</sub> S <sub>2</sub> in Li <sup>+</sup> S batteries: a first-principles study. Journal of Materials Chemistry A, 2015, 3, 8865-8869.	5.2	68
11371	Analysis and Calculation of Electronic Properties and Light Absorption of Defective Sulfur-Doped Silicon and Theoretical Photoelectric Conversion Efficiency. Journal of Physical Chemistry A, 2015, 119, 3753-3761.	1.1	11
11372	Ni cluster nucleation and growth on the anatase TiO <sub>2</sub> (101) surface: a density functional theory study. RSC Advances, 2015, 5, 16582-16591.	1.7	17
11373	D <sub>4h</sub> Ni <sub>4</sub> C(B <sub>4</sub> N <sub>4</sub> H <sub>8</sub> ) <sub>2</sub> : Square sheet sandwich complex containing the planar tetracoordinate carbon. Computational and Theoretical Chemistry, 2015, 1063, 19-23.	1.1	3
11374	Band structure and transport studies on InP nanotube – A first-principles investigation. Superlattices and Microstructures, 2015, 83, 193-209.	1.4	14
11375	Theoretical study of oxygen sorption and diffusion in the volume and on the surface of a $\hat{\Gamma}$ -TiAl alloy. Journal of Experimental and Theoretical Physics, 2015, 120, 257-267.	0.2	19
11376	d <sub>0</sub> half-metallicity of the bulk and surface (001) of full-Heusler alloy RbSrN <sub>2</sub> : A first-principle study. Journal of Magnetism and Magnetic Materials, 2015, 385, 394-401.	1.0	13
11377	Hydrogen diffusion in MgH <sub>2</sub> doped with Ti, Mn and Fe. RSC Advances, 2015, 5, 34894-34899.	1.7	25
11378	Oxygen Defects at Reducible Oxide Surfaces: The Example of Ceria and Vanadia. Springer Series in Surface Sciences, 2015, , 149-190.	0.3	10
11379	van der Waals forces in density functional theory: a review of the vdW-DF method. Reports on Progress in Physics, 2015, 78, 066501.	8.1	615
11380	Ab initio investigation of the adsorption of atomic and molecular hydrogen on AlN nanotubes. Applied Surface Science, 2015, 346, 24-32.	3.1	15
11381	DOPAMINE ADSORPTION CONFIGURATIONS ON ANATASE (101) SURFACE. Surface Review and Letters, 2015, 22, 1550052.	0.5	1
11382	Synergistic effects of nonmetal co-doping with sulfur in anatase TiO <sub>2</sub> : a DFT + U study. Physical Chemistry Chemical Physics, 2015, 17, 3426-3434.	1.3	5
11383	Assessing thermochemical properties of materials through ab initio quantum-mechanical methods: the case of $\hat{\Gamma}$ -Al <sub>2</sub> O <sub>3</sub> . Physical Chemistry Chemical Physics, 2015, 17, 11670-11677.	1.3	51
11384	Thermodynamic modeling of KF-CrF <sub>3</sub> binary system. Chemical Research in Chinese Universities, 2015, 31, 461-465.	1.3	8
11385	Catalytic propane reforming mechanism over Mn-Doped CeO <sub>2</sub> (111). Surface Science, 2015, 640, 119-126.	0.8	14



#	ARTICLE	IF	CITATIONS
11386	The crystal chemistry and the compressibility of silicate-carbonate minerals: Spurrite, galuskinite and tilleyite. <i>Geoscience Frontiers</i> , 2015, 6, 771-777.	4.3	11
11387	Ba <sub>2</sub> GeS <sub>4</sub> and Mg <sub>2</sub> SnS <sub>4</sub> : synthesis, structures, optical properties and electronic structures. <i>RSC Advances</i> , 2015, 5, 33646-33652.	1.7	31
11388	Correlated electron pseudopotentials for 3d-transition metals. <i>Journal of Chemical Physics</i> , 2015, 142, 064110.	1.2	32
11389	Diffusion of Cd and Te adatoms on CdTe(111) surfaces: A computational study using density functional theory. <i>AIP Advances</i> , 2015, 5, .	0.6	5
11390	Mapping the genome of meta-generalized gradient approximation density functionals: The search for B97M-V. <i>Journal of Chemical Physics</i> , 2015, 142, 074111.	1.2	305
11391	Atomistic mechanisms of nonstoichiometry-induced twin boundary structural transformation in titanium dioxide. <i>Nature Communications</i> , 2015, 6, 7120.	5.8	90
11392	Phase-Field Simulation of Orowan Strengthening by Coherent Precipitate Plates in an Aluminum Alloy. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2015, 46, 3287-3301.	1.1	41
11393	Lithium boride sheet and nanotubes: structure and hydrogen storage. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 13821-13828.	1.3	18
11394	Computational chemistry for graphene-based energy applications: progress and challenges. <i>Nanoscale</i> , 2015, 7, 6883-6908.	2.8	72
11395	Density Functional Study of Molecular Hydrogen Adsorption on Small Gold-Copper Binary Clusters. <i>Journal of Cluster Science</i> , 2015, 26, 491-503.	1.7	13
11396	Bonding charge density from atomic perturbations. <i>Journal of Computational Chemistry</i> , 2015, 36, 1008-1014.	1.5	23
11397	Mechanism of Meropenem Hydrolysis by New Delhi Metallo- $\beta$ -Lactamase. <i>ACS Catalysis</i> , 2015, 5, 2577-2586.	5.5	35
11398	Energetics of atomic scale structure changes in graphene. <i>Chemical Society Reviews</i> , 2015, 44, 3143-3176.	18.7	141
11399	Correlated Visible-Light Absorption and Intrinsic Magnetism of SrTiO <sub>3</sub> Due to Oxygen Deficiency: Bulk or Surface Effect?. <i>Inorganic Chemistry</i> , 2015, 54, 3759-3765.	1.9	21
11400	Electronic Structure Calculations for Antiferromagnetism of Cuprates Using SIWB Method for Anions in DV and a Density Functional Theory Confirming from Finite Element Method. <i>Advances in Quantum Chemistry</i> , 2015, 70, 1-29.	0.4	1
11401	Clean Ir(111) and Pt(111) electronic surface states: A first-principle fully relativistic investigation. <i>Surface Science</i> , 2015, 637-638, 106-115.	0.8	26
11402	Facile preparation of semimetallic MoP <sub>2</sub> as a novel visible light driven photocatalyst with high photocatalytic activity. <i>Journal of Materials Chemistry A</i> , 2015, 3, 10360-10367.	5.2	42
11403	Structural, electronic and mechanical properties of CrN: A first principles study. <i>Modern Physics Letters B</i> , 2015, 29, 1550009.	1.0	11



#	ARTICLE	IF	CITATIONS
11404	Synergy between Pd and Au in a Pd@Au(100) bimetallic surface for the water gas shift reaction: a DFT study. <i>RSC Advances</i> , 2015, 5, 47066-47073.	1.7	14
11405	Why Do Boron and Nitrogen Doped 1 <sup>±</sup> - and 1 <sup>3</sup> -Graphyne Exhibit Different Oxygen Reduction Mechanism? A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 11493-11498.	1.5	77
11406	Electron Transport in Graphene-Based Nanosensors for Eu(III) Detection. <i>Journal of Physical Chemistry C</i> , 2015, 119, 12037-12046.	1.5	6
11407	Electronic transport properties of tetracyclopentadienyl modified with C and Si atoms. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2015, 379, 1726-1731.	0.9	2
11408	Flexible Self-Supporting Nanofibers Thin Films Showing Reversible Photochromic Fluorescence. <i>ACS Applied Materials &amp; Interfaces</i> , 2015, 7, 9904-9910.	4.0	63
11409	CO <sub>2</sub> adsorption on single-walled boron nitride nanotubes containing vacancy defects. <i>RSC Advances</i> , 2015, 5, 27412-27420.	1.7	28
11410	Thermodynamic assessment of the cesium-oxygen system by coupling density functional theory and CALPHAD approaches. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015, 49, 67-78.	0.7	9
11411	A facile synthesis of high quality nanostructured CeO <sub>2</sub> and Gd <sub>2</sub> O <sub>3</sub> -doped CeO <sub>2</sub> solid electrolytes for improved electrochemical performance. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14193-14200.	1.3	22
11412	QTAIM-Based Comparison of Agostic Bonds and Intramolecular Charge-Inverted Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4993-5008.	1.1	29
11413	Theoretical insight into the strain effect on the intercalation potential of Li@FePO <sub>4</sub> materials. <i>RSC Advances</i> , 2015, 5, 35667-35674.	1.7	9
11414	The structure and stability of reduced and oxidized mononuclear platinum species on nanostructured ceria from density functional modeling. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14551-14560.	1.3	37
11415	Configurational study of amino-functionalized silica surfaces: A density functional theory modeling. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 59, 21-30.	1.3	5
11416	Theoretical insight into the C-H and C-C scission mechanism of ethane on a tetrahedral Pt <sub>4</sub> subnanocluster. <i>RSC Advances</i> , 2015, 5, 40978-40988.	1.7	4
11417	Sulfisoxazole/cyclodextrin inclusion complex incorporated in electrospun hydroxypropyl cellulose nanofibers as drug delivery system. <i>Colloids and Surfaces B: Biointerfaces</i> , 2015, 128, 331-338.	2.5	98
11418	Electronic structure and thermodynamic properties of Cu <sub>3</sub> V <sub>2</sub> O <sub>8</sub> compound. <i>Phase Transitions</i> , 2015, 88, 970-978.	0.6	7
11419	Multiphysics modelling, quantum chemistry and risk analysis for corrosion inhibitor design and lifetime prediction. <i>Faraday Discussions</i> , 2015, 180, 459-477.	1.6	22
11420	Friction and adhesion of fluorine containing hydrophobic hydrogenated diamond-like carbon (F-H-DLC) coating against magnesium alloy AZ91. <i>Surface and Coatings Technology</i> , 2015, 267, 21-31.	2.2	33
11421	Nanoscale Magnetization Reversal Caused by Electric Field-Induced Ion Migration and Redistribution in Cobalt Ferrite Thin Films. <i>ACS Nano</i> , 2015, 9, 4210-4218.	7.3	60

#	ARTICLE	IF	CITATIONS
11422	SnS <sub>2</sub> nanotubes: a promising candidate for the anode material for lithium ion batteries. RSC Advances, 2015, 5, 32505-32510.	1.7	24
11423	DFT: A Theory Full of Holes?. Annual Review of Physical Chemistry, 2015, 66, 283-304.	4.8	149
11425	Lateral interaction and spectroscopic constants of CO adsorbed on ZnO. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	6
11426	Electronic Structure and Infrared Light Emission in Dislocation-Engineered Silicon. IEEE Nanotechnology Magazine, 2015, 14, 399-403.	1.1	7
11427	A uniformly porous 2D CN (1â€‰%:â€‰%1) network predicted by first-principles calculations. RSC Advances, 2015, 5, 11791-11796.	1.7	6
11428	A benchmark database for adsorption bond energies to transition metal surfaces and comparison to selected DFT functionals. Surface Science, 2015, 640, 36-44.	0.8	396
11429	Structural and electronic properties of Li-ion battery cathode material MoF <sub>3</sub> from first-principles. Journal of Solid State Chemistry, 2015, 227, 25-29.	1.4	4
11430	A first-principles study of transport properties of a gallium arsenide nanoribbon-based molecular device. Materials Science in Semiconductor Processing, 2015, 35, 109-114.	1.9	9
11431	Conductance and spin-filter effects of oxygen-incorporated Au, Cu, and Fe single-atom chains. Journal of Applied Physics, 2015, 117, 043902.	1.1	11
11432	The synergistic mechanism of graphene and MoS <sub>2</sub> for hydrogen generation: insights from density functional theory. Physical Chemistry Chemical Physics, 2015, 17, 11375-11381.	1.3	32
11433	Physiochemical Investigation of Shape-Designed MnO <sub>2</sub> Nanostructures and Their Influence on Oxygen Reduction Reaction Activity in Alkaline Solution. Journal of Physical Chemistry C, 2015, 119, 6604-6618.	1.5	106
11434	Elastic, mechanical, electronic properties and hardness of Nb <sub>2</sub> AsC from first principles. Molecular Physics, 2015, 113, 1501-1507.	0.8	2
11435	Magnetic and magneto-optical properties of doped and co-doped CdTe with (Mn, Fe): Ab-initio study. Journal of Magnetism and Magnetic Materials, 2015, 385, 295-301.	1.0	54
11436	Role of F in Improving the Photocatalytic Activity of Rh-Doped SrTiO <sub>3</sub> . Journal of Physical Chemistry C, 2015, 119, 7215-7224.	1.5	56
11437	Theoretical investigation of magnetic, electronic and optical properties of orthorhombic YFeO <sub>3</sub> : A first-principle study. Materials Science in Semiconductor Processing, 2015, 34, 114-120.	1.9	51
11438	Nine New Phosphorene Polymorphs with Non-Honeycomb Structures: A Much Extended Family. Nano Letters, 2015, 15, 3557-3562.	4.5	275
11439	Effect of irradiation defects on the corrosion behaviors of steels exposed to lead bismuth eutectic in ADS: a first-principles study. Physical Chemistry Chemical Physics, 2015, 17, 12292-12298.	1.3	20
11440	Electronic structure and magnetism on FeSiAl alloy: A DFT study. Journal of Magnetism and Magnetic Materials, 2015, 389, 73-76.	1.0	11

#	ARTICLE	IF	CITATIONS
11441	A panel of peralkylated sulfurâ€“guanidine type bases: Novel pro-ligands for use in biomimetic coordination chemistry. <i>Inorganica Chimica Acta</i> , 2015, 430, 225-238.	1.2	5
11442	Computational Prediction of Metal Organic Frameworks Suitable for Molecular Infiltration as a Route to Development of Conductive Materials. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1586-1591.	2.1	39
11443	Unusual behavior in magnesium-copper cluster matter produced by helium droplet mediated deposition. <i>Journal of Chemical Physics</i> , 2015, 142, 084307.	1.2	11
11444	The non-innocent role of cerium oxide in heterogeneous catalysis: A theoretical perspective. <i>Catalysis Today</i> , 2015, 253, 20-32.	2.2	50
11445	Tuning the Electrical Transport Properties of Multilayered Molybdenum Disulfide Nanosheets by Intercalating Phosphorus. <i>Journal of Physical Chemistry C</i> , 2015, 119, 9560-9567.	1.5	40
11446	The physical properties of Li-doped g-C <sub>3</sub> N <sub>4</sub> monolayer sheet investigated by the first-principles. <i>Materials Research Bulletin</i> , 2015, 66, 156-162.	2.7	72
11447	First-Principles Study on Electronic and Optical Properties of Kesterite and Stannite Cu <sub>2</sub> ZnSnS <sub>4</sub> Photovoltaic Absorbers. <i>Materials Science Forum</i> , 2015, 815, 80-88.	0.3	7
11448	Synthesis and crystal structure of a novel layered barium antimonate Ba <sub>2</sub> Sb <sub>7</sub> O <sub>13</sub> (OH) with mixed-valence antimony. <i>Solid State Sciences</i> , 2015, 44, 27-31.	1.5	3
11449	First-principles calculation of Cu <sub>2</sub> SnS <sub>3</sub> and related compounds. <i>Physica Status Solidi (B): Basic Research</i> , 2015, 252, 1230-1234.	0.7	36
11450	Investigation of Properties of Mg <sub>n</sub> Clusters and Their Hydrogen Storage Mechanism: A Study Based on DFT and a Global Minimum Optimization Method. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3636-3643.	1.1	40
11451	Cubic C <sub>96</sub> : a novel carbon allotrope with a porous nanocube network. <i>Journal of Materials Chemistry A</i> , 2015, 3, 10448-10452.	5.2	47
11452	DFT investigations on the ring-opening polymerization of substituted cyclic carbonates catalyzed by zinc- $\beta$ -diketiminato complexes. <i>Polymer Chemistry</i> , 2015, 6, 3336-3352.	1.9	23
11453	Dynamic motion of an Lu pair inside a C <sub>76</sub> (T <sub>d</sub> ) cage. <i>RSC Advances</i> , 2015, 5, 34383-34389.	1.7	4
11454	Effects of single- and co-substitution of Ti on dehydrogenation of Mg <sub>2</sub> NiH <sub>4</sub> : A first-principles study. <i>Computational Materials Science</i> , 2015, 103, 45-51.	1.4	12
11455	Achieving a high magnetization in sub-nanostructured magnetite films by spin-flipping of tetrahedral Fe <sup>3+</sup> cations. <i>Nano Research</i> , 2015, 8, 2935-2945.	5.8	21
11456	Comparative study of van der Waals corrections to the bulk properties of graphite. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 415502.	0.7	43
11457	Adsorption behavior of Fe atoms on a naphthalocyanine monolayer on Ag(111) surface. <i>Chinese Physics B</i> , 2015, 24, 076802.	0.7	6
11458	A Cu <sub>25</sub> Nanocluster with Partial Cu(0) Character. <i>Journal of the American Chemical Society</i> , 2015, 137, 13319-13324.	6.6	234

#	ARTICLE	IF	CITATIONS
11459	Phonon dispersion and zero-point renormalization of LiNbO <sub>3</sub> from density-functional perturbation theory. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 385402.	0.7	34
11460	In-depth quantum chemical investigation of electro-optical and charge-transport properties of trans-3-(3,4-dimethoxyphenyl)-2-(4-nitrophenyl)prop-2-enitrile. <i>Comptes Rendus Chimie</i> , 2015, 18, 1289-1296.	0.2	28
11461	Epitaxial NbC N1 <sup>~</sup> (001) layers: Growth, mechanical properties, and electrical resistivity. <i>Surface and Coatings Technology</i> , 2015, 277, 136-143.	2.2	35
11462	O <sub>2</sub> → CO <sub>2</sub> Mixed Gas Production Using a Zr-Doped Cu-Based Oxygen Carrier. <i>Industrial &amp; Engineering Chemistry Research</i> , 2015, 54, 9805-9812.	1.8	26
11463	The structural behavior of SrTiO <sub>3</sub> under 400 Å keV Ne <sup>2+</sup> ion irradiation. <i>Applied Physics A: Materials Science and Processing</i> , 2015, 121, 1211-1217.	1.1	0
11464	Rationalization of Au Concentration and Distribution in AuNi@Pt Core-Shell Nanoparticles for Oxygen Reduction Reaction. <i>ACS Catalysis</i> , 2015, 5, 6328-6336.	5.5	49
11465	Equation of state of solid, liquid and gaseous tantalum from first principles. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015, 51, 133-143.	0.7	21
11466	Mechanistic insight into the aerobic oxidation of benzyl alcohol catalyzed by the Cu <sup>II</sup> → TEMPO catalyst in alkaline water solution. <i>RSC Advances</i> , 2015, 5, 83976-83984.	1.7	11
11467	Grafting trimethylaluminum and its halogen derivatives on silica: general trends for <sup>27</sup> Al SS-NMR response from first principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 26937-26945.	1.3	10
11468	Effects of Co Content in Pd-Skin/PdCo Alloys for Oxygen Reduction Reaction: Density Functional Theory Predictions. <i>Journal of Physical Chemistry C</i> , 2015, 119, 24364-24372.	1.5	20
11469	TM atoms on B/N doped defective graphene as a catalyst for oxygen reduction reaction: a theoretical study. <i>RSC Advances</i> , 2015, 5, 82804-82812.	1.7	18
11470	Role of Site Stability in Methane Activation on Pd <sub>x</sub> Ce <sub>1-x</sub> O <sub>2</sub> Surfaces. <i>ACS Catalysis</i> , 2015, 5, 6187-6199.	5.5	69
11471	The electronic structures and photophysical properties of platinum complexes with C <sup>N</sup> N ligands: the influence of the carborane substituent. <i>Dalton Transactions</i> , 2015, 44, 18130-18137.	1.6	28
11472	Influences of Al, Ti and Nb doping on the structure and hydrogen storage property of Mg(BH <sub>4</sub> ) <sub>2</sub> (001) surface – A theoretical study. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 10516-10526.	3.8	12
11473	Toward a Database of Chemically Accurate Barrier Heights for Reactions of Molecules with Metal Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4106-4114.	2.1	67
11474	In Situ Probing of the Active Site Geometry of Ultrathin Nanowires for the Oxygen Reduction Reaction. <i>Journal of the American Chemical Society</i> , 2015, 137, 12597-12609.	6.6	46
11475	Atomic structure of the La/Pt(111) and Ce/Pt(111) surfaces revealed by DFT+U calculations. <i>RSC Advances</i> , 2015, 5, 521-528.	1.7	11
11476	Geometry- and QTAIM-Based Comparison of Intramolecular Charge-Inverted Hydrogen Bonds, M <sup>+</sup> ⋯A <sup>-</sup> (H <sup>+</sup> ⋯Si) ⋯ Agostic Bond, and M <sup>+</sup> ⋯A <sup>-</sup> (I <sup>+</sup> -SiH) ⋯ If Interactions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11384-11396.	1.1	20

#	ARTICLE	IF	CITATIONS
11477	Intramolecularly Group 15 Stabilized Aryltellurenyl Halides and Triflates. <i>Organometallics</i> , 2015, 34, 5341-5360.	1.1	24
11478	How can carbon favor planar multi-coordination in boron-based clusters? Global structures of $CB_xE_y$ ( $E = Al, Ga, x + y = 4$ ). <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 32016-32022.	1.3	11
11479	Failure of single phenolic chains and cross-links: Energetics, mechanisms, and alternative linker design. <i>Polymer</i> , 2015, 80, 265-274.	1.8	5
11480	$Na_4MgM_2Se_6$ ( $M = Si, Ge$ ): The First Noncentrosymmetric Compounds with Special Ethane-like $[M_2Se_6]^{6-}$ Units Exhibiting Large Laser-Damage Thresholds. <i>Inorganic Chemistry</i> , 2015, 54, 10108-10110.	1.9	54
11481	Theoretical investigations of electronic structures, magnetic properties and half-metallicity in Heusler alloys $Zr_2VZ$ ( $Z = Al, Ga, In$ ). <i>Journal of the Korean Physical Society</i> , 2015, 67, 881-888.	0.3	14
11482	Crystal Structures and Electronic Properties of Cesium Xenides at High Pressures. <i>Journal of Physical Chemistry C</i> , 2015, 119, 24996-25002.	1.5	15
11483	Computation assisted design of favored composition for ternary $Mg-Cu-Y$ metallic glass formation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14879-14889.	1.3	3
11484	Nitrogen Activation in a Mars van Krevelen Mechanism for Ammonia Synthesis on $Co_3Mo_3N$ . <i>Journal of Physical Chemistry C</i> , 2015, 119, 28368-28376.	1.5	135
11485	Selective Oxidation of 1,2-Propanediol in Alkaline Anion-Exchange Membrane Electrocatalytic Flow Reactors: Experimental and DFT Investigations. <i>ACS Catalysis</i> , 2015, 5, 6926-6936.	5.5	29
11486	Adsorption studies of Malachite green on 5-sulphosalicylic acid doped tetraethoxysilane (SATEOS) composite material. <i>RSC Advances</i> , 2015, 5, 92788-92798.	1.7	8
11487	Trimerization of Alkynes in the Presence of a Hydrotris(pyrazolyl)borate Iridium Catalyst and the Effect of Substituent Groups on the Reaction Mechanism: A Computational Study. <i>Organometallics</i> , 2015, 34, 4965-4974.	1.1	18
11488	The study of the hydrogen storage capacity of the Ti atoms coated $Si@Ga_{12}$ clusters. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 16278-16287.	3.8	1
11489	Far infrared spectra of solid state l-serine, l-threonine, l-cysteine, and l-methionine in different protonation states. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 150, 301-307.	2.0	22
11490	Pressure evolution of the potential barriers for transformations of layered BN to dense structures. <i>RSC Advances</i> , 2015, 5, 87550-87555.	1.7	3
11491	The effect of manganite nanoparticle addition on the low field magnetoresistance of polyaniline. <i>Journal of Materials Chemistry C</i> , 2015, 3, 12040-12047.	2.7	15
11492	Growth of Ammonium Bisulfate Clusters by Adsorption of Oxygenated Organic Molecules. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11191-11198.	1.1	11
11493	Direct Observation of Sublimation Behaviors in One-Dimensional $In_2Se_3/In_2O_3$ Nanoheterostructures. <i>Analytical Chemistry</i> , 2015, 87, 5584-5588.	3.2	10
11494	Adsorption properties of trifluoroacetic acid on anatase (101) and (001) surfaces: a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 23627-23633.	1.3	6





#	ARTICLE	IF	CITATIONS
11513	First principles-based multiparadigm, multiscale strategy for simulating complex materials processes with applications to amorphous SiC films. <i>Journal of Chemical Physics</i> , 2015, 142, 174703.	1.2	10
11514	Effects of N on Electronic and Mechanical Properties of H-Type SiC. <i>Chinese Physics Letters</i> , 2015, 32, 087103.	1.3	1
11515	On the possibility of contact-induced spin polarization in interfaces of armchair nanotubes with transition metal substrates. <i>Journal of Magnetism and Magnetic Materials</i> , 2015, 396, 102-105.	1.0	2
11516	The interactions between TiO <sub>2</sub> and graphene with surface inhomogeneity determined using density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 29734-29746.	1.3	38
11517	Modelling of oxygen vacancy aggregates in monoclinic HfO <sub>2</sub> : can they contribute to conductive filament formation?. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 415401.	0.7	43
11518	Structure and electronic properties of crystals consisting of graphene layers L 6, L 4, L 3, and L 4. <i>Physics of the Solid State</i> , 2015, 57, 2126-2133.	0.2	31
11519	Structural, Thermodynamic, Elastic, and Electronic Properties of $\beta$ -SnS at High Pressure from First-Principles Investigations. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2015, 70, 949-960.	0.7	2
11520	Characterizing the Greater-Than-Bulk Melting Behavior of Ga-Al Nanoalloys. <i>Journal of Physical Chemistry C</i> , 2015, 119, 24095-24103.	1.5	3
11521	New Insights into Re <sub>3</sub> ( $\frac{1}{4}$ -Cl) <sub>3</sub> Cl <sub>6</sub> Aromaticity. Evidence of $\pi$ - and $\pi$ -Diatropicity. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4326-4330.	2.1	17
11522	First principle investigation on structural and electronic properties of silicon oxycarbide ceramics. <i>Journal of Alloys and Compounds</i> , 2015, 647, 665-669.	2.8	12
11523	Elucidating Hydrogen Oxidation/Evolution Kinetics in Base and Acid by Enhanced Activities at the Optimized Pt Shell Thickness on the Ru Core. <i>ACS Catalysis</i> , 2015, 5, 6764-6772.	5.5	197
11524	Structures, electronic properties and growth strategies of the Fe(ZrO <sub>2</sub> ) <sub>n</sub> (n=6) clusters: Ab initio calculations. <i>Solid State Communications</i> , 2015, 221, 5-8.	0.9	16
11525	Guaiacol Hydrodeoxygenation over Platinum Catalyst: Reaction Pathways and Kinetics. <i>Industrial &amp; Engineering Chemistry Research</i> , 2015, 54, 10638-10644.	1.8	88
11526	Catalytic activities of platinum nanotubes: a density functional study. <i>European Physical Journal B</i> , 2015, 88, 1.	0.6	2
11527	Conservative Tryptophan Mutants of the Protein Tyrosine Phosphatase YopH Exhibit Impaired WPD-Loop Function and Crystallize with Divanadate Esters in Their Active Sites. <i>Biochemistry</i> , 2015, 54, 6490-6500.	1.2	13
11528	Benchmarking density functional theory predictions of framework structures and properties in a chemically diverse test set of metal-organic frameworks. <i>Journal of Materials Chemistry A</i> , 2015, 3, 22432-22440.	5.2	64
11529	Size-dependent properties of transition metal clusters: from molecules to crystals and surfaces - computational studies with the program ParaGauss. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28463-28483.	1.3	16
11530	Density-functional theory investigation of Al pitting corrosion in electrolyte containing chloride ions. <i>Applied Surface Science</i> , 2015, 357, 2028-2038.	3.1	47



#	ARTICLE	IF	CITATIONS
11531	Effects of B and Al on tensile strengths and electronic structure of CuZr: A first-principles study. Computational Condensed Matter, 2015, 5, 1-6.	0.9	1
11532	Hydrogen embrittlement in nickel, visited by first principles modeling, cohesive zone simulation and nanomechanical testing. International Journal of Hydrogen Energy, 2015, 40, 16892-16900.	3.8	93
11533	Calculations of Al dopant in $\alpha$ -quartz using a variational implementation of the Perdew-Zunger self-interaction correction. New Journal of Physics, 2015, 17, 083006.	1.2	26
11534	Electronic structure and soft magnetic properties of Se/FeSiAl (110) films. Applied Surface Science, 2015, 354, 401-407.	3.1	8
11535	DFT Analysis of NO Oxidation Intermediates on Undoped and Doped $\text{LaCoO}_3$ Perovskite. Journal of Physical Chemistry C, 2015, 119, 20488-20494.	1.5	39
11536	Energy of Supported Metal Catalysts: From Single Atoms to Large Metal Nanoparticles. ACS Catalysis, 2015, 5, 5673-5678.	5.5	78
11537	Anchoring Lithium Polysulfides via Affinitive Interactions: Electrostatic Attraction, Hydrogen Bonding, or in Parallel?. Journal of Physical Chemistry C, 2015, 119, 20495-20502.	1.5	53
11538	Performance of a Non-Local van der Waals Density Functional on the Dissociation of $\text{H}_2$ on Metal Surfaces. Journal of Physical Chemistry A, 2015, 119, 12146-12158.	1.1	44
11539	Solution-combustion synthesized aluminium-doped spinel ( $\text{LiAl}_x\text{Mn}_{2-x}\text{O}_4$ ) as a high-performance lithium-ion battery cathode material. Applied Physics A: Materials Science and Processing, 2015, 121, 51-57.	1.1	16
11540	Experimental investigation and thermodynamic description of the Li-Si-Ni ternary system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2015, 51, 13-23.	0.7	3
11541	Fundamental effects of W alloying on various properties of NbH phases. International Journal of Hydrogen Energy, 2015, 40, 12745-12749.	3.8	11
11542	Discovery of $\alpha$ - $\text{MnP}_4$ and the Polymorphism of Manganese Tetrphosphide. Inorganic Chemistry, 2015, 54, 8761-8768.	1.9	8
11543	Influence of Oxygen, Tellurium, and Zinc Substitution on CdSe Nanoribbon: A First-Principles Investigation. Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry, 2015, 45, 1780-1787.	0.6	0
11544	Electronic structures and optical properties of $\alpha$ - $\text{Fe}_2\text{O}_3$ - $x\text{Se}_x$ alloys for solar absorber. Modern Physics Letters B, 2015, 29, 1550050.	1.0	1
11545	Uranyl Carboxyphosphonates Derived from Hydrothermal in Situ Ligand Reaction: Syntheses, Structures, and Computational Investigations. Inorganic Chemistry, 2015, 54, 8617-8624.	1.9	24
11546	Study of the Magnetic Properties of $\text{CdMnTe}_{1-y}\text{N}_y$ and $\text{CdMnTe}$ with Defects by Ab Initio Calculations. Journal of Superconductivity and Novel Magnetism, 2015, 28, 3545-3552.	0.8	4
11547	A Density Functional Theory Study on Mechanism of Electrochemical Oxygen Reduction on $\text{FeN}_3$ -Graphene. Journal of the Electrochemical Society, 2015, 162, F1262-F1267.	1.3	18
11548	Photoelectron spectra and structure of the $\text{Mn}^{n-}$ anions ( $n = 16$ ). Journal of Chemical Physics, 2015, 143, 044306.	1.2	15

#	ARTICLE	IF	CITATIONS
11549	Effect of exchangeâ€ correlation on first-principles-driven lattice thermal conductivity predictions of crystalline silicon. <i>Computational Materials Science</i> , 2015, 110, 115-120.	1.4	74
11550	DFT-based modeling of benzene hydrogenation on Pt at industrially relevant coverage. <i>Journal of Catalysis</i> , 2015, 330, 406-422.	3.1	34
11551	Conformational properties of chiral tobacco alkaloids by DFT calculations and vibrational circular dichroism: ( $\lambda$ )-S-anabasine. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 60, 169-179.	1.3	5
11552	HOMOâ€ LUMO energy gap control in platinum( <i>ii</i> ) biphenyl complexes containing 2,2â€-bipyridine ligands. <i>Dalton Transactions</i> , 2015, 44, 17075-17090.	1.6	19
11553	Structural, electronic and elastic properties of the cubic CaTiO <sub>3</sub> under pressure: A DFT study. <i>AIP Advances</i> , 2015, 5, .	0.6	69
11554	Activation and dissociation of CO <sub>2</sub> on the (001), (011), and (111) surfaces of mackinawite (FeS): A dispersion-corrected DFT study. <i>Journal of Chemical Physics</i> , 2015, 143, 094703.	1.2	46
11555	Ag out-surface diffusion in crystalline SiC with an effective SiO <sub>2</sub> diffusion barrier. <i>Journal of Nuclear Materials</i> , 2015, 464, 294-298.	1.3	3
11556	Investigation of Methacrylic Acid at High Pressure Using Neutron Diffraction. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12147-12154.	1.2	4
11557	Adsorbing a PVDF polymer via noncovalent interactions to effectively tune the electronic and magnetic properties of zigzag SiC nanoribbons. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24038-24047.	1.3	11
11558	First-principles insights on electron transport in V <sub>2</sub> O <sub>5</sub> nanostructures. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2015, 201, 45-50.	1.7	8
11559	Modulation of Electronic Structure of Armchair MoS <sub>2</sub> Nanoribbon. <i>Journal of Physical Chemistry C</i> , 2015, 119, 22164-22171.	1.5	39
11560	Many-body dispersion effects in the binding of adsorbates on metal surfaces. <i>Journal of Chemical Physics</i> , 2015, 143, 102808.	1.2	69
11561	First-principles calculations of the interaction between hydrogen and 3d alloying atom in nickel. <i>Journal of Nuclear Materials</i> , 2015, 465, 254-259.	1.3	8
11562	First-principles study of structural, electronic and Li-ion diffusion properties of N-doped LiFePO <sub>4</sub> (010) surface. <i>Solid State Ionics</i> , 2015, 281, 1-5.	1.3	30
11563	Dissociation of CO <sub>2</sub> on rhodium nanoclusters (Rh <sub>13</sub> ) in various structures supported on unzipped graphene oxide â€ a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 11028-11035.	1.3	10
11564	Four-coordinate nickel( <i>ii</i> ) and copper( <i>ii</i> ) complex based ONO tridentate Schiff base ligands: synthesis, molecular structure, electrochemical, linear and nonlinear properties, and computational study. <i>Dalton Transactions</i> , 2015, 44, 18019-18037.	1.6	62
11565	Operando characterization and DFT modelling of nanospinels: Some examples showing the relationship with catalytic activity. <i>Applied Catalysis A: General</i> , 2015, 504, 631-641.	2.2	11
11566	A visualized probe method for localization of surface oxygen vacancy on TiO <sub>2</sub> : Au in situ reduction. <i>Nanoscale</i> , 2015, 7, 17488-17495.	2.8	14

#	ARTICLE	IF	CITATIONS
11567	Gas adsorption on graphene with different layers: A first-principles study. , 2015, , .		2
11568	Vacancy induced Jahn-Teller distortion in silicon and its influence to the electronic structure. Modern Physics Letters B, 2015, 29, 1550136.	1.0	0
11569	Theoretical study of surface dependence of NH <sub>3</sub> adsorption and decomposition on spinel-type MgAl <sub>2</sub> O <sub>4</sub> . RSC Advances, 2015, 5, 77973-77985.	1.7	4
11570	First-principles study on alkali-metal effect of Li, Na, and K in CuInSe <sub>2</sub> and CuGaSe <sub>2</sub> . Japanese Journal of Applied Physics, 2015, 54, 08KC20.	0.8	38
11571	Modulation of Electronic Structure of Armchair MoS <sub>2</sub> Nanoribbon. Journal of Physical Chemistry A, 2015, , 150902124434000.	1.1	1
11572	Controlling the electronic transport properties of the tetrapyrimidinyl molecule with atom modified sulfur bridge. RSC Advances, 2015, 5, 10675-10679.	1.7	5
11573	In Situ Photoconductivity Kinetic Study of Nano-TiO <sub>2</sub> during the Photocatalytic Oxidation of Formic Acid: Effects of New Recombination and Current Doubling. Journal of Physical Chemistry C, 2015, 119, 21711-21722.	1.5	19
11574	Tuning Thermoelectric Properties of Misfit Layered Cobaltites by Chemically Induced Strain. Journal of Physical Chemistry C, 2015, 119, 21818-21827.	1.5	33
11575	Putting DFT to the trial: First principles pressure dependent analysis on optical properties of cubic perovskite SrZrO <sub>3</sub> . Computational Condensed Matter, 2015, 4, 32-39.	0.9	32
11576	Effects of polar and nonpolar on band structures in ultrathin ZnO/GaN type-II superlattices. Solid State Communications, 2015, 221, 14-17.	0.9	4
11577	Thermally activated surface oxygen defects at the perimeter of Au/TiO <sub>2</sub> : a DFT+U study. Physical Chemistry Chemical Physics, 2015, 17, 25403-25410.	1.3	26
11578	Trapping N <sub>5</sub> rings and N <sub>3</sub> chains on the outer surface of fullerene C <sub>60</sub> : a theoretical study. Journal of Molecular Modeling, 2015, 21, 265.	0.8	5
11579	Prediction of d <sub>0</sub> Half-Metallic Properties in CsMgS <sub>2</sub> Full-Heusler Compound from First-Principle Calculations. Journal of Superconductivity and Novel Magnetism, 2015, 28, 3701-3705.	0.8	12
11580	Using Force-Matched Potentials To Improve the Accuracy of Density Functional Tight Binding for Reactive Conditions. Journal of Chemical Theory and Computation, 2015, 11, 4530-4535.	2.3	28
11581	First-principles study of W-TiC interface cohesion. Surface and Coatings Technology, 2015, 276, 602-605.	2.2	57
11582	Electronic and magnetic properties of C-doped $\alpha$ -Al <sub>2</sub> O <sub>3</sub> by DFT calculations. Computational Materials Science, 2015, 110, 368-374.	1.4	16
11583	Theoretical insights into M-SO bonds in transition metal-sulfur monoxide complexes [N(SPM <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> M(SO)] (M = Fe, Ru, Os): Assessment of density functionals and dispersion interactions. Polyhedron, 2015, 101, 230-238.	1.0	8
11584	Europium Effect on the Electron Transport in Graphene Ribbons. Journal of Physical Chemistry C, 2015, 119, 22486-22495.	1.5	6

#	ARTICLE	IF	CITATIONS
11585	Large-Scale Computational Screening of Binary Intermetallics for Membrane-Based Hydrogen Separation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 26319-26326.	1.5	9
11586	<i>Ab initio</i> molecular dynamics with simultaneous electron and phonon excitations: Application to the relaxation of hot atoms and molecules on metal surfaces. <i>Physical Review B</i> , 2015, 92, .	1.1	76
11587	Theoretical and experimental studies on wide-band-gap p-type conductive BaCuSeF and related compounds. <i>Japanese Journal of Applied Physics</i> , 2015, 54, 08KC07.	0.8	10
11588	First principles calculation of CH <sub>4</sub> decomposition on nickel (111) surface. <i>European Physical Journal B</i> , 2015, 88, 1.	0.6	14
11589	Computational materials design of attractive Fermion system with large negative effective U <sub>eff</sub> in the hole-doped Delafossite of CuAlO <sub>2</sub> , AgAlO <sub>2</sub> and AuAlO <sub>2</sub> : Charge-excitation induced U <sub>eff</sub> < 0. <i>Physica C: Superconductivity and Its Applications</i> , 2015, 519, 168-183.	0.6	4
11590	Structural and electronic properties of Cu-doped Zn <sub>5</sub> (OH) <sub>6</sub> (CO <sub>3</sub> ) <sub>2</sub> from first principles. <i>Journal of Materials Science</i> , 2015, 50, 6794-6807.	1.7	7
11591	Smallest deltahedra silicon dicarbide: C <sub>2</sub> Si <sub>32</sub> . <i>RSC Advances</i> , 2015, 5, 101193-101199.	1.7	5
11592	Transport investigation of branched graphene nanoflakes. <i>Nanotechnology</i> , 2015, 26, 385705.	1.3	7
11593	Lattice distortion induced anomalous ferromagnetism and electronic structure in FCC Fe and Fe-TM (TM = Cr, Ni, Ta and Zr) alloys. <i>Materials Chemistry and Physics</i> , 2015, 162, 748-756.	2.0	17
11594	Theoretical investigation of the interactions in binding pocket of Reverse Transcriptase. <i>Saudi Journal of Biological Sciences</i> , 2015, 22, 719-724.	1.8	0
11595	Competitive Paths for Methanol Decomposition on Ruthenium: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27382-27391.	1.5	25
11596	Reactivity at the Lithium-Metal Anode Surface of Lithium-Sulfur Batteries. <i>Journal of Physical Chemistry C</i> , 2015, 119, 26828-26839.	1.5	140
11597	Computational studies of the effects of ortho- and para- ring activation on the kinetics of S <sub>N</sub> Ar reactions of 1-chloro-2-nitrobenzene and 1-phenoxy-2-nitrobenzene with aniline. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 57-67.	0.9	10
11598	A theoretical study on the interaction of amphetamine and single-walled carbon nanotubes. <i>Applied Surface Science</i> , 2015, 329, 87-93.	3.1	13
11599	The ensemble effect of formic acid oxidation on platinum-gold electrode studied by first-principles calculations. <i>Journal of Power Sources</i> , 2015, 278, 203-212.	4.0	35
11600	Mechanistic Details and Reactivity Descriptors in Oxidation and Acid Catalysis of Methanol. <i>ACS Catalysis</i> , 2015, 5, 666-682.	5.5	49
11601	Phenol Deoxygenation Mechanisms on Fe(110) and Pd(111). <i>ACS Catalysis</i> , 2015, 5, 523-536.	5.5	116
11602	A metal-metal bond passing through the arene ligand: a theoretical study on inverse sandwiches X[ScC <sub>8</sub> H <sub>8</sub> Sc] <sub>n</sub> X (X = F, Cl, Br; n = 1, 2). <i>New Journal of Chemistry</i> , 2015, 39, 1558-1562.	1.4	4

#	ARTICLE	IF	CITATIONS
11603	First principles study of the structural, electronic, mechanical and superconducting properties of WX (X=C, N). Journal of Physics and Chemistry of Solids, 2015, 77, 38-49.	1.9	18
11604	Dissolution energetics and its strain dependence of transition metal alloying elements in tungsten. Journal of Nuclear Materials, 2015, 456, 260-265.	1.3	18
11605	Special quasirandom structures of alon. Computational Materials Science, 2015, 96, 312-318.	1.4	22
11606	Magnesium interatomic potential for simulating plasticity and fracture phenomena. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 015004.	0.8	117
11607	Ab initio study of electronic density of state and photoabsorption of Ga <sub>1-x</sub> MnxAs under pressure. Solid State Communications, 2015, 202, 19-23.	0.9	5
11608	An assessment of theoretical procedures for $\pi$ -conjugation stabilisation energies in enones. Molecular Physics, 2015, 113, 1284-1296.	0.8	19
11609	Modeling Ferro- and Antiferromagnetic Interactions in Metal-Organic Coordination Networks. Journal of Physical Chemistry C, 2015, 119, 547-555.	1.5	23
11610	First-Principles Study of C <sub>2</sub> Oxygenates Synthesis Directly from Syngas over CoCu Bimetallic Catalysts. Journal of Physical Chemistry C, 2015, 119, 216-227.	1.5	47
11611	NO dissociation and reduction by H <sub>2</sub> on Pd(111): A first-principles study. Journal of Catalysis, 2015, 322, 73-83.	3.1	51
11612	Experimental and DFT studies of structure, optical and magnetic properties of (Zn <sub>1-x</sub> Ce <sub>x</sub> Cox)O nanopowders. Journal of Molecular Structure, 2015, 1084, 155-164.	1.8	4
11613	Spinel compounds as multivalent battery cathodes: a systematic evaluation based on ab initio calculations. Energy and Environmental Science, 2015, 8, 964-974.	15.6	430
11614	New insights into assessing the favorable co-doping dopants with various co-doped cases for the band gap engineering of SrTiO <sub>3</sub> . International Journal of Hydrogen Energy, 2015, 40, 1343-1351.	3.8	17
11615	Structural, electronic, elastic and superconducting properties of noble metal nitrides MN <sub>2</sub> (M=Ag, Au, Pt, Ir, Os, Ru, Rh, Ir, Pt, Au, Ag). Journal of Applied Physics, 2015, 118, 043701.	2.9	4
11616	Structure of a novel Mg-rich complex compound in Mg-Co-Y ternary alloys. Scripta Materialia, 2015, 98, 64-67.	2.6	23
11617	Thermodynamic modeling of the CaO-CaF <sub>2</sub> -Al <sub>2</sub> O <sub>3</sub> system aided by first-principles calculations. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2015, 48, 113-122.	0.7	11
11618	Roles of hydrogen bonds and $\pi$ - $\pi$ stacking in the optical detection of nitro-explosives with a luminescent metal-organic framework as the sensor. RSC Advances, 2015, 5, 3045-3053.	1.7	62
11619	Vibrational Circular Dichroism and Theoretical Study of the Conformational Equilibrium in (S)-Nicotine. ChemPhysChem, 2015, 16, 342-352.	1.0	12
11620	Structural formation of binary PtCu clusters: A density functional theory investigation. Computational Materials Science, 2015, 98, 278-286.	1.4	39

#	ARTICLE	IF	CITATIONS
11621	Effect of carbon types on the generation and morphology of GaN polycrystals grown using the Na flux method. <i>CrystEngComm</i> , 2015, 17, 1030-1036.	1.3	11
11622	A Gupta potential for magnesium in hcp phase. <i>Computational Materials Science</i> , 2015, 98, 328-332.	1.4	11
11623	Remarkable NO oxidation on single supported platinum atoms. <i>Scientific Reports</i> , 2014, 4, 7238.	1.6	78
11624	Pentaatomic planar tetracoordinate silicon with 14 valence electrons: A large-scale global search of $\text{SiXnYmq}$ ( $n < 10$ ; $m < 10$ ; $q < 10$ , $A \pm 1$ , $a \leq 2$ ; X, Y = main group elements from H to Br). <i>Computational Chemistry</i> , 2015, 36, 355-360.		
11625	First principles study of structural stability, electronic structure and mechanical properties of ReN and TcN. <i>Journal of Physics and Chemistry of Solids</i> , 2015, 78, 118-126.	1.9	10
11626	Catalytic properties of Au electrodes modified by an underlayer of Pd. <i>Surface Science</i> , 2015, 631, 235-247.	0.8	23
11627	Theoretical study of electronic structure, phase transition, elastic, and thermodynamic properties of ReN. <i>Physica B: Condensed Matter</i> , 2015, 458, 124-131.	1.3	6
11628	Diamond polytypes under high pressure: A first-principles study. <i>Computational Materials Science</i> , 2015, 98, 129-135.	1.4	12
11629	First-principles calculations of hydrogen solution and diffusion in tungsten: Temperature and defect-trapping effects. <i>Acta Materialia</i> , 2015, 84, 426-435.	3.8	96
11630	Metal-metal bonding in the actinide elements: Conceptual synthesis of a pure two-electron $\text{U-U}$ single bond in a constrained geometry of $\text{U}_2(\text{OH})_{10}$ . <i>Inorganica Chimica Acta</i> , 2015, 424, 267-273.	1.2	9
11631	On the solid-state NMR spectra of naproxen. <i>Chemical Physics Letters</i> , 2015, 619, 230-235.	1.2	15
11632	Strain effects on oxygen migration in perovskites. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2715-2721.	1.3	70
11633	Titanium Oxynitride Interlayer to Influence Oxygen Reduction Reaction Activity and Corrosion Stability of Pt and Pt-Ni Alloy. <i>ChemSusChem</i> , 2015, 8, 361-376.	3.6	9
11634	Influence of oxygen nonstoichiometry and doping with 2p-, 3p-, 6p- and 3d-elements on electronic structure, optical properties and photocatalytic activity of rutile and anatase: Ab initio approaches. <i>Journal of Photochemistry and Photobiology C: Photochemistry Reviews</i> , 2015, 22, 58-83.	5.6	28
11635	Elasticity of superhydrous phase, B, $\text{Mg}_{10}\text{Si}_3\text{O}_{14}(\text{OH})_4$ . <i>Physics of the Earth and Planetary Interiors</i> , 2015, 238, 42-50.	0.7	15
11636	Assessment of various density functionals for intermolecular N-H...Sn interactions: The test case of poly(trimethyltin cyanide). <i>Computational and Theoretical Chemistry</i> , 2015, 1051, 110-122.	1.1	12
11637	Thiophene derivatives as novel functional additives for high-voltage LiCoO <sub>2</sub> operations in lithium ion batteries. <i>Electrochimica Acta</i> , 2015, 151, 429-436.	2.6	56
11638	Exploring electronic transport properties of AlN nanoribbon molecular device - A first-principles investigation. <i>Solid State Sciences</i> , 2015, 39, 45-51.	1.5	15



#	ARTICLE	IF	CITATIONS
11639	Fine precipitation scenarios of AlZnMg(Cu) alloys revealed by advanced atomic-resolution electron microscopy study Part II: Fine precipitation scenarios in AlZnMg(Cu) alloys. <i>Materials Characterization</i> , 2015, 99, 142-149.	1.9	50
11640	Structure and bonding analysis of intermediate model heme-imidazole and heme-thiolate enzymes complexed with formate, acetate and nitrate: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2015, 1051, 137-143.	1.1	1
11641	First principles study of oxygen adsorption on the anatase TiO <sub>2</sub> (101) surface. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2015, 67, 59-64.	1.3	12
11642	New First Order Raman-active Modes in Few Layered Transition Metal Dichalcogenides. <i>Scientific Reports</i> , 2014, 4, 4215.	1.6	367
11643	Giant barocaloric effect enhanced by the frustration of the antiferromagnetic phase in Mn <sub>3</sub> GaN. <i>Nature Materials</i> , 2015, 14, 73-78.	13.3	226
11644	Ab-initio study of planar strain on electronic structure properties of graphene sheets with nanoholes. <i>Indian Journal of Physics</i> , 2015, 89, 23-29.	0.9	6
11645	Computational study of unsaturated and saturated cyclic (alkyl) (amino) carbene borane complexes. <i>Computational and Theoretical Chemistry</i> , 2015, 1051, 17-23.	1.1	3
11646	The defect-induced changes of the electronic and magnetic properties in the inverse Heusler alloy Ti <sub>2</sub> CoAl. <i>Journal of Solid State Chemistry</i> , 2015, 221, 311-317.	1.4	26
11647	Elastic, phonon and thermodynamic properties of ZnAl <sub>2</sub> O <sub>4</sub> and ZnAl <sub>2</sub> S <sub>4</sub> compounds from first-principles calculations. <i>Solid State Sciences</i> , 2015, 40, 7-12.	1.5	4
11648	DFT study on the adsorption and dissociation of H <sub>2</sub> on Pd <sub>n</sub> (n=4, 6, 13, 19, 55) clusters. <i>Journal of Molecular Structure</i> , 2015, 1080, 105-110.	1.8	32
11649	First principles study on the electronic and optical properties of Al- and Si-doped ZnO with GGA and mBJ approximations. <i>Optical and Quantum Electronics</i> , 2015, 47, 1869-1880.	1.5	17
11650	Recent Progresses in Understanding of Co-Based Fischer-Tropsch Catalysis by Means of Transient Kinetic Studies and Theoretical Analysis. <i>Catalysis Letters</i> , 2015, 145, 145-161.	1.4	59
11651	Formation mechanism of precipitate T1 in AlCuLi alloys. <i>Journal of Alloys and Compounds</i> , 2015, 624, 22-26.	2.8	71
11652	Structural stability and bonding nature of Li-Sn carbon nanocomposites as Li-ion battery anodes: first principles approach. <i>RSC Advances</i> , 2015, 5, 123-129.	1.7	9
11653	Theoretical studies of the pressure-induced phase transition and elastic properties of BeS. <i>Journal of Alloys and Compounds</i> , 2015, 623, 304-310.	2.8	77
11654	Calculating accurate barriers for olefin insertion and related reactions. <i>Journal of Organometallic Chemistry</i> , 2015, 775, 39-49.	0.8	56
11655	Ab initio study of Si doping effects in Pd-Ni-P bulk metallic glass. <i>Journal of Non-Crystalline Solids</i> , 2015, 409, 49-53.	1.5	7
11656	Decolorization by <i>Caldicellulosiruptor saccharolyticus</i> with dissolved hydrogen under extreme thermophilic conditions. <i>Chemical Engineering Journal</i> , 2015, 262, 847-853.	6.6	22



#	ARTICLE	IF	CITATIONS
11657	On the nature of hydrogen bonds to platinum( $\langle \text{scp} \rangle$ ) which interaction can predict their strength?. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 812-816.	1.3	22
11658	Thermodynamic modeling of the Ca-In and Ca-Sb systems supported with first-principles calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015, 48, 35-42.	0.7	8
11659	Can metal-free silicon-doped hexagonal boron nitride nanosheets and nanotubes exhibit activity toward CO oxidation?. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 888-895.	1.3	88
11660	Electronic structures and magnetism of $Rh_3Z$ ( $Z=Al, Ga, In, Si, Ge, Sn, Pb, Sb$ ) with DO 3 structures. <i>Journal of Magnetism and Magnetic Materials</i> , 2015, 378, 16-23.	1.0	44
11661	In search of an intrinsic chemical bond. <i>Computational and Theoretical Chemistry</i> , 2015, 1053, 31-37.	1.1	28
11662	Structural stability, electronic structure and mechanical properties of platinum group metal nitrides PGMN (PGM=Os, Ir, Pt). <i>International Journal of Refractory Metals and Hard Materials</i> , 2015, 48, 382-397.	1.7	3
11663	First principles treatment of structural, optical, and thermoelectric properties of $Li_7MnN_4$ as electrode for a Li secondary battery. <i>Materials Research Bulletin</i> , 2015, 61, 306-314.	2.7	2
11664	Effects of group II elements on the cold stretch formability of Mg-Zn alloys. <i>Acta Materialia</i> , 2015, 83, 294-303.	3.8	120
11665	Electronic structure and surface properties of $PrMnO_3$ (001): A density functional theory study. <i>Solid State Communications</i> , 2015, 201, 31-35.	0.9	17
11666	Vibrational and thermodynamic properties of orthorhombic $CaSnO_3$ from DFT and DFPT calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2015, 77, 85-91.	1.9	48
11667	Adsorption and diffusion of oxygen on $\hat{1}^3$ -TiAl(0 0 1) and (1 0 0) surfaces. <i>Computational Materials Science</i> , 2015, 97, 55-63.	1.4	32
11668	Effect of Ce and Cu co-doping on the structural, morphological, and optical properties of ZnO nanocrystals and first principle investigation of their stability and magnetic properties. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2015, 66, 209-220.	1.3	28
11669	Highly active $Fe_2O_3$ -doped $TiO_2$ photocatalyst for degradation of trichloroethylene in air under UV and visible light irradiation: Experimental and computational studies. <i>Applied Catalysis B: Environmental</i> , 2015, 165, 209-221.	10.8	117
11670	Adsorption of organic molecules at the $TiO_2(110)$ surface: The effect of van der Waals interactions. <i>Surface Science</i> , 2015, 632, 142-153.	0.8	57
11671	Investigations about the effect of annealing temperatures in the presence of oxygen flow on optical and electronic properties of titanium nano-layers by using Kramers-Kronig and DFT methods. <i>Materials Science in Semiconductor Processing</i> , 2015, 30, 1-8.	1.9	18
11672	Ab-initio study of the structure and thermodynamic properties of $TiSiN$ at external pressure. <i>Computational Materials Science</i> , 2015, 96, 33-38.	1.4	5
11673	The Effects of Conducting Polymers on Formic Acid Oxidation at Pt Nanoparticles. <i>Electrochimica Acta</i> , 2015, 162, 230-236.	2.6	11
11674	In situ photogenerated defects on surface-complex $BiOCl$ (0 1 0) with high visible-light photocatalytic activity: A probe to disclose the charge transfer in $BiOCl$ (0 1 0)/surface-complex system. <i>Applied Catalysis B: Environmental</i> , 2015, 163, 205-213.	10.8	60

#	ARTICLE	IF	CITATIONS
11675	First Principles Calculations on Oxide-Based Heterogeneous Catalysts and Photocatalysts: Problems and Advances. <i>Catalysis Letters</i> , 2015, 145, 80-94.	1.4	49
11676	A possible critical temperature mechanism for H blistering nucleation/dissociation in metals. <i>Solid State Communications</i> , 2015, 201, 43-48.	0.9	5
11677	Structural, optoelectronic, infrared and Raman spectra from first principles calculations of $\beta$ -Cd(OH) <sub>2</sub> . <i>Journal of Physics and Chemistry of Solids</i> , 2015, 76, 45-50.	1.9	16
11678	Generalized stacking fault in FePt nanoparticles and effects of extended defects on magnetocrystalline anisotropy energy. <i>Journal of Magnetism and Magnetic Materials</i> , 2015, 374, 525-529.	1.0	7
11679	Polar and nonpolar structures of BiCrO <sub>3</sub> from first-principles calculations. <i>Computational Materials Science</i> , 2015, 96, 219-222.	1.4	4
11680	Average structure and local configuration of excess oxygen in UO <sub>2+x</sub> . <i>Scientific Reports</i> , 2014, 4, 4216.	1.6	35
11681	Electronic properties of orthorhombic BaSn <sub>2</sub> S <sub>5</sub> single crystal. <i>Indian Journal of Physics</i> , 2015, 89, 437-443.	0.9	1
11682	The effects of stepped sites and ruthenium adatom decoration on methanol dehydrogenation over platinum-based catalyst surfaces. <i>Catalysis Today</i> , 2015, 242, 230-239.	2.2	10
11683	Heterojunction Hybrid Devices from Vapor Phase Grown MoS <sub>2</sub> . <i>Scientific Reports</i> , 2014, 4, 5458.	1.6	80
11684	Combined experimental and computational study of CO oxidation promoted by Nb in manganese oxide octahedral molecular sieves. <i>Applied Catalysis B: Environmental</i> , 2015, 163, 361-369.	10.8	46
11685	Arithmetic extraction of elastic constants of cubic crystals from first-principles calculations of stress. <i>Computational Materials Science</i> , 2015, 96, 117-123.	1.4	2
11686	Tunable Two-color Luminescence and Host-guest Energy Transfer of Fluorescent Chromophores Encapsulated in Metal-Organic Frameworks. <i>Scientific Reports</i> , 2014, 4, 4337.	1.6	119
11687	First-principles study of Si <sub>3</sub> N <sub>2</sub> . <i>Computational Materials Science</i> , 2015, 96, 140-145.	1.4	6
11688	Structural, thermodynamic, and mechanical properties of bulk La and A-La <sub>2</sub> O <sub>3</sub> . <i>Journal of Alloys and Compounds</i> , 2015, 618, 615-622.	2.8	24
11689	Ab Initio Study of Binary and Ternary Nb <sub>3</sub> (X,Y) Al <sub>15</sub> Intermetallic Phases (X,Y=Al, Ge, Si, Sn). <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2015, 46, 566-576.	1.1	29
11690	Tuning band structure and electronic transport properties of ZrN nanotube – A first-principles investigation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 1018-1026.	2.0	3
11691	Dual emission behavior of phenyleneethynylene gold(I) complexes dictated by intersystem crossing: A theoretical perspective. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 137, 259-266.	2.0	3
11692	Statistical model and first-principles simulation on concentration of He V cluster and He bubble formation in $\delta$ -Fe and W. <i>Journal of Nuclear Materials</i> , 2015, 456, 162-173.	1.3	20

#	ARTICLE	IF	CITATIONS
11693	Mechanical and thermodynamic properties of ZrO <sub>2</sub> under high-pressure phase transition: A first-principles study. <i>Journal of Alloys and Compounds</i> , 2015, 622, 504-512.	2.8	31
11694	Theoretical study of $ht-[(\text{ph})\text{Pt}(\frac{1}{4}\text{-PN})(\frac{1}{4}\text{-NP})\text{PtMe}_2](\text{CF}_3\text{CO}_2)$ structure as a heavy dimer complex and comparison of results with experimental X-ray data. <i>Arabian Journal of Chemistry</i> , 2016, 9, S259-S263.	2.3	1
11695	Theoretical investigations of interactions between boron nitride nanotubes and drugs. , 2016, , 59-77.		9
11696	Energetics, atomic structure, and magnetism of rare earth-doped GaN bulk and nanoparticles. , 2016, , 103-126.		1
11697	Atomic Scale Simulations of Relationship between Macroscopic Mechanical Properties and Microscopic Defect Evolution in Ultrafine-grained Metals. <i>Materials Transactions</i> , 2016, 57, 1476-1481.	0.4	1
11699	Theoretical and computational methods for nanoalloy structure and thermodynamics. <i>Frontiers of Nanoscience</i> , 2016, , 75-129.	0.3	7
11700	First-Principles Study of Chemical and Topological Short-Range Orders in the Mgâ€“Si Liquid Alloys. <i>Metals</i> , 2016, 6, 78.	1.0	6
11701	Pressure Prediction of Electronic, Anisotropic Elastic, Optical, and Thermal Properties of Quaternary $(\text{M}_{2/3}\text{Ti}_{1/3})_{\text{AlC}_2}$ (M = Cr, Mo, and Ti). <i>Advances in Condensed Matter Physics</i> , 2016, 2016, 1-18.	0.4	4
11702	Computational Chemistry of Zeolite Catalysis. , 2016, , 111-135.		3
11703	Interaction of Hydrogen with Au Modified by Pd and Rh in View of Electrochemical Applications. <i>Computation</i> , 2016, 4, 26.	1.0	6
11704	Pressure-Induced Phase Transition and Mechanical Properties of Mg <sub>2</sub> Sr Intermetallics. <i>Materials</i> , 2016, 9, 902.	1.3	1
11705	The Effects of Al and Ti Additions on the Structural Stability, Mechanical and Electronic Properties of D <sub>8m</sub> -Structured Ta <sub>5</sub> Si <sub>3</sub> . <i>Metals</i> , 2016, 6, 127.	1.0	6
11706	The origin of the conductivity maximum in molten salts. II. SnCl <sub>2</sub> and HgBr <sub>2</sub> . <i>Journal of Chemical Physics</i> , 2016, 145, 094504.	1.2	12
11707	Computational Tools for the Study of Biomolecules. <i>Computer Aided Chemical Engineering</i> , 2016, , 583-648.	0.3	7
11708	Enhanced photocatalytic activity of anatase-TiO <sub>2</sub> nanoparticles by fullerene modification: A theoretical and experimental study. <i>Applied Surface Science</i> , 2016, 387, 750-758.	3.1	95
11709	Robust vanadium pentoxide electrodes for sodium and calcium ion batteries: thermodynamic and diffusion mechanical insights. <i>Journal of Materials Chemistry A</i> , 2016, 4, 12516-12525.	5.2	26
11710	$\langle \text{DFT} \rangle$ Predictions of Crystal Structure, Electronic Structure, Compressibility, and Elastic Properties of Hfâ€“Alâ€“C Carbides. <i>Journal of the American Ceramic Society</i> , 2016, 99, 3449-3457.	1.9	22
11711	Lithium-Ion Model Behavior in an Ethylene Carbonate Electrolyte Using Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , 2016, 120, 16322-16332.	1.5	83

#	ARTICLE	IF	CITATIONS
11712	Synthesis of C <sub>4</sub> and C <sub>8</sub> Chemicals from Ethanol on MgO-Incorporated Faujasite Catalysts with Balanced Confinement Effects and Basicity. <i>ChemSusChem</i> , 2016, 9, 736-748.	3.6	27
11714	Understanding the Structural Evolution and Redox Mechanism of a NaFeO <sub>2</sub> -NaCoO <sub>2</sub> Solid Solution for Sodium-Ion Batteries. <i>Advanced Functional Materials</i> , 2016, 26, 6047-6059.	7.8	132
11715	Enhanced Catalytic Activity in Liquid-Exfoliated FeOCl Nanosheets as a Fenton-Like Catalyst. <i>Chemistry - A European Journal</i> , 2016, 22, 9321-9329.	1.7	59
11716	Formation of Oxazoles from Elusive Gold(I) $\pi$ -Oxocarbenes: A Mechanistic Study. <i>Chemistry - A European Journal</i> , 2016, 22, 9827-9834.	1.7	33
11717	Nitrogen-Rich Manganese Oxynitrides with Enhanced Catalytic Activity in the Oxygen Reduction Reaction. <i>Angewandte Chemie</i> , 2016, 128, 8095-8099.	1.6	8
11718	DFT Study of Synergistic Catalysis of the Water-Gas-Shift Reaction on Cu-Au Bimetallic Surfaces. <i>ChemCatChem</i> , 2016, 8, 1208-1217.	1.8	14
11719	Predicting the electronic and optical properties of IB metals doped monoclinic BiVO <sub>4</sub> : First principle calculations. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 388-395.	1.0	12
11720	H <sub>2</sub> S adsorption and decomposition on the gradually reduced $\gamma$ -Fe <sub>2</sub> O <sub>3</sub> (001) surface: A DFT study. <i>Applied Surface Science</i> , 2016, 387, 720-731.	3.1	53
11721	Electrostatic surface potential analysis of the $\gamma$ -Fe <sub>2</sub> O <sub>3</sub> (001) surface: A DFT study. <i>Applied Surface Science</i> , 2016, 387, 720-731.		
11721	ion in the gas phase, the condensed phase and a novel extrapolation to the solid state. <i>Computational and Theoretical Chemistry</i> , 2016, 1090, 225-233.		
11722	First-Principles Study on Doping of SnSe <sub>2</sub> Monolayers. <i>ChemPhysChem</i> , 2016, 17, 375-379.	1.0	30
11723	Strongly Enhanced Long-Lived Persistent Room Temperature Phosphorescence Based on the Formation of Metal-Organic Hybrids. <i>Advanced Optical Materials</i> , 2016, 4, 897-905.	3.6	241
11724	Sampling free energy surfaces as slices by combining umbrella sampling and metadynamics. <i>Journal of Computational Chemistry</i> , 2016, 37, 1413-1424.	1.5	36
11725	Electro-optical properties of the perfect reflector material: Poly(3-thiophene boronic acid) semiconducting polymer. <i>Polymer Engineering and Science</i> , 2016, 56, 707-714.	1.5	2
11726	Transient spectroscopic characterization of the ring-opening reaction of tetrahydrochromeno[2,3-dimethyl]indole. <i>Journal of Physical Organic Chemistry</i> , 2016, 29, 221-226.	0.9	0
11727	Hexagonal FeS nanosheets with high-energy (001) facets: Counter electrode materials superior to platinum for dye-sensitized solar cells. <i>Nano Research</i> , 2016, 9, 2862-2874.	5.8	38
11728	Novel fluorine-free 2,2-bis(4,5-dimethylimidazole) additive for lithium-ion poly(methyl methacrylate) solid polymer electrolytes. <i>RSC Advances</i> , 2016, 6, 67150-67156.	1.7	15
11729	Dendrite-Free Lithium Deposition Induced by Uniformly Distributed Lithium Ions for Efficient Lithium Metal Batteries. <i>Advanced Materials</i> , 2016, 28, 2888-2895.	11.1	877
11730	Insight into the effect of surface structure on H <sub>2</sub> adsorption and activation over different CuO(1 1 1) surfaces: A first-principle study. <i>Computational Materials Science</i> , 2016, 122, 191-200.	1.4	27

#	ARTICLE	IF	CITATIONS
11731	First-principles study of vacancy, interstitial, noble gas atom interstitial and vacancy clusters in bcc-W. <i>Computational Materials Science</i> , 2016, 123, 121-130.	1.4	54
11732	Effects of chemical substitution on the structural and optical properties of $\text{Li}_{1-x}\text{Ag}_x\text{Ni}_x\text{WO}_4$ (0 ≤ x ≤ 0.08) solid solutions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21966-21975.	1.3	24
11733	Mechanism of Oxygen Vacancy on Impeded Phase Transformation and Electrochemical Activation in Inactive $\text{Li}_2\text{MnO}_3$ . <i>ChemElectroChem</i> , 2016, 3, 943-949.	1.7	44
11734	Skin Bond Electron Relaxation Dynamics of Germanium Manipulated by Interactions with $\text{H}_2$ , $\text{O}_2$ , $\text{H}_2\text{O}$ , $\text{H}_2\text{O}_2$ , HF, and Au. <i>ChemPhysChem</i> , 2016, 17, 310-316.	1.0	5
11735	$\text{Sr}_2\text{Pd}_4\text{Al}_5$ : Synthesis, Crystal and Electronic Structures, and Chemical Bonding of a Polar Intermetallic Compound. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 1108-1114.	1.0	8
11736	$\text{TiO}$ , a Novel Stable Polymorph of Titanium Monoxide. <i>Angewandte Chemie</i> , 2016, 128, 1684-1689.	1.6	3
11737	Variation of Band Gap and Lattice Parameters of $\text{Al}_x\text{Ga}_{1-x}\text{O}_3$ Powder Produced by Solution Combustion Synthesis. <i>Journal of the American Ceramic Society</i> , 2016, 99, 2467-2473.	1.9	87
11738	Rock-salt structure lithium deuteride formation in liquid lithium with high-concentrations of deuterium: a first-principles molecular dynamics study. <i>Nuclear Fusion</i> , 2016, 56, 016020.	1.6	10
11739	Gold deposited on a $\text{Ge}(0001)$ surface: DFT calculations. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 435001.	0.7	0
11740	First-principles study of the structural and dynamic properties of the liquid and amorphous $\text{Li-Si}$ alloys. <i>Journal of Chemical Physics</i> , 2016, 144, 034502.	1.2	16
11741	Mechanical properties of bimetallic one-dimensional structures. <i>Proceedings of SPIE</i> , 2016, . .	0.8	0
11742	Modeling surface motion effects in $\text{N}_2$ dissociation on $\text{W}(110)$ : Ab initio molecular dynamics calculations and generalized Langevin oscillator model. <i>Journal of Chemical Physics</i> , 2016, 144, 244708.	1.2	19
11743	Effect of Alloying Element X on Transformation Strains and Phase Stabilities between $\alpha'$ and $\beta$ ; Ti-Nb-X (X = Al, Sn, Zr, Ta) Ternary Alloys from First-Principles Calculations. <i>Materials Transactions</i> , 2016, 57, 263-268.	0.4	9
11744	Controlling Factors for the Formation of Guinier-Preston Zones in Al-Cu Alloys: An Atomistic Study. <i>Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals</i> , 2016, 80, 575-584.	0.2	8
11745	Ab initio calculation study on the site of hydrogen in $\text{Al-Zn-Mg}$ alloys. <i>Keikinzoiku/Journal of Japan Institute of Light Metals</i> , 2016, 66, 339-344.	0.1	1
11746	Searching for Highly Active Catalysts for Hydrogen Evolution Reaction Based on O-Terminated MXenes through a Simple Descriptor. <i>Chemistry of Materials</i> , 2016, 28, 9026-9032.	3.2	247
11747	Theoretical Study of the Structural, Energetic, and Electronic Properties of 55-Atom Metal Nanoclusters: A DFT Investigation within van der Waals Corrections, Spin-Orbit Coupling, and PBE+U of 42 Metal Systems. <i>Journal of Physical Chemistry C</i> , 2016, 120, 28844-28856.	1.5	75
11748	Mapping the electrostatic force field of single molecules from high-resolution scanning probe images. <i>Nature Communications</i> , 2016, 7, 11560.	5.8	95

#	ARTICLE	IF	CITATIONS
11749	Platinum single-atom and cluster catalysis of the hydrogen evolution reaction. <i>Nature Communications</i> , 2016, 7, 13638.	5.8	1,521
11750	Strain-induced quasi-one-dimensional rare-earth silicide structures on Si(111). <i>Physical Review B</i> , 2016, 94, .	1.1	9
11751	<i>Ab initio</i> study of deformed As, Sb, and Bi with an application to thin films. <i>Physical Review B</i> , 2016, 94, .	1.1	11
11752	Spintronic and Electronic Phenomena in Organic Molecules Measured with $\frac{1}{4}$ SR. <i>Journal of the Physical Society of Japan</i> , 2016, 85, 091011.	0.7	7
11753	Insights on finite size effects in <i>ab initio</i> study of CO adsorption and dissociation on Fe 110 surface. <i>Journal of Applied Physics</i> , 2016, 120, .	1.1	18
11754	Communication: Near-locality of exchange and correlation density functionals for 1- and 2-electron systems. <i>Journal of Chemical Physics</i> , 2016, 144, 191101.	1.2	20
11755	Self-consistent implementation of meta-GGA functionals for the ONETEP linear-scaling electronic structure package. <i>Journal of Chemical Physics</i> , 2016, 145, 204114.	1.2	18
11756	Phonon-mediated superconductivity in borophenes. <i>Applied Physics Letters</i> , 2016, 108, .	1.5	83
11757	Influence of surface vacancy defects on the carburisation of Fe 110 surface by carbon monoxide. <i>Journal of Chemical Physics</i> , 2016, 145, 044710.	1.2	12
11758	Electron-hole pair effects in methane dissociative chemisorption on Ni(111). <i>Journal of Chemical Physics</i> , 2016, 145, 044704.	1.2	51
11759	First-principles study of structure, initial lattice expansion, and pressure-composition-temperature hysteresis for substituted $\text{LaNi}_5$ and $\text{TiMn}_2$ alloys. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2016, 24, 085007.	0.8	8
11760	Tuning the charge states of $\text{CrW}_2\text{O}_9$ clusters deposited on perfect and defective $\text{MgO}(001)$ surfaces with different color centers: A comprehensive DFT study. <i>Journal of Chemical Physics</i> , 2016, 144, 174706.	1.2	4
11761	Magnetic ordering temperature of nanocrystalline Gd: enhancement of magnetic interactions via hydrogenation-induced negative pressure. <i>Scientific Reports</i> , 2016, 6, 22553.	1.6	37
11762	On the small angle twist sub-grain boundaries in $\text{Ti}_3\text{AlC}_2$ . <i>Scientific Reports</i> , 2016, 6, 23943.	1.6	8
11763	Interaction of methanol and its dehydrogenation species with Pt-alloy surfaces. <i>AIP Conference Proceedings</i> , 2016, , .	0.3	1
11764	Effective optical constants of silver nanofilms calculated in wide frequency range. <i>Proceedings of SPIE</i> , 2016, , .	0.8	1
11765	Pressure dependence of band-gap and phase transitions in bulk $\text{CuX}$ ( $X = \text{Cl}, \text{Br}, \text{I}$ ). <i>AIP Conference Proceedings</i> , 2016, , .	0.3	1
11766	First-principles study on the half-metallic properties of the d0 quaternary Heusler compounds: $\text{KCaCBr}$ and $\text{KCaCl}$ . <i>AIP Advances</i> , 2016, 6, 105308.	0.6	10



#	ARTICLE	IF	CITATIONS
11767	Structure and optical properties of aSiAl and aSiAlH <sub>x</sub> magnetron sputtered thin films. APL Materials, 2016, 4, .	2.2	8
11768	Application of van der Waals functionals to the calculation of dissociative adsorption of N <sub>2</sub> on W(110) for static and dynamic systems. Journal of Chemical Physics, 2016, 144, 084702.	1.2	12
11769	Crystallographic and optical properties and band structures of CuInSe <sub>2</sub> , CuIn <sub>3</sub> Se <sub>5</sub> , and CuIn <sub>5</sub> Se <sub>8</sub> phases in Cu-poor Cu <sub>2</sub> Se-In <sub>2</sub> Se <sub>3</sub> pseudo-binary system. Japanese Journal of Applied Physics, 2016, 55, 04ES15.	0.8	59
11770	Understanding the Formation Mechanism of Two-Dimensional Atomic Islands on Crystal Surfaces by the Condensing Potential Model. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2016, 71, 321-324.	0.7	0
11771	CO adsorption on small Au <sub>n</sub> ( <i>n</i> = 1-4) structures supported on hematite. I. Adsorption on iron terminated Fe <sub>2</sub> O <sub>3</sub> (0001) surface. Journal of Chemical Physics, 2016, 144, 044704.	1.2	10
11772	Zero-Kelvin Compression Isotherms of the Elements 1 % Z % 92 to 100 GPa. Journal of Physical and Chemical Reference Data, 2016, 45, .	1.9	28
11773	The LDA+U calculation of electronic band structure of GaAs. AIP Conference Proceedings, 2016, , .	0.3	2
11774	Self-interaction corrections applied to Mg-porphyrin, C60, and pentacene molecules. Journal of Chemical Physics, 2016, 144, 164117.	1.2	34
11775	Electronic structure of cubic ScF <sub>3</sub> from first-principles calculations. Low Temperature Physics, 2016, 42, 556-560.	0.2	9
11776	A computational ab initio study of surface diffusion of sulfur on the CdTe (111) surface. AIP Advances, 2016, 6, 085002.	0.6	1
11777	Effect of Organic Cations on Hydrogen Oxidation Reaction of Carbon Supported Platinum. Journal of the Electrochemical Society, 2016, 163, F1503-F1509.	1.3	29
11778	A Database of the Structural and Electronic Properties of Prussian Blue, Prussian White, and Berlin Green Compounds through Density Functional Theory. Inorganic Chemistry, 2016, 55, 12851-12862.	1.9	92
11779	Enhancing Sodium Ion Battery Performance by Strongly Binding Nanostructured Sb <sub>2</sub> S <sub>3</sub> on Sulfur-Doped Graphene Sheets. ACS Nano, 2016, 10, 10953-10959.	7.3	344
11780	Calibrating Reaction Enthalpies: Use of Density Functional Theory and the Correlation Consistent Composite Approach in the Design of Photochromic Materials. Journal of Physical Chemistry A, 2016, 120, 9982-9997.	1.1	6
11781	Electric-field-driven magnetization switching and nonlinear magnetoelasticity in Au/FeCo/MgO heterostructures. Scientific Reports, 2016, 6, 29815.	1.6	48
11782	Density functional theory study of lithium diffusion at the interface between olivine-type LiFePO <sub>4</sub> and LiMnPO <sub>4</sub> . Journal Physics D: Applied Physics, 2016, 49, 505601.	1.3	13
11783	Electron mean free path in elemental metals. Journal of Applied Physics, 2016, 119, .	1.1	630
11784	Effect of transition metal impurities on the strength of grain boundaries in vanadium. Journal of Applied Physics, 2016, 120, .	1.1	16



#	ARTICLE	IF	CITATIONS
11785	Insight into the effect of surface coverage and structure over different Co surfaces on the behaviors of H <sub>2</sub> adsorption and activation. International Journal of Hydrogen Energy, 2016, 41, 23022-23032.	3.8	9
11786	Rungs 1 to 4 of DFT Jacob's ladder: Extensive test on the lattice constant, bulk modulus, and cohesive energy of solids. Journal of Chemical Physics, 2016, 144, 204120.	1.2	191
11787	Enhanced superconductivity by strain and carrier-doping in borophene: A first principles prediction. Applied Physics Letters, 2016, 109, .	1.5	105
11788	Electronic structure and thermoelectric properties of half-Heusler compounds with eight electron valence count KScX (X = C and Ge). Journal of Applied Physics, 2016, 119, .	1.1	31
11789	Electronic structures and edge effects of Ga <sub>2</sub> S <sub>2</sub> nanoribbons. Chinese Physics B, 2016, 25, 107101.	0.7	1
11790	Quantum chemistry mechanism study on preventing slag bonding via modifying the material surface properties. Asia-Pacific Journal of Chemical Engineering, 2016, 11, 874-883.	0.8	5
11791	Analyzing relationships between surface perturbations and local chemical reactivity of metal sites: Alkali promotion of O <sub>2</sub> dissociation on Ag(111). Journal of Chemical Physics, 2016, 144, 234704.	1.2	13
11792	The magnetism and spin-dependent electronic transport properties of boron nitride atomic chains. Journal of Chemical Physics, 2016, 145, 044301.	1.2	9
11793	Communication: Simple and accurate uniform electron gas correlation energy for the full range of densities. Journal of Chemical Physics, 2016, 145, 021101.	1.2	41
11794	The electronic, structural and magnetic properties of La <sup>1/3</sup> Sr <sup>1/3</sup> MnO <sub>3</sub> film with oxygen vacancy: a first principles investigation. Scientific Reports, 2016, 6, 22422.	1.6	4
11795	Thermal equation of state of silicon carbide. Applied Physics Letters, 2016, 108, .	1.5	33
11796	DFT-D2 simulations of water adsorption and dissociation on the low-index surfaces of mackinawite (FeS). Journal of Chemical Physics, 2016, 144, 174704.	1.2	33
11797	Direct-to-indirect bandgap transitions in $\alpha$ -silicon nanowires. Journal of Applied Physics, 2016, 119, .	1.1	18
11798	Perspective: How good is DFT for water?. Journal of Chemical Physics, 2016, 144, 130901.	1.2	571
11799	Mechanism of stabilization and magnetization of impurity-doped zigzag graphene nanoribbons. Journal of Applied Physics, 2016, 120, .	1.1	6
11800	Phthalocyanine adsorption on Au(110): 1D ordering and adaptive reconstruction. Journal of Physics Condensed Matter, 2016, 28, 434001.	0.7	4
11801	Pressure-induced phase transitions in the $\text{CdC}_2\text{S}_4$ spinel. Physical Review B, 2016, 94, .	1.1	16
11803	Energy band gap and spectroscopic studies in $\text{Mn}^{1-x}\text{Cu}_x\text{WO}_4$ (0 ≤ x ≤ 0.125). AIP Conference Proceedings, 2016, .	0.3	0

#	ARTICLE	IF	CITATIONS
11804	Investigating the effects of phosphorus in a binary-phase TiAl-Ti3Al alloy by first-principles: from site preference, interfacial energetics to mechanical properties. <i>European Physical Journal B</i> , 2016, 89, 1.	0.6	2
11805	The first-principles study of Al <sub>12</sub> X (X = Sc-Zn) clusters and their adsorption of H, O and N. <i>AIP Advances</i> , 2016, 6, .	0.6	6
11806	LCAO-based theoretical study of PbTiO <sub>3</sub> crystal to search for parity and time reversal violating interaction in solids. <i>Journal of Chemical Physics</i> , 2016, 145, 054115.	1.2	26
11807	Synthesis of Functional Ionic Liquids and their Application for the Direct Saccharification of Cellulose. <i>Journal of Chemical Engineering of Japan</i> , 2016, 49, 466-474.	0.3	6
11808	Ligand effects on the structure and vibrational properties of the thiolated Au <sub>18</sub> cluster. <i>Progress in Natural Science: Materials International</i> , 2016, 26, 510-515.	1.8	25
11809	Alloying effects of refractory elements in the dislocation of Ni-based single crystal superalloys. <i>Progress in Natural Science: Materials International</i> , 2016, 26, 636-642.	1.8	6
11810	Cohesive energy and structural parameters of binary oxides of groups IIA and IIIB from diffusion quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2016, 144, 174707.	1.2	36
11811	Hydrocarbon adsorption in an aqueous environment: A computational study of alkyls on Cu(111). <i>Journal of Chemical Physics</i> , 2016, 145, 074702.	1.2	20
11812	Reaction paths of phosphine dissociation on silicon (001). <i>Journal of Chemical Physics</i> , 2016, 144, 014705.	1.2	36
11813	Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. <i>Journal of Chemical Physics</i> , 2016, 145, 234306.	1.2	25
11814	BH-DFTB/DFT calculations for iron clusters. <i>AIP Advances</i> , 2016, 6, .	0.6	22
11815	Magnetism in molybdenum disulphide monolayer with sulfur substituted by 3d transition metals. <i>Journal of Applied Physics</i> , 2016, 120, 144305.	1.1	11
11816	Ferroelasticity and domain physics in two-dimensional transition metal dichalcogenide monolayers. <i>Nature Communications</i> , 2016, 7, 10843.	5.8	125
11817	In-situ real-space imaging of single crystal surface reconstructions via electron microscopy. <i>Applied Physics Letters</i> , 2016, 109, 201601.	1.5	17
11818	Infrared absorption of 1-chloro-2-methyl-2-propyl [ $\dot{\text{a}}\dots\text{C}(\text{CH}_3)_2\text{CH}_2\text{Cl}$ ] and 2-chloro-2-methylpropyl [ $\dot{\text{a}}\dots\text{CH}_2\text{C}(\text{CH}_3)_2\text{Cl}$ ] radicals produced in the addition reactions of Cl with isobutene ( <i>i</i> -C <sub>4</sub> H <sub>8</sub> ) in solid <i>i</i> -hydrogen. <i>Journal of Chemical Physics</i> , 2016, 145, 134302.	1.2	4
11819	Locality of correlation in density functional theory. <i>Journal of Chemical Physics</i> , 2016, 145, 054112.	1.2	35
11820	Density-Functional Study of the La <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> (001) and (011) Surfaces and Bulk. <i>Journal of Physical Chemistry C</i> , 2016, 120, 7522-7531.	1.5	11
11821	Uncovering the Roles of Oxygen in Cr(III) Photoredox Catalysis. <i>Journal of the American Chemical Society</i> , 2016, 138, 5451-5464.	6.6	131

#	ARTICLE	IF	CITATIONS
11822	Carbene-mediated self-assembly of diamondoids on metal surfaces. <i>Nanoscale</i> , 2016, 8, 8966-8975.	2.8	20
11823	Access to highly active Niâ€‘Pd bimetallic nanoparticle catalysts for Câ€‘C coupling reactions. <i>Catalysis Science and Technology</i> , 2016, 6, 5567-5579.	2.1	73
11824	Boron diffusion in bcc-Fe studied by first-principles calculations. <i>Chinese Physics B</i> , 2016, 25, 036601.	0.7	8
11825	A dataset of highly accurate homolytic NiË;Br bond dissociation energies obtained by Means of W2 theory. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 52-60.	1.0	28
11826	Evaluation of modern DFT functionals and G3n-RAD composite methods in the modelization of organic singlet diradicals. <i>Journal of Molecular Modeling</i> , 2016, 22, 76.	0.8	12
11827	Selenideâ€‘Based Electrocatalysts and Scaffolds for Water Oxidation Applications. <i>Advanced Materials</i> , 2016, 28, 77-85.	11.1	544
11828	Phase diagram and physical properties of iridium tetraboride from first principles. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 12569-12575.	1.3	15
11829	Catalytic water dissociation by greigite Fe <sub>3</sub> S <sub>4</sub> surfaces: density functional theory study. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2016, 472, 20160080.	1.0	17
11830	Cationic half-sandwich Ru(II) complexes containing (N,N)-bound Schiff-base ligands: Synthesis, crystal structure analysis and spectroscopic studies. <i>Journal of Molecular Structure</i> , 2016, 1118, 48-55.	1.8	3
11831	Early Oxidation Processes on the Greigite Fe<sub>3</sub>S<sub>4</sub>(001) Surface by Water: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2016, 120, 8616-8629.	1.5	32
11832	Bicarbonate Hydrogenation Catalyzed by Iron: How the Choice of Solvent Can Reverse the Reaction. <i>ACS Catalysis</i> , 2016, 6, 2923-2929.	5.5	29
11833	Theoretical Study of Hydrogenation Catalysis of Phosphorus Compound and Prediction of Catalyst with High Activity and Wide Application Scope. <i>ACS Catalysis</i> , 2016, 6, 4859-4870.	5.5	26
11834	First principles study of the open-framework compound [Me 4 N] 2 Mn[Sn 4 Se 10 ]: Magnetic and half-metallic properties. <i>Chinese Journal of Physics</i> , 2016, 54, 379-384.	2.0	1
11835	Hybrid density functional studies of C-anion-doped anatase TiO2. <i>Chemical Physics Letters</i> , 2016, 650, 19-28.	1.2	11
11836	Microalloying-induced large plasticity in La-Al-C bulk metallic glass. <i>Journal of Non-Crystalline Solids</i> , 2016, 447, 55-58.	1.5	2
11837	First-principles calculations of structural, elastic, and electronic properties of trigonal ZnSnO3 under pressure. <i>Materials Chemistry and Physics</i> , 2016, 180, 75-81.	2.0	24
11838	Chemisorption of oxygen and subsequent reactions on low index surfaces of Î²â€‘Mo2C: Insights from first-principles thermodynamics and kinetics. <i>Journal of Molecular Catalysis A</i> , 2016, 417, 53-63.	4.8	12
11839	Crystal structures, DFT calculations and Hirshfeld surface analyses of three new cobalt(III) Schiff base complexes derived from meso-1,2-diphenyl-1,2-ethylenediamine. <i>Journal of Molecular Structure</i> , 2016, 1122, 123-133.	1.8	27

#	ARTICLE	IF	CITATIONS
11840	Electric field effects on the electronic properties of the silicene-amine interface. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15639-15644.	1.3	6
11841	Hydrogen bonding at C=Se acceptors in selenoureas, selenoamides and selones. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 317-325.	0.5	23
11842	Adsorption of some important tautomers of 5-amino tetrazole on the (001) and (101) surfaces of anatase: Theoretical study. <i>Journal of Molecular Structure</i> , 2016, 1121, 203-214.	1.8	6
11843	Theoretical study of stability and reaction mechanism of CuO supported on ZrO <sub>2</sub> during chemical looping combustion. <i>Applied Surface Science</i> , 2016, 367, 485-492.	3.1	55
11844	Theoretical insight into the enhanced CH <sub>4</sub> desorption via H <sub>2</sub> O adsorption on different rank coal surfaces. <i>Journal of Energy Chemistry</i> , 2016, 25, 677-682.	7.1	30
11845	An ab initio molecular dynamics study of D <sub>2</sub> dissociation on CO-precovered Ru(0001). <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21190-21201.	1.3	3
11846	Structural, electronic, elastic, optical, and vibrational properties of HfXSb (X=Co, Rh, Ru) half-Heusler compounds: an ab initio study. <i>Indian Journal of Physics</i> , 2016, 90, 1233-1241.	0.9	20
11847	On the adaptability of 1/1 cubic approximant structure in the Mg-Al-Zn system with the particular example of Mg <sub>32</sub> Al <sub>12</sub> Zn <sub>37</sub> . <i>Journal of Alloys and Compounds</i> , 2016, 656, 159-165.	2.8	9
11848	Field emission properties of Ge-doped GaN nanowires. <i>Journal of Alloys and Compounds</i> , 2016, 681, 324-329.	2.8	14
11849	First-principles simulation on Seebeck coefficient in silicon and silicon carbide nanosheets. <i>Japanese Journal of Applied Physics</i> , 2016, 55, 06GJ07.	0.8	5
11850	Density Functional Theory. <i>Graduate Texts in Physics</i> , 2016, , 99-110.	0.1	1
11851	DRIFT and DFT study of cerium addition on SO <sub>2</sub> of Manganese-based Catalysts for low temperature SCR. <i>Journal of Molecular Catalysis A</i> , 2016, 421, 102-108.	4.8	113
11852	Sr <sub>2</sub> SmNbO <sub>6</sub> perovskite: Synthesis, characterization and density functional theory calculations. <i>Materials Chemistry and Physics</i> , 2016, 179, 55-64.	2.0	14
11853	Exchange-Correlation Functionals via Local Interpolation along the Adiabatic Connection. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2598-2610.	2.3	40
11854	Electronic structure of Mn <sub>0.25</sub> TaS <sub>2</sub> . <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2016, 208, 74-77.	0.8	1
11855	Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12530-12538.	1.5	25
11856	The charge states of Au on gold-substituted Ce <sub>1-x</sub> O <sub>2</sub> (111) surfaces with multiple oxygen vacancies. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15884-15893.	1.3	16
11857	The terahertz spectroscopic investigation and vibration analysis of triadimefon. <i>Proceedings of SPIE</i> , 2016, , .	0.8	0

#	ARTICLE	IF	CITATIONS
11858	Doped penta-graphene and hydrogenation of its related structures: a structural and electronic DFT-D study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15505-15509.	1.3	37
11859	<i>In situ</i> growth of Ag nanoparticles on $\text{Ag}_2\text{WO}_4$ under electron irradiation: probing the physical principles. <i>Nanotechnology</i> , 2016, 27, 225703.	1.3	30
11860	Synergistic Effects in Bimetallic Palladium-Copper Catalysts Improve Selectivity in Oxygenate Coupling Reactions. <i>Journal of the American Chemical Society</i> , 2016, 138, 6805-6812.	6.6	94
11861	<i>Ab initio</i> threshold displacement energies in iron. <i>Materials Research Letters</i> , 2016, 4, 219-225.	4.1	68
11862	Asymmetric mixing behavior and stability of the predicted phases in the W-Cu system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2016, 53, 116-121.	0.7	9
11863	Efficacies of dopants in thermoelectric BiOCuSe. <i>Materials Chemistry and Physics</i> , 2016, 177, 73-78.	2.0	5
11864	First-Principles Kinetic Study on the Effect of the Zeolite Framework on 1-Butanol Dehydration. <i>ACS Catalysis</i> , 2016, 6, 4081-4094.	5.5	44
11865	Interlayer coupling in two-dimensional titanium carbide MXenes. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20256-20260.	1.3	120
11866	An Efficient Strategy for Controlled Band Gap Engineering of $\text{KTaO}_3$ . <i>Journal of Physical Chemistry C</i> , 2016, 120, 6920-6929.	1.5	63
11867	Hydrogen sensitive field-effect transistor based on germanene nanoribbon and optical properties of hydrogenated germanene. <i>Journal of Computational Electronics</i> , 2016, 15, 381-388.	1.3	16
11868	How Much Can Density Functional Approximations (DFA) Fail? The Extreme Case of the $\text{FeO}_4$ Species. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1525-1533.	2.3	33
11869	<i>Ab initio</i> study of energetics and magnetism of sigma phase in Co-Mo and Fe-Mo systems. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2016, 24, 025009.	0.8	7
11870	Graphene Monoxide Bilayer As a High-Performance on/off Switching Media for Nanoelectronics. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 10477-10482.	4.0	10
11871	DFT Insights into the Competitive Adsorption of Sulfur- and Nitrogen-Containing Compounds and Hydrocarbons on Co-Promoted Molybdenum Sulfide Catalysts. <i>ACS Catalysis</i> , 2016, 6, 2904-2917.	5.5	66
11872	Thermoelectric properties of SnSe nanoribbons: a theoretical aspect. <i>Materials Research Express</i> , 2016, 3, 035013.	0.8	13
11873	Hydrogen storage in Li-doped fullerene-intercalated hexagonal boron nitrogen layers. <i>Frontiers of Physics</i> , 2016, 11, 1.	2.4	15
11874	Theoretical analysis of the combined effects of sulfur vacancies and analyte adsorption on the electronic properties of single-layer $\text{MoS}_2$ . <i>Nanotechnology</i> , 2016, 27, 185701.	1.3	55
11875	Theoretical and experimental study of the phase formation for $\text{Ti}_2\text{YAl}$ and $\text{Ti}_2\text{Y}\hat{=}\text{Ga}$ ( $\text{Y}=\text{Co, Fe; Y}=\text{Cr, Fe}$ ). <i>Intermetallics</i> , 2016, 73, 26-30.	1.8	49

#	ARTICLE	IF	CITATIONS
11876	Spectral properties of bisphenol F based on quantum chemical calculations. <i>Vacuum</i> , 2016, 128, 198-204.	1.6	7
11877	A PW91-like exchange with a simple analytical form. <i>Chemical Physics Letters</i> , 2016, 651, 268-273.	1.2	16
11878	On the Potential of Using the Al <sub>7</sub> Superatom as an Excess Electron Acceptor To Construct Materials with Excellent Nonlinear Optical Properties. <i>Inorganic Chemistry</i> , 2016, 55, 4421-4427.	1.9	18
11879	First-principles modeling of 3 <i>d</i> -transition-metal-atom adsorption on silicene: a linear-response DFT+U approach. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 135301.	0.7	13
11880	Hydrostatic pressure driven spin, volume and band gap collapses in SmFeO <sub>3</sub> : a GGA + U study. <i>Philosophical Magazine</i> , 2016, 96, 1613-1622.	0.7	6
11881	Hydrogen effect on electronic and magnetic properties of Cd <sub>1-x</sub> MnxTe: Ab initio study. <i>Solid State Communications</i> , 2016, 239, 44-48.	0.9	4
11882	Synthesis and structure of dithizonato complexes of antimony(III), copper(II) and tin(IV). <i>Journal of Coordination Chemistry</i> , 2016, 69, 788-800.	0.8	4
11883	High catalytic activity of oxygen-induced (200) surface of Ta <sub>2</sub> O <sub>5</sub> nanolayer towards durable oxygen evolution reaction. <i>Nano Energy</i> , 2016, 25, 60-67.	8.2	36
11884	Computational Investigation of Fe-Cu Bimetallic Catalysts for CO <sub>2</sub> Hydrogenation. <i>Journal of Physical Chemistry C</i> , 2016, 120, 9364-9373.	1.5	49
11885	Interaction between single vacancies in graphene sheet: An ab initio calculation. <i>Solid State Communications</i> , 2016, 240, 5-9.	0.9	11
11886	Global hybrid exchange energy functional with correct asymptotic behavior of the corresponding potential. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	7
11887	Enhancing performance of PEM fuel cells: Using the Au nanoplatelet/Nafion interface to enable CO oxidation under ambient conditions. <i>Journal of Catalysis</i> , 2016, 339, 31-37.	3.1	14
11888	The nature of M-PNR2 bonds in the electrophilic phosphinidene complexes [(L)(CO) <sub>3</sub> M{PNR <sub>2</sub> }] <sup>+</sup> (L = Tj ETQqO O 0 rgBT /Overlock 10 T Organometallic Chemistry, 2016, 813, 84-94.	0.8	3
11889	Cation synergies affect ammonia adsorption over VOX and (V,W)OX dispersed on $\hat{\pm}$ -Al <sub>2</sub> O <sub>3</sub> (0001) and $\hat{\pm}$ -Fe <sub>2</sub> O <sub>3</sub> (0001). <i>Surface Science</i> , 2016, 651, 41-50.	0.8	7
11890	Computational Study of Excess Electron Mobility in High-Pressure Liquid Benzene. <i>Journal of Physical Chemistry C</i> , 2016, 120, 8490-8501.	1.5	27
11891	A broken-symmetry density functional study of structures, energies, and protonation states along the catalytic O-H bond cleavage pathway in ba <sub>3</sub> cytochrome c oxidase from <i>Thermus thermophilus</i> . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21162-21171.	1.3	21
11892	Equation of state for technetium from X-ray diffraction and first-principle calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2016, 95, 6-11.	1.9	5
11893	Development of a second-nearest-neighbor modified embedded atom method potential for silicon-phosphorus binary system. <i>Computational Materials Science</i> , 2016, 120, 1-12.	1.4	5



#	ARTICLE	IF	CITATIONS
11894	First-principles study of the effect of boron on grain boundary in NiAl. Computational Materials Science, 2016, 121, 1-5.	1.4	10
11895	First-Principles studies of silicon underpotential deposition on defective graphene and its relevance for lithium-ion battery materials. Electrochimica Acta, 2016, 208, 92-101.	2.6	14
11896	Stationary Full Li-Ion Batteries with Interlayer-Expanded V6O13 Cathodes and Lithiated Graphite Anodes. Electrochimica Acta, 2016, 203, 171-177.	2.6	42
11897	Ab initio study of the structural and electronic properties of Nb2AlC. Computational Condensed Matter, 2016, 6, 1-4.	0.9	5
11898	Chemisorption of Acetophenone on Si(111)-7 Å <sup>2</sup> 7. Polar Aromatic Molecule on Electronically Complex Surface. Journal of Physical Chemistry C, 2016, 120, 9200-9206.	1.5	2
11899	First-principles study of Mn alloying into Fe3AlC: Towards the improvement of ductility. Journal of Alloys and Compounds, 2016, 681, 283-292.	2.8	6
11900	Control of valence and conduction band energies in layered transition metal phosphates via surface functionalization. Physical Chemistry Chemical Physics, 2016, 18, 14122-14128.	1.3	5
11901	Strain-Induced Electronic Structure Changes in Stacked van der Waals Heterostructures. Nano Letters, 2016, 16, 3314-3320.	4.5	122
11902	Atomically Dispersed Pd, Ni, and Pt Species in Ceria-Based Catalysts: Principal Differences in Stability and Reactivity. Journal of Physical Chemistry C, 2016, 120, 9852-9862.	1.5	99
11903	Aminofluorination of Cyclopropanes: A Multifold Approach through a Common, Catalytically Generated Intermediate. Journal of the American Chemical Society, 2016, 138, 6598-6609.	6.6	139
11904	DFT MODELING OF BENZOYL PEROXIDE ADSORPTION ON $\sqrt{3}\times\sqrt{3}$ -R <sub>3</sub> O <sub>2</sub> (0001) SURFACE. Surface Review and Letters, 2016, 23, 1650037.	0.5	1
11905	Analytical interatomic potential for a molybdenum-erbium system. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 045018.	0.8	2
11906	Magnetic BiMn phase synthesis prediction: First-principles calculation, thermodynamic modeling and nonequilibrium chemical partitioning. Computational Materials Science, 2016, 120, 117-126.	1.4	5
11907	Theoretical Prediction and Synthesis of CS <sub>x</sub> F <sub>y</sub> Thin Films. Journal of Physical Chemistry C, 2016, 120, 9527-9534.	1.5	6
11908	Relative edge energy in the stability of transition metal nanoclusters of different motifs. Nanoscale, 2016, 8, 12834-12842.	2.8	5
11909	New insight into the structure of the C <sub>60</sub> Sc <sub>20</sub> cluster: bonding, vibrational and optical properties. Physical Chemistry Chemical Physics, 2016, 18, 12434-12437.	1.3	7
11910	The high-pressure semiconducting phase of LiBC. Europhysics Letters, 2016, 114, 16001.	0.7	8
11911	Electronic and magnetic properties of TbNi4Si: Ab initio calculations, mean field approximation and Monte Carlo simulation. Journal of Solid State Chemistry, 2016, 241, 38-46.	1.4	3



#	ARTICLE	IF	CITATIONS
11912	Effect of the Exchange-Correlation Potential on the Transferability of Brønsted–Evans–Polanyi Relationships in Heterogeneous Catalysis. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2121-2126.	2.3	20
11913	CO oxidation by MoS <sub>2</sub> -supported Au <sub>19</sub> nanoparticles: effects of vacancy formation and tensile strain. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 13232-13238.	1.3	14
11914	Density functional theory calculations of hydrogen dissociative adsorption on platinum-involved alloy surfaces. <i>Surface and Coatings Technology</i> , 2016, 306, 35-40.	2.2	9
11915	First-principles study on the electronic and optical properties of Si and Al co-doped zinc oxide for solar cell devices. <i>Applied Physics A: Materials Science and Processing</i> , 2016, 122, 1.	1.1	10
11916	Theoretical study of the effect of N-oxides on the performances of energetic compounds. <i>Journal of Molecular Modeling</i> , 2016, 22, 83.	0.8	15
11917	Theoretical insight into the sensitive mechanism of multilayer-shaped cocrystal explosives: compression and slide. <i>Journal of Molecular Modeling</i> , 2016, 22, 108.	0.8	2
11918	Comparative DFT and DFT-D studies on structural, electronic, vibrational and absorption properties of crystalline ammonium perchlorate. <i>RSC Advances</i> , 2016, 6, 48489-48497.	1.7	11
11919	Optical spectra of zigzag carbon nanotubes. <i>Optik</i> , 2016, 127, 6952-6960.	1.4	11
11920	Rectifications in organic single-molecule diodes alkanethiolate-terminated heterocyclics. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2016, 380, 923-926.	0.9	11
11921	Rare-earth pnictides and chalcogenides from first-principles. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 223001.	0.7	24
11922	Energetics of a Li Atom adsorbed on B/N doped graphene with monovacancy. <i>Journal of Solid State Chemistry</i> , 2016, 240, 67-75.	1.4	22
11923	Theoretical studies of the adsorption of hydroxymethylidyne (COH) on Pt-alloy surfaces using density functional theory. <i>Physica Scripta</i> , 2016, 91, 025803.	1.2	5
11924	Density Functional Theory Methods for Computing and Predicting Mechanical Properties. <i>Springer Series in Materials Science</i> , 2016, , 131-158.	0.4	0
11925	Role of Ti doping and Al and B vacancies in the dehydrogenation of Al(BH <sub>4</sub> ) <sub>3</sub> . <i>Journal of Chemical Sciences</i> , 2016, 128, 1651-1662.	0.7	3
11926	Peierls–Distorted Ru–Chains and Boron Dumbbells in Nb <sub>2</sub> Ru <sub>2</sub> and Ta <sub>2</sub> Ru <sub>2</sub> from First-Principles Calculations and Experiments. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 4104-4110.	1.0	6
11927	Electronic and Magnetic Properties of Co- and Mn-codoped ZnO by Density Functional Theory. <i>Chinese Physics Letters</i> , 2016, 33, 097102.	1.3	7
11928	N–Mg dual-acceptor co-doping in CuCrO <sub>2</sub> studied by first-principles calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2016, 380, 3861-3865.	0.9	10
11929	Magnetic MAX phases from theory and experiments; a review. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 433003.	0.7	84

#	ARTICLE	IF	CITATIONS
11930	Beyond energies: geometry predictions with the XYG3 type of doubly hybrid density functionals. Chemical Communications, 2016, 52, 13840-13860.	2.2	18
11931	Electronic and optical properties study on Fe B co-doped anatase TiO <sub>2</sub> . Chemical Physics, 2016, 477, 52-60.	0.9	7
11932	Ab initio study of structural and electronic properties of single crystal and core/shell II-VI semiconductor nanowires. Computational Materials Science, 2016, 123, 158-163.	1.4	1
11933	The effect of concentration of H <sub>2</sub> physisorption on the current-voltage characteristic of armchair BN nanotubes in CNT-BNNT-CNT set. Pramana - Journal of Physics, 2016, 87, 1.	0.9	8
11934	Effect of doping on structural and opto-electronic properties of tin dioxide layers produced by chemical deposition. Optik, 2016, 127, 11235-11241.	1.4	4
11935	Electronic and magnetic properties of spiral spin-density-wave states in transition-metal chains. Physical Review B, 2016, 94, .	1.1	4
11936	Insight into CH <sub>x</sub> formation in Fischer-Tropsch synthesis on the hexahedron Co catalyst: Effect of surface structure on the preferential mechanism and existence form. Applied Catalysis A: General, 2016, 525, 76-84.	2.2	18
11937	DFT + U investigation on the adsorption and initial decomposition of methylamine by a Pt single-atom catalyst supported on rutile (110) TiO <sub>2</sub> . Applied Surface Science, 2016, 389, 411-418.	3.1	14
11938	Data for molecular dynamics simulations of B-type cytochrome c oxidase with the Amber force field. Data in Brief, 2016, 8, 1209-1214.	0.5	13
11939	Influences of interstitial nitrogen with high electronegativity on structure and hydrogen storage properties of Mg-based metal hydride: A theoretical study. International Journal of Hydrogen Energy, 2016, 41, 18550-18561.	3.8	18
11940	Synthesis and radiation tolerance of Lu <sup>2+</sup> Ce Ti <sub>2</sub> O <sub>7</sub> pyrochlores. Journal of Nuclear Materials, 2016, 480, 182-188.	1.3	11
11941	Hydrolysis of Me <sub>3</sub> SiCH <sub>2</sub> groups on a double-chelating bis(ferrocenediyl)diphosphine coordinating to a Pt(0) center. Polyhedron, 2016, 110, 114-118.	1.0	0
11942	Density functional theory study of the electronic structure and the thermoelectric properties of strained Mn <sub>4</sub> Si <sub>7</sub> . Journal of the Korean Physical Society, 2016, 69, 402-405.	0.3	2
11943	Theoretical study of disorder-order transition of sodium borohydride. Computational Materials Science, 2016, 124, 87-91.	1.4	3
11944	On the crystalline structure of orthorhombic SrRuO <sub>3</sub> : A benchmark study of DFT functionals. Computational Materials Science, 2016, 124, 78-86.	1.4	4
11945	Optical properties of titanium and iron doped 3C-SiC behaviors TB-mBJ. Chinese Journal of Physics, 2016, 54, 960-967.	2.0	11
11946	Manipulating charge density waves in charge-carrier doping: A first-principles investigation. Physical Review B, 2016, 94, .	1.1	3
11947	Adsorption of water and ethanol on noble and transition-metal substrates: a density functional investigation within van der Waals corrections. Physical Chemistry Chemical Physics, 2016, 18, 29526-29536.	1.3	30

#	ARTICLE	IF	CITATIONS
11948	Surface and shape modification of mackinawite (FeS) nanocrystals by cysteine adsorption: a first-principles DFT-D2 study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32007-32020.	1.3	35
11949	Enhanced molecular adsorption of ethylene on reduced anatase TiO <sub>2</sub> (001): role of surface O-vacancies. <i>RSC Advances</i> , 2016, 6, 92241-92251.	1.7	13
11950	Towards understanding the differences in irradiation effects of He, Ne and Ar plasma by investigating the physical origin of their clustering in tungsten. <i>Nuclear Fusion</i> , 2016, 56, 106002.	1.6	16
11951	Impact of uniaxial compressive strain on physical and electronic parameters of a 10Ånm germanene nanoribbon field effect transistor. <i>Superlattices and Microstructures</i> , 2016, 100, 198-208.	1.4	17
11952	Nanostructural adsorption of vanadium oxide on functionalized graphene: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29208-29217.	1.3	8
11953	Crystal structures and superconductivity of technetium hydrides under pressure. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28791-28796.	1.3	15
11954	First principle calculations of photocatalytic properties of bismuth oxyhalides considering van der Waals correction. , 2016, , .		1
11955	Towards visible-light water splitting Photocatalysts: Band engineering of two-dimensional A <sub>5</sub> B <sub>4</sub> O <sub>15</sub> perovskites. <i>Nano Energy</i> , 2016, 28, 390-396.	8.2	29
11956	Dependence of Adenine Raman Spectrum on Excitation Laser Wavelength: Comparison between Experiment and Theoretical Simulations. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8114-8122.	1.1	7
11957	Insight into the mechanism about the initiation, growth and termination of the C chain in syngas conversion on the Co(0001) surface: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27272-27283.	1.3	30
11958	Optoelectronic properties of naphtho[2, 1-b:6, 5-b']difuran derivatives for photovoltaic application: a computational study. <i>Journal of Molecular Modeling</i> , 2016, 22, 248.	0.8	24
11959	Indium-defect interactions in FCC and BCC metals studied using the modified embedded atom method. <i>Hyperfine Interactions</i> , 2016, 237, 1.	0.2	1
11960	Nanoscale Patterns on Polar Oxide Surfaces. <i>Chemistry of Materials</i> , 2016, 28, 7433-7443.	3.2	20
11961	Correlation energy, correlated electron density, and exchange-correlation potential in some spherically confined atoms. <i>Journal of Computational Chemistry</i> , 2016, 37, 2677-2686.	1.5	6
11962	Implementation Strategies for Orbital-dependent Density Functionals. <i>Brazilian Journal of Physics</i> , 2016, 46, 636-642.	0.7	2
11963	First principle molecular dynamics simulations of oxygen reduction reaction on Pt(111) in aqueous environment. <i>Catalysis Communications</i> , 2016, 87, 74-77.	1.6	1
11964	Photocatalytic Properties of g-C <sub>6</sub> N <sub>6</sub> /g-C <sub>3</sub> N <sub>4</sub> Heterostructure: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24023-24029.	1.5	78
11965	Anomalous enhancement of Seebeck coefficients of the graphene/hexagonal boron nitride composites. <i>Japanese Journal of Applied Physics</i> , 2016, 55, 1102A9.	0.8	4

#	ARTICLE	IF	CITATIONS
11966	Raman and IR Spectra of Ice Ih and Ice XI with an Assessment of DFT Methods. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11043-11051.	1.2	18
11967	Tunability of the two-dimensional electron gas at the LaAlO <sub>3</sub> /SrTiO <sub>3</sub> interface by strain-induced ferroelectricity. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28474-28484.	1.3	25
11968	Selective hydrogenation of biomass-derived 2(5H)-furanone over Pt-Ni and Pt-Co bimetallic catalysts: From model surfaces to supported catalysts. <i>Journal of Catalysis</i> , 2016, 344, 148-156.	3.1	26
11969	Chemical Trend of Superconducting Critical Temperatures in Hole-Doped CuBO <sub>2</sub> , CuAlO <sub>2</sub> , CuGaO <sub>2</sub> , and CuInO <sub>2</sub> . <i>Journal of the Physical Society of Japan</i> , 2016, 85, 094711.	0.7	7
11970	Phase-controlled synthesis and comparative study of 1- and 2-WP 2 submicron particles as efficient electrocatalysts for hydrogen evolution. <i>Electrochimica Acta</i> , 2016, 216, 304-311.	2.6	17
11971	Effect of carbon segregation on performance of inhomogeneous SiCyO <sub>6/5</sub> as anode materials for lithium-ion battery: A first-principles study. <i>Journal of Power Sources</i> , 2016, 334, 39-43.	4.0	27
11972	Possible martensitic transformation in Heusler alloy Mn <sub>2</sub> PdSn from first principles. <i>Journal of Magnetism and Magnetic Materials</i> , 2016, 419, 543-546.	1.0	3
11973	Cuboctahedral vs. octahedral platinum nanoclusters: insights into the shape-dependent catalytic activity for fuel cell applications. <i>Catalysis Science and Technology</i> , 2016, 6, 7913-7923.	2.1	27
11974	Hybridization of inorganic CoB noncrystal with graphene and its Kubas-enhanced hydrogen adsorption at room temperature. <i>RSC Advances</i> , 2016, 6, 93238-93244.	1.7	7
11975	Fast-Dissolving, Prolonged Release, and Antibacterial Cyclodextrin/Limonene-Inclusion Complex Nanofibrous Webs via Polymer-Free Electrospinning. <i>Journal of Agricultural and Food Chemistry</i> , 2016, 64, 7325-7334.	2.4	92
11976	Dichlorophosphanyl isocyanate <sup>13</sup> C spectroscopy, conformation and molecular structure in the gas phase and the solid state. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26245-26253.	1.3	12
11977	Strain controlled ferromagnetic <sup>1</sup> ferrimagnetic transition and vacancy formation energy of defective graphene. <i>Nanotechnology</i> , 2016, 27, 435206.	1.3	9
11978	Room-Temperature Phosphorescence of Crystalline Metal-Free Organoboron Complex. <i>ChemPhysChem</i> , 2016, 17, 4033-4036.	1.0	25
11979	First-principles phase diagram calculations for the carbonate quasibinary systems CaCO <sub>3</sub> -ZnCO <sub>3</sub> , CdCO <sub>3</sub> -ZnCO <sub>3</sub> , CaCO <sub>3</sub> -CdCO <sub>3</sub> and MgCO <sub>3</sub> -ZnCO <sub>3</sub> . <i>Chemical Geology</i> , 2016, 443, 137-145.	1.4	11
11980	Sintering of Pt Nanoparticles via Volatile PtO <sub>2</sub> : Simulation and Comparison with Experiments. <i>ACS Catalysis</i> , 2016, 6, 7098-7108.	5.5	72
11981	Pt <sub>3</sub> Ti (Ti <sub>19</sub> @Pt <sub>60</sub> )-Based Cuboctahedral Core-Shell Nanocluster Favors a Direct over Indirect Oxygen Reduction Reaction. <i>ACS Energy Letters</i> , 2016, 1, 797-805.	8.8	33
11982	Adsorption of H <sub>2</sub> , Cl <sub>2</sub> , and HCl molecules on 1-Cr <sub>2</sub> O <sub>3</sub> (0001) surfaces: A density functional theory investigation. <i>Surface Science</i> , 2016, 653, 211-221.	0.8	11
11983	Experimental and Computational Studies of the Single-Molecule Conductance of Ru(II) and Pt(II) <i>trans</i> -Bis(acetylide) Complexes. <i>Organometallics</i> , 2016, 35, 2944-2954.	1.1	49

#	ARTICLE	IF	CITATIONS
11984	Promotional Effects of Cesium Promoter on Higher Alcohol Synthesis from Syngas over Cesium-Promoted Cu/ZnO/Al <sub>2</sub> O <sub>3</sub> Catalysts. ACS Catalysis, 2016, 6, 5771-5785.	5.5	79
11985	Stacking fault energy of face-centered cubic metals: thermodynamic and <i>ab initio</i> approaches. Journal of Physics Condensed Matter, 2016, 28, 395001.	0.7	43
11986	Two-Component Orderly Molecular Hybrids of Diphenylanthracene: Modulation of Solid-State Aggregation toward Tunable Photophysical Properties and Highly Enhanced Electrochemiluminescence. Advanced Optical Materials, 2016, 4, 2139-2147.	3.6	45
11987	Novel room-temperature spin-valve-like magnetoresistance in magnetically coupled nano-column Fe <sub>3</sub> O <sub>4</sub> /Ni heterostructure. Nanoscale, 2016, 8, 15737-15743.	2.8	9
11988	Relativistic and electron correlation effects on NMR J-coupling of Sn and Pb containing molecules. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	16
11989	Structural, Electronic, and Li Migration Properties of RE-Doped (RE = Ce, La) LiCoO <sub>2</sub> for Li-ion Batteries: A First-Principles Investigation. Journal of Physical Chemistry C, 2016, 120, 18428-18434.	1.5	48
11990	Molecular Simulation of Nanosized Tubular Clay Minerals. Developments in Clay Science, 2016, , 331-359.	0.3	3
11991	A phase width for CaGaSn. Crystal structure of mixed intermetallic Ca <sub>4</sub> Ga <sub>4+x</sub> Sn <sub>4</sub> <sup>x</sup> and SmGaxSn <sub>3</sub> <sup>x</sup> , stability, geometry and electronic structure. Journal of Solid State Chemistry, 2016, 242, 63-70.	1.4	0
11992	DFT study of structural, electronic, thermo-elastic properties and plausible origin of superconductivity due to quantum degenerate states in LaTiO <sub>3</sub> . Journal of Theoretical and Computational Chemistry, 2016, 15, 1650044.	1.8	13
11993	Growth and characterization of Ba <sub>3</sub> InB <sub>9</sub> O <sub>18</sub> single crystals. Chemical Physics Letters, 2016, 660, 136-142.	1.2	1
11994	The hydrogen storage capacity of Sc atoms decorated porous boron fullerene B <sub>40</sub> : A DFT study. International Journal of Hydrogen Energy, 2016, 41, 16992-16999.	3.8	74
11995	Electronic properties of red and black phosphorous and their potential application as photocatalysts. RSC Advances, 2016, 6, 80872-80884.	1.7	33
11996	DFT Studies of the Selective C=O Hydrogenolysis and Ring-Opening of Biomass-Derived Tetrahydrofurfuryl Alcohol over Rh(111) surfaces. Journal of Physical Chemistry C, 2016, 120, 19124-19134.	1.5	17
11999	The structural, electro-optical, charge transport and nonlinear optical properties of 2-[(3,5-dimethyl-1-phenyl-1H-pyrazol-4-yl)methylidene]indan-1,3-dione. Optik, 2016, 127, 10148-10157.	1.4	31
12000	Anatomizing the Impact of High Dielectric Gate Materials on the Charge Transport in Graphene Field Effect Transistors. Materials Today: Proceedings, 2016, 3, 1933-1938.	0.9	3
12001	First-principles study of sulfur atom doping and adsorption on $\hat{\Gamma}$ -Fe <sub>2</sub> O <sub>3</sub> (0001) film. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 3149-3154.	0.9	7
12002	Vibrational and electronic profiles, molecular docking and biological prediction of 5-methoxy-1-[(5-methoxy-1H-indol-2-yl)methyl]-1H-indole: Experimental and theoretical investigations. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650046.	1.8	0
12003	Deformation mechanisms of D022 ordered intermetallic phase in superalloys. Acta Materialia, 2016, 118, 350-361.	3.8	41

#	ARTICLE	IF	CITATIONS
12004	Synthesis, electrochemical and DFT study of octahedral bis( $\eta^2$ -diketonato)-titanium(IV) complexes. <i>Inorganica Chimica Acta</i> , 2016, 453, 247-256.	1.2	15
12005	Can the state of platinum species be unambiguously determined by the stretching frequency of an adsorbed CO probe molecule?. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22108-22121.	1.3	113
12006	Recent application of calculations of metal complexes based on density functional theory. <i>RSC Advances</i> , 2016, 6, 77375-77395.	1.7	47
12007	Theoretical Modeling of $^{99}\text{Tc}$ NMR Chemical Shifts. <i>Inorganic Chemistry</i> , 2016, 55, 8341-8347.	1.9	10
12008	Band inversion and topological aspects in a TiNi monolayer. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22154-22159.	1.3	26
12009	Na <sub>0.282</sub> V <sub>2</sub> O <sub>5</sub> : A high-performance cathode material for rechargeable lithium batteries and sodium batteries. <i>Journal of Power Sources</i> , 2016, 328, 241-249.	4.0	37
12010	Theoretical and Experimental Insight on Ag <sub>2</sub> CrO <sub>4</sub> Microcrystals: Synthesis, Characterization, and Photoluminescence Properties. <i>Inorganic Chemistry</i> , 2016, 55, 8961-8970.	1.9	31
12011	First-principles studies on switching properties of azobenzene based molecular device. <i>Chemical Physics Letters</i> , 2016, 660, 27-32.	1.2	14
12012	Correlation between local structures and glass forming ability of liquid Mg <sub>x</sub> Zn <sub>1-x</sub> alloys. <i>Journal of Non-Crystalline Solids</i> , 2016, 447, 262-266.	1.5	3
12013	Effect of the third element on the structure of liquid Mg <sub>65</sub> Cu <sub>25</sub> Y <sub>10</sub> alloy. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2016, 380, 2786-2790.	0.9	1
12014	Is Spillover Relevant for Hydrogen Adsorption and Storage in Porous Carbons Doped with Palladium Nanoparticles?. <i>Journal of Physical Chemistry C</i> , 2016, 120, 17357-17364.	1.5	51
12015	C <sub>2</sub> H <sub>4</sub> adsorption on Cu(210), revisited: bonding nature and coverage effects. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 23621-23627.	1.3	6
12016	High-Temperature Quantum Anomalous Hall Effect in $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ Topological Insulators. <i>Physical Review Letters</i> , 2016, 117, 056804.	2.9	71
12017	Formation and Stability of Low-Dimensional Structures for Group VIII B and IB Transition Metals: The Role of $d^4$ Hybridization. <i>Advanced Science</i> , 2016, 3, 1500314.	5.6	7
12018	Effect of Surface Chemistry on Water Interaction with Cu(111). <i>Langmuir</i> , 2016, 32, 8061-8070.	1.6	16
12019	Computational study of the threshold energy for the 1,2-interchange of X and R (X, R = halogens.) <i>Tj ETQq1 1 0.784314 rgBT /Overlook Canadian Journal of Chemistry</i> , 2016, 94, 1038-1043.	0.6	5
12020	A comparative examination of density functional performance against the ISOL24/11 isomerization energy benchmark. <i>Computational and Theoretical Chemistry</i> , 2016, 1090, 147-152.	1.1	23
12021	Electronic and magnetic properties of Cr-Mn-Ni-Al compound with LiMgPdSb-type structure. <i>Solid State Communications</i> , 2016, 244, 38-42.	0.9	6



#	ARTICLE	IF	CITATIONS
12022	Phase stability, electronic structure and equation of state of cubic TcN from first-principles calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2016, 380, 3144-3148.	0.9	3
12023	Ab-initio investigation of the finite-temperatures structural, elastic, and thermodynamic properties of Ti <sub>3</sub> AlC <sub>2</sub> and Ti <sub>3</sub> SiC <sub>2</sub> . <i>Computational Materials Science</i> , 2016, 124, 420-427.	1.4	9
12024	DFT-D2 Study of the Adsorption and Dissociation of Water on Clean and Oxygen-Covered {001} and {011} Surfaces of Mackinawite (FeS). <i>Journal of Physical Chemistry C</i> , 2016, 120, 21441-21450.	1.5	34
12025	Large energy product enhancement in perpendicularly coupled MnBi/CoFe magnetic bilayers. <i>Physical Review B</i> , 2016, 94, .	1.1	15
12026	The hydrogen storage properties of Na decorated small boron cluster B <sub>6</sub> Na <sub>8</sub> . <i>Chemical Physics Letters</i> , 2016, 661, 161-167.	1.2	14
12027	Towards easily tunable hydrogen storage via a hydrogen-induced glass-to-glass transition in Mg-based metallic glasses. <i>Acta Materialia</i> , 2016, 120, 68-74.	3.8	68
12028	First-principles determination of grain boundary strengthening in tungsten: Dependence on grain boundary structure and metallic radius of solute. <i>Acta Materialia</i> , 2016, 120, 315-326.	3.8	143
12029	First-principles study of the interaction between helium and the defects in tantalum. <i>Journal of Nuclear Materials</i> , 2016, 480, 202-206.	1.3	16
12030	Stability and effects of carbon-induced surface reconstructions in cobalt Fischer-Tropsch synthesis. <i>Surface Science</i> , 2016, 653, 82-87.	0.8	11
12031	The structure of the bulk and the (001) surface of V <sub>2</sub> O <sub>5</sub> . A DFT+U study. <i>Materials Research Express</i> , 2016, 3, 085005.	0.8	15
12032	Kinetic-energy-density dependent semilocal exchange-correlation functionals. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1641-1694.	1.0	78
12033	Three-dimensional porous structural MoP <sub>2</sub> nanoparticles as a novel and superior catalyst for electrochemical hydrogen evolution. <i>Journal of Power Sources</i> , 2016, 328, 551-557.	4.0	88
12034	Evaluation of sulfur spinel compounds for multivalent battery cathode applications. <i>Energy and Environmental Science</i> , 2016, 9, 3201-3209.	15.6	121
12035	Effects of the Grafting of Lanthanum Complexes on a Silica Surface on the Reactivity: Influence on Ethylene, Propylene, and 1,3-Butadiene Homopolymerization. <i>Inorganic Chemistry</i> , 2016, 55, 10024-10033.	1.9	5
12036	Pt <sub>38</sub> cluster on OH- and COOH-functionalised graphene as a model for Pt/C-catalysts. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 25693-25704.	1.3	7
12037	Effect of Complex-Valued Optimal Orbitals on Atomization Energies with the Perdew-Zunger Self-Interaction Correction to Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4296-4302.	2.3	29
12038	Three-dimensional imaging of shear bands in bulk metallic glass composites. <i>Journal of Microscopy</i> , 2016, 264, 304-310.	0.8	9
12039	Transition Metal-Promoted V <sub>2</sub> CO <sub>2</sub> (MXenes): A New and Highly Active Catalyst for Hydrogen Evolution Reaction. <i>Advanced Science</i> , 2016, 3, 1600180.	5.6	279



#	ARTICLE	IF	CITATIONS
12040	TM@gt-C<sub>3</sub>N<sub>3</sub> monolayers: high-temperature ferromagnetism and high anisotropy. <i>Journal of Materials Chemistry C</i> , 2016, 4, 8253-8262.	2.7	26
12041	On the Structure Sensitivity of Formic Acid Decomposition on Cu Catalysts. <i>Topics in Catalysis</i> , 2016, 59, 1580-1588.	1.3	37
12042	Embedded atom approach for goldâ€“silicon system from ab initio molecular dynamics simulations using the force matching method. <i>Bulletin of Materials Science</i> , 2016, 39, 1339-1347.	0.8	2
12043	Structural and Electronic Property Study of (ZnO)<sub>n</sub>, <i>n</i> 168: Transition from Zinc Oxide Molecular Clusters to Ultrasmall Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2016, 120, 20400-20418.	1.5	53
12044	Room temperature<i>d</i><sup>0</sup>ferromagnetism in hole doped Y<sub>2</sub>O<sub>3</sub>: widening the choice of host to tailor DMS. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 336001.	0.7	12
12045	Confirmation of a de novo structure prediction for an atomically precise monolayer-coated silver nanoparticle. <i>Science Advances</i> , 2016, 2, e1601609.	4.7	39
12046	Density functional theories study on optoelectronic properties of arsenic-doped GaN nanowires. <i>Optical and Quantum Electronics</i> , 2016, 48, 1.	1.5	6
12047	Geometric, stability, and electronic properties of gold-doped Pd clusters (Pd n Au, n=3~20). <i>Journal of Nanoparticle Research</i> , 2016, 18, 1.	0.8	3
12048	Electronic bonding analyses and mechanical strengths of incompressible tetragonal transition metal dinitrides TMN <sub>2</sub> (TM=Ti, Zr, and Hf). <i>Scientific Reports</i> , 2016, 6, 36911.	1.6	22
12049	Theoretical study of physical and thermodynamic properties of Al <sub>n</sub> M clusters*. <i>European Physical Journal D</i> , 2016, 70, 1.	0.6	11
12050	On the Mechanism of the Improved Operation Voltage of Rhombohedral Nickel Hexacyanoferrate as Cathodes for Sodium-Ion Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 33619-33625.	4.0	89
12051	In Situ and Ex Situ TEM Study of Lithiation Behaviours of Porous Silicon Nanostructures. <i>Scientific Reports</i> , 2016, 6, 31334.	1.6	43
12052	Scaling relationships for nonadiabatic energy relaxation times in warm dense matter: toward understanding the equation of state. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32466-32476.	1.3	14
12053	Solid-State <sup>27</sup>Al NMR Spectroscopy of the Î³-Al<sub>13</sub> Keggin Containing Al Coordinated by a Terminal Hydroxyl Ligand. <i>Inorganic Chemistry</i> , 2016, 55, 12270-12280.	1.9	13
12054	Structural effects of substitutional impurities on MoO <sub>3</sub> bilayers: A first principles study. <i>Journal of the Korean Physical Society</i> , 2016, 69, 1439-1444.	0.3	2
12055	Pressure induced elastic softening in framework aluminosilicate- albite (NaAlSi <sub>3</sub> O <sub>8</sub> ). <i>Scientific Reports</i> , 2016, 6, 34815.	1.6	19
12056	Reaction and Mechanistic Studies of Heterogeneous Hydroamination over Supportâ€“stabilized Gold Nanoparticles. <i>ChemCatChem</i> , 2016, 8, 3121-3130.	1.8	17
12057	Double-Hole-Mediated Codoping on KNbO<sub>3</sub> for Visible Light Photocatalysis. <i>Inorganic Chemistry</i> , 2016, 55, 9620-9631.	1.9	30

#	ARTICLE	IF	CITATIONS
12058	Potassium and Water Coadsorption on TiO <sub>2</sub> (110): OH-Induced Anchoring of Potassium and the Generation of Single-Site Catalysts. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3866-3872.	2.1	14
12059	Ligand effects on the optical and chiroptical properties of the thiolated Au <sub>18</sub> cluster. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27738-27744.	1.3	33
12060	Synergistic effect of Li <sup>+</sup> and K <sup>+</sup> Ti co-doping on the dehydrogenation properties of NaAlH <sub>4</sub> : an ab initio study. <i>RSC Advances</i> , 2016, 6, 89895-89900.	1.7	0
12061	The adsorption behaviors of CO and H <sub>2</sub> on FeO surface: A density functional theory study. <i>Powder Technology</i> , 2016, 303, 100-108.	2.1	35
12062	Direct Gap Semiconductors Pb <sub>2</sub> BiS <sub>2</sub> I <sub>3</sub> , Sn <sub>2</sub> BiS <sub>2</sub> I <sub>3</sub> , and Sn <sub>2</sub> BiSI <sub>5</sub> . <i>Chemistry of Materials</i> , 2016, 28, 7332-7343.	3.2	33
12063	Local structure in the disordered solid solution of <i>cis</i> - and <i>trans</i> -perinones. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 416-433.	0.5	12
12064	State-of-the-art Sn <sup>2+</sup> -based ternary oxides as photocatalysts for water splitting: electronic structures and optoelectronic properties. <i>Catalysis Science and Technology</i> , 2016, 6, 7656-7670.	2.1	45
12065	EPW: Electron-phonon coupling, transport and superconducting properties using maximally localized Wannier functions. <i>Computer Physics Communications</i> , 2016, 209, 116-133.	3.0	777
12066	Trimerization of Acetylene Catalyzed by Ir(PH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> PH <sub>2</sub> )Cl(cod): A Computational Study. <i>Bulletin of the Chemical Society of Japan</i> , 2016, 89, 584-594.	2.0	1
12067	Assessing Hubbard-corrected AM05+U and PBEsol+U density functionals for strongly correlated oxides CeO <sub>2</sub> and Ce <sub>2</sub> O <sub>3</sub> . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26816-26826.	1.3	25
12068	Magnetism in $\text{SrPt}_2\text{Al}_2$ : A combined <i>ab initio</i> and model study. <i>Physical Review B</i> , 2016, 94, .	2.1	25
12069	Source function and plane waves: Toward complete bader analysis. <i>Journal of Computational Chemistry</i> , 2016, 37, 2133-2139.	1.5	8
12070	The effect of water molecules on the thiol collector interaction on the galena (PbS) and sphalerite (ZnS) surfaces: A DFT study. <i>Applied Surface Science</i> , 2016, 389, 103-111.	3.1	77
12071	Experimental and theoretical investigations of the polar intermetallics SrPt <sub>3</sub> Al <sub>2</sub> and Sr <sub>2</sub> Pd <sub>2</sub> Al. <i>Journal of Solid State Chemistry</i> , 2016, 242, 143-150.	1.4	17
12072	Theoretical study of electronic and mechanical properties of Fe <sub>2</sub> B. <i>RSC Advances</i> , 2016, 6, 73576-73580.	1.7	13
12073	First-principles study of intercalation of alkali ions in FeSe for solid-state batteries. <i>Chemical Physics Letters</i> , 2016, 659, 230-233.	1.2	18
12074	Nondirected C-H Activation of Arenes with Cp*Ir(III) Acetate Complexes: An Experimental and Computational Study. <i>Organometallics</i> , 2016, 35, 2435-2445.	1.1	13
12075	The investigation of pressure effect on the optical properties, spontaneous polarization and effective mass of BaHfO <sub>3</sub> : ab initio study. <i>Optical and Quantum Electronics</i> , 2016, 48, 1.	1.5	5

#	ARTICLE	IF	CITATIONS
12076	Titanium $\hat{I}_{\pm}$ transformation pathway and a predicted metastable structure. Physical Review B, 2016, 93, .	1.1	8
12077	Quantum spin Hall effect in $\hat{I}_{\pm}$ structures. Physical Review B, 2016, 93, .	1.1	8
12078	Real-space method for first-principles electron transport calculations: Self-energy terms of electrodes for large systems. Physical Review B, 2016, 93, .	1.1	10
12079	Stacking fault energetics of $\hat{I}_{\pm}$ and $\hat{I}^3$ -cerium investigated with ab initio calculations. Physical Review B, 2016, 93, .	1.1	4
12080	Atomic size effects studied by transport in single silicide nanowires. Physical Review B, 2016, 93, .	1.1	14
12081	Self-assembly of nanoscale lateral segregation profiles. Physical Review B, 2016, 93, .	1.1	7
12082	Structural transition in the magnetoelectric $\text{ZnC}_2\text{S}_4$ spinel. Physical Review B, 2016, 93, .	1.1	16
12083	Vibrational properties of $\text{LiNbO}_3$ mixed crystals. Physical Review B, 2016, 93, .	1.1	26
12084	Rare-earth silicide thin films on the Si(111) surface. Physical Review B, 2016, 93, .	1.1	28
12085	Charge compensation in extremely large magnetoresistance materials LaSb and LaBi revealed by first-principles calculations. Physical Review B, 2016, 93, .	1.1	82
12086	Surface electron density models for accurate <i>ab initio</i> molecular dynamics with electronic friction. Physical Review B, 2016, 93, .	1.1	54
12087	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. Physical Review Letters, 2016, 116, 057002.	2.9	132
12088	Submolecular Resolution Imaging of Molecules by Atomic Force Microscopy: The Influence of the Electrostatic Force. Physical Review Letters, 2016, 116, 096102.	2.9	51
12089	Hydrogen Incorporation in Crystalline Jadeite: Insight from First Principles Calculations. Acta Geologica Sinica, 2016, 90, 939-945.	0.8	1
12090	Isolated Chromium(VI) Oxide Species Supported on Al-Modified Silica: A Molecular Description. Journal of Physical Chemistry C, 2016, 120, 17594-17603.	1.5	19
12091	First principles calculations on oxygen vacant hydrated $\hat{I}_{\pm}$ - $\text{MnO}_2$ for activating water oxidation and its self-healing mechanism. Physical Chemistry Chemical Physics, 2016, 18, 22196-22202.	1.3	7
12092	First Principles Simulations of Cyclic Voltammograms on Stepped Pt(553) and Pt(533) Electrode Surfaces. ChemElectroChem, 2016, 3, 1609-1617.	1.7	47
12093	Reduced graphene oxide enhancing the photoelectrochemical properties of poly(3-hexylthiophene). Carbon, 2016, 109, 57-64.	5.4	6

#	ARTICLE	IF	CITATIONS
12094	Density Functional Theory Studies of the Methanol Decomposition Reaction on Graphene-Supported Pt <sub>13</sub> Nanoclusters. Journal of Physical Chemistry C, 2016, 120, 17408-17417.	1.5	23
12095	Reactivity and Selectivity Descriptors for the Activation of C-H Bonds in Hydrocarbons and Oxygenates on Metal Oxides. Journal of Physical Chemistry C, 2016, 120, 16741-16760.	1.5	75
12096	First principles calculation of the stacking fault in (111) low-temperature metastable alumina. Journal of Structural Chemistry, 2016, 57, 294-300.	0.3	3
12097	SiN Coatings Deposited by Reactive High Power Impulse Magnetron Sputtering: Process Parameters Influencing the Nitrogen Content. ACS Applied Materials & Interfaces, 2016, 8, 20385-20395.	4.0	28
12098	New cytotoxic trichothecene macrolide epimers from endophytic Myrothecium roridum IFB-E012. Journal of Antibiotics, 2016, 69, 652-655.	1.0	10
12099	Direct growth by arc discharge and computational study of zinc sulfide nanotubes. Journal of Materials Science, 2016, 51, 9716-9722.	1.7	1
12100	First-principles study of the stability and diffusion properties of hydrogen in zirconium carbide. Journal of Nuclear Materials, 2016, 479, 130-136.	1.3	14
12101	Atomic investigation on reversible lithium storage in amorphous silicon oxycarbide as a high power anode material. Journal of Materials Chemistry A, 2016, 4, 12328-12333.	5.2	54
12102	Tuning chemical bonding of MnO <sub>2</sub> through transition-metal doping for enhanced CO oxidation. Journal of Catalysis, 2016, 341, 82-90.	3.1	132
12104	First-principles prediction of structural, mechanical and magnetic properties in Ni <sub>2</sub> MnAl. Computational Materials Science, 2016, 123, 52-58.	1.4	12
12105	Origin of the magnetization and compensation temperature in rare-earth orthoferrites and orthochromates. Physical Review B, 2016, 93, .	1.1	59
12106	Potentially superhard hcp Cr <sub>3</sub> N <sub>2</sub> compound studied at high pressure. Physical Review B, 2016, 93, .	1.1	11
12107	Better band gaps with asymptotically corrected local exchange potentials. Physical Review B, 2016, 93, .	1.1	17
12108	STM and DFT study on formation and characterization of Ba-incorporated phases on a Ge(001) surface. Physical Review B, 2016, 93, .	1.1	7
12109	Potentially superhard hcp Cr <sub>3</sub> N <sub>2</sub> compound studied at high pressure. Physical Review B, 2016, 93, .	1.1	33
12110	Chemomechanical Origin of Hydrogen Trapping at Grain Boundaries in fcc Metals. Physical Review Letters, 2016, 116, 075502.	2.9	81
12111	Nonvortical Rashba Spin Structure on a Surface with C <sub>1h</sub> Symmetry. Physical Review Letters, 2016, 117, 016803.	2.9	15
12112	Assessment of DFT Functionals for QTAIM Topological Analysis of Halogen Bonds with Benzene. Journal of Physical Chemistry A, 2016, 120, 9071-9080.	1.1	37

#	ARTICLE	IF	CITATIONS
12113	Cu <sub>2</sub> ZnSnS <sub>4</sub> Nanocrystals as Highly Active and Stable Electrocatalysts for the Oxygen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24265-24270.	1.5	17
12114	First-principles calculations of the electronic and structural properties of GaSb. <i>Semiconductors</i> , 2016, 50, 1280-1286.	0.2	8
12115	Edge preference and band gap characters of MoS <sub>2</sub> and WS <sub>2</sub> nanoribbons. <i>Surface Science</i> , 2016, 653, 107-112.	0.8	51
12116	Fe doped LaGaO <sub>3</sub> : good white light emitters. <i>RSC Advances</i> , 2016, 6, 100230-100238.	1.7	35
12117	Metal-free half-metallicity in a high energy phase C-doped gh-C <sub>3</sub> N <sub>4</sub> system: a high Curie temperature planar system. <i>Journal of Materials Chemistry C</i> , 2016, 4, 11530-11539.	2.7	32
12118	Catalysis on solid acids: Mechanism and catalyst descriptors in oligomerization reactions of light alkenes. <i>Journal of Catalysis</i> , 2016, 344, 553-569.	3.1	80
12119	A Radical Mechanism for the Vanadium-Catalyzed Deoxydehydration of Glycols. <i>Inorganic Chemistry</i> , 2016, 55, 11372-11382.	1.9	16
12120	Band gap engineering of ZnO substituted with nitrogen and fluorine, ZnO <sub>1-3x</sub> N <sub>2x</sub> F <sub>x</sub> : a hybrid density functional study. <i>RSC Advances</i> , 2016, 6, 99088-99095.	1.7	5
12121	Assessing exchange-correlation functional performance for structure and property predictions of oxyfluoride compounds from first principles. <i>Physical Review B</i> , 2016, 94, .	1.1	27
12122	DFT Study on the Interaction of Tris(benzene-1,2-dithiolato)molybdenum Complex with Water. A Hydrolysis Mechanism Involving a Feasible Seven-Coordinate Aquomolybdenum Intermediate. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9636-9646.	1.1	5
12123	Synthesis of sodium polyhydrides at high pressures. <i>Nature Communications</i> , 2016, 7, 12267.	5.8	79
12124	Theoretical Study of Cu/Mg Core-shell Nanocluster Formation. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9612-9617.	1.1	5
12125	The mechanism of large second harmonic generation enhancement activated by Zn <sup>2+</sup> substitution. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32931-32936.	1.3	31
12126	The effect of oxygen vacancies on water wettability of transition metal based SrTiO <sub>3</sub> and rare-earth based Lu <sub>2</sub> O <sub>3</sub> . <i>RSC Advances</i> , 2016, 6, 109234-109240.	1.7	40
12127	Theoretical Investigation on Porphyrin-Based Small Molecules as Donor Materials for Photovoltaic Applications. <i>Journal of Physical Chemistry C</i> , 2016, 120, 27148-27158.	1.5	15
12128	Synthesis and coordination chemistry of (PNEt <sub>2</sub> ) <sub>2</sub> -bridged [2]ferrocenophanes. <i>Dalton Transactions</i> , 2016, 45, 19034-19044.	1.6	11
12129	Giant perpendicular magnetic anisotropy energies in CoPt thin films: impact of reduced dimensionality and imperfections. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 496002.	0.7	3
12130	Mechanistic aspects of the activation of C-H bond in C <sub>2</sub> H <sub>6</sub> by Th atom: bonding analysis and reaction coefficients. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	1

#	ARTICLE	IF	CITATIONS
12131	Structural stability and electronic properties of multi-functionalized two-dimensional chromium carbides. <i>Thin Solid Films</i> , 2016, 619, 131-136.	0.8	33
12132	<sup>125</sup> Te NMR provides evidence of autoassociation of organo-ditellurides in solution. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30740-30747.	1.3	16
12133	Surface energies of elemental crystals. <i>Scientific Data</i> , 2016, 3, 160080.	2.4	583
12134	Enigmatic HCl + Au(111) Reaction: A Puzzle for Theory and Experiment. <i>Journal of Physical Chemistry C</i> , 2016, 120, 25760-25779.	1.5	48
12135	Irradiation Specified Conformational Change in a Small Organic Compound and Its Effect on Electrical Properties. <i>Journal of Physical Chemistry C</i> , 2016, 120, 25557-25563.	1.5	20
12136	Scaling Atomic Partial Charges of Carbonate Solvents for Lithium Ion Solvation and Diffusion. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5709-5718.	2.3	64
12137	First-Principle Characterization of the Adsorption Configurations of Cyanoacrylic Dyes on TiO <sub>2</sub> Film for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8813-8822.	1.1	13
12138	Valence band electronic structure of Pd based ternary chalcogenide superconductors. <i>Physica C: Superconductivity and Its Applications</i> , 2016, 531, 98-102.	0.6	2
12139	Local heterojunctions of atomic Pt clusters boost the oxygen reduction activity of Ru <sub>core</sub> @Pd <sub>shell</sub> nanocrystallites. <i>Journal of Materials Chemistry A</i> , 2016, 4, 17848-17856.	5.2	3
12140	Cooperative Effects in Clusters and Oligonuclear Complexes of Transition Metals in Isolation. <i>Structure and Bonding</i> , 2016, , 1-40.	1.0	5
12141	The diffusion behavior of Cr and Re in nickel-based superalloys at an atomic level. <i>Computational and Theoretical Chemistry</i> , 2016, 1097, 33-39.	1.1	4
12142	Structure and Electronic Properties of Fe <sub>2</sub> SH <sub>3</sub> Compound under High Pressure. <i>Inorganic Chemistry</i> , 2016, 55, 11434-11439.	1.9	50
12143	Quantum chemistry calculations of technetium and rhenium compounds with application in radiopharmacy: review. <i>RSC Advances</i> , 2016, 6, 107127-107140.	1.7	12
12144	A first-principles study of the linear and nonlinear optical properties of isoxazole derivatives. <i>Journal of Theoretical and Computational Chemistry</i> , 2016, 15, 1650060.	1.8	3
12145	Periodic DFT Characterization of NO <sub>x</sub> Adsorption in Cu-Exchanged SSZ-13 Zeolite Catalysts. <i>Journal of Physical Chemistry C</i> , 2016, 120, 27934-27943.	1.5	29
12146	Structural phase transition and spin reorientation of LaFeO <sub>3</sub> films under epitaxial strain. <i>RSC Advances</i> , 2016, 6, 100526-100531.	1.7	14
12147	Theoretical study of the optical and charge transport properties of ĩ-conjugated three-coordinate organoboron compounds as organic light-emitting diodes materials. <i>RSC Advances</i> , 2016, 6, 108209-108216.	1.7	4
12148	Oscillatory magnetic anisotropy and spin-reorientation induced by heavy-metal cap in Cu/FeCo/ M ( ) Tj ETQq1 1 0.784314 rgBT /Overlo	1.1	8



#	ARTICLE	IF	CITATIONS
12149	Assessment of quantum chemical methods for the calculation of homolytic N–F bond dissociation energies. <i>Chemical Data Collections</i> , 2016, 5-6, 28-35.	1.1	5
12150	Investigation of a solid oxide fuel cells catalyst LaSrNiO <sub>4</sub> : Electronic structure, surface segregation, and oxygen adsorption. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 21497-21502.	3.8	5
12151	Oxidation of InP nanowires: a first principles molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 31101-31106.	1.3	3
12152	Modification of silica-supported tungsten neosilyl oxo precatalysts: impact of substituted phenol on activity and stability in olefin metathesis. <i>Catalysis Science and Technology</i> , 2016, 6, 8532-8539.	2.1	11
12153	Self-supported three-dimensional mesoporous semimetallic WP <sub>2</sub> nanowire arrays on carbon cloth as a flexible cathode for efficient hydrogen evolution. <i>Nanoscale</i> , 2016, 8, 19779-19786.	2.8	84
12154	Role of Dispersion in Metallophilic Hg–M Interactions (M = Cu, Ag, Au) within Coinage Metal Complexes of Bis(6-diphenylphosphinoacenaphth-5-yl)mercury. <i>Inorganic Chemistry</i> , 2016, 55, 11513-11521.	1.9	24
12155	Octahedral Ni-nanocluster (Ni <sub>85</sub> ) for Efficient and Selective Reduction of Nitric Oxide (NO) to Nitrogen (N <sub>2</sub> ). <i>Scientific Reports</i> , 2016, 6, 25590.	1.6	15
12156	Assembling non-ferromagnetic materials to ferromagnetic architectures using metal-semiconductor interfaces. <i>Scientific Reports</i> , 2016, 6, 34404.	1.6	10
12157	Charge self-consistency in density functional theory combined with dynamical mean field theory: $k$ -space reoccupation and orbital order. <i>Physical Review B</i> , 2016, 94, .	1.1	29
12158	Insight into the Thermal Ring-Opening Polymerization of Phospha[1]ferrocenophanes. <i>Chemistry - A European Journal</i> , 2016, 22, 16838-16849.	1.7	20
12159	Optimizing the sputter deposition process of polymers for the Storing Matter technique using PMMA. <i>Journal of Mass Spectrometry</i> , 2016, 51, 889-899.	0.7	0
12160	Design of a p-Type Electrode for Enhancing Electronic Conduction in High-Mn, Li-Rich Oxides. <i>Chemistry of Materials</i> , 2016, 28, 8201-8209.	3.2	24
12161	Nanocluster-Assembled Materials. <i>Series in Materials Science and Engineering</i> , 2016, , 113-148.	0.1	3
12162	Structure, Vibrational Spectra and <sup>11</sup> B-NMR Chemical Shift of Na <sub>8</sub> [AlSiO <sub>4</sub> ] <sub>6</sub> (B(OH) <sub>4</sub> ) <sub>2</sub> : Comparison of Theory and Experiment. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7503-7509.	1.1	2
12163	Competition between Two High-Density Assemblies of Poly(phenyl)thiols on Au(111). <i>Journal of Physical Chemistry C</i> , 2016, 120, 25462-25472.	1.5	19
12164	Pressure dependency of localization degree in heavy fermion CeIn <sub>3</sub> : A density functional theory analysis. <i>Scientific Reports</i> , 2016, 6, 31734.	1.6	14
12165	Effects of ZnO Quantum Dots Decoration on the Field Emission Behavior of Graphene. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 31856-31862.	4.0	11
12166	The stability and catalytic activity of W <sub>13</sub> @Pt <sub>42</sub> core-shell structure. <i>Scientific Reports</i> , 2016, 6, 35464.	1.6	7



#	ARTICLE	IF	CITATIONS
12167	CO <sub>2</sub> capture in amine solutions: modelling and simulations with non-empirical methods. Journal of Physics Condensed Matter, 2016, 28, 503003.	0.7	8
12168	Dimers of heavy p-elements of groups IV–VI: Electronic, vibrational, and magnetic properties. JETP Letters, 2016, 103, 471-475.	0.4	5
12170	A heterogeneous mechanism for the catalytic decomposition of hydroperoxides and oxidation of alkanes over CeO <sub>2</sub> nanoparticles: A combined theoretical and experimental study. Journal of Catalysis, 2016, 344, 334-345.	3.1	13
12171	Structural and elastic properties of BiOCu <sub>1-x</sub> S with Cu vacancies. Materials Today: Proceedings, 2016, 3, 2877-2882.	0.9	2
12172	Spin-orbital effects in metal-dichalcogenide semiconducting monolayers. Scientific Reports, 2016, 6, 24093.	1.6	60
12173	Gaseous NH <sub>3</sub> Confers Porous Pt Nanodendrites Assisted by Halides. Scientific Reports, 2016, 6, 26196.	1.6	11
12174	A DFT kinetic study on 1,3-dipolar cycloaddition reactions in solution. Physical Chemistry Chemical Physics, 2016, 18, 30815-30823.	1.3	32
12175	Optimized effective potentials at a glance: the effective exchange potential of Becke–Johnson applied to molecules. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	1
12176	Density functional study of molecular interactions in secondary structures of proteins. Biophysics and Physicobiology, 2016, 13, 27-35.	0.5	17
12177	Electronic origin of strain effects on solute stabilities in iron. Journal of Applied Physics, 2016, 120, 075902.	1.1	2
12178	Theoretical Analysis of Pseudodegenerate Zero-Energy Modes in Vacancy-Centered Hexagonal Armchair Nanographene. Journal of the Physical Society of Japan, 2016, 85, 084703.	0.7	8
12179	Peptide Reactivity of Isothiocyanates – Implications for Skin Allergy. Scientific Reports, 2016, 6, 21203.	1.6	22
12180	Optical and magnetic properties of Mn doped 4H-SiC: First principal calculations. , 2016, , .		2
12182	Hydrogen-induced atomic structure evolution of the oxygen-chemisorbed Cu(110) surface. Journal of Chemical Physics, 2016, 145, 234704.	1.2	7
12183	<i>Ab initio</i> tensorial electronic friction for molecules on metal surfaces: Nonadiabatic vibrational relaxation. Physical Review B, 2016, 94, .	1.1	74
12184	<i>Ab Initio</i> Elastic Properties calculation of Gold (Au). Journal of Physics: Conference Series, 2016, 739, 012068.	0.3	0
12185	A DFT based equilibrium study of a chemical mixture Tachyhydrite and their lower hydrates for long term heat storage. Journal of Physics: Conference Series, 2016, 745, 032003.	0.3	5
12186	First-principles study of Cl-terminated silicon nanoribbons electronic properties. Journal of Physics: Conference Series, 2016, 758, 012002.	0.3	0

#	ARTICLE	IF	CITATIONS
12187	Communication: Energy transfer and reaction dynamics for DCl scattering on Au(111): An <i>ab initio</i> molecular dynamics study. <i>Journal of Chemical Physics</i> , 2016, 145, 011102.	1.2	32
12188	Stability of atomic oxygen chemisorption on Pt-alloy surfaces. <i>Surface and Interface Analysis</i> , 2016, 48, 181-185.	0.8	3
12189	Thermal decomposition of diethyl ketone triperoxide in methyl methacrylate: Theoretical and experimental study of the initial solvation state and its influence on the polymerization process. <i>Journal of Applied Polymer Science</i> , 2016, 133, .	1.3	0
12190	Mechanistic Insight into the Intramolecular Benzylic C-H Nitrene Insertion Catalyzed by Bimetallic Paddlewheel Complexes: Influence of the Metal Centers. <i>Chemistry - A European Journal</i> , 2016, 22, 7288-7297.	1.7	14
12191	Photoluminescence and Photocatalytic Properties of Ag <sub>3</sub> PO <sub>4</sub> Microcrystals: An Experimental and Theoretical Investigation. <i>ChemPlusChem</i> , 2016, 81, 202-212.	1.3	70
12192	First-principles based computational study on nucleation and growth mechanisms of U on Mo(110) surface solvated in an eutectic LiCl-KCl molten salt. <i>International Journal of Energy Research</i> , 2016, 40, 1381-1388.	2.2	13
12193	Hyperconjugative and Electrostatic Interactions as Anomeric Triggers in Archetypical 1,4-Dioxane Derivatives. <i>ChemPhysChem</i> , 2016, 17, 530-540.	1.0	4
12194	Energy storage performance of V <sub>n+1</sub> C <sub>n</sub> monolayer as electrode material studied by first-principles calculations. <i>RSC Advances</i> , 2016, 6, 54999-55006.	1.7	18
12195	Theoretical Investigation of Donor-Acceptor Copolymers Based on C-, Si-, and Ge-Bridged Thieno[3,2-b]dithiophene for Organic Solar Cell Applications. <i>Journal of Electronic Materials</i> , 2016, 45, 5427-5435.	1.0	0
12196	Reduction of chromia-silica catalysts: A molecular picture. <i>Journal of Catalysis</i> , 2016, 340, 122-135.	3.1	42
12197	Stable and metallic borophene nanoribbons from first-principles calculations. <i>Journal of Materials Chemistry C</i> , 2016, 4, 6380-6385.	2.7	75
12198	Overview of band-edge and defect related luminescence in aluminum nitride. <i>Journal of Luminescence</i> , 2016, 178, 267-281.	1.5	53
12199	Adsorption structures and energetics of molecules on metal surfaces: Bridging experiment and theory. <i>Progress in Surface Science</i> , 2016, 91, 72-100.	3.8	121
12200	Quantum Monte Carlo analysis of a charge ordered insulating antiferromagnet: the Ti <sub>4</sub> O <sub>7</sub> Magnéli phase. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18323-18335.	1.3	27
12201	±,²-Substituent effect of dialkylphosphinic acids on lanthanide extraction. <i>RSC Advances</i> , 2016, 6, 56004-56008.	1.7	16
12202	The stacking of antiferrofluorite Fe <sub>2</sub> P <sub>2</sub> layer on the electronic structure of the ternary compounds CaFe <sub>2</sub> P <sub>2</sub> , BaFe <sub>2</sub> P <sub>2</sub> and EuFe <sub>2</sub> P <sub>2</sub> . <i>Computational Materials Science</i> , 2016, 122, 177-182.	1.4	2
12203	CO <sub>2</sub> Activation on Ni <sub>3</sub> Al <sub>2</sub> O <sub>3</sub> Catalysts by First-Principles Calculations: From Ideal Surfaces to Supported Nanoparticles. <i>ACS Catalysis</i> , 2016, 6, 4501-4505.	5.5	92
12204	FeO <sub>2</sub> and FeOOH under deep lower-mantle conditions and Earth's oxygen-hydrogen cycles. <i>Nature</i> , 2016, 534, 241-244.	13.7	245

#	ARTICLE	IF	CITATIONS
12205	DFT simulations of $^{7}\text{Li}$ solid state NMR spectral parameters and $^{7}\text{Li}$ ion migration barriers in $\text{Li}_2\text{ZrO}_3$ . RSC Advances, 2016, 6, 41015-41024.	1.7	5
12206	Transition-metal embedded carbon nitride monolayers: high-temperature ferromagnetism and half-metallicity. Nanoscale, 2016, 8, 14117-14126.	2.8	49
12207	Study on the crystal structure of $(\text{Gd}_{2-x}\text{Ce}_x)\text{Ti}_2\text{O}_7$ pyrochlore. Advances in Applied Ceramics, 2016, 115, 411-416.		
12208	Theoretical Simulation of isocyanate (NCO) adsorption on the Ag(001) surface. Journal of the Korean Physical Society, 2016, 68, 1192-1199.	0.3	4
12209	Water exit pathways and proton pumping mechanism in B-type cytochrome c oxidase from molecular dynamics simulations. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 1594-1606.	0.5	15
12210	First-principles calculations of crystal and electronic structures and thermodynamic stabilities of $\text{LaNi}_5\text{H}$ , $\text{LaNi}_5\text{AlH}$ and $\text{LaNi}_5\text{AlMnH}$ hydrogen storage compounds. International Journal of Hydrogen Energy, 2016, 41, 12194-12204.	1.8	7
12211	Experimental and theoretical studies on the linear and nonlinear optical properties of lead phosphate crystals $\text{LiPbPO}_4$ . Physical Chemistry Chemical Physics, 2016, 18, 19123-19129.	1.3	61
12212	First-principles study of nitrogen and carbon monoxide adsorptions on silicene. International Journal of Modern Physics B, 2016, 30, 1650176.	1.0	7
12213	Doping of helium at Fe/W interfaces from first principles calculation. Journal of Alloys and Compounds, 2016, 686, 160-167.	2.8	28
12214	The in vitro antitumor activity of arene-ruthenium(II) curcuminoid complexes improves when decreasing curcumin polarity. Journal of Inorganic Biochemistry, 2016, 162, 44-51.	1.5	49
12215	Adsorption of gold subnano-structures on a magnetite(111) surface and their interaction with CO. Physical Chemistry Chemical Physics, 2016, 18, 18169-18179.	1.3	14
12216	Nitrate reduction pathways on Cu single crystal surfaces: Effect of oxide and $\text{Cl}^-$ . Nano Energy, 2016, 29, 457-465.	8.2	124
12217	Ab-initio study of surface oxide formation in Pt(111) electrocatalyst under influences of $\text{O}_2$ -containing intermediates of oxygen reduction reaction. Journal of Applied Electrochemistry, 2016, 46, 1031-1038.	1.5	4
12218	Unraveling the Coupled Processes of (De)hydration and Structural Changes in Na-Saturated Montmorillonite. Journal of Physical Chemistry C, 2016, 120, 15282-15287.	1.5	16
12219	Silica-Supported Tungsten Neosilyl Oxo Precatalysts: Impact of the Podality on Activity and Stability in Olefin Metathesis. Organometallics, 2016, 35, 2188-2196.	1.1	31
12220	A computational study on the adsorption configurations and reactions of $\text{SiH}_x$ ( $x = 1-4$ ) on clean and H-covered Si(100) surfaces. Applied Surface Science, 2016, 387, 546-556.	3.1	4
12221	Polymer-free nanofibers from vanillin/cyclodextrin inclusion complexes: high thermal stability, enhanced solubility and antioxidant property. Food and Function, 2016, 7, 3141-3153.	2.1	87
12222	Chiral vectors-tunable electronic property of $\text{MoS}_2$ nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 84, 196-201.	1.3	6

#	ARTICLE	IF	CITATIONS
12223	How does the B,F-monodoping and B/F-codoping affect the photocatalytic water-splitting performance of $g\text{-C}_{3}\text{N}_{4}$ ? Physical Chemistry Chemical Physics, 2016, 18, 19217-19226.	1.3	99
12224	Preparation, structure and properties of $\text{Na}_{2}\text{Mn}_{3}(\text{SO}_{4})_{4}$ : a new potential candidate with high voltage for Na-ion batteries. Journal of Materials Chemistry A, 2016, 4, 11870-11877.	5.2	24
12225	Ultralong Persistent Room Temperature Phosphorescence of Metal Coordination Polymers Exhibiting Reversible pH-Responsive Emission. ACS Applied Materials & Interfaces, 2016, 8, 15489-15496.	4.0	153
12226	Tuning the electronic and photophysical properties of platinum(II) complexes through ancillary ligand modification: a theoretical study. Molecular Simulation, 2016, 42, 1035-1041.	0.9	3
12227	Quantum-chemical study of nitrogen and magnesium co-doping in $\hat{\pm}\text{-Cr}_{2}\text{O}_{3}$ . Modern Physics Letters B, 2016, 30, 1650219.	1.0	1
12228	Twin boundary activated $\hat{\pm}\hat{\Delta}\hat{\Gamma}\hat{\Gamma}\%$ phase transformation in titanium under shock compression. Acta Materialia, 2016, 115, 1-9.	3.8	28
12229	Laser lap welding quality of steel/aluminum dissimilar metal joint and its electronic simulations. International Journal of Advanced Manufacturing Technology, 2016, 86, 2231-2242.	1.5	11
12230	Theoretical study on the $\text{H}_{2}\text{S}$ activation by $\text{PtCH}_{2}$ + in the gas phase. Structural Chemistry, 2016, 27, 1363-1371.	1.0	1
12231	Complex Precipitation Sequences of Al-Cu-Li-(Mg) Alloys Characterized in Relation to Thermal Ageing Processes. Acta Metallurgica Sinica (English Letters), 2016, 29, 94-103.	1.5	34
12232	First-principles study on the stability and electronic structure of Mg/ZrB <sub>2</sub> interfaces. Science China Materials, 2016, 59, 28-37.	3.5	29
12233	Influence mechanism of $\text{H}_{2}\text{S}$ on the reactivity of Ni-based oxygen carriers for chemical-looping combustion. Chemical Engineering Journal, 2016, 295, 461-467.	6.6	25
12234	First principle calculations on the adsorption of molecular $\text{H}_{2}$ in the largest pore of $\text{Co}[\text{Fe}(\text{CN})_{5}\text{NO}]$ and $\text{Ni}[\text{Fe}(\text{CN})_{5}\text{NO}]$ metal nitroprussides. Effect of the charged cavities on the adsorption and $\text{H}_{2}$ -host interactions. Computational Materials Science, 2016, 114, 102-111.	1.4	3
12235	Size-selective electrocatalytic activity of $(\text{Pt})_{n}/\text{MoS}_{2}$ for oxygen reduction reaction. Catalysis Science and Technology, 2016, 6, 6389-6395.	2.1	16
12236	Intrinsic reactivity of Ni, Pd and Pt surfaces in dry reforming and competitive reactions: Insights from first principles calculations and microkinetic modeling simulations. Journal of Catalysis, 2016, 343, 196-207.	3.1	156
12237	Electronic Structure of Third-Row Elements in Different Local Symmetries Studied by Valence-to-Core X-ray Emission Spectroscopy. Inorganic Chemistry, 2016, 55, 5328-5336.	1.9	15
12238	Short-range effect at the semi-coherent metal/its native oxide interface. Applied Surface Science, 2016, 378, 451-459.	3.1	3
12239	Yttrium dispersion on capped carbon nanotube: Promising materials for hydrogen storage applications. International Journal of Hydrogen Energy, 2016, 41, 1053-1059.	3.8	16
12240	Jahn-Teller distortion in $\text{tris}[4,4,4\text{-trifluoro-1-(2-thienyl)-1,3-butanedionato}]$ manganese(III) isomers: An X-ray and computational study. Journal of Molecular Structure, 2016, 1119, 48-53.	1.8	11

#	ARTICLE	IF	CITATIONS
12241	Hydrogen diffusion in bulk MgB <sub>2</sub> . Scripta Materialia, 2016, 117, 86-91.	2.6	6
12242	Assessing the concept of structure sensitivity or insensitivity for sub-nanometer catalyst materials. Surface Science, 2016, 652, 7-19.	0.8	36
12243	Au-induced deep groove nanowire structure on the Ge(001) surface: DFT calculations. Surface Science, 2016, 651, 164-174.	0.8	7
12244	The process of dissociative adsorption of fluorine on Ge(001) surface. Applied Surface Science, 2016, 384, 263-271.	3.1	3
12245	Reduction effect of Fe <sub>2</sub> O <sub>3</sub> on carbon deposition and CO oxidation during chemical-looping combustion. Chemical Engineering Journal, 2016, 301, 257-265.	6.6	52
12246	Adsorption of H <sub>2</sub> S on Cr <sub>2</sub> O <sub>3</sub> (0001) surfaces: A density functional theory investigation. Corrosion Science, 2016, 111, 1-12.	3.0	10
12247	Electronic transport properties and CO adsorption characteristics on TiO <sub>2</sub> molecular device – A first-principles study. Microelectronic Engineering, 2016, 162, 51-56.	1.1	13
12248	Structural and mechanical properties of alkali hydrides investigated by the first-principles calculations and principal component analysis. Solid State Sciences, 2016, 58, 30-36.	1.5	6
12249	Chiral vectors-tunable electronic property of MoS <sub>2</sub> nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 83, 232-237.	1.3	6
12250	Synthesis and structure of a new halophosphate Sr <sub>3</sub> P <sub>3</sub> O <sub>10</sub> Cl with the flexible [P <sub>3</sub> O <sub>10</sub> ] <sup>5-</sup> anions. Solid State Sciences, 2016, 55, 159-163.	1.5	7
12251	Atomic-Scale Mapping of Layer-by-Layer Hydrogen Etching and Passivation of SiC(0001) Substrates. Journal of Physical Chemistry C, 2016, 120, 10361-10367.	1.5	20
12252	Saturation of electrical resistivity of solid iron at Earth's core conditions. SpringerPlus, 2016, 5, 256.	1.2	26
12253	Studies of synergy between metal-support interfaces and selective hydrogenation of HMF to DMF in water. Journal of Catalysis, 2016, 340, 248-260.	3.1	101
12254	Challenging Dogmas: Hydrogen Bond Revisited. Journal of Physical Chemistry A, 2016, 120, 4550-4559.	1.1	23
12255	Cu Deposited on CeO <sub>x</sub> -Modified TiO <sub>2</sub> (110): Synergistic Effects at the Metal-Oxide Interface and the Mechanism of the WGS Reaction. ACS Catalysis, 2016, 6, 4608-4615.	5.5	43
12256	Microwave-Assisted Synthesis of Pd <sub>x</sub> Au <sub>100-x</sub> Alloy Nanoparticles: A Combined Experimental and Theoretical Assessment of Synthetic and Compositional Effects upon Catalytic Reactivity. ACS Catalysis, 2016, 6, 4882-4893.	5.5	54
12257	The structure-dependent enhancement of the oxygen reduction reaction performance of Co-based low Pt catalysts through Au addition. Journal of Materials Chemistry A, 2016, 4, 11023-11029.	5.2	15
12258	Corrosion inhibition effect of novel methyl benzimidazolium ionic liquid for carbon steel in HCl medium. Journal of Molecular Liquids, 2016, 221, 368-380.	2.3	78

#	ARTICLE	IF	CITATIONS
12259	Comparisons between adsorption and diffusion of alkali, alkaline earth metal atoms on silicene and those on silicane: Insight from first-principles calculations. <i>Chinese Physics B</i> , 2016, 25, 067103.	0.7	17
12260	A computational study of a phenolic based polymer with a spring-like structure. <i>Chemical Physics Letters</i> , 2016, 655-656, 76-79.	1.2	0
12261	Density function theoretical study on the complex involved in Th atom-activated C-C bond in C <sub>2</sub> H <sub>6</sub> . <i>Chinese Physics B</i> , 2016, 25, 063102.	0.7	3
12262	Single-layered platinum nanocage: a highly selective and efficient catalyst for fuel cells. <i>Journal of Materials Chemistry A</i> , 2016, 4, 12756-12767.	5.2	33
12263	Enthalpies of formation of TM-X compounds (X=Al, Ga, Si, Ge, Sn). Comparison of ab-initio values and experimental data. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2016, 54, 16-34.	0.7	12
12264	Mono- and Dinuclear Manganese Carbonyls Supported by 1,8-Disubstituted (L = Py, SMe, SH) Anthracene Ligand Scaffolds. <i>Inorganic Chemistry</i> , 2016, 55, 5127-5138.	1.9	13
12265	Synthesis, antifungal evaluation and optical properties of silver molybdate microcrystals in different solvents: a combined experimental and theoretical study. <i>Dalton Transactions</i> , 2016, 45, 10736-10743.	1.6	49
12266	Insight into the Formation of Highly Strained [1]Ferrocenophanes with Boron in Bridging Position. <i>Organometallics</i> , 2016, 35, 2156-2164.	1.1	13
12267	CO gas optoelectronic sensor using semiconductor graphene nanoribbons: A first-principles study. <i>Physica Status Solidi (B): Basic Research</i> , 2016, 253, 559-565.	0.7	3
12268	Engel-Vosko generalized gradient approximation within DFT investigations of optoelectronic and thermoelectric properties of copper thioantimonates(III) and thioarsenate(III) for solar energy conversion. <i>Physica Status Solidi (B): Basic Research</i> , 2016, 253, 583-590.	0.7	11
12269	New description of metastable hcp phase for unaries Fe and Mn: Coupling between first-principles calculations and CALPHAD modeling. <i>Physica Status Solidi (B): Basic Research</i> , 2016, 253, 1830-1836.	0.7	34
12270	Advances in DFT. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 801-801.	1.0	2
12271	High coverage CO adsorption and dissociation on the Co(0001) and Co(100) surfaces from DFT and thermodynamics. <i>Applied Catalysis A: General</i> , 2016, 523, 209-220.	2.2	22
12272	A density functional theory study of propylene epoxidation on RuO <sub>2</sub> (110) surface. <i>Applied Surface Science</i> , 2016, 385, 99-105.	3.1	17
12273	Introducing DDEC6 atomic population analysis: part 2. Computed results for a wide range of periodic and nonperiodic materials. <i>RSC Advances</i> , 2016, 6, 45727-45747.	1.7	351
12274	Characterization of LSMO/C60 spinterface by first-principle calculations. <i>Organic Electronics</i> , 2016, 37, 55-60.	1.4	6
12275	É-TiO, a Novel Stable Polymorph of Titanium Monoxide. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 1652-1657.	7.2	42
12276	Nitrogen-Rich Manganese Oxynitrides with Enhanced Catalytic Activity in the Oxygen Reduction Reaction. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 7963-7967.	7.2	52



#	ARTICLE	IF	CITATIONS
12277	Theoretical Study of Pd <sub>11</sub> Si <sub>6</sub> Nanosheet Compounds Including Seven-Coordinate Si Species and Its Ge Analogues. <i>Chemistry - A European Journal</i> , 2016, 22, 1076-1087.	1.7	13
12278	The electro-optical and charge transport study of imidazolidin derivative: Quantum chemical investigations. <i>Journal of Saudi Chemical Society</i> , 2016, 20, 680-685.	2.4	17
12279	An Effective Approach to Improving Cadmium Telluride (111)A Surface by Molecular-Beam-Epitaxy Growth of Tellurium Monolayer. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 726-735.	4.0	2
12280	Problems, successes and challenges for the application of dispersion-corrected density-functional theory combined with dispersion-based implicit solvent models to large-scale hydrophobic self-assembly and polymorphism. <i>Molecular Simulation</i> , 2016, 42, 494-510.	0.9	13
12281	Elastic constants of beryllium: a first-principles investigation. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 075401.	0.7	112
12282	Bond dissociation energies from the topology of the charge density using gradient bundle analysis. <i>Physica Scripta</i> , 2016, 91, 023012.	1.2	9
12283	A comparison of mechanical properties between Al and Al3Mg. <i>International Journal of Modern Physics B</i> , 2016, 30, 1550243.	1.0	7
12284	Site preference and diffusion of hydrogen during hydrogenation of Mg: A first-principles study. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 3508-3516.	3.8	12
12285	Chalcogen bonding interactions between reducible sulfur and selenium compounds and models of zinc finger proteins. <i>Journal of Inorganic Biochemistry</i> , 2016, 157, 94-103.	1.5	12
12286	Lanthanide-doped LaSi <sub>3</sub> N <sub>5</sub> based phosphors: Ab initio study of electronic structures, band gaps, and energy level locations. <i>Journal of Luminescence</i> , 2016, 172, 83-91.	1.5	11
12287	Structure sensitivity in the non-scalable regime explored via catalysed ethylene hydrogenation on supported platinum nanoclusters. <i>Nature Communications</i> , 2016, 7, 10389.	5.8	115
12288	Comparative density functional theory and density functional tight binding study of 2-anthracic acid on TiO <sub>2</sub> . <i>Chemical Physics Letters</i> , 2016, 643, 16-20.	1.2	14
12289	Mechanical properties of the interface structure of nanodiamond composite films: First-principles studies. <i>Applied Surface Science</i> , 2016, 363, 522-531.	3.1	2
12290	The "bimodal effect" of the bulk modulus of rare-earth titanate pyrochlore. <i>Computational Materials Science</i> , 2016, 114, 233-235.	1.4	7
12291	First-principles investigation on mechanical behaviors of W-Cr/Ti binary alloys. <i>Journal of Nuclear Materials</i> , 2016, 468, 105-112.	1.3	22
12292	A DFT study of ethanol adsorption and decomposition on $\alpha$ -Al <sub>2</sub> O <sub>3</sub> (0001) surface. <i>Applied Surface Science</i> , 2016, 363, 636-643.	3.1	24
12293	Crystal structures and mechanical properties of M (Mg, Sr, Ba, La) x Ca <sub>1-x</sub> B <sub>6</sub> solid solution: A first principles study. <i>Ceramics International</i> , 2016, 42, 6632-6639.	2.3	10
12294	DFT modelling of hydrogen sulphide adsorption on $\alpha$ -Cr <sub>2</sub> O <sub>3</sub> (0001) surface. <i>Surface Science</i> , 2016, 647, 78-83.	0.8	15



#	ARTICLE	IF	CITATIONS
12295	First principles modeling of Mo <sub>6</sub> S <sub>9</sub> nanowires via condensation of Mo <sub>4</sub> S <sub>6</sub> clusters and the effect of iodine doping on structural and electronic properties. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5471-5476.	1.3	2
12296	Microalloying for the controllable delay of precipitate formation in metal alloys. <i>Acta Materialia</i> , 2016, 106, 117-128.	3.8	32
12297	Behaviour of the surface hydroxide groups of exfoliated kaolinite in the gas phase and during water adsorption. <i>Dalton Transactions</i> , 2016, 45, 2523-2535.	1.6	9
12298	DFT study on the galvanic interaction between pyrite (100) and galena (100) surfaces. <i>Applied Surface Science</i> , 2016, 367, 270-276.	3.1	51
12299	New ternary tantalum borides containing boron dumbbells: Experimental and theoretical studies of Ta <sub>2</sub> OsB <sub>2</sub> and TaRuB. <i>Journal of Solid State Chemistry</i> , 2016, 242, 28-33.	1.4	10
12300	Oxygen character in the density of states as an indicator of the stability of Li-ion battery cathode materials. <i>Solid State Ionics</i> , 2016, 286, 83-89.	1.3	43
12301	Insights into the Effect of Pt Atomic Ensemble on HCOOH Oxidation over Pt-Decorated Au Bimetallic Catalyst To Maximize Pt Utilization. <i>Journal of Physical Chemistry C</i> , 2016, 120, 2234-2246.	1.5	45
12302	Ab initio study of electronic, magnetic, elastic and optical properties of full Heusler Co <sub>2</sub> MnSb. <i>Indian Journal of Physics</i> , 2016, 90, 909-916.	0.9	31
12303	Glide of dislocations in $\{111\}$ slip system: an atomistic study. <i>Philosophical Magazine</i> , 2016, 96, 71-83.	0.7	5
12304	Magnetism of Nd-Fe films as a model of grain boundary phase in Nd-Fe-B permanent magnets. <i>Applied Physics Express</i> , 2016, 9, 013002.	1.1	37
12305	Synthesis, modeling and photovoltaic properties of a benzothiadiazole based molecule for dye-sensitized solar cells. <i>Journal of Materials Science: Materials in Electronics</i> , 2016, 27, 4501-4507.	1.1	16
12306	Primary damage in tungsten using the binary collision approximation, molecular dynamic simulations and the density functional theory. <i>Physica Scripta</i> , 2016, T167, 014018.	1.2	16
12307	Density functional theory calculations of lithium alloying with Ge <sub>10</sub> H <sub>16</sub> atomic cluster. <i>Chinese Chemical Letters</i> , 2016, 27, 437-440.	4.8	3
12308	Coexistence of flat bands and Dirac bands in a carbon-Kagome-lattice family. <i>Carbon</i> , 2016, 99, 65-70.	5.4	42
12309	pH and Alkali Cation Effects on the Pt Cyclic Voltammogram Explained Using Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2016, 120, 457-471.	1.5	145
12310	Crystal phase competition by addition of a second metal cation in solid solution metal-organic frameworks. <i>Dalton Transactions</i> , 2016, 45, 4327-4337.	1.6	13
12311	Lattice dynamics of bismuth-deficient BiFeO <sub>3</sub> from first principles. <i>Computational Materials Science</i> , 2016, 111, 374-379.	1.4	6
12312	Quercetin/ $\beta$ -cyclodextrin inclusion complex embedded nanofibres: Slow release and high solubility. <i>Food Chemistry</i> , 2016, 197, 864-871.	4.2	115

#	ARTICLE	IF	CITATIONS
12313	Phosphorene ribbons as anode materials with superhigh rate and large capacity for Li-ion batteries. <i>Journal of Power Sources</i> , 2016, 302, 215-222.	4.0	46
12314	The acid–base and redox reactivity of CeO <sub>2</sub> nanoparticles: Influence of the Hubbard U term in DFT + U studies. <i>Surface Science</i> , 2016, 648, 212-219.	0.8	18
12315	The ferrite/oxide interface and helium management in nano-structured ferritic alloys from the first principles. <i>Acta Materialia</i> , 2016, 103, 474-482.	3.8	68
12316	Examining the Performance of Refractory Conductive Ceramics as Plasmonic Materials: A Theoretical Approach. <i>ACS Photonics</i> , 2016, 3, 43-50.	3.2	126
12317	Methanol formation from CO <sub>2</sub> catalyzed by Fe <sub>3</sub> S <sub>4</sub> {111}: formate versus hydrocarboxyl pathways. <i>Faraday Discussions</i> , 2016, 188, 161-180.	1.6	29
12318	Crystal structure, equation of state, and elasticity of hydrous aluminosilicate phase, topaz-OH (Al <sub>2</sub> SiO <sub>4</sub> (OH) <sub>2</sub> ) at high pressures. <i>Physics of the Earth and Planetary Interiors</i> , 2016, 251, 24-35.	0.7	18
12319	New Cu(II) complex with acetylpyridine benzoyl hydrazone: experimental and theoretical analysis. <i>Journal of Coordination Chemistry</i> , 2016, 69, 330-342.	0.8	10
12320	Design of new disulfide-based organic compounds for the improvement of self-healing materials. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1758-1770.	1.3	139
12321	Steam Reforming of Ethylene Glycol over MgAl <sub>2</sub> O <sub>4</sub> Supported Rh, Ni, and Co Catalysts. <i>ACS Catalysis</i> , 2016, 6, 315-325.	5.5	45
12322	Adsorption of guaiacol on Fe (110) and Pd (111) from first principles. <i>Surface Science</i> , 2016, 648, 227-235.	0.8	36
12323	Total Synthesis of (âˆ™)-Hymenoseetin. <i>Journal of Organic Chemistry</i> , 2016, 81, 215-228.	1.7	26
12324	Al-rich beta zeolites. Distribution of Al atoms in the framework and related protonic and metal-ion species. <i>Journal of Catalysis</i> , 2016, 333, 102-114.	3.1	86
12325	Kinetic Monte Carlo simulations of the water gas shift reaction on Cu(1 1 1) from density functional theory based calculations. <i>Journal of Catalysis</i> , 2016, 333, 217-226.	3.1	53
12326	Performance of some DFT functionals with dispersion on modeling of the translational isomers of a solvent-switchable [2]rotaxane. <i>Journal of Molecular Structure</i> , 2016, 1107, 31-38.	1.8	13
12327	The structure and thermodynamic properties of liquid Al–Si alloys by ab initio molecular dynamics simulation. <i>Journal of Non-Crystalline Solids</i> , 2016, 433, 31-37.	1.5	15
12328	Unraveling the origins of conduction band valley degeneracies in Mg <sub>2</sub> Si <sup>1-x</sup> S <sub>x</sub> thermoelectrics. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 939-946.	1.3	12
12329	Effects of Zr alloying on cohesion properties of Cu/W interfaces. <i>Journal of Alloys and Compounds</i> , 2016, 661, 553-556.	2.8	34
12330	Structural stability, electronic, mechanical and superconducting properties of CrC and MoC. <i>Materials Chemistry and Physics</i> , 2016, 169, 71-81.	2.0	30

#	ARTICLE	IF	CITATIONS
12331	Crystal structure, electronic and magnetic properties of double perovskite Ba <sub>2</sub> FeWO <sub>6</sub> : A combined experimental–theoretical study. <i>Physica B: Condensed Matter</i> , 2016, 481, 217-223.	1.3	11
12332	A Two-Dimensional Liquid Structure Explains the Elevated Melting Temperatures of Gallium Nanoclusters. <i>Nano Letters</i> , 2016, 16, 21-26.	4.5	18
12333	First-principles study of defect formation in the photovoltaic semiconductor Cu <sub>2</sub> SnS <sub>3</sub> for comparison with Cu <sub>2</sub> ZnSnS <sub>4</sub> and CuInSe <sub>2</sub> . <i>Japanese Journal of Applied Physics</i> , 2016, 55, 04ES08.	0.8	9
12334	N and Ti adatom dynamics on stoichiometric polar TiN(111) surfaces. <i>Surface Science</i> , 2016, 649, 72-79.	0.8	32
12335	The C–H bond dissociation enthalpies in fused N-heterocyclic compounds. <i>Russian Journal of Physical Chemistry A</i> , 2016, 90, 610-621.	0.1	2
12336	Tri-iodide Reduction Activity of Shape- and Composition-Controlled PtFe Nanostructures as Counter Electrodes in Dye-Sensitized Solar Cells. <i>Chemistry of Materials</i> , 2016, 28, 2110-2119.	3.2	51
12337	Density Functional Theory Study of Elemental Mercury Adsorption on Fe <sub>2</sub> O <sub>3</sub> [104] and Its Effect on Carbon Deposit during Chemical Looping Combustion. <i>Energy &amp; Fuels</i> , 2016, 30, 3413-3418.	2.5	12
12338	Shape Evolution of Metal Nanoparticles in Water Vapor Environment. <i>Nano Letters</i> , 2016, 16, 2628-2632.	4.5	92
12339	Underlying mechanisms of the synergistic role of Li <sub>2</sub> MnO <sub>3</sub> and LiNi <sub>1/3</sub> Co <sub>1/3</sub> Mn <sub>1/3</sub> O <sub>2</sub> in high-Mn, Li-rich oxides. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11411-11421.	1.3	22
12340	Ab initio study of oxygen adsorption on the NiTi(1 1 0) surface and the surface phase diagram. <i>Corrosion Science</i> , 2016, 106, 137-146.	3.0	13
12341	Electronic structure and thermodynamic properties of platinum–lead oxides PbPt <sub>2</sub> O <sub>4</sub> and Pb <sub>2</sub> PtO <sub>4</sub> by <i>ab initio</i> methods. <i>Phase Transitions</i> , 2016, 89, 1090-1102.	0.6	2
12342	Silver/hydroxyapatite foam as a highly selective catalyst for acetaldehyde production via ethanol oxidation. <i>Catalysis Today</i> , 2016, 276, 19-27.	2.2	29
12343	A DFT+U study of the Mars Van Krevelen mechanism of CO oxidation on Au/TiO <sub>2</sub> catalysts. <i>Applied Catalysis A: General</i> , 2016, 519, 27-33.	2.2	39
12344	Geometrical isomers of tris(β <sup>2</sup> -diketonato)metal(III) complexes for M = Cr or Co: Synthesis, X-ray structures and DFT study. <i>Inorganica Chimica Acta</i> , 2016, 447, 59-65.	1.2	11
12345	Effect of metallation, substituents and inter/intra-molecular polarization on electronic couplings for hole transport in stacked porphyrin dyads. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21122-21132.	1.3	8
12346	A DFT study to unravel the ligand exchange kinetics and thermodynamics of Os <sup>VIII</sup> oxo/hydroxido/aqua complexes in aqueous matrices. <i>Dalton Transactions</i> , 2016, 45, 7028-7041.	1.6	4
12347	A solid phase honey-like channel method for synthesizing urea-ammonium chloride cocrystals on industrial scale. <i>Journal of Crystal Growth</i> , 2016, 442, 110-113.	0.7	5
12348	NO Reduction by H <sub>2</sub> on the Rh(111) and Rh(221) Surfaces: A Mechanistic and Kinetic Study. <i>Journal of Physical Chemistry C</i> , 2016, 120, 5410-5419.	1.5	28

#	ARTICLE	IF	CITATIONS
12349	Mode specificity for the dissociative chemisorption of H <sub>2</sub> O on Cu(111): a quantum dynamics study on an accurately fitted potential energy surface. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8537-8544.	1.3	33
12350	Manipulation resolves non-trivial structure of corrole monolayer on Ag(111). <i>Nanotechnology</i> , 2016, 27, 025704.	1.3	10
12351	Density functional theoretical studies on the methanol adsorption and decomposition on Ru(0001) surfaces. <i>Chemical Research in Chinese Universities</i> , 2016, 32, 234-241.	1.3	4
12352	Effect and controlling mechanism of vanadium on Fe-Al interface reaction in Zn bath. <i>Surface and Coatings Technology</i> , 2016, 306, 408-417.	2.2	8
12353	Surface-Mediated Hydrogen Bonding of Proteinogenic $\alpha$ -Amino Acids on Silicon. <i>Accounts of Chemical Research</i> , 2016, 49, 942-951.	7.6	26
12354	Pt-Doped NiFe <sub>2</sub> O <sub>4</sub> Spinel as a Highly Efficient Catalyst for H <sub>2</sub> Selective Catalytic Reduction of NO at Room Temperature. <i>ACS Combinatorial Science</i> , 2016, 18, 195-202.	3.8	34
12355	Hexagonal Planar CdS Monolayer Sheet for Visible Light Photocatalysis. <i>Journal of Physical Chemistry C</i> , 2016, 120, 7052-7060.	1.5	132
12356	Origin of Indium Diffusion in High- $\kappa$ Oxide HfO <sub>2</sub> . <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 7595-7600.	4.0	28
12357	Long-afterglow metal-organic frameworks: reversible guest-induced phosphorescence tunability. <i>Chemical Science</i> , 2016, 7, 4519-4526.	3.7	376
12358	Density functional theory study of nitrogen atoms and molecules interacting with Fe(1 1 1) surfaces. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2016, 382, 105-109.	0.6	6
12359	Automatized Parameterization of the Density-Functional Tight-Binding Method. II. Two-center Integrals. <i>Journal of the Chinese Chemical Society</i> , 2016, 63, 57-68.	0.8	13
12360	Active sites and mechanisms for H <sub>2</sub> O decomposition over Pd catalysts. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E1973-82.	3.3	171
12361	Site preferences and effects of X (X = Mn, Fe, Co, Cu) on the properties of NiAl: A first-principles study. <i>Modern Physics Letters B</i> , 2016, 30, 1650133.	1.0	4
12362	A quantum-chemical approach to Ni and Fe codoping in SnO <sub>2</sub> . <i>Journal of Theoretical and Computational Chemistry</i> , 2016, 15, 1650016.	1.8	1
12363	Structural features and thermal properties of W/Cu compounds using tight-binding potential calculations. <i>Journal of Materials Science</i> , 2016, 51, 5948-5961.	1.7	18
12364	Theoretical Study on Free Fatty Acid Elimination Mechanism for Waste Cooking Oils to Biodiesel over Acid Catalyst. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 66, 41-46.	1.3	9
12365	Dimethyl ether electro-oxidation on platinum surfaces. <i>Nano Energy</i> , 2016, 29, 428-438.	8.2	17
12366	Orientation of trimethylolethane cyclic phosphite in rhodium complexes: Structure of [Rh(CH <sub>3</sub> COCHCOCH <sub>3</sub> )(CO)(P(OCH <sub>2</sub> ) <sub>3</sub> CCH <sub>3</sub> )]. <i>Polyhedron</i> , 2016, 111, 161-166.	1.0	1

#	ARTICLE	IF	CITATIONS
12367	Complexes with Tunable Intramolecular Ferrocene to Ti <sup>IV</sup> Electronic Transitions: Models for Solid State Fe <sup>II</sup> to Ti <sup>IV</sup> Charge Transfer. <i>Inorganic Chemistry</i> , 2016, 55, 2200-2211.	1.9	27
12368	The Design of "Neutral" Carbanions with Intramolecular Charge Compensation. <i>Journal of Organic Chemistry</i> , 2016, 81, 1885-1898.	1.7	8
12369	Electron Detachment and Subsequent Structural Changes of Water Clusters. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1065-1073.	1.1	5
12370	Adsorption and coupling of 4-aminophenol on Pt(111) surfaces. <i>Surface Science</i> , 2016, 646, 5-12.	0.8	8
12371	First principle study of the surface reactivity of layered lithium oxides LiMO <sub>2</sub> (M = Ni, Mn, Co). <i>Surface Science</i> , 2016, 649, 46-55.	0.8	24
12372	Correlation of Methane Activation and Oxide Catalyst Reducibility and Its Implications for Oxidative Coupling. <i>ACS Catalysis</i> , 2016, 6, 1812-1821.	5.5	134
12373	Effect of particle size on the surface activity of TiC-Ni composite coating via the interfacial valence electron localization. <i>RSC Advances</i> , 2016, 6, 18793-18799.	1.7	12
12374	The role of carboxylic acid in cobalt Fischer-Tropsch synthesis catalyst deactivation. <i>Catalysis Today</i> , 2016, 275, 127-134.	2.2	13
12375	Predicting <sup>17</sup> O NMR chemical shifts of polyoxometalates using density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8235-8241.	1.3	4
12376	Novel $\hat{1}\pm$ - and $\hat{1}^2$ -type boron sheets: Theoretical insight into their structures, thermodynamic stability, and work functions. <i>Chemical Physics Letters</i> , 2016, 648, 81-86.	1.2	12
12377	H <sub>2</sub> S adsorption on graphene in the presence of sulfur: A density functional theory study. <i>Computational Materials Science</i> , 2016, 117, 110-119.	1.4	65
12378	First-principles study of transition metal (Ti, Nb)-doped NaAlH <sub>4</sub> . <i>International Journal of Hydrogen Energy</i> , 2016, 41, 3517-3526.	3.8	6
12379	Oxygen vacancies as active sites for H <sub>2</sub> S dissociation on the rutile TiO <sub>2</sub> (110) surface: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 6706-6712.	1.3	42
12380	Ab Initio Study of Carbon Impurities in Cu <sub>2</sub> ZnSnS <sub>4</sub> . <i>IEEE Journal of Photovoltaics</i> , 2016, 6, 562-570.	1.5	3
12381	Optical band gaps of zigzag CNTs. <i>Optik</i> , 2016, 127, 3940-3942.	1.4	13
12382	Adsorption of ethyl xanthate on ZnS(110) surface in the presence of water molecules: A DFT study. <i>Applied Surface Science</i> , 2016, 370, 11-18.	3.1	76
12383	Surface segregation phenomena in extended and nanoparticle surfaces of Cu-Au alloys. <i>Surface Science</i> , 2016, 649, 39-45.	0.8	11
12384	No need for external orthogonality in subsystem density-functional theory. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21001-21009.	1.3	21

#	ARTICLE	IF	CITATIONS
12385	High-Pressure Phase Stability and Superconductivity of Pnictogen Hydrides and Chemical Trends for Compressed Hydrides. <i>Chemistry of Materials</i> , 2016, 28, 1746-1755.	3.2	68
12386	Theoretical study on the surface stabilities, electronic structures and water adsorption behavior of the Ta <sub>3</sub> N <sub>5</sub> (110) surface. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7938-7945.	1.3	8
12387	Water-soluble, heterometallic chalcogenide oligomers as building blocks for functional films. <i>Inorganic Chemistry Frontiers</i> , 2016, 3, 689-701.	3.0	3
12388	Shuffling-controlled versus strain-controlled deformation twinning: The case for HCP Mg twin nucleation. <i>International Journal of Plasticity</i> , 2016, 82, 32-43.	4.1	71
12389	The Nature of Secondary Interactions at Electrophilic Metal Sites of Molecular and Silica-Supported Organolutetium Complexes from Solid-State NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2016, 138, 3831-3843.	6.6	35
12390	Screening for high-spin metal organic frameworks (MOFs): density functional theory study on DUT-8(M <sub>1</sub> ,M <sub>2</sub> ) (with M <sub>i</sub> = V, Cu). <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8075-8080.	1.3	23
12391	Fundamental properties of GaN(0001) films grown directly on Gd <sub>2</sub> O <sub>3</sub> (0001) platforms: ab-initio structural simulations. <i>Optical and Quantum Electronics</i> , 2016, 48, 1.	1.5	2
12392	Intrinsic magnetic properties of ZnO nanoislands: Insight from first-principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2016, 380, 1324-1328.	0.9	4
12393	Calculation of alloying effect on formation enthalpy of TiCu intermetallics from first-principles calculations for designing Ti-Cu-system metallic glasses. <i>Philosophical Magazine Letters</i> , 2016, 96, 27-34.	0.5	7
12394	Phase Transition of MoS <sub>2</sub> Bilayer Structures. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3776-3780.	1.5	33
12395	Facile preparation of semimetallic WP <sub>2</sub> as a novel photocatalyst with high photoactivity. <i>RSC Advances</i> , 2016, 6, 15724-15730.	1.7	23
12396	First principle calculations of the adsorption of molecular H <sub>2</sub> in Cu[Fe(CN) <sub>5</sub> NO] metal nitroprussides. An insight into H <sub>2</sub> -host interactions. <i>Computational Materials Science</i> , 2016, 117, 54-64.	1.4	1
12397	Defect Physics and Chemistry in Layered Mixed Transition Metal Oxide Cathode Materials: (Ni,Co,Mn) vs (Ni,Co,Al). <i>Chemistry of Materials</i> , 2016, 28, 1325-1334.	3.2	78
12398	The hydrogen storage properties of the Ti decorated benzene-Ti-graphene sandwich-type structures. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 1035-1043.	3.8	21
12399	Kinetic and Theoretical Insights into the Mechanism of Alkanol Dehydration on Solid Brønsted Acid Catalysts. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3371-3389.	1.5	42
12400	Incorrect DFT-GGA predictions of the stability of non-stoichiometric/polar dielectric surfaces: the case of Cu <sub>2</sub> O(111). <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 6729-6733.	1.3	46
12401	Kohn-Sham density functional theory prediction of fracture in silicon carbide under mixed mode loading. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2016, 24, 035004.	0.8	7
12402	Anisotropic and temperature-dependent growth mechanism of S-phase precipitates in Al-Cu-Mg alloy in relation with GPB zones. <i>Transactions of Nonferrous Metals Society of China</i> , 2016, 26, 1-11.	1.7	23



#	ARTICLE	IF	CITATIONS
12403	Structural, electronic and optical properties of TcX <sub>2</sub> (X = S, Se, Te) from first principles calculations. Computational Materials Science, 2016, 115, 177-183.	1.4	18
12404	The nature of B and N bonding in iminoboryl complexes of rhodium and iridium cis,mer-[ $(L)_3(Br)_2M(BNSiMe_3)$ ] ( $L = PMe_3, CO$ ): Dispersion corrected DFT study. Journal of Organometallic Chemistry, 2016, 803, 21-29.	0.8	1
12405	Periodic density functional theory study of structural and electronic properties of single-walled zinc oxide and carbon nanotubes. Journal of Solid State Chemistry, 2016, 237, 36-47.	1.4	23
12406	The effects of post-deposition ion-beam bombardment with oxygen on the Co surface in modifying the magnetic properties of Co thin films. Microelectronic Engineering, 2016, 152, 41-47.	1.1	4
12407	Breakthrough of the p-type doping bottleneck in ZnO by inserting an ultrathin ZnX (X = S, Se and Te) layer doped with N or Ag/Zn. Journal Physics D: Applied Physics, 2016, 49, 095104.	1.3	5
12408	The transformation pathways for virtual long period stacking-ordered Mg: First-principles study. Computational Materials Science, 2016, 114, 1-12.	1.4	2
12409	Density functional theory studies of HCOOH decomposition on Pd(111). Surface Science, 2016, 650, 111-120.	0.8	70
12410	Nano-scale polar/nonpolar oxide heterostructures for photocatalysis. Nanoscale, 2016, 8, 6057-6063.	2.8	14
12411	Methanol dissociation on bimetallic surfaces: validity of the general Brønsted-Evans-Polanyi relationship for O-H bond cleavage. RSC Advances, 2016, 6, 18695-18702.	1.7	10
12412	Development of an exchange correlation functional with uncertainty quantification capabilities for density functional theory. Journal of Computational Physics, 2016, 311, 173-195.	1.9	29
12413	HCOOH decomposition on Pt(111): A DFT study. Surface Science, 2016, 648, 201-211.	0.8	54
12414	Li <sub>2</sub> S Film Formation on Lithium Anode Surface of Li-S batteries. ACS Applied Materials & Interfaces, 2016, 8, 4700-4708.	4.0	70
12415	The photocatalytic properties of ultrathin bismuth oxychloride nanosheets: a first principles study. Physical Chemistry Chemical Physics, 2016, 18, 7261-7268.	1.3	43
12416	Systematic theoretical investigation of structure and electronic properties of pure copper and lithium doped copper clusters. Molecular Physics, 2016, 114, 1644-1656.	0.8	5
12417	Deposition Morphology and Magnetism of Co, Pt Adatoms and Small CoPt Adclusters on Ni(100) Substrate. Journal of Cluster Science, 2016, 27, 947-964.	1.7	2
12418	The comparative theoretical study of the LaBO <sub>3</sub> (001) (B = Mn, Fe, Co, and Ni) surface properties and oxygen adsorption mechanisms. Ionics, 2016, 22, 1153-1158.	1.2	6
12419	Structure, Ionization, and Fragmentation of Neutral and Positively Charged Hydrogenated Carbon Clusters: C <sub>n</sub> H <sub>m</sub> <sup>q+</sup> ( $n = 1-5, m = 1-5$ ) Tj. J. Chem. Phys. 143, 084701 (2015)	1.3	96
12420	The Impact of Specifically Adsorbed Ions on the Copper-Catalyzed Electroreduction of CO <sub>2</sub> . Journal of the Electrochemical Society, 2016, 163, F477-F484.	1.3	92



#	ARTICLE	IF	CITATIONS
12421	Buckminsterfullerene's movability on the Fe(001) surface. Journal of Magnetism and Magnetic Materials, 2016, 410, 41-46.	1.0	3
12422	Low-Cost Al <sub>2</sub> O <sub>3</sub> Coating Layer As a Preformed SEI on Natural Graphite Powder To Improve Coulombic Efficiency and High-Rate Cycling Stability of Lithium-Ion Batteries. ACS Applied Materials & Interfaces, 2016, 8, 6512-6519.	4.0	89
12423	Simultaneously Controllable Doping Sites and the Activity of a W <sup>δ</sup> -N Codoped TiO <sub>2</sub> Photocatalyst. ACS Catalysis, 2016, 6, 2745-2753.	5.5	84
12424	A DFT-based comparative equilibrium study of thermal dehydration and hydrolysis of CaCl <sub>2</sub> hydrates and MgCl <sub>2</sub> hydrates for seasonal heat storage. Physical Chemistry Chemical Physics, 2016, 18, 10059-10069.	1.3	32
12425	Nanostructured Co <sub>x</sub> Ni <sub>1-x</sub> bimetallic alloys for high efficient and ultrafast adsorption: experiments and first-principles calculations. RSC Advances, 2016, 6, 9209-9220.	1.7	12
12426	Electronic and optical properties of titanium-doped GaN nanowires. Materials and Design, 2016, 96, 409-415.	3.3	95
12427	Assessing the potential of Mg-doped Cr <sub>2</sub> O <sub>3</sub> as a novel <i>p</i> -type transparent conducting oxide. Journal of Physics Condensed Matter, 2016, 28, 125501.	0.7	21
12428	Ni-containing Cu/SiO <sub>2</sub> catalyst for the chemoselective synthesis of ethanol via hydrogenation of dimethyl oxalate. Catalysis Today, 2016, 276, 28-35.	2.2	46
12429	Density function theory study of water gas shift reaction on 2Cu/ZnO		

#	ARTICLE	IF	CITATIONS
12439	Hydrogen Recombination and Dimer Formation on Graphite from Ab Initio Molecular Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5032-5040.	1.1	10
12440	Solution Combustion Synthesis, Characterization, and Photoelectrochemistry of $\text{CuNb}_2\text{O}_6$ and $\text{ZnNb}_2\text{O}_6$ Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2016, 120, 16024-16034.	1.5	56
12441	Stabilities, Electronic and Optical Properties of $\text{SnSe}_2(1\bar{1}0)$ Alloys: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2016, 120, 5839-5847.	1.5	45
12442	Density functional theory study of Li binding to graphene. <i>RSC Advances</i> , 2016, 6, 26540-26545.	1.7	21
12443	A comprehensive first-principles study of pure elements: Vacancy formation and migration energies and self-diffusion coefficients. <i>Acta Materialia</i> , 2016, 109, 128-141.	3.8	117
12444	On the applicability of hybrid functionals for predicting fundamental properties of metals. <i>Solid State Communications</i> , 2016, 234-235, 10-13.	0.9	36
12445	Self-Organized Supported Clusters of L-Methionine. <i>Journal of Physical Chemistry C</i> , 2016, 120, 6534-6542.	1.5	2
12446	Unraveling the Origin of Instability in Ni-Rich $\text{LiNi}_{1-x}\text{Co}_x\text{Mn}_x\text{O}_2$ (NCM) Cathode Materials. <i>Journal of Physical Chemistry C</i> , 2016, 120, 6383-6393.	1.5	154
12447	Structure, electronic, mechanical and optical properties of ternary $\text{YAl}_3\text{C}_3$ carbide. <i>Journal of Solid State Chemistry</i> , 2016, 237, 336-342.	1.4	9
12448	Gold as a 6p-Element in Dense Lithium Aurides. <i>Journal of the American Chemical Society</i> , 2016, 138, 4046-4052.	6.6	101
12449	Insight into the Vibrational and Thermodynamic Properties of Layered Lithium Transition-Metal Oxides $\text{LiMO}_2$ (M = Co, Ni, Mn): A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2016, 120, 5876-5882.	1.5	28
12450	Electronic Structure of Zn-Modified Zeolite: A Density Functional Theory Study of Ferrierite. <i>Journal of Physical Chemistry C</i> , 2016, 120, 6031-6038.	1.5	10
12451	Resolution of the Band Gap Prediction Problem for Materials Design. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1198-1203.	2.1	200
12452	$^{57}\text{Fe}$ emission Mössbauer spectroscopy following dilute implantation of $^{57}\text{Mn}$ into $\text{In}_2\text{O}_3$ . <i>Hyperfine Interactions</i> , 2016, 237, 1.	0.2	2
12453	New perspectives in organolanthanide chemistry from redox to bond metathesis: insights from theory. <i>Chemical Society Reviews</i> , 2016, 45, 2516-2543.	18.7	44
12454	High-Pressure Synthesis and Characterization of Incompressible Titanium Pernitride. <i>Chemistry of Materials</i> , 2016, 28, 1616-1620.	3.2	83
12455	Structural, Electronic, Vibrational, and Topological Analysis of Single-Walled Zinc Oxide Nanotubes. <i>Journal of Physical Chemistry C</i> , 2016, 120, 6814-6823.	1.5	28
12456	Reducing the $\text{V}_2\text{O}_3(0001)$ surface through electron bombardment – a quantitative structure determination with I/V-LEED. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3124-3130.	1.3	8

#	ARTICLE	IF	CITATIONS
12457	Chemical speciation via X-ray emission spectroscopy in the tender X-ray range. <i>Journal of Analytical Atomic Spectrometry</i> , 2016, 31, 450-457.	1.6	21
12458	Two-component molecular cocrystals of 9-acetylanthracene with highly tunable one-/two-photon fluorescence and aggregation induced emission. <i>Journal of Materials Chemistry C</i> , 2016, 4, 2527-2534.	2.7	71
12459	Germanene nanoribbon tunneling field effect transistor (GeNR-TFET) with a 10 nm channel length: analog performance, doping and temperature effects. <i>Semiconductor Science and Technology</i> , 2016, 31, 045009.	1.0	27
12460	Efficient visible light photocatalytic oxidation of NO with hierarchical nanostructured 3D flower-like BiOCl <sub>x</sub> Br <sub>1-x</sub> solid solutions. <i>Journal of Alloys and Compounds</i> , 2016, 671, 318-327.	2.8	66
12461	Some new members of MAX family including light-elements: Nanolayered Hf <sub>2</sub> XY (X= Al, Si, P and Y=B, C). <i>Tj ETQq0.0.0 rgBT /Overlock 1</i>	1.5	23
12462	Ab initio molecular dynamics simulations of the O <sub>2</sub> /Pt(1 1 1) interaction. <i>Catalysis Today</i> , 2016, 260, 60-65.	2.2	23
12463	Thermal desorption of molecular oxygen from SnO <sub>2</sub> (110) surface: Insights from first-principles calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2016, 89, 15-22.	1.9	14
12464	Bottom-up design of 2D organic photocatalysts for visible-light driven hydrogen evolution. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 034004.	0.7	13
12465	Syntheses, spectroscopic investigation and electronic properties of two sulfonamide derivatives: A combined experimental and quantum chemical approach. <i>Journal of Molecular Structure</i> , 2016, 1108, 496-507.	1.8	26
12466	New routes for improving adhesion at the metal/Al <sub>2</sub> O <sub>3</sub> (0001) interface. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3032-3039.	1.3	16
12467	Stability, adsorption, and diffusion of hydrogen in Pd <sub>3</sub> Ag phases. <i>Journal of Membrane Science</i> , 2016, 503, 124-131.	4.1	14
12468	A user guide for SLUSCHI: Solid and Liquid in Ultra Small Coexistence with Hovering Interfaces. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2016, 52, 88-97.	0.7	23
12469	Complex of manganese (II) with curcumin: Spectroscopic characterization, DFT study, model-based analysis and antiradical activity. <i>Journal of Molecular Structure</i> , 2016, 1109, 139-145.	1.8	12
12470	Prediction of the Half-Metallic Properties of Zr <sub>2</sub> VZ (Z = Si, Ge, Sn, and Pb) Heusler Alloys Based on Density Functional Theory. <i>Journal of Superconductivity and Novel Magnetism</i> , 2016, 29, 493-500.	0.8	6
12471	Robust half-metallic properties in inverse Heusler alloys composed of 4d transition metal elements: Zr <sub>2</sub> RhZ (Z=Al, Ga, In). <i>Journal of Magnetism and Magnetic Materials</i> , 2016, 402, 190-195.	1.0	51
12472	Density functional theory study of O-H and C-H bond scission of methanol catalyzed by a chemisorbed oxygen layer on Cu(111). <i>Surface Science</i> , 2016, 646, 288-297.	0.8	16
12473	Unravelling the hydrogen absorption process in Pd overlayers on a Au(111) surface. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3659-3668.	1.3	10
12474	First-principles calculations of transition metal solute interactions with hydrogen in tungsten. <i>Nuclear Fusion</i> , 2016, 56, 026004.	1.6	33

#	ARTICLE	IF	CITATIONS
12475	Benchmarking semiempirical, Hartree-Fock, DFT, and MP2 methods against the ionization energies and electron affinities of short- through long-chain [n]acenes and [n]phenacenes. <i>Canadian Journal of Chemistry</i> , 2016, 94, 251-258.	0.6	8
12476	High thermoelectric performance from optimization of hole-doped $\text{CuInTe}_2$ . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5925-5931.	1.3	36
12477	Novel superhard $\text{B}_6\text{C}_6\text{O}$ phases predicted from first principles. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1859-1863.	1.3	44
12478	Effect of Mg doping on optical and electrical properties of $\text{SnO}_2$ thin films: An experiment and first-principles study. <i>Ceramics International</i> , 2016, 42, 5299-5303.	2.3	26
12479	Stability and nucleation of $\text{Ir}_n$ ( $n = 1-5$ ) clusters on different $\text{Al}_2\text{O}_3$ surfaces: A density functional theory study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2016, 380, 718-725.	0.9	8
12480	Theoretical study of the $\text{NO}$ , $\text{NO}_2$ , $\text{CO}$ , $\text{SO}_2$ , and $\text{NH}_3$ adsorptions on multi-diameter single-wall $\text{MoS}_2$ nanotube. <i>Journal Physics D: Applied Physics</i> , 2016, 49, 045106.	1.3	22
12481	Theoretical investigations on enhancing the performance of terminally diketopyrrolopyrrole-based small-molecular donors in organic solar cell applications. <i>Journal of Molecular Modeling</i> , 2016, 22, 15.	0.8	11
12482	Non-equilibrium properties of interatomic potentials in cascade simulations in tungsten. <i>Journal of Nuclear Materials</i> , 2016, 470, 119-127.	1.3	63
12483	Electronic structure, photovoltage, and photocatalytic hydrogen evolution with $\text{p-CuBi}_2\text{O}_4$ nanocrystals. <i>Journal of Materials Chemistry A</i> , 2016, 4, 2936-2942.	5.2	158
12484	$\text{Ce}^{3+}$ -doped $\text{Li}_4\text{Ti}_5\text{O}_{12}$ with $\text{CeO}_2$ surface modification by a sol-gel method for high-performance lithium-ion batteries. <i>Electrochimica Acta</i> , 2016, 189, 147-157.	2.6	66
12485	Synthesis, structure, and catalytic properties of copper, palladium and cobalt complexes containing an N,O-type bidentate thiazoline ligand. <i>Inorganica Chimica Acta</i> , 2016, 443, 22-27.	1.2	34
12486	Catalytic Activity for Oxygen Reduction Reaction on $\text{CoN}_2$ -Graphene: A Density Functional Theory Study. <i>Journal of the Electrochemical Society</i> , 2016, 163, F160-F165.	1.3	15
12487	Tailoring the substitution on the surface of $\text{Fe}_{13}/\text{Pt}_{42}$ core-shell nanoparticles by Au atoms. <i>Materials and Design</i> , 2016, 92, 794-801.	3.3	1
12488	Density functional study on positively charged six-coordinate $\text{FeO}_2$ porphyrin complex for a trigger of $\text{O}_2$ dissociation. <i>Chemical Physics Letters</i> , 2016, 643, 119-125.	1.2	3
12489	Characterization of Phosphate Species on Hydrated Anatase $\text{TiO}_2$ Surfaces. <i>Langmuir</i> , 2016, 32, 997-1008.	1.6	18
12490	Linear and Nonlinear Optical Response in Silver Nanoclusters: Insight from a Computational Investigation. <i>Journal of Physical Chemistry A</i> , 2016, 120, 507-518.	1.1	31
12491	Orientation of Cyano-Substituted Bipyridine $\text{Re}(\text{I})$ -Tricarbonyl Electrocatalysts Bound to Conducting Au Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1657-1665.	1.5	46
12492	Surface segregation and oxidation of $\text{Pt}_3\text{Ni}(1\ 1\ 1)$ alloys under oxygen environment. <i>Catalysis Today</i> , 2016, 260, 3-7.	2.2	26

#	ARTICLE	IF	CITATIONS
12493	Soluteâ€“grain boundary interaction and segregation formation in Al: First principles calculations and molecular dynamics modeling. Computational Materials Science, 2016, 112, 18-26.	1.4	32
12494	Competitive adsorption of nitrogen and sulphur compounds on a multisite model of NiMoS catalyst: A theoretical study. Journal of Catalysis, 2016, 333, 78-93.	3.1	52
12495	Interatomic Potentials Including Chemistry. Springer Series in Materials Science, 2016, , 107-194.	0.4	1
12496	A template for a planar tetracoordinate heavier group 14 atom: a global study of $C_{2q}Si_{2q}X_q$ ( $X = C, Si, Ge, Sn, Pb; q = +1, 0, \sim 1$ ). Dalton Transactions, 2016, 45, 56-60.	1.6	24
12497	Dehydrogenation of ammonia borane catalyzed by pristine and defective h-BN sheets. Applied Surface Science, 2016, 362, 562-571.	3.1	24
12498	Optical properties of SiC nanosheet. Optik, 2016, 127, 1867-1870.	1.4	30
12499	Ab initio derived reaction mechanism for the dry reforming of methane on Rh doped pyrochlore catalysts. Journal of Catalysis, 2016, 333, 59-70.	3.1	31
12500	Understanding the effects of a multi-functionalized additive on the cathodeâ€“electrolyte interfacial stability of Ni-rich materials. Journal of Power Sources, 2016, 302, 431-438.	4.0	82
12501	Structural, electronic, mechanical and magnetic properties of rare-earth nitrides REN (RE=Ce, Pr, Nd): A first principles study. Materials Science in Semiconductor Processing, 2016, 41, 17-25.	1.9	4
12502	Phase stability, mechanical and thermodynamic properties of orthorhombic and trigonal $MgSiN_2$ : an <i>ab initio</i> study. Phase Transitions, 2016, 89, 480-513.	0.6	69
12503	Density function theoretical and experimental study of $NH_3^+$ NO adsorptions on $MnO/TiO_2$ surface. Computational Materials Science, 2016, 112, 238-244.	1.4	24
12504	Understanding the thermodynamic pathways of $SnO$ -to- $SnO_x$ phase transition. Computational Materials Science, 2016, 111, 359-365.	1.4	22
12505	One-Pot Synthesis of $Au_{11}(PPh_2)_7Br_3$ for the Highly Chemoselective Hydrogenation of Nitrobenzaldehyde. ACS Catalysis, 2016, 6, 92-99.	5.5	75
12506	Facet Dependence of $CO_2$ Reduction Paths on Cu Electrodes. ACS Catalysis, 2016, 6, 219-229.	5.5	420
12507	Accessing Realistic Models for the $WO_3/SiO_2$ Industrial Catalyst through the Design of Organometallic Precursors. ACS Catalysis, 2016, 6, 1-18.	5.5	54
12508	Biogenic approaches using citrus extracts for the synthesis of metal nanoparticles: the role of flavonoids in gold reduction and stabilization. New Journal of Chemistry, 2016, 40, 1420-1429.	1.4	24
12509	Direct atomic-scale evidence for shearâ€“dilatation correlation in metallic glasses. Scripta Materialia, 2016, 112, 37-41.	2.6	28
12510	Influence of Ag substitution on the local structure and glass-forming ability of $Al_{86}Ni_{(8-x)}Y_{6}Ag_x$ ( $x = 0, 1, 2$ ) liquids. Physics and Chemistry of Liquids, 2016, 54, 98-109.	0.4	7

#	ARTICLE	IF	CITATIONS
12511	Can DFT and ab initio methods describe all aspects of the potential energy surface of cycloreversion reactions?. <i>Molecular Physics</i> , 2016, 114, 21-33.	0.8	21
12512	First-principles study of NiAl alloyed with Co. <i>Computational Materials Science</i> , 2016, 111, 34-40.	1.4	28
12513	Electronic and Magnetic Properties of Linear and Dimerized Titanium Nanochains Under Compressive and Tensile Strain. <i>Journal of Cluster Science</i> , 2016, 27, 183-191.	1.7	3
12514	Deep HDS of FCC gasoline over alumina supported CoMoS catalyst: Inhibiting effects of carbon monoxide and water. <i>Applied Catalysis B: Environmental</i> , 2016, 183, 317-327.	10.8	28
12515	Phase equilibria and solidification characteristics of the Al–Sc–Si alloys. <i>Journal of Materials Science</i> , 2016, 51, 1644-1658.	1.7	13
12516	Influence of trap connectivity on H diffusion: Vacancy trapping. <i>Acta Materialia</i> , 2016, 103, 334-340.	3.8	38
12517	Long-range intercluster interactions of solute nanoprecipitates in Mg–Y alloys: A first-principles study. <i>Journal of Alloys and Compounds</i> , 2016, 657, 662-670.	2.8	14
12518	Nuclear quantum tunnelling and carrier delocalization effects to bridge the gap between hopping and bandlike behaviors in organic semiconductors. <i>Nanoscale Horizons</i> , 2016, 1, 53-59.	4.1	49
12519	Characterisation and mechanistic study of the oxidative addition reactions of [Ir(cod)(sacac)]. <i>Journal of Organometallic Chemistry</i> , 2016, 801, 80-86.	0.8	4
12520	DFT calculations on electro-oxidations and dissolutions of Pt and Pt–Au nanoparticles. <i>Catalysis Today</i> , 2016, 262, 100-109.	2.2	25
12521	Theoretical insight on reactivity trends in CO <sub>2</sub> electroreduction across transition metals. <i>Catalysis Science and Technology</i> , 2016, 6, 1042-1053.	2.1	57
12522	Stabilization of primary mobile radiation defects in MgF <sub>2</sub> crystals. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2016, 374, 24-28.	0.6	42
12523	DPP containing A organic dyes toward highly efficient dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2016, 125, 27-35.	2.0	25
12524	Experimental and theoretical optical properties of methylammonium lead halide perovskites. <i>Nanoscale</i> , 2016, 8, 6317-6327.	2.8	385
12525	Electronic Structure of Crystalline Buckyballs: fcc-C <sub>60</sub> . <i>Journal of Electronic Materials</i> , 2016, 45, 339-348.	1.0	26
12526	Half-Metallicity and Tetragonal Deformation of Ti <sub>2</sub> RhAl, Ti <sub>2</sub> RhGa, and Ti <sub>2</sub> RhIn: A First-Principle Study. <i>Journal of Superconductivity and Novel Magnetism</i> , 2016, 29, 349-356.	0.8	18
12527	Electronic Structure Change in DNA Caused by Base Pair Motions and Its Effect on Charge Transfer in DNA Chains. <i>Australian Journal of Chemistry</i> , 2016, 69, 300.	0.5	1
12528	Modulation of magnetic properties of bilayer SnSe with transition-metals doping in the interlayer. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2016, 75, 106-111.	1.3	14

#	ARTICLE	IF	CITATIONS
12529	Molecular entrapment of volatile organic compounds (VOCs) by electrospun cyclodextrin nanofibers. <i>Chemosphere</i> , 2016, 144, 736-744.	4.2	75
12530	Bond-bending isomerism of Au <sub>2</sub> I <sub>3</sub> <sup>+</sup> : competition between covalent bonding and aurophilicity. <i>Chemical Science</i> , 2016, 7, 475-481.	3.7	16
12531	Cu atoms suppress misfit dislocations at the $\text{I}^{2\text{Å}^3}/\text{Al}$ interface in Al-Mg-Si alloys. <i>Scripta Materialia</i> , 2016, 110, 6-9.	2.6	35
12532	Quantum and classical dynamics of reactive scattering of H <sub>2</sub> from metal surfaces. <i>Chemical Society Reviews</i> , 2016, 45, 3658-3700.	18.7	137
12533	The structure and electronic properties of dislocations studied by first-principles and molecular dynamics. <i>Molecular Simulation</i> , 2016, 42, 102-109.	0.9	3
12534	Including protein density relaxation effects in first-principles embedding calculations of cofactor excitation energies. <i>Molecular Physics</i> , 2017, 115, 526-537.	0.8	9
12535	Certain doping concentrations caused half-metallic graphene. <i>Journal of Saudi Chemical Society</i> , 2017, 21, 111-117.	2.4	24
12536	Defect engineering toward strong photocatalysis of Nb-doped anatase TiO <sub>2</sub> : Computational predictions and experimental verifications. <i>Applied Catalysis B: Environmental</i> , 2017, 206, 520-530.	10.8	62
12537	Synthesis, Crystal Structure, Magnetic Properties, and Stability of the Manganese-Rich $\alpha\text{-Mn}_3\text{AlC}$ Phase. <i>Inorganic Chemistry</i> , 2017, 56, 1045-1048.	1.9	13
12538	Semi-Dirac semimetal in silicene oxide. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3820-3825.	1.3	40
12539	Effects of boron on the mechanical properties of the TiAl-Ti <sub>3</sub> Al Alloy: A first-principles investigation. <i>Modern Physics Letters B</i> , 2017, 31, 1750002.	1.0	0
12540	Electrocatalyst Design for Direct Borohydride Oxidation Guided by First Principles. <i>Journal of Physical Chemistry C</i> , 2017, 121, 2872-2881.	1.5	13
12541	Improper electric polarization in simple perovskite oxides with two magnetic sublattices. <i>Nature Communications</i> , 2017, 8, 14025.	5.8	53
12542	Adsorption of oxygen and CO oxidation on Au/anatase(001) catalysts. A DFT+U study. <i>New Journal of Chemistry</i> , 2017, 41, 2073-2080.	1.4	12
12543	Ionicity and birefringence of $\text{LiNH}_4\text{SO}_4$ crystals: ab initio DFT study, X-ray spectroscopy measurements. <i>RSC Advances</i> , 2017, 7, 6889-6901.	1.7	20
12544	Vapor-phase $\text{I}^{\text{I}}$ molecular recognition: a fast and solvent-free strategy towards the formation of co-crystalline hollow microtube with 1D optical waveguide and up-conversion emission. <i>Journal of Materials Chemistry C</i> , 2017, 5, 1632-1637.	2.7	48
12545	Ultrasml CuCo <sub>2</sub> S <sub>4</sub> Nanocrystals: All-in-One Theragnosis Nanoplatform with Magnetic Resonance/Near-Infrared Imaging for Efficiently Photothermal Therapy of Tumors. <i>Advanced Functional Materials</i> , 2017, 27, 1606218.	7.8	106
12546	The effects of metalloid elements (P, C, B) on the properties of Co-based amorphous alloys studied by ab initio molecular dynamics simulations. <i>Computational Materials Science</i> , 2017, 130, 76-83.	1.4	6



#	ARTICLE	IF	CITATIONS
12547	Switching between Inner- and Outer-Sphere PCET Mechanisms of Small-Molecule Activation: Superoxide Dismutation and Oxygen/Superoxide Reduction Reactivity Deriving from the Same Manganese Complex. <i>Journal of the American Chemical Society</i> , 2017, 139, 1472-1484.	6.6	37
12548	Theoretical investigations on phase stability, elastic constants and electronic structures of Ga <sub>3</sub> Zr polymorphs under high pressure. <i>Journal of Alloys and Compounds</i> , 2017, 696, 1010-1018.	2.8	3
12549	Improving visible light photocatalytic activity of KTaO <sub>3</sub> using cation-anion dopant pair. <i>Solar Energy Materials and Solar Cells</i> , 2017, 159, 590-598.	3.0	31
12550	Density functional theory is straying from the path toward the exact functional. <i>Science</i> , 2017, 355, 49-52.	6.0	711
12551	Electronic, magnetic and spectroscopic properties of doped Mn <sub>1-x</sub> A <sub>x</sub> WO <sub>4</sub> (A = Co, Ni and Fe) multiferroic: an experimental and DFT study. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 075901.		
12552	Principles and simulations of high-resolution STM imaging with a flexible tip apex. <i>Physical Review B</i> , 2017, 95, .	1.1	76
12553	Intrinsic Origins of Crack Generation in Ni-rich LiNi <sub>0.8</sub> Co <sub>0.1</sub> Mn <sub>0.1</sub> O <sub>2</sub> Layered Oxide Cathode Material. <i>Scientific Reports</i> , 2017, 7, 39669.	1.6	225
12554	Substituent effect on the transport properties of dihydroazulene-based molecular optical switch: A way to tune the switching properties. <i>Computational and Theoretical Chemistry</i> , 2017, 1103, 48-55.	1.1	1
12555	Structural stability, phase transition, and hydrogen diffusion of PdCu phases with additions of Nb and Cr. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 3051-3057.	3.8	5
12556	Exploring metal decorated Porphyrin-like Porous Fullerene as catalyst for oxygen reduction reaction: A DFT study. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 2278-2287.	3.8	47
12557	Structural and chemical contributions on solubility of silicon and carbon in ferrite studied by first-principles calculations. <i>Journal of Alloys and Compounds</i> , 2017, 695, 2717-2722.	2.8	4
12558	Spin-Polarization-Induced Preedge Transitions in the Sulfur K-Edge XAS Spectra of Open-Shell Transition-Metal Sulfates: Spectroscopic Validation of $\pi$ -Bond Electron Transfer. <i>Inorganic Chemistry</i> , 2017, 56, 1080-1093.	1.9	7
12559	Cooperativity and Dynamics Increase the Performance of NiFe Dry Reforming Catalysts. <i>Journal of the American Chemical Society</i> , 2017, 139, 1937-1949.	6.6	322
12560	Layered structure of the near-surface region of oxidized chalcopyrite (CuFeS <sub>2</sub> ): hard X-ray photoelectron spectroscopy, X-ray absorption spectroscopy and DFT+U studies. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2749-2759.	1.3	21
12561	Mechanistic insights into the formation of butene isomers from 1-butanol in H-ZSM-5: DFT based microkinetic modelling. <i>Catalysis Science and Technology</i> , 2017, 7, 1055-1072.	2.1	30
12562	Role of Charge Transfer in Catalytic Hydrogen Oxidation over Platinum. <i>Journal of Physical Chemistry C</i> , 2017, 121, 2696-2701.	1.5	3
12563	Tuning chemical compositions of bimetallic AuPd catalysts for selective catalytic hydrogenation of halogenated quinolines. <i>Journal of Materials Chemistry A</i> , 2017, 5, 3260-3266.	5.2	40
12564	Structural and optical characteristics of pre- and post-annealed sol-gel derived CoCu-oxide coatings. <i>Journal of Alloys and Compounds</i> , 2017, 701, 222-235.	2.8	12

#	ARTICLE	IF	CITATIONS
12565	Designing magnetic compensated states in tetragonal Mn 3 Ge-based Heusler alloys. <i>Journal of Magnetism and Magnetic Materials</i> , 2017, 429, 40-44.	1.0	12
12566	Function of CN group in organic sensitizers: The first principle study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 179, 227-232.	2.0	4
12567	Superpolyhedron-Built Second Harmonic Generation Materials Exhibit Large Mid-Infrared Conversion Efficiencies and High Laser-Induced Damage Thresholds. <i>Chemistry of Materials</i> , 2017, 29, 1796-1804.	3.2	84
12568	Revisiting CO Activation on Co Catalysts: Impact of Step and Kink Sites from DFT. <i>ACS Catalysis</i> , 2017, 7, 1984-1992.	5.5	64
12569	Global optimization of neutral and charged 20- and 55-atom silver and gold clusters at the DFTB level. <i>Computational and Theoretical Chemistry</i> , 2017, 1107, 102-114.	1.1	35
12570	Quantum Chemical Methods for the Prediction of Energetic, Physical, and Spectroscopic Properties of Ionic Liquids. <i>Chemical Reviews</i> , 2017, 117, 6696-6754.	23.0	181
12571	Ligand Influence on Local Magnetic Moments in Fe-Based Metal-Organic Networks. <i>Journal of Physical Chemistry C</i> , 2017, 121, 4253-4260.	1.5	12
12572	Dehydrogenation of goethite in Earth's deep lower mantle. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 1498-1501.	3.3	83
12573	Molecular Dynamics Simulation: From Ab Initio to Coarse Grained, 2017, , 337-396.		2
12574	Quantum mechanical investigation into the electronic transport properties of a memantine-functionalized gold nanopore biosensor for natural and mutated DNA nucleobase detection. <i>RSC Advances</i> , 2017, 7, 8474-8483.	1.7	6
12575	The prospects of phosphorene as an anode material for high-performance lithium-ion batteries: a fundamental study. <i>Nanotechnology</i> , 2017, 28, 075401.	1.3	48
12576	Comprehensive SPHYB and B3LYP-DFT Studies of Two Types of Ferrocene. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2017, 643, 420-431.	0.6	10
12577	A first-principles study on electronic structures and elastic properties of metal doped $\delta$ -Fe(N) high nitrogen steel. <i>Journal of Iron and Steel Research International</i> , 2017, 24, 103-110.	1.4	4
12578	First-Principles Study of Novel Two-Dimensional $(\text{C}_{4}\text{H}_{9}\text{NH}_{3})_{2}\text{PbX}_{4}$ Perovskites for Solar Cell Absorbers. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 876-883.	2.1	61
12579	Properties of the exotic metastable ST12 germanium allotrope. <i>Nature Communications</i> , 2017, 8, 13909.	5.8	29
12580	Structural, electronic, optical and mechanical properties of InP alloyed with Zn, Si, Sn and S under pressure: First-principles calculation. <i>Journal of Alloys and Compounds</i> , 2017, 700, 98-105.	2.8	17
12581	Electronic structure of stoichiometric and reduced ZnO from periodic relativistic all electron hybrid density functional calculations using numeric atom-centered orbitals. <i>Journal of Computational Chemistry</i> , 2017, 38, 523-529.	1.5	18
12582	A DFT study on the modification mechanism of (Cr, C) co-doping for the electronic and optical properties of anatase TiO <sub>2</sub> . <i>Computational Materials Science</i> , 2017, 129, 295-303.	1.4	25

#	ARTICLE	IF	CITATIONS
12583	Half-metallic ferromagnetism in KCaN X ( X = O, S, and Se) quaternary Heusler compounds: A first-principles study. <i>Superlattices and Microstructures</i> , 2017, 105, 39-47.	1.4	10
12584	How Strained are [1]Ferrocenophanes?. <i>Organometallics</i> , 2017, 36, 614-621.	1.1	18
12585	Multireference Perturbation Theory with Cholesky Decomposition for the Density Matrix Renormalization Group. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 451-459.	2.3	88
12586	Structural, mechanical, thermal and electronic properties of novel ternary carbide Al <sub>4</sub> Si <sub>2</sub> C <sub>5</sub> under high pressure by DFT calculation. <i>International Journal of Modern Physics B</i> , 2017, 31, 1750012.	1.0	2
12587	Electrocatalytic Activities of Oxygen Reduction Reaction on Pd/C and Pd <sup>δ</sup> -B/C Catalysts. <i>Journal of Physical Chemistry C</i> , 2017, 121, 3416-3423.	1.5	91
12588	Adsorption and decomposition of dimethyl methylphosphonate on pristine and mono-vacancy defected graphene: A first principles study. <i>Applied Surface Science</i> , 2017, 418, 318-327.	3.1	9
12589	Structural, mechanical and thermodynamic properties of ZrO <sub>2</sub> polymorphs by first-principles calculation. <i>Physica B: Condensed Matter</i> , 2017, 511, 10-19.	1.3	15
12590	Does the S-H Bond Always Break after Adsorption of an Alkylthiol on Au(111)?. <i>Chemistry - A European Journal</i> , 2017, 23, 1402-1408.	1.7	23
12591	Novel Graphene-like Co <sub>2</sub> VAI (111): Case Study on Magnetoelectronic and Optical Properties by First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 3978-3986.	1.5	67
12592	Is the Metallic Phosphorus Carbide (P <sub>2</sub> O-PC) Monolayer Stable? An Answer from a Theoretical Perspective. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 747-754.	2.1	47
12593	First principles study of structural and magnetic properties of transition metal nitrides TMN (TM = Tj ETQq0 0 0 rgBT/Overlock 10 Tf 50	0.6	9
12594	Study of Pressure Effects on the Elastic Stability and Optical Treatment of Co <sub>2</sub> VAI using GGA+U. <i>Silicon</i> , 2017, 9, 431-437.	1.8	0
12595	A simple method to approximate electrode potential-dependent activation energies using density functional theory. <i>Catalysis Today</i> , 2017, 288, 63-73.	2.2	77
12596	The electronic structure, optical absorption and photocatalytic water splitting of (Fe <sup>δ</sup> + <sup>δ</sup> Ni)-codoped TiO <sub>2</sub> : A DFT +U study. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 4966-4976.	3.8	22
12597	The migration behavior of the fourth period transition metals in liquid Al: An ab initio molecular dynamics study. <i>Computational Materials Science</i> , 2017, 130, 183-190.	1.4	7
12598	Hydrolytic Stability of 3-Aminopropylsilane Coupling Agent on Silica and Silicate Surfaces at Elevated Temperatures. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 8344-8353.	4.0	41
12599	On-Surface Site-Selective Cyclization of Corrole Radicals. <i>ACS Nano</i> , 2017, 11, 3383-3391.	7.3	24
12600	Dislocation mechanisms and 3D twin architectures generate exceptional strength-ductility-toughness combination in CrCoNi medium-entropy alloy. <i>Nature Communications</i> , 2017, 8, 14390.	5.8	344

#	ARTICLE	IF	CITATIONS
12601	Adsorption modes of 1,3-thiazol-2-amine on the TiO <sub>2</sub> (001) and (101) anatase surfaces. <i>Structural Chemistry</i> , 2017, 28, 1151-1162.	1.0	4
12602	The electronic structure and optical absorption of rutile TiO <sub>2</sub> with La and N dopants from first-principles calculation. <i>Computational Materials Science</i> , 2017, 131, 178-186.	1.4	12
12603	Acid Gas Adsorption on Metal-Organic Framework Nanosheets as a Model of an All-Surface Material. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1341-1350.	2.3	23
12604	Combination of Inelastic Neutron Scattering Experiments and ab Initio Quantum Calculations for the Study of the Hydration Properties of Oriented Saponites. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5029-5040.	1.5	21
12605	A van der Waals Inclusive Density Functional Theory Study of the Nature of Bonding for Thiophene Adsorption on Ni(100) and Cu(100) Surfaces. <i>Journal of Physical Chemistry C</i> , 2017, 121, 6090-6103.	1.5	19
12606	Insights into the enhanced Ce-N triple bond in the HCe <sub>2</sub> N molecule. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 8216-8222.	1.3	10
12607	Borophene nanosheet molecular device for detection of ethanol - A first-principles study. <i>Computational and Theoretical Chemistry</i> , 2017, 1105, 52-60.	1.1	62
12608	A new stable antiferromagnetic semiconductor: The case of inverse Heusler compound Ti <sub>2</sub> CrSn. <i>Intermetallics</i> , 2017, 85, 149-155.	1.8	3
12609	Interfacial and Alloying Effects on Activation of Ethanol from First-Principles. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5603-5611.	1.5	24
12610	Irradiation-induced void evolution in iron: A phase-field approach with atomistic derived parameters. <i>Chinese Physics B</i> , 2017, 26, 026102.	0.7	6
12611	Recurring polyhedral motifs in the amorphous indium gallium zinc oxide network. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2017, 214, 1600471.	0.8	4
12612	Localized orbital corrections for density functional calculations on transition metal containing systems. <i>Coordination Chemistry Reviews</i> , 2017, 344, 205-213.	9.5	8
12613	First-principles exploration of sp-electron digital magnetic heterostructures: The case for CaO $\hat{\Gamma}$ -doped with 2p-block elements boron, carbon, and nitrogen. <i>Computational Materials Science</i> , 2017, 130, 91-97.	1.4	3
12614	Efficient Spin-Flip Excitation of a Nickelocene Molecule. <i>Nano Letters</i> , 2017, 17, 1877-1882.	4.5	55
12615	Ab initio study of the structural, electronic, elastic and thermal conductivity properties of SrClF with pressure effects. <i>Philosophical Magazine</i> , 2017, 97, 743-758.	0.7	8
12616	Theoretical Investigation of 2D Layered Materials as Protective Films for Lithium and Sodium Metal Anodes. <i>Advanced Energy Materials</i> , 2017, 7, 1602528.	10.2	196
12617	Computational investigation on structural and electronic properties of various metal complexes of (2,2',6',6'-terpyridine)-4-mercaptopbenzoic acid ligand. <i>Applied Surface Science</i> , 2017, 418, 275-279.	3.1	4
12618	Decarbonylation and hydrogenation reaction of furfural on Pd/Cu(111) surface. <i>Journal of Fuel Chemistry and Technology</i> , 2017, 45, 34-42.	0.9	15

#	ARTICLE	IF	CITATIONS
12619	Modelling of the charge carrier mobility in disordered linear polymer materials. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 7760-7771.	1.3	29
12620	Graphene contacts to a HfSe <sub>2</sub> /SnS <sub>2</sub> heterostructure. <i>Journal of Chemical Physics</i> , 2017, 146, 064701.	1.2	8
12621	TNUâ€9 Zeolite: Aluminum Distribution and Extraâ€Framework Sites of Divalent Cations. <i>Chemistry - A European Journal</i> , 2017, 23, 8857-8870.	1.7	15
12622	Adsorption of CO on Low-Energy, Low-Symmetry Pt Nanoparticles: Energy Decomposition Analysis and Prediction via Machine-Learning Models. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5612-5619.	1.5	58
12623	Stability of the crystal structure of $\hat{1}\pm$ -BiFeO <sub>3</sub> . <i>Journal of the Korean Physical Society</i> , 2017, 70, 394-400.	0.3	6
12624	First principles study of inert-gas (helium, neon, and argon) interactions with hydrogen in tungsten. <i>Journal of Nuclear Materials</i> , 2017, 487, 128-134.	1.3	17
12625	Design of Chemoresponsive Liquid Crystals through Integration of Computational Chemistry and Experimental Studies. <i>Chemistry of Materials</i> , 2017, 29, 3563-3571.	3.2	33
12626	Energetics of $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi mathvariant="normal"} \rangle \text{H} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:math} \rangle$ clusters from density functional and coupled cluster theories. <i>Physical Review B</i> , 2017, 95, .	1.1	2
12627	â€œAb initioâ€ synthesis of zeolites for preestablished catalytic reactions. <i>Science</i> , 2017, 355, 1051-1054.	6.0	204
12628	Gas-phase COS activation by U <sup>+</sup> : Reaction mechanisms and bonding analysis. <i>Journal of Theoretical and Computational Chemistry</i> , 2017, 16, 1750010.	1.8	0
12629	Harmonic Vibrational Frequencies: Approximate Global Scaling Factors for TPSS, M06, and M11 Functional Families Using Several Common Basis Sets. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2265-2273.	1.1	141
12630	Dynamic Phase Engineering of Bendable Transition Metal Dichalcogenide Monolayers. <i>Nano Letters</i> , 2017, 17, 2473-2481.	4.5	41
12631	Atomistic Origin of Deformation Twinning in Biomineral Aragonite. <i>Physical Review Letters</i> , 2017, 118, 105501.	2.9	25
12632	First-principles investigation of the equation of state and elastic properties of perovskite-type SrW(O,N) <sub>3</sub> under hydrostatic pressures up to 139 GPa. <i>European Physical Journal B</i> , 2017, 90, 1.	0.6	1
12633	Low-lying Ptn cluster structures (n = 6â€10) from global optimizations based on DFT potential energy surfaces: Sensitivity of the chemical ordering with the functional. <i>Computational and Theoretical Chemistry</i> , 2017, 1107, 136-141.	1.1	15
12634	Low conductance of nickel atomic junctions in hydrogen atmosphere. <i>Frontiers of Physics</i> , 2017, 12, 1.	2.4	5
12635	Tuning the electronic and magnetic properties of porous graphene-like carbon nitride through 3d transition-metal doping. <i>Carbon</i> , 2017, 117, 120-125.	5.4	52
12636	Reinvestigation of Mechanical Properties and Shear-Induced Atomic Deformation of Tetragonal Superhard Semiconducting OsB <sub>4</sub> . <i>Journal of Physical Chemistry C</i> , 2017, 121, 6290-6299.	1.5	7

#	ARTICLE	IF	CITATIONS
12637	Structures and Properties of As(OH) <sub>3</sub> Adsorption Complexes on Hydrated Mackinawite (FeS) Surfaces: A DFT-D2 Study. Environmental Science & Technology, 2017, 51, 3461-3470.	4.6	49
12638	Dopant activation mechanism of Bi wire- $\delta$ -doping into Si crystal, investigated with wavelength dispersive fluorescence x-ray absorption fine structure and density functional theory. Journal of Physics Condensed Matter, 2017, 29, 155001.	0.7	3
12639	Introducing <i>ab initio</i> based neural networks for transition-rate prediction in kinetic Monte Carlo simulations. Physical Review B, 2017, 95, .	1.1	18
12640	Control of the dipole layer of polar organic molecules adsorbed on metal surfaces via different charge-transfer channels. Physical Review B, 2017, 95, .	1.1	8
12641	Influence of sulfur vacancy on thiophene hydrodesulfurization mechanism at different MoS <sub>2</sub> edges: A DFT study. Chemical Engineering Science, 2017, 164, 292-306.	1.9	59
12642	Utilizing super-atom orbital ideas to understand properties of silver clusters inside ZSM-5 zeolite. RSC Advances, 2017, 7, 4950-4959.	1.7	21
12643	Equilibrium Shape of Metal Nanoparticles under Reactive Gas Conditions. Journal of Physical Chemistry C, 2017, 121, 5629-5634.	1.5	48
12644	Most effective way to improve the hydrogen storage abilities of Na-decorated BN sheets: applying external biaxial strain and an electric field. Physical Chemistry Chemical Physics, 2017, 19, 5570-5578.	1.3	23
12645	A free-standing platinum monolayer as an efficient and selective catalyst for the oxygen reduction reaction. Journal of Materials Chemistry A, 2017, 5, 5303-5313.	5.2	41
12646	Covalent surface modification with electron-donating/accepting $\pi$ -conjugated chains to effectively tune the electronic and magnetic properties of zigzag SiC nanoribbons. Journal of Materials Chemistry C, 2017, 5, 2022-2032.	2.7	7
12647	Tuning of intrinsic antiferromagnetic to ferromagnetic ordering in microporous $\delta$ -MnO <sub>2</sub> by inducing tensile strain. Physical Chemistry Chemical Physics, 2017, 19, 3770-3776.	1.3	5
12648	DFT study of hydrogen and helium defects at the (112̄,1) twin boundary in hcp scandium. International Journal of Modern Physics B, 2017, 31, 1750080.	1.0	2
12649	The Role of Low-Coordinated Sites on the Adsorption of Glycerol on Defected Pt <sub>n</sub> /Pt(111) Substrates: A Density Functional Investigation within the D3 van der Waals Correction. Journal of Physical Chemistry C, 2017, 121, 3445-3454.	1.5	14
12650	High temperature ferromagnetism in $\pi$ -conjugated two-dimensional metal-organic frameworks. Chemical Science, 2017, 8, 2859-2867.	3.7	86
12651	Full atomistic reaction mechanism with kinetics for CO reduction on Cu(100) from <i>ab initio</i> molecular dynamics free-energy calculations at 298 K. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 1795-1800.	3.3	414
12652	CO Oxidation by Molecular and Atomic Oxygen on Ag(100): A Density Functional Theory Study. Journal of Physical Chemistry C, 2017, 121, 2635-2642.	1.5	20
12653	Towards highly active Pd/CeO <sub>2</sub> for alkene hydrogenation by tuning Pd dispersion and surface properties of the catalysts. Nanoscale, 2017, 9, 3140-3149.	2.8	35
12654	Structural, Electronic, and Mechanical Properties of CoN and NiN: An <i>Ab Initio</i> Study. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2017, 72, 321-330.	0.7	5



#	ARTICLE	IF	CITATIONS
12655	A Density Functional Theory Investigation of Ni <sub>n</sub> , Pd <sub>n</sub> , and Pt <sub>n</sub> Clusters ( $n=1-4$ ) Adsorbed on Buckminsterfullerene. <i>ChemPhysChem</i> , 2017, 18, 1376-1384.	1.0	2
12656	In-situ Conversion of Multiwalled Carbon Nanotubes to Graphene Nanosheets: An Increasing Capacity Anode for Li Ion Batteries. <i>Electrochimica Acta</i> , 2017, 231, 255-263.	2.6	14
12657	Epitaxial NiWO <sub>4</sub> films on Ni(110): Experimental and theoretical study of surface stability. <i>Surface Science</i> , 2017, 659, 20-30.	0.8	12
12658	Testing the CP-correction procedure with different DFT methods on H-bonding complexes of $\beta$ -carrabiose with water molecules. <i>Journal of Molecular Modeling</i> , 2017, 23, 31.	0.8	8
12659	Ni <sup>II</sup> formate complexes with bi- and tridentate nitrogen-donor ligands: synthesis, characterization, and magnetic and thermal properties. <i>Dalton Transactions</i> , 2017, 46, 3963-3979.	1.6	8
12660	Surface ferromagnetism in HfO <sub>2</sub> by excess oxygen. <i>Solid State Communications</i> , 2017, 252, 33-39.	0.9	5
12661	Electronic study of carbon nanotube (6,0) doped with transition metals: Copper, silver and gold. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2017, 17, 71-79.	0.1	0
12662	Quantum-chemical investigation on 5-fluorouracil anticancer drug. <i>Structural Chemistry</i> , 2017, 28, 1093-1109.	1.0	10
12663	Tunable thermal expansion in framework materials through redox intercalation. <i>Nature Communications</i> , 2017, 8, 14441.	5.8	95
12664	Selective hydrogenation of CO on Fe <sub>3</sub> S <sub>4</sub> {111}: a computational study. <i>Faraday Discussions</i> , 2017, 197, 325-336.	1.6	7
12665	Mechanistic Insights into Ethylene Transformations on Ir(111) by Density Functional Calculations and Microkinetic Modeling. <i>ChemPhysChem</i> , 2017, 18, 906-916.	1.0	10
12666	X-ray crystallographic analysis and DFT calculations of three $\epsilon$ -propylene linker™ dimers linked by one polystep reaction. <i>Journal of Molecular Structure</i> , 2017, 1137, 126-135.	1.8	2
12667	Stabilization of body-centred cubic iron under inner-core conditions. <i>Nature Geoscience</i> , 2017, 10, 312-316.	5.4	91
12668	Influence of a ZrO <sub>2</sub> Support and Its Surface Structures on the Stability and Nucleation of Pt <sub>n</sub> ( $n=1-5$ ) Clusters: A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2017, 121, 2132-2141.	1.2	25
12669	Composition dependent band offsets of ZnO and its ternary alloys. <i>Scientific Reports</i> , 2017, 7, 41567.	1.6	42
12670	Adsorption dynamics of molecular nitrogen at an Fe(111) surface. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 7370-7379.	1.3	9
12671	Probing the electronic structures of Co <sub>n</sub> ( $n=1-5$ ) clusters on $\beta$ -Al <sub>2</sub> O <sub>3</sub> surfaces using first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3679-3687.	1.3	18
12672	Why Porous Materials Have Selective Adsorptions: A Rational Aspect from Electrodynamics. <i>Inorganic Chemistry</i> , 2017, 56, 2614-2620.	1.9	12



#	ARTICLE	IF	CITATIONS
12673	Identifying and Visualizing the Edge Terminations of Single-Layer MoSe <sub>2</sub> Island Epitaxially Grown on Au(111). ACS Nano, 2017, 11, 1689-1695.	7.3	48
12674	Strain Gated Bilayer Molybdenum Disulfide Field Effect Transistor with Edge Contacts. Scientific Reports, 2017, 7, 41593.	1.6	17
12675	Selective Oxidation and Functionalization of 6-Diphenylphosphinoacenaphthyl-5-tellurenyl Species 6-Ph <sub>2</sub> P-Ace-5-TeX (X = Mes, Cl, O <sub>3</sub> SCF <sub>3</sub> ). Various Types of P-E-Te(II,IV) Bonding Situations (E = O, S, Se). Organometallics, 2017, 36, 1566-1579.	1.1	18
12676	Geometrical and electronic structures of small Co-Mo nanoclusters. RSC Advances, 2017, 7, 4933-4940.	1.7	6
12677	TiPdSn: A half Heusler compound with high thermoelectric performance. Europhysics Letters, 2017, 117, 47002.	0.7	50
12678	First-principles study of defect formation in the photovoltaic semiconductors Cu <sub>2</sub> GeS <sub>3</sub> and Cu <sub>2</sub> ZnGeS <sub>4</sub> for comparison with Cu <sub>2</sub> SnS <sub>3</sub> , Cu <sub>2</sub> ZnSnS <sub>4</sub> , and CuInSe <sub>2</sub> . Japanese Journal of Applied Physics, 2017, 56, 04CS08.	0.8	14
12679	Experimental and thermodynamic investigation of Al-Cu-Nd ternary system. Materials Chemistry and Physics, 2017, 195, 94-104.	2.0	3
12680	Theoretical Elucidation of Potential Enantioselectivity in a Pd-Catalyzed Aromatic C-H Coupling Reaction. Journal of Organic Chemistry, 2017, 82, 4900-4906.	1.7	13
12681	Structure and Optical Properties of Small (TiO <sub>2</sub> ) <sub>n</sub> Nanoparticles, $n = 21-24$ . Journal of Physical Chemistry C, 2017, 121, 9528-9536.	1.5	7
12682	Mechanism of Electron Excitation and Emission from a Nanoribbon under Pulsed Laser Irradiation: Time-Dependent First-Principles Study. Journal of the Physical Society of Japan, 2017, 86, 035003.	0.7	3
12683	Controllable embedding of sulfur in high surface area nitrogen doped three dimensional reduced graphene oxide by solution drop impregnation method for high performance lithium-sulfur batteries. Journal of Power Sources, 2017, 353, 298-311.	4.0	71
12684	Pressure-Induced Stable Beryllium Peroxide. Inorganic Chemistry, 2017, 56, 5233-5238.	1.9	17
12685	Enhanced Stability of Cu Clusters of Low Atomicity against Oxidation. Effect on the Catalytic Redox Process. ACS Catalysis, 2017, 7, 3560-3568.	5.5	58
12686	MoS <sub>2</sub> edges and heterophase interfaces: energy, structure and phase engineering. 2D Materials, 2017, 4, 025080.	2.0	16
12687	Unusual magnetic properties of Au-Mn nanowires on copper and silicon substrates. Physica Status Solidi (B): Basic Research, 2017, 254, 1600850.	0.7	2
12688	Antibacterial electrospun zein nanofibrous web encapsulating thymol/cyclodextrin-inclusion complex for food packaging. Food Chemistry, 2017, 233, 117-124.	4.2	179
12689	Exploring high dimensional free energy landscapes: Temperature accelerated sliced sampling. Journal of Chemical Physics, 2017, 146, .	1.2	45
12690	Synthesis and properties of CS <sub>x</sub> F <sub>y</sub> thin films deposited by reactive magnetron sputtering in an Ar/SF <sub>6</sub> discharge. Journal of Physics Condensed Matter, 2017, 29, 195701.	0.7	9

#	ARTICLE	IF	CITATIONS
12691	Investigation of electronic properties and spin-orbit coupling effects on passivated stanene nanosheet: A first-principles study. Superlattices and Microstructures, 2017, 107, 118-126.	1.4	18
12692	Low thermal conductivity of monolayer ZnO and its anomalous temperature dependence. Physical Chemistry Chemical Physics, 2017, 19, 12882-12889.	1.3	55
12693	Adsorption of Formic Acid on Pd(111) Catalyst in the Gas Phase. Progress in Reaction Kinetics and Mechanism, 2017, 42, 30-35.	1.1	1
12694	Chiro-optic and nonlinear optical studies of bridged triarylamine heterohelicenes; A DFT study. Journal of Molecular Structure, 2017, 1142, 1-10.	1.8	6
12695	Ab initio investigation of Jahn-Teller-distortion-tuned Li-ion migration in $\hat{\text{I}}\text{-MnO}_2$ . Journal of Materials Chemistry A, 2017, 5, 9618-9626.	5.2	23
12696	First-principles study of the thermoelectric properties of intermetallic compound YbAl <sub>3</sub> . Intermetallics, 2017, 87, 27-30.	1.8	12
12697	Importance of the Kinetic Energy Density for Band Gap Calculations in Solids with Density Functional Theory. Journal of Physical Chemistry A, 2017, 121, 3318-3325.	1.1	126
12698	Single Pd Atoms on $\hat{\text{I}}\text{-Al}_2\text{O}_3$ (010) Surface do not Catalyze NO Oxidation. Scientific Reports, 2017, 7, 560.	1.6	19
12699	An approximate full-dimensional quantum dynamics study of the mode specificity in the dissociative chemisorption of $\text{D}_2$ on rigid Cu(111). Physical Chemistry Chemical Physics, 2017, 19, 11960-11967.	1.3	9
12700	Ultra-low magnetic damping of perovskite $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ thin films. Applied Physics Letters, 2017, 110, .	1.5	45
12701	Chip-Scale Mass Manufacturable High-Q Silicon Microdisks. Advanced Materials Technologies, 2017, 2, 1600299.	3.0	11
12702	Mechanism of Methanol Decomposition on the $\text{Pt}_3\text{Ni}(111)$ Surface: DFT Study. Journal of Physical Chemistry C, 2017, 121, 9348-9360.	1.5	46
12703	First-Principles Study on CO Removing Mechanism on Pt-Decorated Oxygen-Rich Anode Surfaces ( $\text{Pt}_2/\text{o-MO}_2(110)$ , M = Ru and Ir) in DMFC. Journal of Physical Chemistry C, 2017, 121, 9825-9832.	1.5	14
12704	A layered wide-gap oxyhalide semiconductor with an infinite $\text{ZnO}_2$ square planar sheet: $\text{Sr}_2\text{ZnO}_2\text{Cl}_2$ . Chemical Communications, 2017, 53, 3826-3829.	2.2	13
12705	Absorption of visible light by GaAs and GaN nanosheets. Optik, 2017, 141, 60-65.	1.4	9
12706	Benchmark Relative Energies for Large Water Clusters with the Generalized Energy-Based Fragmentation Method. Journal of Chemical Theory and Computation, 2017, 13, 2696-2704.	2.3	34
12707	Electronic, magnetic, mechanical, half-metallic and highly dispersive zero-gap half-metallic properties of rare-earth-element-based quaternary Heusler compounds. Journal of Alloys and Compounds, 2017, 718, 63-74.	2.8	67
12708	Hydrolysis of cephalexin and meropenem by New Delhi metallo- $\hat{\text{I}}^2$ -lactamase: the substrate protonation mechanism is drug dependent. Physical Chemistry Chemical Physics, 2017, 19, 13111-13121.	1.3	32

#	ARTICLE	IF	CITATIONS
12709	Terahertz spectroscopy and solid-state density functional theory calculations of structural isomers: Nicotinic acid, isonicotinic acid and 2-picolinic acid. <i>Modern Physics Letters B</i> , 2017, 31, 1750149.	1.0	12
12710	Mechanical, Dynamical and Thermodynamic Properties of Al-3wt%Mg from First Principles. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2017, 72, 527-534.	0.7	1
12711	Crystal structure and mechanical properties of a new ternary phase in Mg-Zn-Y alloy solidified under high pressure. <i>Journal of Alloys and Compounds</i> , 2017, 717, 214-218.	2.8	19
12712	Ab initio investigation of supported Au-Mn nanowires. <i>Modern Physics Letters B</i> , 2017, 31, 1750142.	1.0	7
12713	Raman studies in tetragonal structure PbTeO <sub>3</sub> . <i>Solid State Communications</i> , 2017, 260, 1-5.	0.9	0
12714	Fabrication and characterizations of nitrogen-doped BaSi <sub>2</sub> epitaxial films grown by molecular beam epitaxy. <i>Journal of Crystal Growth</i> , 2017, 471, 37-41.	0.7	0
12715	Nanotubular Gamma Alumina with High-Energy External Surfaces: Synthesis and High Performance for Catalysis. <i>ACS Catalysis</i> , 2017, 7, 4083-4092.	5.5	41
12716	Phase evolution of lithium intercalation dynamics in 2H-MoS <sub>2</sub> . <i>Nanoscale</i> , 2017, 9, 7533-7540.	2.8	83
12717	Rhodium-rhodium interactions in [Rh( $\eta^2$ -diketonato)(CO) <sub>2</sub> ] complexes. <i>Journal of Molecular Structure</i> , 2017, 1144, 280-289.	1.8	13
12718	Spectroscopic and Reactivity Comparisons of a Pair of bTAML Complexes with Fe <sup>V</sup> -O and Fe <sup>IV</sup> -O Units. <i>Inorganic Chemistry</i> , 2017, 56, 6352-6361.	1.9	51
12719	Importance of Dispersion on the Stability of the Concave-Bound CpM (M = Fe, Ru, Os) Complexes of Sumanene. <i>Organometallics</i> , 2017, 36, 2036-2041.	1.1	4
12720	Strained rocksalt ScN: <i>ab initio</i> studies of electronic structure and lattice-dynamical properties. <i>Materials Research Express</i> , 2017, 4, 055001.	0.8	2
12721	Gold(I)-Catalysed Asymmetric Hydroamination of Alkenes: A Silver- and Solvent-Dependent Enantiodivergent Reaction. <i>Chemistry - A European Journal</i> , 2017, 23, 10777-10788.	1.7	31
12722	Effect of task specific thiocyanate based ionic liquids on relative volatility of cyclohexane and benzene azeotropic mixture. <i>Journal of Molecular Liquids</i> , 2017, 238, 208-214.	2.3	14
12723	Active Tetrahedral Iron Sites of $\eta^3$ -Fe <sub>2</sub> O <sub>3</sub> Catalyzing NO Reduction by NH <sub>3</sub> . <i>Environmental Science and Technology Letters</i> , 2017, 4, 246-250.	3.9	47
12724	The electronic, optical, and thermodynamical properties of tetragonal, monoclinic, and orthorhombic M <sub>3</sub> N <sub>4</sub> (M = Si, Ge, Sn): A first-principles study. <i>Chinese Physics B</i> , 2017, 26, 046303.	0.7	1
12725	5,9-Dioxa-13b-Oxophosphanaphtho[3,2,1-de]anthracenes Prepared by Tandem Phospha-Friedel-Crafts Reaction as Hole-/Exciton-Blocking Materials for OLEDs. <i>Organometallics</i> , 2017, 36, 2622-2631.	1.1	9
12726	Insights into Frustrated and Regular peri-Substituted (Ace-)Naphthylaminoboranes and (Ace-)Naphthylphosphinoboranes. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 3302-3311.	1.0	12

#	ARTICLE	IF	CITATIONS
12727	Adsorption and decomposition of HMX and CL <sub>20</sub> on Al(111) surface by DFT investigation. <i>Surface and Interface Analysis</i> , 2017, 49, 441-449.	0.8	9
12728	Electronic structure study of screw dislocation core energetics in Aluminum and core energetics informed forces in a dislocation aggregate. <i>Journal of the Mechanics and Physics of Solids</i> , 2017, 104, 115-143.	2.3	18
12729	The Importance of Being Inconsistent. <i>Annual Review of Physical Chemistry</i> , 2017, 68, 555-581.	4.8	93
12730	Interaction of alcohols on monolayer stanane nanosheet: A first-principles investigation. <i>Applied Surface Science</i> , 2017, 419, 9-15.	3.1	26
12731	The Two-Dimensional A <sub>x</sub> Cd <sub>x</sub> Bi <sub>4-x</sub> Q <sub>6</sub> (A = K, Rb, Cs; Q =) Tj ETQq0 0 0 rgBT /Overl Society, 2017, 139, 6978-6987.	6.6	18
12732	Electronic structures, magnetic properties and half-metallicity in the Heusler alloy Hf <sub>2</sub> VAI. <i>Chinese Journal of Physics</i> , 2017, 55, 1466-1472.	2.0	15
12733	Dramatic Increase in the Rate of Olefin Insertion by Coordination of Lewis Acids to the Oxo Ligand in Oxorhenium(V) Hydrides. <i>Organometallics</i> , 2017, 36, 2042-2051.	1.1	18
12734	First-principles study of Pd-skin/Pd <sub>3</sub> Fe(111) electrocatalyst for oxygen reduction reaction. <i>Journal of Applied Electrochemistry</i> , 2017, 47, 747-754.	1.5	8
12735	Experimental and theoretical DFT+ D investigations regarding to various morphology of cuprous oxide nanoparticles: Growth mechanism of ionic liquid-assisted synthesis and photocatalytic activities. <i>Chemical Engineering Journal</i> , 2017, 324, 347-357.	6.6	31
12736	Structural, phononic and electronic properties of Ge-doped $\hat{1}^3$ -graphynes: A first-principles study. <i>Solid State Communications</i> , 2017, 258, 38-44.	0.9	11
12737	Electronegativity determination of individual surface atoms by atomic force microscopy. <i>Nature Communications</i> , 2017, 8, 15155.	5.8	46
12738	Tuning electronic states of catalytic sites enhances SCR activity of hexagonal WO <sub>3</sub> by Mo framework substitution. <i>Catalysis Science and Technology</i> , 2017, 7, 2467-2473.	2.1	8
12739	Magnetic behavior of Mn-doped silicon carbide nanosheet. <i>International Journal of Modern Physics B</i> , 2017, 31, 1750163.	1.0	9
12740	Electrochemical oxygen reduction mechanism on FeN <sub>2</sub> -graphene. <i>Journal of Molecular Modeling</i> , 2017, 23, 170.	0.8	9
12741	Density functional theory insights into ternary layered boride MoAlB. <i>Acta Materialia</i> , 2017, 132, 69-81.	3.8	113
12742	Interatomic potential to study plastic deformation in tungsten-rhenium alloys. <i>Journal of Applied Physics</i> , 2017, 121, .	1.1	38
12743	First-principle study of graphyne-like BN sheet: Electronic structure and optical properties. <i>Computational Materials Science</i> , 2017, 136, 12-19.	1.4	44
12744	First-principles study of noble gas stability in ThO <sub>2</sub> . <i>Journal of Nuclear Materials</i> , 2017, 490, 181-187.	1.3	13

#	ARTICLE	IF	CITATIONS
12745	Structure, Stability, and (Non)Reactivity of the Low-Index Surfaces of Crystalline $B_2O_3$ . Journal of Physical Chemistry C, 2017, 121, 11346-11354.	1.5	10
12746	HCl dissociating on a rigid Au(111) surface: A six-dimensional quantum mechanical study on a new potential energy surface based on the RPBE functional. Journal of Chemical Physics, 2017, 146, 164706.	1.2	20
12747	Evaluation of Non-covalent Binding Energies and Optoelectronic Properties of New $CuBr_2(C_6H_7N)_2$ Complex: DFT Approaches. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 180-191.	0.6	2
12748	High intrinsic catalytic activity of two-dimensional boron monolayers for the hydrogen evolution reaction. Nanoscale, 2017, 9, 533-537.	2.8	116
12749	Stability and electronic properties of $CuAlO_2$ . overflow="scroll" > < mml:mrow > < mml:mo > ( < /mml:mo > < mml:mn > 11 < /mml:mn > < mml:mrow > < mml:mover > Tj ETQq010 0 rgBT14 Overlock	0.0	0
12750	Current Applied Physics, 2017, 17, 126-129. Structural, mechanical, dynamical and electronic properties and high-pressure behavior of $Mo_2GeC$ : A first-principles study. Computational Materials Science, 2017, 137, 306-313.	1.4	7
12751	Adsorption of $NO_2$ molecules on armchair phosphorene nanosheet for nano sensor applications – A first-principles study. Journal of Molecular Graphics and Modelling, 2017, 75, 365-374.	1.3	46
12752	Migrating and clustering of He atoms in $Ti_3SiC_2$ : First-principles calculations. Computational Materials Science, 2017, 137, 327-331.	1.4	9
12753	Adsorption and desorption of propane on Pd (111): A van der Waals density functional study. Energy binding sites and geometries. Surface Science, 2017, 664, 82-86.	0.8	2
12754	Exploring surface landscapes with molecules: rotationally induced diffraction of $H_2$ on $LiF(001)$ under fast grazing incidence conditions. Physical Chemistry Chemical Physics, 2017, 19, 16317-16322.	1.3	8
12755	Bimetallic core-based cuboctahedral core-shell nanoclusters for the formation of hydrogen peroxide ( $2e^-$ reduction) over water ( $4e^-$ reduction): role of core metals. Nanoscale, 2017, 9, 9537-9547.	2.8	20
12756	Vibrational Excitation of $H_2$ Scattering from Cu(111): Effects of Surface Temperature and of Allowing Energy Exchange with the Surface. Journal of Physical Chemistry C, 2017, 121, 13617-13633.	1.5	26
12757	Hydrogen-Bonding Evolution during the Polymorphic Transformations in $CH_3NH_3PbBr_3$ : Experiment and Theory. Chemistry of Materials, 2017, 29, 5974-5981.	3.2	80
12758	Intermediate selectivity in the oxidation of phenols using plasmonic Au/ZnO photocatalysts. Nanoscale, 2017, 9, 9359-9364.	2.8	8
12759	The geometric and electronic transitions in body-centered-tetragonal C8: A first principle study. Carbon, 2017, 120, 89-94.	5.4	17
12760	Enhancing Dissociative Adsorption of Water on Cu(111) via Chemisorbed Oxygen. Journal of Physical Chemistry C, 2017, 121, 12117-12126.	1.5	17
12761	Systematic Investigation into $Mg^{2+}/Li^{+}$ Dual-Cation Transport in Chevrel Phases Using Computational and Experimental Approaches. Journal of Physical Chemistry C, 2017, 121, 12617-12623.	1.5	14
12762	Ferromagnetism and the Optical Properties of Mn-Doped CdSe with the Wurtzite Structure. Journal of Superconductivity and Novel Magnetism, 2017, 30, 3109-3115.	0.8	4

#	ARTICLE	IF	CITATIONS
12763	DFT study of adsorption and diffusion of atomic hydrogen on metal surfaces. <i>Applied Surface Science</i> , 2017, 420, 1-8.	3.1	59
12764	O <sub>3</sub> and SO <sub>2</sub> sensing concept on extended surface of B <sub>12</sub> N <sub>12</sub> nanocages modified by Nickel decoration: A comprehensive DFT study. <i>Solid State Sciences</i> , 2017, 69, 22-30.	1.5	87
12765	Initial stages of Lutetium growth on Si (111)-7 $\times$ 7 probed by STM and core-level photoelectron spectroscopy. <i>Surface Science</i> , 2017, 663, 81-87.	0.8	1
12766	A DFT+U study on the oxidative chlorination of CH <sub>4</sub> at ceria: the role of HCl. <i>Catalysis Science and Technology</i> , 2017, 7, 2498-2505.	2.1	11
12767	Analysis of a Li-Ion Nanobattery with Graphite Anode Using Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12959-12971.	1.5	41
12768	Quantum Chemical Spin Densities for Radical Cations of Photosynthetic Pigment Models. <i>Photochemistry and Photobiology</i> , 2017, 93, 815-833.	1.3	9
12769	Oxygen-Rich Lithium Oxide Phases Formed at High Pressure for Potential Lithium-Air Battery Electrode. <i>Advanced Science</i> , 2017, 4, 1600453.	5.6	22
12770	Electronic optical, properties and widening band gap of graphene with Ge doping. <i>Optical and Quantum Electronics</i> , 2017, 49, 1.	1.5	39
12771	DFT study of methanol adsorption on PtCo(111). <i>Applied Surface Science</i> , 2017, 420, 383-389.	3.1	21
12772	Using defects to store energy in materials – a computational study. <i>Scientific Reports</i> , 2017, 7, 3403.	1.6	13
12773	Graph Theoretical Representation, Analysis and Synthesis of Amorphous Metal Oxide Networks. <i>MRS Advances</i> , 2017, 2, 2639-2644.	0.5	0
12774	Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals. <i>Molecular Physics</i> , 2017, 115, 2315-2372.	0.8	1,401
12775	Recent Progress in the Development of Semiconductor-Based Photocatalyst Materials for Applications in Photocatalytic Water Splitting and Degradation of Pollutants. <i>Advanced Sustainable Systems</i> , 2017, 1, 1700006.	2.7	144
12776	Substrate induced reconstruction and activation of platinum clusters: A systematic DFT study. <i>Applied Surface Science</i> , 2017, 422, 1075-1081.	3.1	8
12777	Supramolecular coordination polymers of La(III), Ce(III), Sm(III), Gd(III) and Eu(III) decorated with rigid 5-hydroxy-1,3-benzenedicarboxylate and flexible hexane-1,6-dicarboxylate linkers: Syntheses, structures, DFT study, luminescence and magnetic properties. <i>Polyhedron</i> , 2017, 134, 153-165.	1.0	5
12778	Exploring the Mechanism of Spontaneous and Lithium-Assisted Graphitic Phase Formation in SiC Nanocrystallites of a High Capacity Li-Ion Battery Anode. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15106-15113.	1.5	16
12779	Comparative single atom heterogeneous catalysts (SAHCs) on different platforms: a theoretical approach. <i>Catalysis Science and Technology</i> , 2017, 7, 4285-4293.	2.1	36
12780	Chemical reactivity descriptors evaluation for determining catalytic activity, redox potential, and oxygen binding of metallophthalocyanines. <i>Chemical Papers</i> , 2017, 71, 2185-2194.	1.0	1



#	ARTICLE	IF	CITATIONS
12781	First-principles study of fission product stability and clustering in ThO <sub>2</sub> . Computational Materials Science, 2017, 137, 186-194.	1.4	3
12782	Band offsets of Ag <sub>2</sub> ZnSnSe <sub>4</sub> /CdS heterojunction: An experimental and first-principles study. Journal of Applied Physics, 2017, 121, .	1.1	22
12783	Uranyl Carbonate Complexes in Aqueous Solution and Their Ligand NMR Chemical Shifts and <sup>17</sup> O Quadrupolar Relaxation Studied by ab Initio Molecular Dynamics. Inorganic Chemistry, 2017, 56, 7384-7396.	1.9	21
12784	Ground-State Crystal Structure of Strontium Peroxide Predicted from First Principles. Inorganic Chemistry, 2017, 56, 7545-7549.	1.9	7
12785	Three-dimensional Pentagon Carbon with a genesis of emergent fermions. Nature Communications, 2017, 8, 15641.	5.8	104
12786	Phosphomolybdic acid supported atomically dispersed transition metal atoms (M = Fe, Co, Ni, Cu, Ru.) Tj ETQq1 1 0.784314 rgBT /Overl Advances, 2017, 7, 24925-24932.	1.7	23
12787	Response of the physical properties of $\hat{\Gamma}$ -Y <sub>6</sub> WO <sub>12</sub> and Y <sub>6</sub> UO <sub>12</sub> to pressure. Computational Materials Science, 2017, 134, 201-205.	1.4	5
12788	First-principles study on surface properties of t-LiFeSO <sub>4</sub> F: Showing a potential way to enhance electronic conductivity. Chemical Physics Letters, 2017, 684, 177-185.	1.2	1
12789	Crystal structure of radium sulfate: An X-ray powder diffraction and density functional theory study. Journal of Solid State Chemistry, 2017, 253, 15-20.	1.4	18
12790	Thermal Ring-Opening Polymerization of Planar-Chiral Sila[1]ferrocenophanes. Organometallics, 2017, 36, 2182-2189.	1.1	15
12791	Modeling of diameter-dependent Fe and Co ultrathin nanowires from first-principles calculations. Physical Chemistry Chemical Physics, 2017, 19, 15412-15423.	1.3	17
12792	Enhancing Enantiomeric Separation with Strain: The Case of Serine on Cu(531). Journal of the American Chemical Society, 2017, 139, 8167-8173.	6.6	12
12793	Tunable Type-I and Type-II Dirac Fermions in Graphene with Nitrogen Line Defects. Journal of Physical Chemistry C, 2017, 121, 12476-12482.	1.5	10
12794	Kinetic and mechanistic investigation for the copolymerization of CO <sub>2</sub> and cyclohexene oxide catalyzed by zinc complexes. Polymer Chemistry, 2017, 8, 3632-3640.	1.9	15
12795	Predicted structural evolution and detailed insight into configuration correlation, mechanical properties of silicon-boron binary compounds. RSC Advances, 2017, 7, 16109-16118.	1.7	19
12796	Comparative studies about CO methanation over Ni(211) and Zr-modified Ni(211) surfaces: Qualitative insight into the effect of surface structure and composition. Molecular Catalysis, 2017, 438, 1-14.	1.0	19
12797	Study of Potential Change, Charge Distribution, Voltage Drop, Band Lineup, and Transmission Spectrum of Molecular Break Junction Under Low Bias. Journal of Physical Chemistry C, 2017, 121, 12903-12910.	1.5	3
12798	Mechanistic Insight into C-C Coupling over Fe-Cu Bimetallic Catalysts in CO <sub>2</sub> Hydrogenation. Journal of Physical Chemistry C, 2017, 121, 13164-13174.	1.5	91



#	ARTICLE	IF	CITATIONS
12799	First principle study of electronic and optical properties of molecular ion (BF <sub>4</sub> <sup>-</sup> ) substituted hybrid perovskite (CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> ). AIP Conference Proceedings, 2017, , .	0.3	2
12800	van Hove singularities and tight-binding model in high-temperature superconductor H <sub>3</sub> Se. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 2526-2530.	0.9	4
12801	Structure-reactivity relationship in isolated Zr sites present in Zr-zeolite and ZrO <sub>2</sub> for the Meerwein-Ponndorf-Verley reaction. Catalysis Science and Technology, 2017, 7, 2865-2873.	2.1	52
12802	Novel structural phases and the electrical properties of Si <sub>3</sub> B under high pressure. Physical Chemistry Chemical Physics, 2017, 19, 16206-16212.	1.3	9
12803	Tunable Mechanoresponsive Self-Assembly of an Amide-Linked Dyad with Dual Sensitivity of Photochromism and Mechanochromism. Advanced Functional Materials, 2017, 27, 1701210.	7.8	125
12804	Evaluating the accuracy of theoretical one-bond <sup>13</sup> C- <sup>13</sup> C scalar couplings and their ability to predict structure in a natural product. Magnetic Resonance in Chemistry, 2017, 55, 979-989.	1.1	17
12805	Reaction Mechanism of Cu(I)-Mediated Reductive CO <sub>2</sub> Coupling for the Selective Formation of Oxalate: Cooperative CO <sub>2</sub> Reduction To Give Mixed-Valence Cu <sub>2</sub> (CO <sub>2</sub> ) <sup>+</sup> and Nucleophilic-Like Attack. Inorganic Chemistry, 2017, 56, 6809-6819.	1.9	39
12806	Mechanistic insights on the reduction of glutathione disulfide by protein disulfide isomerase. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E4724-E4733.	3.3	49
12807	DFT study of coadsorption of water and oxygen on galena (PbS) surface: An insight into the oxidation mechanism of galena. Applied Surface Science, 2017, 420, 714-719.	3.1	41
12808	Efficient Strategy for Enhancement of Visible Light Photocatalytic Activity of NaTaO <sub>3</sub> by a Significant Extent. Journal of Physical Chemistry C, 2017, 121, 12980-12990.	1.5	20
12809	First-principles study on intrinsic defects of SnSe. RSC Advances, 2017, 7, 27612-27618.	1.7	69
12810	Geometrical and magnetic structure of iron oxide clusters (FeO) for n > 10. Computational Materials Science, 2017, 137, 134-143.	1.4	16
12811	Revisiting the polytopal rearrangements in penta-coordinate d <sup>7</sup> -metallocomplexes: modified Berry pseudorotation, octahedral switch, and butterfly isomerization. Chemical Science, 2017, 8, 5512-5525.	3.7	18
12812	The mechanical and thermodynamic properties of <sup>12</sup> C-Si <sub>1-x</sub> C. RSC Advances, 2017, 7, 28499-28505.	1.7	13
12813	Simulation Investigation of Siligene Nanoribbon as a Novel Gas Sensor with Strain Engineering: Sensitivity and Selectivity of Current-Voltage Characteristic. ECS Journal of Solid State Science and Technology, 2017, 6, M83-M87.	0.9	1
12814	Glycerol adsorption on a defected Pt <sub>6</sub> /Pt(100) substrate: a density functional theory investigation within the D <sub>3</sub> van der Waals correction. RSC Advances, 2017, 7, 17122-17127.	1.7	5
12815	Reliable Estimation of Prediction Uncertainty for Physicochemical Property Models. Journal of Chemical Theory and Computation, 2017, 13, 3297-3317.	2.3	47
12816	Comparison of DFT, MP2/CBS, and CCSD(T)/CBS methods for a dual-level QM/MM Monte Carlo simulation approach calculating the free energy of activation of reactions in solution and water: a case study. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	8

#	ARTICLE	IF	CITATIONS
12817	Nonstoichiometric [012] dislocation in strontium titanate. <i>Acta Materialia</i> , 2017, 135, 103-111.	3.8	13
12818	Free Energy Reconstruction from Logarithmic Mean-Force Dynamics Using Multiple Nonequilibrium Trajectories. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3106-3119.	2.3	12
12819	Can DFT and ab initio methods adequately describe binding energies in strongly interacting C <sub>6</sub> H <sub>6</sub> -C <sub>2</sub> X <sub>2</sub> complexes?. <i>Chemical Physics</i> , 2017, 493, 12-19.	0.9	7
12820	Selective and Efficient Removal of Volatile Organic Compounds by Channel-type Gamma-Cyclodextrin Assembly through Inclusion Complexation. <i>Industrial &amp; Engineering Chemistry Research</i> , 2017, 56, 7345-7354.	1.8	25
12821	Effect of zeolite confinement on the conversion of 1-butanol to butene isomers: mechanistic insights from DFT based microkinetic modelling. <i>Catalysis Science and Technology</i> , 2017, 7, 2978-2997.	2.1	27
12822	Template-Grown MoS <sub>2</sub> Nanowires Catalyze the Hydrogen Evolution Reaction: Ultralow Kinetic Barriers with High Active Site Density. <i>ACS Catalysis</i> , 2017, 7, 5097-5102.	5.5	78
12823	Intramolecularly Coordinated 2-aminomethylphenyltellurium Compounds. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 3435-3445.	1.0	5
12824	Thermochemical and electrochemical CO <sub>2</sub> reduction on octahedral Cu nanocluster: Role of solvent towards product selectivity. <i>Journal of Catalysis</i> , 2017, 349, 118-127.	3.1	52
12825	Molecular Dynamics Simulation of a RNA Aptasensor. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4071-4080.	1.2	34
12826	Dirac Nodal Lines and Tilted Semi-Dirac Cones Coexisting in a Striped Boron Sheet. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1707-1713.	2.1	81
12827	First-principles investigation of chemical stability and proton conductivity of M-doped BaZrO <sub>3</sub> (M=K, Rb, and Cs). <i>Journal of the American Ceramic Society</i> , 2017, 100, 2997-3003.	1.9	19
12828	Adsorption studies of alcohol molecules on monolayer MoS <sub>2</sub> nanosheet—A first-principles insights. <i>Applied Surface Science</i> , 2017, 413, 109-117.	3.1	65
12829	B2-disorder phase boundary calculations in Fe rich region of Fe-Si binary system with tetrahedron approximation of CVM. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2017, 56, 207-214.	0.7	2
12830	ZrB <sub>2</sub> : Adjusting the phase structure to improve the brittle fracture and electronic properties. <i>Ceramics International</i> , 2017, 43, 8763-8768.	2.3	73
12831	Effect of exchange-correlation functionals on the density functional theory simulation of phase transformation of fast-ion conductors: A case study in the Li garnet oxide Li <sub>7</sub> La <sub>3</sub> Zr <sub>2</sub> O <sub>12</sub> . <i>Computational Materials Science</i> , 2017, 134, 132-136.	1.4	1
12832	Edge eigen-stress and eigen-displacement of armchair molybdenum disulfide nanoribbons. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017, 381, 1568-1572.	0.9	4
12833	Pressure effects on electronic, anisotropic elastic and thermal properties of Ti <sub>3</sub> AC <sub>2</sub> (A=Si, Ge and Sn) by ab initio calculations. <i>Results in Physics</i> , 2017, 7, 1055-1065.	2.0	6
12834	Perpendicular magnetization of Co <sub>2</sub> FeAl full-Heusler alloy films induced by Pt insertion. <i>Journal of Materials Science: Materials in Electronics</i> , 2017, 28, 9606-9611.	1.1	2

#	ARTICLE	IF	CITATIONS
12835	First principles study of the n-channel thiophene based heterocyclic chalcones. <i>Optik</i> , 2017, 138, 349-358.	1.4	34
12836	Ordering effect on the mechanical, electronic and magnetic properties of the $\hat{I}^2$ -based non-canonical approximant phases: $\hat{I}^2$ -Al <sub>50</sub> Cu <sub>33</sub> Fe <sub>17</sub> , $\hat{I}$ -Al <sub>50</sub> Cu <sub>44</sub> Fe <sub>6</sub> and $\hat{I}^{\dagger}$ -Al <sub>47.5</sub> Cu <sub>49.5</sub> Fe <sub>3</sub> . <i>Philosophical Magazine</i> , 2017, 97, 1024-1046.	0.7	1
12837	Effect of strain on electronic and magnetic properties of Fe-doped monolayer SnS 2. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017, 381, 1732-1737.	0.9	19
12838	Activation mechanism of ammonium ions on sulfidation of malachite ( $\hat{\alpha}$ "201) surface by DFT study. <i>Applied Surface Science</i> , 2017, 410, 126-133.	3.1	50
12839	Acidic gases (CO <sub>2</sub> , NO <sub>2</sub> and SO <sub>2</sub> ) capture and dissociation on metal decorated phosphorene. <i>Applied Surface Science</i> , 2017, 410, 505-512.	3.1	42
12840	Application of pristine and Ni-decorated B 12 P 12 nano-clusters as superior media for acetylene and ethylene adsorption: DFT calculations. <i>Computational and Theoretical Chemistry</i> , 2017, 1109, 1-9.	1.1	69
12841	Cohesion strength and atomic structure of W-Cu graded interfaces. <i>Fusion Engineering and Design</i> , 2017, 117, 20-23.	1.0	17
12842	Temperature-dependent dissolution and diffusion of H isotopes in iron for nuclear energy applications: First-principles and vibration spectrum predictions. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 11560-11573.	3.8	11
12843	Enhanced spectral response of semiconducting BaSi 2 films by oxygen incorporation. <i>Thin Solid Films</i> , 2017, 629, 17-21.	0.8	14
12844	A comparative first-principles study of the structural and electronic properties of the liquid Li $\hat{\alpha}$ "Si and Li $\hat{\alpha}$ "Ge alloys. <i>Journal of Chemical Physics</i> , 2017, 146, 064502.	1.2	2
12845	Edge Engineering of MoS <sub>2</sub> Nanoribbons as High Performance Electrode Material for Na $\hat{\alpha}$ "ion Battery: A First-Principle Study. <i>Chinese Journal of Chemistry</i> , 2017, 35, 896-902.	2.6	13
12846	Novel bipolar magnetic semiconducting and fully compensated ferrimagnetic semiconducting characters in newly designed LiMgPdSn-type compounds: KCaCX (X=AO, S, and Se). <i>Journal of Alloys and Compounds</i> , 2017, 710, 1-7.	2.8	19
12847	Composition-directed Fe <sub>X</sub> Mo <sub>2</sub> X <sub>P</sub> bimetallic catalysts for hydrodeoxygenation reactions. <i>Catalysis Science and Technology</i> , 2017, 7, 1857-1867.	2.1	48
12848	Effect of the Ni size on CH <sub>4</sub> /CO <sub>2</sub> reforming over Ni/MgO catalyst: A DFT study. <i>Chinese Journal of Chemical Engineering</i> , 2017, 25, 1442-1448.	1.7	22
12849	Comparative study of CO adsorption on planar and tetrahedral Pt nanoclusters supported on TiO <sub>2</sub> (110) stoichiometric and reduced surfaces. <i>Molecular Catalysis</i> , 2017, 433, 403-413.	1.0	7
12850	Evidence of a Cu <sup>2+</sup> $\hat{\alpha}$ "Alkane Interaction in Cu-Zeolite Catalysts Crucial for the Selective Catalytic Reduction of NO <sub>x</sub> with Hydrocarbons. <i>ACS Catalysis</i> , 2017, 7, 3501-3509.	5.5	28
12851	A kinetic model of water adsorption, clustering and dissociation on the Fe <sub>3</sub> S <sub>4</sub> {001} surface. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12045-12055.	1.3	16
12852	Probing structure, electronic property, and hydrogen adsorption for the alkali auride series. <i>European Physical Journal Plus</i> , 2017, 132, 1.	1.2	2

#	ARTICLE	IF	CITATIONS
12853	Synergetic control of band gap and structural transformation for optimizing TiO <sub>2</sub> photocatalysts. Applied Catalysis B: Environmental, 2017, 210, 513-521.	10.8	37
12854	Edge dominated electronic properties of MoS <sub>2</sub> /graphene hybrid 2D materials: edge state, electron coupling and work function. Journal of Materials Chemistry C, 2017, 5, 4845-4851.	2.7	28
12855	A density functional theory study on the carbon chain growth of ethanol formation on Cu-Co (111) and (211) surfaces. Applied Surface Science, 2017, 412, 374-384.	3.1	27
12856	Electronic properties of MgZnPt <sub>2</sub> at extremely high temperatures and pressures. Chinese Journal of Physics, 2017, 55, 1011-1017.	2.0	0
12857	First-principles investigation on the geometries, stabilities and defective properties of fluoride surfaces. Computational Materials Science, 2017, 133, 159-166.	1.4	8
12858	Prediction on structural, mechanical and thermal properties of Al <sub>4</sub> SiC <sub>4</sub> , Al <sub>4</sub> C <sub>3</sub> and 4H-SiC under high pressure by first-principles calculation. Modern Physics Letters B, 2017, 31, 1750080.	1.0	10
12859	Bonding interactions in Li/Na oxides, peroxides and superoxides and their implication to the performance of the Li/Na-air batteries. Solid State Ionics, 2017, 303, 24-28.	1.3	3
12860	Ab initio study of (Fe, Ni) doped GaAs: Magnetic, electronic properties and Faraday rotation. Superlattices and Microstructures, 2017, 106, 163-169.	1.4	3
12861	Investigation of V-shaped extended defects in a 4H-SiC epitaxial film. Philosophical Magazine, 2017, 97, 657-670.	0.7	5
12862	Realization of quantum anomalous Hall effect in graphene from $\pi$ codoping-induced stable atomic adsorption. Physical Review B, 2017, 95, .	1.1	13
12863	CO and NO monitoring using pristine germanene nanosheets: DFT study. Journal of Molecular Liquids, 2017, 234, 355-363.	2.3	31
12864	Chemical states of 3d transition metal impurities in a liquid lead-bismuth eutectic analyzed using first principles calculations. Physical Chemistry Chemical Physics, 2017, 19, 9945-9956.	1.3	16
12865	The structural and organic magnetoresistance response of poly(9-vinyl carbazole) using low applied magnetic fields and magnetic nanoparticle addition. Journal of Materials Chemistry C, 2017, 5, 3779-3787.	2.7	7
12866	Influence of alloying elements on stability and adhesion ability of TiAl/TiO <sub>2</sub> interface by first-principles calculations. Intermetallics, 2017, 85, 80-89.	1.8	31
12867	Thermodynamics of GaN(s)-NH <sub>3</sub> (v)+N <sub>2</sub> (v)+H <sub>2</sub> (v) system – Electronic aspects of the processes at GaN(0001) surface. Surface Science, 2017, 662, 12-33.	0.8	12
12868	Proton Transfer in Mixed Clusters of Methanesulfonic Acid, Methylamine, and Oxalic Acid: Implications for Atmospheric Particle Formation. Journal of Physical Chemistry A, 2017, 121, 2377-2385.	1.1	42
12869	Dipole-Moment Reversal in a Polar Organic Monolayer Probed by Sum and Difference Frequency Spectroscopy. Journal of Physical Chemistry C, 2017, 121, 6692-6700.	1.5	4
12870	Surface Characterization of Mechanochemically Modified Exfoliated Halloysite Nanoscrolls. Langmuir, 2017, 33, 3534-3547.	1.6	14

#	ARTICLE	IF	CITATIONS
12871	Towards high visible light photocatalytic activity in rare earth and N co-doped SrTiO <sub>3</sub> : a first principles evaluation and prediction. RSC Advances, 2017, 7, 16282-16289.	1.7	28
12872	Effect of intervalley interaction on band topology of commensurate graphene/EuO heterostructures. Physical Review B, 2017, 95, .	1.1	26
12873	Counterintuitive Adsorption of [PW <sub>11</sub> O <sub>39</sub> ] <sup>7-</sup> on Au(100). Inorganic Chemistry, 2017, 56, 3961-3969.	1.9	18
12874	Investigation of sub-10nm cylindrical surrounding gate germanium nanowire field effect transistor with different cross-section areas. Superlattices and Microstructures, 2017, 105, 110-116.	1.4	19
12875	Reaction pathway of CH <sub>4</sub> /CO <sub>2</sub> reforming over Ni <sub>8</sub> /MgO(100). Surface Science, 2017, 660, 22-30.	0.8	13
12876	Crystallographic, optical, and electronic properties of (Cu,Li)InS <sub>2</sub> system. Thin Solid Films, 2017, 633, 172-178.	0.8	7
12877	Rare earth separations by selective borate crystallization. Nature Communications, 2017, 8, 14438.	5.8	125
12878	Ab Initio Investigations of Structural, Elastic, Mechanical, Electronic, Magnetic, and Optical Properties of Half-Heusler Compounds RhCrZ (Z = Si, Ge). Journal of Superconductivity and Novel Magnetism, 2017, 30, 2481-2488.	0.8	49
12879	Room-Temperature Magneto-dielectric Effect in LaGa <sub>0.7</sub> Fe <sub>0.3</sub> O <sub>3+<math>\delta</math></sub> ; Origin and Impact of Excess Oxygen. Inorganic Chemistry, 2017, 56, 3809-3819.	1.9	14
12880	Accurate, Large-Scale Density Functional Melting of Hg: Relativistic Effects Decrease Melting Temperature by 160 K. Journal of Physical Chemistry Letters, 2017, 8, 1407-1412.	2.1	21
12881	Intrinsic air stability mechanisms of two-dimensional transition metal dichalcogenide surfaces: basal versus edge oxidation. 2D Materials, 2017, 4, 025050.	2.0	87
12882	Switching properties of quinquephenylene molecular device – A first-principles approach. Chemical Physics Letters, 2017, 675, 131-136.	1.2	16
12883	Semilocal exchange hole with an application to range-separated density functionals. Physical Review B, 2017, 95, .	1.1	19
12884	Structural phase transition, electronic, elastic, and vibrational properties of LiAl intermetallic compound: insights from first-principles calculations. Canadian Journal of Physics, 2017, 95, 691-698.	0.4	4
12885	Chiral penta-graphene nanotubes: Structure, bonding and electronic properties. Computational and Theoretical Chemistry, 2017, 1108, 70-75.	1.1	21
12886	Atomistic modeling study of a strain-free stress driven grain boundary migration mechanism. Scripta Materialia, 2017, 134, 52-56.	2.6	10
12887	Efficient noble metal nanocatalysts supported on HfC(001) for O <sub>2</sub> dissociation. AIP Advances, 2017, 7, .	0.6	6
12888	Atomically modified thin interface in metal-dielectric hetero-integrated systems: control of electronic properties. Journal of Physics Condensed Matter, 2017, 29, 145503.	0.7	0

#	ARTICLE	IF	CITATIONS
12889	First-Principles Investigation on Interaction of NH <sub>3</sub> Gas on a Silicene Nanosheet Molecular Device. IEEE Nanotechnology Magazine, 2017, 16, 445-452.	1.1	33
12890	Experimental study and thermodynamic modeling of the Al-Sc-Zr system. Computational Materials Science, 2017, 133, 82-92.	1.4	18
12891	Colloidal synthesis of tungsten oxide quantum dots for sensitive and selective H <sub>2</sub> S gas detection. Sensors and Actuators B: Chemical, 2017, 248, 1029-1036.	4.0	46
12892	Benchmark Study of Density Functional Theory for Neutral Gold Clusters, Au <sub>n</sub> (n = 2-8). Journal of Physical Chemistry A, 2017, 121, 2410-2419.	1.1	34
12893	Layer effect on catalytic activity of Pd-Cu bimetal for CO oxidation. Applied Catalysis A: General, 2017, 538, 66-73.	2.2	8
12894	Effect of flue gas components on the adsorption of sulfur oxides on CaO(1 0 0). Fuel, 2017, 197, 541-550.	3.4	19
12895	The adsorption and activation of formic acid on different anatase TiO <sub>2</sub> surfaces. Journal of Energy Chemistry, 2017, 26, 738-742.	7.1	6
12896	In situ growth of ceramic quantum dots in polyaniline host via water vapor flow diffusion as potential electrode materials for energy applications. Journal of Solid State Chemistry, 2017, 250, 60-67.	1.4	18
12897	Theoretical insight into Cobalt subnano-clusters adsorption on $\sqrt{3}\times\sqrt{3}$ -Al <sub>2</sub> O <sub>3</sub> (0001). Journal of Solid State Chemistry, 2017, 246, 176-185.	1.4	5
12898	Atomic-Scale Structural Evolution of Rh(110) during Catalysis. ACS Catalysis, 2017, 7, 664-674.	5.5	20
12899	Microstructure, mechanical properties, and electronic simulations of steel/aluminum alloy joint during deep penetration laser welding. International Journal of Advanced Manufacturing Technology, 2017, 89, 377-387.	1.5	9
12900	Li ion diffusion dynamics on Li oxides and peroxides surfaces. Materials Letters, 2017, 188, 208-211.	1.3	2
12901	Formation of New Phases to Improve the Visible-Light Photocatalytic Activity of TiO <sub>2</sub> (B) Via Introducing Alien Elements. Journal of Physical Chemistry C, 2017, 121, 52-59.	1.5	1
12902	First-Principles Investigations on Structural, Elastic, Dynamical, and Thermal Properties of Earth-Abundant Nitride Semiconductor CaZn <sub>2</sub> N <sub>2</sub> under Pressure. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2017, 72, 39-49.	0.7	8
12903	First-Principles Study of Pressure-Induced Phase Transition in CuGaO <sub>2</sub> . Brazilian Journal of Physics, 2017, 47, 42-45.	0.7	0
12904	Rational design of bis(4-methoxyphenyl)amine-based molecules with different $\pi$ -bridges as hole-transporting materials for efficient perovskite solar cells. Dyes and Pigments, 2017, 139, 283-291.	2.0	13
12905	Photoelectrochemical Properties and Behavior of $\sqrt{3}\times\sqrt{3}$ -SnWO <sub>4</sub> Photoanodes Synthesized by Hydrothermal Conversion of WO <sub>3</sub> Films. ACS Applied Materials & Interfaces, 2017, 9, 1459-1470.	4.0	42
12906	The structural, elastic, electronic and dynamical properties of chalcopyrite semiconductor BeGeAs <sub>2</sub> from first-principles calculations. Applied Physics A: Materials Science and Processing, 2017, 123, 1.	1.1	3



#	ARTICLE	IF	CITATIONS
12907	Ab initio study of interaction of helium with edge and screw dislocations in tungsten. Nuclear Instruments & Methods in Physics Research B, 2017, 393, 150-154.	0.6	17
12908	Valence band electronic structure of Nb <sub>2</sub> Pd <sub>1.2</sub> Se <sub>5</sub> and Nb <sub>2</sub> Pd <sub>0.95</sub> S <sub>5</sub> superconductors. Physica B: Condensed Matter, 2017, 509, 31-35.	1.3	2
12909	Electronic properties and stability phase diagrams for cubic BN surfaces. Molecular Simulation, 2017, 43, 267-275.	0.9	4
12910	Mechanistic investigation of cis and trans oxidative addition to acetylacetonato-1,5-cyclooctadieneiridium(I). Polyhedron, 2017, 123, 252-258.	1.0	0
12911	Elucidating the GTP Hydrolysis Mechanism in FeoB: A Hydrophobic Amino-Acid Substituted GTPase. ACS Catalysis, 2017, 7, 902-906.	5.5	18
12912	Activating Basal Planes and S-terminated Edges of MoS <sub>2</sub> toward More Efficient Hydrogen Evolution. Advanced Functional Materials, 2017, 27, 1604943.	7.8	131
12913	Structural, electronic, mechanical, dielectric and optical properties of TiSiO <sub>4</sub> : First-principles study. Solid State Communications, 2017, 251, 43-49.	0.9	27
12914	Identification of Second Shell Coordination in Transition Metal Species Using Theoretical XANES: Example of Ti <sup>IV</sup> (C, Si, Ge) Complexes. Journal of Physical Chemistry A, 2017, 121, 162-167.	1.1	7
12915	The Fine Line between a Two-phase and Solid-solution Phase Transformation and Highly Mobile Phase Interfaces in Spinel Li <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> . Advanced Energy Materials, 2017, 7, 1601781.	10.2	33
12916	Computational study on C-B homolytic bond dissociation enthalpies of organoboron compounds. New Journal of Chemistry, 2017, 41, 1346-1362.	1.4	12
12917	Methanol decomposition on low index and stepped CeO <sub>2</sub> surfaces from GGA+ U. Applied Surface Science, 2017, 394, 509-518.	3.1	8
12918	Influence of point defects on optical properties of GaN-based materials by first principle study. Computational Materials Science, 2017, 129, 49-54.	1.4	14
12919	Edge-Modified Graphene Nanoribbons: Appearance of Robust Spiral Magnetism. Journal of Physical Chemistry C, 2017, 121, 1371-1376.	1.5	12
12920	Characterization and oxidative addition reactions for iridium cod complexes. Journal of Coordination Chemistry, 2017, 70, 10-24.	0.8	1
12921	Catalytic selectivity of Rh/TiO <sub>2</sub> catalyst in syngas conversion to ethanol: probing into the mechanism and functions of TiO <sub>2</sub> support and promoter. Catalysis Science and Technology, 2017, 7, 1073-1085.	2.1	31
12922	Accurate Dissociation of Chemical Bonds Using DFT-in-DFT Embedding Theory with External Orbital Orthogonality. Journal of Physical Chemistry A, 2017, 121, 256-264.	1.1	24
12923	The power of exact conditions in electronic structure theory. Chemical Physics Letters, 2017, 669, 54-70.	1.2	34
12924	First-principles investigation of the energetics of point defects at a grain boundary in tungsten. Nuclear Instruments & Methods in Physics Research B, 2017, 393, 144-149.	0.6	18



#	ARTICLE	IF	CITATIONS
12925	Dual-Functional N Dopants in Edges and Basal Plane of MoS <sub>2</sub> Nanosheets Toward Efficient and Durable Hydrogen Evolution. <i>Advanced Energy Materials</i> , 2017, 7, 1602086.	10.2	286
12926	Bi <sub>24</sub> Ga <sub>20</sub> O <sub>39</sub> for visible light photocatalytic reduction of Cr(VI): Controlled synthesis, facet-dependent activity and DFT study. <i>Chemical Engineering Journal</i> , 2017, 314, 249-256.	6.6	91
12927	A coupled experimental and thermodynamic study of the Al-Cr and Al-Cr-Mg systems. <i>Journal of Alloys and Compounds</i> , 2017, 698, 1038-1057.	2.8	26
12928	Promoting the oxygen reduction reaction with gold at step/edge sites of Ni@AuPt core-shell nanoparticles. <i>Catalysis Science and Technology</i> , 2017, 7, 596-606.	2.1	27
12929	Properties improvement of poly(o-methoxyaniline) based supercapacitors: experimental and theoretical behaviour study of self-doping effect. <i>Electrochimica Acta</i> , 2017, 228, 57-65.	2.6	6
12930	Adsorbing the 3d-transition metal atoms to effectively modulate the electronic and magnetic behaviors of zigzag SiC nanoribbons. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3694-3705.	1.3	9
12931	Water-gas-shift reaction on reduced gold-substituted Ce <sub>1-x</sub> O <sub>2</sub> (111) surfaces: the role of Au charge. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2201-2206.	1.3	10
12932	Mg fragments and Al bonded networks in liquid Mg-Al alloys. <i>Computational Materials Science</i> , 2017, 129, 115-122.	1.4	13
12933	First-principles calculations on the structural and electronic properties of cubic KCaF <sub>3</sub> and NaCaF <sub>3</sub> (001) surfaces. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017, 381, 890-895.	0.9	11
12934	X-ray Spectroscopy of Thin Film Free-Base Corroles: A Combined Theoretical and Experimental Characterization. <i>Journal of Physical Chemistry C</i> , 2017, 121, 2192-2200.	1.5	14
12935	Effects of High and Low Salt Concentration in Electrolytes at Lithium-Metal Anode Surfaces. <i>Journal of Physical Chemistry C</i> , 2017, 121, 182-194.	1.5	128
12936	First-principles modeling of metal (ii) ferrocyanide: electronic property, magnetism, bulk moduli, and the role of C <sub>4</sub> N <sup>+</sup> defect. <i>Journal Physics D: Applied Physics</i> , 2017, 50, 035004. 1.3		3
12937	Fermi surface and band structure of BiPd from ARPES studies. <i>Physica C: Superconductivity and Its Applications</i> , 2017, 534, 13-18.	0.6	3
12938	Morphological effects of Au <sub>13</sub> clusters on the adsorption of CO <sub>2</sub> over anatase TiO <sub>2</sub> (101). <i>Applied Surface Science</i> , 2017, 399, 469-479.	3.1	21
12939	Modeling the active sites of Co-promoted MoS <sub>2</sub> particles by DFT. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2017-2024.	1.3	25
12940	Theoretical study on [3]- and [4]radialene complexes CpM(C <sub>2n</sub> H <sub>2n</sub> ) (n=3, 4; M=Sc <sup>1/4</sup> Ni): Special metal-aromatic interaction along with metal-alkene bonds. <i>Journal of Organometallic Chemistry</i> , 2017, 828, 75-82.	0.8	4
12941	Investigation of structural, electronic and anisotropic elastic properties of Ru-doped WB <sub>2</sub> compound by increased valence electron concentration. <i>Materials Chemistry and Physics</i> , 2017, 189, 90-95.	2.0	21
12942	Fundamental effects of hydrogen on cohesion properties of Cu/W interfaces. <i>Solid State Communications</i> , 2017, 250, 79-83.	0.9	25

#	ARTICLE	IF	CITATIONS
12943	On the Preferred Active Sites of Promoted MoS <sub>2</sub> for Hydrodesulfurization with Minimal Organonitrogen Inhibition. ACS Catalysis, 2017, 7, 501-509.	5.5	78
12944	Exchange-Hole Dipole Dispersion Model for Accurate Energy Ranking in Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2017, 13, 441-450.	2.3	56
12945	Computational Criteria for Evaluating Polysulfide Cohesion, Solvation, and Stabilization: Approach for Screening Effective Anchoring Substrates. Journal of Physical Chemistry C, 2017, 121, 308-314.	1.5	10
12946	The effects of disorder on the normal state and superconducting properties of Nb <sub>3</sub> Sn. Superconductor Science and Technology, 2017, 30, 025006.	1.8	9
12947	Effects of reduced dimensionality on the properties of magnesium hydroxide and calcium hydroxide nanostructures. Physical Chemistry Chemical Physics, 2017, 19, 1963-1974.	1.3	9
12948	Ethene hydrogenation vs. dimerization over a faujasite-supported [Rh(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> ] complex. A computational study of mechanism. Catalysis Science and Technology, 2017, 7, 102-113.	2.1	18
12949	Two-dimensional thio- and seleno-cyanates of Mo and W. Journal of Physics Condensed Matter, 2017, 29, 485703.	0.7	0
12950	Contrasting the Role of Ni/Al <sub>2</sub> O <sub>3</sub> Interfaces in Water-Gas Shift and Dry Reforming of Methane. Journal of the American Chemical Society, 2017, 139, 17128-17139.	6.6	172
12951	Exchange-correlation energies of atoms from efficient density functionals: influence of the electron density. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 245004.	0.6	0
12952	The effects of He clusters on the mechanical properties of Ti <sub>3</sub> AlC <sub>2</sub> (A = Ge, Si): first-principles studies. RSC Advances, 2017, 7, 48437-48443.	1.7	4
12953	Optical Gaps in Pristine and Heavily Doped Silicon Nanocrystals: DFT versus Quantum Monte Carlo Benchmarks. Journal of Chemical Theory and Computation, 2017, 13, 6061-6067.	2.3	11
12954	L <sub>2</sub> and XA ordering competition in titanium-based full-Heusler alloys. Journal of Materials Chemistry C, 2017, 5, 11559-11564.	2.7	42
12955	Hydrogen penetration and diffusion on Mg <sub>17</sub> Al <sub>12</sub> (110) surface: A density functional theory investigation. International Journal of Hydrogen Energy, 2017, 42, 26013-26019.	3.8	11
12956	Experimental and theoretical assessment of the mechanism of hydrogen transfer in alkane-alkene coupling on solid acids. Journal of Catalysis, 2017, 354, 287-298.	3.1	7
12957	Platinum electrocatalysts with plasmonic nano-cores for photo-enhanced oxygen-reduction. Nano Energy, 2017, 41, 233-242.	8.2	41
12958	Crystal structure, theoretical and experimental electronic structure and DNA/BSA protein interactions of nickel(II) N <sub>2</sub> O <sub>2</sub> tetradentate Schiff base complexes. Polyhedron, 2017, 138, 88-102.	1.0	13
12959	Real-Space Bonding Indicator Analysis of the Donor-Acceptor Complexes X <sub>3</sub> BNY <sub>3</sub> , X <sub>3</sub> AlNY <sub>3</sub> , X <sub>3</sub> BPY <sub>3</sub> , and X <sub>3</sub> AlPY <sub>3</sub> (X, Y = H, Me, Cl). Journal of Physical Chemistry A, 2017, 121, 7717-7725.	1.1	13
12960	Enhancing the solar energy conversion efficiency of solution-deposited Bi <sub>2</sub> S <sub>3</sub> thin films by annealing in sulfur vapor at elevated temperature. Sustainable Energy and Fuels, 2017, 1, 2134-2144.	2.5	25

#	ARTICLE	IF	CITATIONS
12961	Identification of Distinct Copper Species in Cu-CHA Samples Using NO as Probe Molecule. A Combined IR Spectroscopic and DFT Study. <i>Topics in Catalysis</i> , 2017, 60, 1653-1663.	1.3	19
12962	Introducing DDEC6 atomic population analysis: part 3. Comprehensive method to compute bond orders. <i>RSC Advances</i> , 2017, 7, 45552-45581.	1.7	327
12963	Superconductivity in ultra-thin carbon nanotubes and carbyne-nanotube composites: An ab-initio approach. <i>Carbon</i> , 2017, 125, 509-515.	5.4	11
12964	First-principles study of Ga-vacancy induced magnetism in $\hat{I}^2$ -Ga <sub>2</sub> O <sub>3</sub> . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 28928-28935.	1.3	17
12965	First-principles investigation of H <sub>2</sub> S adsorption and dissociation on titanium carbide surfaces. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27116-27122.	1.3	8
12966	First-principles study of helium clustering at initial stage in ThO <sub>2</sub> . <i>Chinese Physics B</i> , 2017, 26, 097101.	0.7	5
12967	Exchange-Hole Dipole Dispersion Model for Accurate Energy Ranking in Molecular Crystal Structure Prediction II: Nonplanar Molecules. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5332-5342.	2.3	31
12968	Remarkably Strong Chemisorption of Nitric Oxide on Insulating Oxide Films Promoted by Hybrid Structure. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21482-21490.	1.5	10
12969	Complete Separation of Carriers in the GeS/SnS Lateral Heterostructure by Uniaxial Tensile Strain. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 40969-40977.	4.0	34
12970	Superconductivity of Pressure-Stabilized Vanadium Hydrides. <i>Inorganic Chemistry</i> , 2017, 56, 13759-13765.	1.9	42
12971	First principles study towards the influence of interstitial nitrogen on the hydrogen storage properties of the Mg <sub>2</sub> Ni (0 1 0) surface. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 24868-24876.	3.8	7
12972	Aqueous oxidation of iron monosulfide (FeS) in the presence of glycine. <i>Journal of Electroanalytical Chemistry</i> , 2017, 804, 165-170.	1.9	1
12973	The anisotropic size effect of the electrical resistivity of metal thin films: Tungsten. <i>Journal of Applied Physics</i> , 2017, 122, .	1.1	61
12974	Local structure and oxide-ion conduction mechanism in apatite-type lanthanum silicates. <i>Science and Technology of Advanced Materials</i> , 2017, 18, 644-653.	2.8	6
12975	Epitaxial Growth of ZnGa <sub>2</sub> O <sub>4</sub> : A New, Deep Ultraviolet Semiconductor Candidate. <i>Crystal Growth and Design</i> , 2017, 17, 6071-6078.	1.4	61
12976	Critical Intermediate Structure That Directs the Crystalline Texture and Surface Morphology of Organo-Lead Trihalide Perovskite. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 36897-36906.	4.0	20
12977	Impact of Intrinsic Structural Properties on the Hydration of 2:1 Layer Silicates. <i>ACS Earth and Space Chemistry</i> , 2017, 1, 608-620.	1.2	10
12978	Indole-based conjugated macromolecules as a redox-mediated electrolyte for an ultrahigh power supercapacitor. <i>Energy and Environmental Science</i> , 2017, 10, 2441-2449.	15.6	68

#	ARTICLE	IF	CITATIONS
12979	Hot carrier-enhanced interlayer electron-hole pair multiplication in 2D semiconductor heterostructure photocells. <i>Nature Nanotechnology</i> , 2017, 12, 1134-1139.	15.6	74
12980	A systematic investigation of the geometries, electronic and magnetic properties of $Al_nAs_q$ ( $n = 1, 0, +1$ ; $q = 16$ ) clusters: a DFT calculation. <i>Molecular Physics</i> , 2017, 115, 3033-3043.	0.8	3
12981	Evaluation of the Factors Impacting the Accuracy of $^{13}C$ NMR Chemical Shift Predictions using Density Functional Theory: The Advantage of Long-Range Corrected Functionals. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5798-5819.	2.3	77
12982	Quantitative DFT modeling of product concentration in organometallic reactions: Cu-mediated pentafluoroethylation of benzoic acid chlorides as a case study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29344-29353.	1.3	22
12983	Metastable Stacking-Polymorphism in $Ge_2Sb_2Te_5$ . <i>Inorganic Chemistry</i> , 2017, 56, 11990-11997.	1.9	16
12984	Strain and Ligand Effects on $CO_2$ Reduction Reactions over Cu-Metal Heterostructure Catalysts. <i>Journal of Physical Chemistry C</i> , 2017, 121, 22139-22146.	1.5	46
12985	Two isomeric solid carbon nitrides with 1:1 stoichiometry which exhibit strong mechanical anisotropy. <i>New Journal of Chemistry</i> , 2017, 41, 13140-13148.	1.4	8
12986	Ab initio coverage-dependent microkinetic modeling of benzene hydrogenation on Pd(111). <i>Catalysis Science and Technology</i> , 2017, 7, 5267-5283.	2.1	19
12987	Persistent Self-Association of Solute Molecules in Solution. <i>Journal of Physical Chemistry B</i> , 2017, 121, 10118-10124.	1.2	38
12988	Particle formation and growth from oxalic acid, methanesulfonic acid, trimethylamine and water: a combined experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 28286-28301.	1.3	42
12989	Jahn-Teller distortion affected Li ion migration in spinel $TiO_2$ . <i>Solid State Ionics</i> , 2017, 312, 17-20.	1.3	2
12990	Diffusion coefficient of hydrogen interstitial atom in $\delta$ -Fe, $\beta$ -Fe and $\mu$ -Fe crystals by first-principle calculations. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 27438-27445.	3.8	88
12991	Surface Modification of Perfect and Hydroxylated $TiO_2$ Rutile (110) and Anatase (101) with Chromium Oxide Nanoclusters. <i>ACS Omega</i> , 2017, 2, 6795-6808.	1.6	18
12992	Fragment approach to the electronic structure of boron allotrope. <i>Physical Review B</i> , 2017, 95, .		
12993	Ab initio nonadiabatic molecular dynamics investigation on the dynamics of photogenerated spin hole current in Cu-doped $MoS_2$ . <i>Physical Review B</i> , 2017, 96, .		32
12994	Strain effects on oxygen vacancy formation energy in perovskites. <i>Solid State Ionics</i> , 2017, 311, 105-117.	1.3	36
12995	First principle study of edge topological defect-modulated electronic and magnetic properties in zigzag graphene nanoribbons. <i>Chinese Physics B</i> , 2017, 26, 103103.	0.7	5
12996	A Density Functional Theory Study of New Boron Nanotubes. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2017, 72, 1145-1150.	0.7	1

#	ARTICLE	IF	CITATIONS
12997	Quantum chemical and kinetic study of the CCl <sub>2</sub> self-recombination reaction. Computational and Theoretical Chemistry, 2017, 1121, 1-10.	1.1	2
12998	Investigations of half-Heusler compounds CrScZ (Z = P, As, Sb): a density functional theory study. Materials Research Express, 2017, 4, 106519.	0.8	1
12999	Investigation on electronic properties of functionalized arsenene nanoribbon and nanotubes: A first-principles study. Chemical Physics, 2017, 495, 35-41.	0.9	29
13000	Lattice constant changes leading to significant changes of the spin-gapless features and physical nature in a inverse Heusler compound Zr <sub>2</sub> MnGa. Journal of Magnetism and Magnetic Materials, 2017, 444, 313-318.	1.0	13
13001	Computational Studies of Versatile Heterogeneous Palladium-Catalyzed Suzuki, Heck, and Sonogashira Coupling Reactions. ACS Sustainable Chemistry and Engineering, 2017, 5, 8475-8490.	3.2	46
13002	Insights into the radiation behavior of Ln <sub>2</sub> TiO <sub>5</sub> (Ln = La-Y) from defect energetics. Computational Materials Science, 2017, 139, 295-300.	1.4	9
13003	Thermo-controllable self-assembled structures of single-layer 4,4'-diamino-p-terphenyl molecules on Au (110) surface. Chinese Physics B, 2017, 26, 086801.	0.7	5
13004	Benzthiazoline-2-thione (BTT) revisited: An experimental and theoretical endeavor to understand UV-spectra. Chemical Physics Letters, 2017, 686, 88-96.	1.2	7
13005	Theoretical Studies on the Growth Mechanism of Chemical Vapor Deposition of Graphene on Metal Surface. , 2017, , 205-241.		0
13006	Stability and superconducting properties of GaH <sub>5</sub> at high pressure. Physica B: Condensed Matter, 2017, 525, 36-40.	1.3	4
13007	Initial-Stage Oxidation of Ni <sub>3</sub> Al(100) and -(110) from Ab Initio Thermodynamics. Journal of Physical Chemistry C, 2017, 121, 19191-19200.	1.5	12
13008	Steam Reforming of Acetic Acid over Co-Supported Catalysts: Coupling Ketonization for Greater Stability. ACS Sustainable Chemistry and Engineering, 2017, 5, 9136-9149.	3.2	25
13009	Pressure-induced stable BeN <sub>4</sub> as a high-energy density material. Journal of Power Sources, 2017, 365, 155-161.	4.0	43
13010	Theoretical Study of the CO <sub>2</sub> Adsorption by Zeolitic Imidazolate Frameworks (ZIFs). Journal of Physical Chemistry C, 2017, 121, 20259-20265.	1.5	19
13011	Addressed realization of multication complex arrangements in metal-organic frameworks. Science Advances, 2017, 3, e1700773.	4.7	47
13012	In situ atomic-scale imaging of the metal/oxide interfacial transformation. Nature Communications, 2017, 8, 307.	5.8	79
13013	Ab initio electronic transport and thermoelectric properties of solids from full and range-separated hybrid functionals. Journal of Chemical Physics, 2017, 147, 114101.	1.2	32
13014	Conformation-based signal transfer and processing at the single-molecule level. Nature Nanotechnology, 2017, 12, 1071-1076.	15.6	37

#	ARTICLE	IF	CITATIONS
13015	Towards understanding MgO/Fe interface formation: Adsorption of O and Mg atoms on an Fe(001) surface. <i>Physical Review B</i> , 2017, 96, .	1.1	6
13016	Study of reaction mechanism of methane conversion over Ni-based oxygen carrier in chemical looping reforming. <i>Fuel</i> , 2017, 210, 866-872.	3.4	37
13017	Computational Investigation of the Geometrical and Electronic Structures of $VGe_n$ ( $n = 1-4$ ) Clusters by Density Functional Theory and Multiconfigurational CASSCF/CASPT2 Method. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7787-7796.	1.1	19
13018	Electronic Interactions of Size-Selected Oxide Clusters on Metallic and Thin Film Oxide Supports. <i>Journal of Physical Chemistry C</i> , 2017, 121, 22234-22247.	1.5	12
13019	Interaction of curcumin in a drug delivery system including a composite with poly(lactic-co-glycolic) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 <i>Materials Chemistry B</i> , 2017, 5, 8070-8082.	2.9	45
13020	Arsenene/ $Ca(OH)_2$ van der Waals heterostructure: strain tunable electronic and photocatalytic properties. <i>RSC Advances</i> , 2017, 7, 44394-44400.	1.7	36
13021	First-principles calculations of $Co_7W_6$ doped with Re: Site occupancy and electronic properties. <i>Computational Condensed Matter</i> , 2017, 13, 36-40.	0.9	4
13022	Influence of oxygen partial pressure on the adsorption and diffusion during oxide growth: ZnO(0001) surface. <i>Physical Review B</i> , 2017, 96, .	1.1	6
13023	Structural, electronic, optical and elastic properties of the cubic perovskite $PbHfO_3$ through modified Becke-Johnson potential. <i>Chinese Journal of Physics</i> , 2017, 55, 2514-2522.	2.0	5
13024	First-Principles Investigation of Lithium Polysulfide Structure and Behavior in Solution. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21105-21117.	1.5	53
13025	Tris(trimethylsilyl) Phosphite as an Efficient Electrolyte Additive To Improve the Surface Stability of Graphite Anodes. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 32851-32858.	4.0	52
13026	The development of a promising photosensitive Schottky barrier diode using a novel $Cd$ based coordination polymer. <i>Dalton Transactions</i> , 2017, 46, 13531-13543.	1.6	49
13027	An unsaturated metal site-promoted approach to construct strongly coupled noble metal/ $HfNb_3O_8$ nanosheets for efficient thermo/photo-catalytic reduction. <i>Nanoscale</i> , 2017, 9, 14654-14663.	2.8	30
13028	Hydrogen assisted synthesis of branched nickel nanostructures: a combined theoretical and experimental study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26718-26727.	1.3	13
13029	Subatomic electronic feature from dynamic motion of Si dimer defects in Bi nanolines on Si(001). <i>Physical Review B</i> , 2017, 96, .	1.1	2
13030	Magnetic two-dimensional $C_3N_2$ carbonitrides: semiconductors, metals and half-metals. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26743-26748.	1.3	15
13031	Site preferences in hetero-metallic $[Fe_9^xNi_x]$ clusters: a combined crystallographic, spectroscopic and theoretical analysis. <i>Dalton Transactions</i> , 2017, 46, 12835-12844.	1.6	4
13032	Diffusion in energy materials: Governing dynamics from atomistic modelling. <i>Applied Physics Reviews</i> , 2017, 4, .	5.5	22



#	ARTICLE	IF	CITATIONS
13033	3D Foam Struttred Graphene Carbon Nitride with Highly Stable Optoelectronic Properties. <i>Advanced Functional Materials</i> , 2017, 27, 1703711.	7.8	87
13034	A General Route to Include Pauli Repulsion and Quantum Dispersion Effects in QM/MM Approaches. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4854-4870.	2.3	62
13035	Lattice-Directed Construction of Metal-Organic Molecular Wires of Pentacene on the Au(110) Surface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21650-21657.	1.5	14
13036	Tuning the Electronic Properties of Single-Atom Pt Catalysts by Functionalization of the Carbon Support Material. <i>Journal of Physical Chemistry C</i> , 2017, 121, 20802-20812.	1.5	23
13037	Uric Acid as an Electrochemically Active Compound for Sodium-Ion Batteries: Stepwise Na <sup>3+</sup> -Storage Mechanisms of $\pi$ -Conjugation and Stabilized Carbon Anion. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 33934-33940.	4.0	13
13038	Effects of Y Dopant on Lattice Distortion and Electrical Properties of In <sub>3</sub> SbTe <sub>2</sub> Phase-Change Material. <i>Physica Status Solidi - Rapid Research Letters</i> , 2017, 11, 1700275.	1.2	6
13039	Top-down synthesis strategies: Maximum noble-metal atom efficiency in catalytic materials. <i>Chinese Journal of Catalysis</i> , 2017, 38, 1588-1596.	6.9	15
13040	Effect of Sr doping on the electronic band structure and optical properties of ZnO: A first principle calculation. <i>Journal of Applied Physics</i> , 2017, 122, .	1.1	14
13041	Atomic-scale study of the amorphous-to-crystalline phase transition mechanism in GeTe thin films. <i>Scientific Reports</i> , 2017, 7, 8234.	1.6	14
13042	Morphology and Electronic Properties of $\pi$ -Ditridecylperylene-3,4,9,10-tetracarboxylic Diimide Layered Aggregates: From Structural Predictions to Charge Transport. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21857-21864.	1.5	14
13043	Structure of Carbon-Coated C12A7 Electride via Solid-State NMR and DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 22268-22273.	1.5	9
13044	Finite-temperature H behaviors in tungsten and molybdenum: first-principles total energy and vibration spectrum calculations. <i>Nuclear Fusion</i> , 2017, 57, 126024.	1.6	8
13045	Tetragonal-prism-like Guinier-Preston-Bagaryatsky zones in an AlCuMg alloy. <i>Materials Characterization</i> , 2017, 132, 139-144.	1.9	20
13046	First-Principles Study of Chemical Mixtures of CaCl <sub>2</sub> and MgCl <sub>2</sub> Hydrates for Optimized Seasonal Heat Storage. <i>Journal of Physical Chemistry C</i> , 2017, 121, 20576-20590.	1.5	22
13047	Structural, optical and electronic properties of indium sulfide compositions under influence of copper impurity produced by chemical method. <i>Results in Physics</i> , 2017, 7, 3380-3389.	2.0	11
13048	Implementation and Application of the Frozen Density Embedding Theory with the Algebraic Diagrammatic Construction Scheme for the Polarization Propagator up to Third Order. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4711-4725.	2.3	21
13049	Structure sensitive photocatalytic reduction of nitroarenes over TiO <sub>2</sub> . <i>Scientific Reports</i> , 2017, 7, 8783.	1.6	173
13050	Catalytic activation of O <sub>2</sub> molecule by transition metal atoms deposited on the outer surface of BN nanocluster. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 77, 218-224.	1.3	27



#	ARTICLE	IF	CITATIONS
13052	Manipulating the Magnetic Moment of Palladium Clusters by Adsorption and Dissociation of Molecular Hydrogen. <i>Journal of Physical Chemistry C</i> , 2017, 121, 20756-20762.	1.5	12
13053	Modeling butadiene adsorption on oxidized graphene surface using density functional theory. <i>AIP Conference Proceedings</i> , 2017, . .	0.3	1
13054	Raman study of electron-phonon coupling in thin films of the spinel oxide superconductor $\text{LiTi}_2\text{O}_4$ . <i>Physical Review B</i> , 2017, 96, .		
13055	Cryogenic Photochemical Synthesis and Electronic Spectroscopy of Cyanotetracetylene. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7374-7384.	1.1	11
13056	Hydrogen adsorption and dissociation on the TM-doped (TM=Ti, Nb) Mg55 nanoclusters: A DFT study. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 24797-24810.	3.8	31
13057	Oxygen adsorption at heterophase boundaries of the oxygenated Cu(110). <i>Surface Science</i> , 2017, 666, 28-43.	0.8	11
13058	First-principles analysis of solute diffusion in dilute bcc Fe- $\text{X}$ alloys. <i>Physical Review B</i> , 2017, 96, .	1.1	63
13059	A structural and computational study of citrulline in biochemical reactions. <i>Structural Chemistry</i> , 2017, 28, 1581-1589.	1.0	4
13060	Controlling activation barrier by carbon nanotubes as nano-chemical reactors. <i>Journal of Molecular Modeling</i> , 2017, 23, 229.	0.8	2
13061	The design of a macromolecular depressant for galena based on DFT studies and its application. <i>Minerals Engineering</i> , 2017, 112, 50-56.	1.8	35
13062	Defect induced charge trapping in C-doped $\text{Al}_2\text{O}_3$ . <i>Journal of Applied Physics</i> , 2017, 122, 025702.	1.1	6
13063	3R and 2H polytypes of MoS <sub>2</sub> : DFT and DFPT calculations of structural, optoelectronic, vibrational and thermodynamic properties. <i>Journal of Physics and Chemistry of Solids</i> , 2017, 111, 25-33.	1.9	35
13064	Electric-field noise from carbon-atom diffusion on a Au(110) surface: First-principles calculations and experiments. <i>Physical Review A</i> , 2017, 95, .	1.0	20
13065	Compositional phase stability of strongly correlated electron materials within DFT+ $\text{U}$ . <i>Physical Review B</i> , 2017, 95, .	1.1	11
13066	Two-dimensional electron systems in $\text{A}_x\text{Ti}_{1-x}\text{O}$ perovskites ( $\text{A} = \text{Ca, Sr, Ba, Pb}$ ). <i>Physical Review B</i> , 2017, 95, .		
13067	Catalytic nitridation preparation of high-performance $\text{Si}_3\text{N}_4$ (w)-SiC composite using $\text{Fe}_2\text{O}_3$ nano-particle catalyst: Experimental and DFT studies. <i>Journal of the European Ceramic Society</i> , 2017, 37, 4467-4474.	2.8	23
13068	The relationship between atomic structure and magnetic property of amorphous Fe <sub>78</sub> Si <sub>9</sub> B <sub>13</sub> alloy at different pressures. <i>Journal of Magnetism and Magnetic Materials</i> , 2017, 443, 216-221.	1.0	15
13069	A Cd-based MOF as a photosensitive Schottky diode: experimental and theoretical studies. <i>Dalton Transactions</i> , 2017, 46, 11239-11249.	1.6	66

#	ARTICLE	IF	CITATIONS
13070	Thickness dependent semiconductor-to-metal transition of two-dimensional polyaniline with unique work functions. <i>Nanoscale</i> , 2017, 9, 12025-12031.	2.8	24
13071	DFT studies of elemental mercury oxidation mechanism by gaseous advanced oxidation method: Co-interaction with H <sub>2</sub> O <sub>2</sub> on Fe <sub>3</sub> O <sub>4</sub> (111) surface. <i>Applied Surface Science</i> , 2017, 426, 647-655.	3.1	11
13072	First principles investigations of electronics, magnetic, and thermoelectric properties of rare earth based PrYO <sub>3</sub> (Y=Cr, V) perovskites. <i>Current Applied Physics</i> , 2017, 17, 1539-1546.	1.1	93
13073	Density Functional Theory Calculation of the Absorption Properties of Brown Carbon Chromophores Generated by Catechol Heterogeneous Ozonolysis. <i>ACS Earth and Space Chemistry</i> , 2017, 1, 353-360.	1.2	25
13074	Substitution reactions of iron(II) carbamoyl-thioether complexes related to mono-iron hydrogenase. <i>Dalton Transactions</i> , 2017, 46, 10814-10829.	1.6	15
13075	Theab initiostudy of unconventional superconductivity in CeCoIn <sub>5</sub> and FeSe. <i>New Journal of Physics</i> , 2017, 19, 063039.	1.2	25
13076	Boron doping effect on the interface interaction and mechanical properties of graphene reinforced copper matrix composite. <i>Applied Surface Science</i> , 2017, 425, 811-822.	3.1	23
13077	Synergetic effect of oxygen vacancy and Pd site on the interaction between Pd/Anatase TiO <sub>2</sub> (101) and formaldehyde: A density functional theory study. <i>Catalysis Today</i> , 2017, 297, 151-158.	2.2	38
13078	Spectroscopic and microbiological characterization of labdane diterpene 15,16-epoxy-4-hydroxy-labda-13(16),14-dien-3,12-dione isolated from the stems of <i>Croton jacobinensis</i> . <i>Journal of Molecular Structure</i> , 2017, 1147, 335-344.	1.8	11
13079	Hole Polaron Diffusion in the Final Discharge Product of Lithium Sulfur Batteries. <i>Journal of Physical Chemistry C</i> , 2017, 121, 17169-17175.	1.5	15
13080	Elastic Effects in Adsorbate Adsorbate Interactions of C and S on a Stepped Ru Surface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 16761-16769.	1.5	2
13081	Nanosheet Supported Single-Metal Atom Bifunctional Catalyst for Overall Water Splitting. <i>Nano Letters</i> , 2017, 17, 5133-5139.	4.5	395
13082	Structural and magnetic properties and DFT analysis of ZnO:(Al,Er) nanoparticles. <i>RSC Advances</i> , 2017, 7, 32931-32941.	1.7	28
13083	Surface interaction of H <sub>2</sub> S, SO <sub>2</sub> , and SO <sub>3</sub> on fullerene-like gallium nitride (GaN) nanostructure semiconductor. <i>Solid State Communications</i> , 2017, 265, 6-11.	0.9	19
13084	Influence of adsorbate and defect on structural and electronic properties of ultrathin silver nanotube. <i>Journal of Physics and Chemistry of Solids</i> , 2017, 111, 135-141.	1.9	1
13085	Liquid Exfoliation Few-Layer SnSe Nanosheets with Tunable Band Gap. <i>Journal of Physical Chemistry C</i> , 2017, 121, 17530-17537.	1.5	75
13086	Excess Li-Ion Storage on Reconstructed Surfaces of Nanocrystals To Boost Battery Performance. <i>Nano Letters</i> , 2017, 17, 6018-6026.	4.5	53
13087	Band Structure of Topological Insulator BiSbTe <sub>1.25</sub> Se <sub>1.75</sub> . <i>Scientific Reports</i> , 2017, 7, 4567.	1.6	16

#	ARTICLE	IF	CITATIONS
13088	Ab Initio Density Functional Calculations and Infra-Red Study of CO Interaction with Pd Atoms on $\gamma$ -Al <sub>2</sub> O <sub>3</sub> (010) Surface. <i>Scientific Reports</i> , 2017, 7, 6231.	1.6	9
13089	Simulation and understanding of atomic and molecular quantum crystals. <i>Reviews of Modern Physics</i> , 2017, 89, .	16.4	94
13090	Anisotropic surface physicochemical properties of spodumene and albite crystals: Implications for flotation separation. <i>Applied Surface Science</i> , 2017, 426, 1005-1022.	3.1	56
13091	Effects of solute concentration on the stacking fault energy in copper alloys at finite temperatures. <i>Journal of Alloys and Compounds</i> , 2017, 726, 601-607.	2.8	36
13092	The effect of silicon on spangle size in hot-dipped 55 wt%Al-Zn coatings. <i>Surface and Coatings Technology</i> , 2017, 327, 110-117.	2.2	5
13093	Effects of substitution of X (X=rhenium, chromium and zirconium) on the properties of Co <sub>7</sub> Mo <sub>6</sub> $\sqrt{2}$ phase: A first-principles study. <i>Materialwissenschaft Und Werkstofftechnik</i> , 2017, 48, 570-576.	0.5	0
13094	Band Gap Tuning Of ZnO 1-3x N 2x F x Alloys: A First Principles Study. <i>Materials Today: Proceedings</i> , 2017, 4, 5700-5705.	0.9	1
13095	The interaction of CO molecules on Au-Rh bimetallic nanoclusters supported on a thin film of Al <sub>2</sub> O <sub>3</sub> /NiAl(100). <i>RSC Advances</i> , 2017, 7, 13362-13371.	1.7	6
13096	DFT-Supported Threshold Ionization Study of Chromium Biphenyl Complexes: Unveiling the Mechanisms of Substituent Influence on Redox Properties of Sandwich Compounds. <i>Chemistry - A European Journal</i> , 2017, 23, 13669-13675.	1.7	10
13097	Ab Initio Molecular Dynamics Studies of Pb <sub>m</sub> Sb <sub>n</sub> (m+n=9) Alloy Clusters. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2017, 48, 4905-4913.	1.1	3
13098	Zn <sup>2+</sup> , Mg <sup>2+</sup> , and Li <sup>+</sup> -TMP Bases for the Successive Regioselective Metalations of the 1,5-Naphthyridine Scaffold (TMP=2,2,6,6-tetramethylpiperidyl). <i>Chemistry - A European Journal</i> , 2017, 23, 13046-13050.	1.7	36
13099	Robustness of topological states with respect to lattice instability in the nonsymmorphic topological insulator KHgSb. <i>Physical Review B</i> , 2017, 96, .	1.1	3
13100	General Synthesis of Dual Carbon-Confined Metal Sulfides Quantum Dots Toward High-Performance Anodes for Sodium-Ion Batteries. <i>Advanced Functional Materials</i> , 2017, 27, 1702046.	7.8	259
13101	Computational study of fluoroquinolone binding to Mg(H <sub>2</sub> O) <sub>6</sub> <sup>2+</sup> and its applicability to future drug design. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25428.	1.0	5
13102	Validation of density functionals for pancake-bonded $\text{I}_2$ -dimers; dispersion is not enough. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24761-24768.	1.3	32
13103	Photoluminescence properties of TADF-emitting three-coordinate silver( <sup>i</sup> ) halide complexes with diphosphine ligands: a comparison study with copper( <sup>i</sup> ) complexes. <i>Dalton Transactions</i> , 2017, 46, 12446-12455.	1.6	37
13104	Monitoring and manipulating single molecule rotors on the Bi(111) surface by the scanning tunneling microscopy. <i>RSC Advances</i> , 2017, 7, 34262-34266.	1.7	1
13105	Homologous Series of 2D Chalcogenides CsAgBiQ (Q = S, Se) with Ion-Exchange Properties. <i>Journal of the American Chemical Society</i> , 2017, 139, 12601-12609.	6.6	22

#	ARTICLE	IF	CITATIONS
13106	Catalytic Activity for Oxygen Reduction Reaction on CoN <sub>2</sub> -Embedded Graphene: A Density Functional Theory Study. <i>Journal of the Electrochemical Society</i> , 2017, 164, F1122-F1129.	1.3	26
13107	Canonical orbital contributions to the magnetic fields induced by global and local diatropic and paratropic ring currents. <i>Journal of Computational Chemistry</i> , 2017, 38, 2594-2604.	1.5	16
13108	Effect of pressure on structural, elastic and mechanical properties of transition metal hydrides Mg <sub>7</sub> TmH <sub>16</sub> (TM = Sc, Ti, V, Y, Zr and Nb): First-principles investigation. <i>Journal of Physics and Chemistry of Solids</i> , 2017, 111, 229-237.	1.9	7
13109	Dissociative adsorption dynamics of nitrogen on a Fe(111) surface. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24626-24635.	1.3	9
13110	A key role of tensile strain and surface termination in formation and properties of La <sub>0.7</sub> Sr <sub>0.3</sub> MnO <sub>3</sub> composites with carbon nanotubes. <i>Computational Materials Science</i> , 2017, 139, 125-131.	1.4	1
13111	Performance of a nonempirical exchange functional from density matrix expansion: comparative study with different correlations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21707-21713.	1.3	20
13112	Metal-mediated diradical tuning for DNA replication arrest via template strand scission. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E7405-E7414.	3.3	11
13113	Structure and dynamics of CaO films: A computational study of an effect of external static electric field. <i>Physical Review B</i> , 2017, 95, .	1.1	2
13114	Increased thermal stability of activated N <sub>2</sub> adsorbed on K-promoted Ni{110}. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21848-21855.	1.3	3
13115	Insight into the preferred formation mechanism of long-chain hydrocarbons in Fischer-Tropsch synthesis on Hcp Co(10 $\bar{1}1$ ) surfaces from DFT and microkinetic modeling. <i>Catalysis Science and Technology</i> , 2017, 7, 3758-3776.	2.1	39
13116	Visible light absorption of (Fe, C/N) co-doped NaTaO <sub>3</sub> : DFT + U *. <i>Chinese Physics B</i> , 2017, 26, 087102.	0.7	5
13117	Si allotropes and group IV clathrates investigated under high pressures. <i>Japanese Journal of Applied Physics</i> , 2017, 56, 05FA07.	0.8	4
13118	Polyamorphic Transformations in Fe-Ni Liquids: Implications for Chemical Evolution of Terrestrial Planets. <i>Journal of Geophysical Research: Solid Earth</i> , 2017, 122, 9745-9754.	1.4	10
13119	Amorphous chalcogenides as random octahedrally bonded solids: I. Implications for the first sharp diffraction peak, photodarkening, and Boson peak. <i>Journal of Chemical Physics</i> , 2017, 147, 114505.	1.2	9
13120	Dissociation reaction of B <sub>2</sub> H <sub>6</sub> on TiN surfaces during atomic layer deposition: first-principles study. <i>RSC Advances</i> , 2017, 7, 55750-55755.	1.7	11
13121	Exploring multiband tunneling for uncoupled particles: A polynomial view. <i>Journal of Applied Physics</i> , 2017, 122, .	1.1	2
13122	Appearance and disappearance of ferromagnetism in ultrathin $\text{LaMnO}_3$ on $\text{SrTiO}_3$ substrate: A viewpoint from first principles. <i>Physical Review B</i> , 2017, 96, .	1.1	27
13123	Machine learning unifies the modeling of materials and molecules. <i>Science Advances</i> , 2017, 3, e1701816.	4.7	488

#	ARTICLE	IF	CITATIONS
13124	Low-temperature binding of NO adsorbed on MIL-100(Al)â€”A case study for the application of high resolution pulsed EPR methods and DFT calculations. <i>Journal of Chemical Physics</i> , 2017, 147, 224701.	1.2	12
13125	Assessing the performance of self-consistent hybrid functional for band gap calculation in oxide semiconductors. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 454004.	0.7	33
13126	In-plane magnetization-induced quantum anomalous Hall effect in atomic crystals of group-V elements. <i>Physical Review B</i> , 2017, 96, .	1.1	25
13127	Effect of solid electrolyte interphase on the reactivity of polysulfide over lithium-metal anode. <i>Electrochimica Acta</i> , 2017, 258, 1320-1328.	2.6	13
13128	Spin states of Mn(III) meso-tetraphenylporphyrin chloride assessed by density functional methods. <i>Journal of Molecular Modeling</i> , 2017, 23, 363.	0.8	2
13129	First-principles calculation of Zr doping on cohesion properties of TiC/W interfaces. <i>Fusion Engineering and Design</i> , 2017, 125, 85-88.	1.0	7
13130	Decomposition of Ionic Liquids at Lithium Interfaces. 1. <i>Ab Initio</i> Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 28214-28234.	1.5	68
13131	Graphitic nanofilms of zinc-blende materials: <i>ab initio</i> calculations. <i>Materials Research Express</i> , 2017, 4, 125018.	0.8	1
13132	Quantifying confidence in density functional theory predictions of magnetic ground states. <i>Physical Review B</i> , 2017, 96, .	1.1	24
13133	Structural superlubricity of platinum on graphite under ambient conditions: The effects of chemistry and geometry. <i>Applied Physics Letters</i> , 2017, 111, .	1.5	23
13134	Structural phase transitions of Ga(Mn)N under high pressure. <i>Journal of Physics: Conference Series</i> , 2017, 901, 012030.	0.3	1
13135	First-principles study of the interactions of hydrogen with low-index surfaces of PdCu ordered alloy. <i>Progress in Natural Science: Materials International</i> , 2017, 27, 709-713.	1.8	6
13136	Atomic-Scale Origin of the Quasi-One-Dimensional Metallic Conductivity in Strontium Niobates with Perovskite-Related Layered Structures. <i>ACS Nano</i> , 2017, 11, 12519-12525.	7.3	8
13137	Structural, electronic, magnetic, half-metallic, mechanical, and thermodynamic properties of the quaternary Heusler compound FeCrRuSi: A first-principles study. <i>Scientific Reports</i> , 2017, 7, 16183.	1.6	59
13138	$H_2$ diffractive scattering under fast grazing incidence using a DFT-based potential energy surface. <i>Physical Review B</i> , 2017, 96, .	1.1	7
13139	Decomposition of Ionic Liquids at Lithium Interfaces. 2. Gas Phase Computations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 28235-28248.	1.5	24
13140	Surface Reactivity of $Li_2MnO_3$ : First-Principles and Experimental Study. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 44222-44230.	4.0	20
13141	Ground-State Gas-Phase Structures of Inorganic Molecules Predicted by Density Functional Theory Methods. <i>ACS Omega</i> , 2017, 2, 8373-8387.	1.6	14

#	ARTICLE	IF	CITATIONS
13142	Hydrogen accumulation around dislocation loops and edge dislocations: from atomistic to mesoscopic scales in BCC tungsten. <i>Physica Scripta</i> , 2017, T170, 014073.	1.2	15
13143	Organocalcium-mediated nucleophilic alkylation of benzene. <i>Science</i> , 2017, 358, 1168-1171.	6.0	180
13144	Theoretical calculation pKa values of phthalhydrazide derivatives in its aqueous solutions. <i>Russian Journal of Physical Chemistry B</i> , 2017, 11, 722-728.	0.2	4
13145	Carbon nanotubes as excitonic insulators. <i>Nature Communications</i> , 2017, 8, 1461.	5.8	51
13146	Tailoring perpendicular magnetic anisotropy with graphene oxide membranes. <i>RSC Advances</i> , 2017, 7, 52938-52944.	1.7	3
13147	A theoretical quest for high temperature superconductivity on the example of low-dimensional carbon structures. <i>Scientific Reports</i> , 2017, 7, 15815.	1.6	7
13148	Structural and Mechanical Properties of TiN-TiC-TiO System: First Principle Study. <i>Communications in Theoretical Physics</i> , 2017, 68, 678.	1.1	6
13149	Segregation of Native Defects to the Grain Boundaries in Methylammonium Lead Iodide Perovskite. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5935-5942.	2.1	56
13150	Chemical Cosubstitution-Oriented Design of Rare-Earth Borates as Potential Ultraviolet Nonlinear Optical Materials. <i>Journal of the American Chemical Society</i> , 2017, 139, 18397-18405.	6.6	187
13151	Hydrogen-bearing iron peroxide and the origin of ultralow-velocity zones. <i>Nature</i> , 2017, 551, 494-497.	13.7	113
13152	The cohesive energy of superheavy element copernicium determined from accurate relativistic coupled-cluster theory. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32286-32295.	1.3	15
13153	Effect of Extended Benzannelation Orientation on Bergman and Related Cyclizations of Isomeric Quinoxalenediynes. <i>Journal of Organic Chemistry</i> , 2017, 82, 13297-13312.	1.7	8
13154	Structure and Properties of one- and Two-Dimensional Clusters of Groups IV-VI of Heavy N-Elements. <i>Russian Physics Journal</i> , 2017, 60, 1218-1225.	0.2	1
13155	Mechanical properties, Born effective charge tensors and high frequency dielectric constants of the eight phases of BaTiO <sub>3</sub> . <i>Moscow University Physics Bulletin (English Translation of Vestnik) Tj ETQq1 1 0.784314 rgrBf /Overlock 10 T 5</i>		
13156	Oxidation Mechanism and Protection Strategy of Ultrathin Indium Selenide: Insight from Theory. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4368-4373.	2.1	62
13157	Iced photochemical reduction to synthesize atomically dispersed metals by suppressing nanocrystal growth. <i>Nature Communications</i> , 2017, 8, 1490.	5.8	322
13158	Heterogeneous Hydroamination over Supported Ionic Liquid-Stabilized Copper Ions and Its Mechanistic Study. <i>ChemistrySelect</i> , 2017, 2, 10387-10392.	0.7	3
13159	Electronic Structure Reconfiguration toward Pyrite NiS <sub>2</sub> via Engineered Heteroatom Defect Boosting Overall Water Splitting. <i>ACS Nano</i> , 2017, 11, 11574-11583.	7.3	310



#	ARTICLE	IF	CITATIONS
13160	From Type-II Triply Degenerate Nodal Points and Three-Band Nodal Rings to Type-II Dirac Points in Centrosymmetric Zirconium Oxide. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5792-5797.	2.1	61
13161	Quasi-chemical theory of $F_2^{+}(aq)$ : The "no split occupancies rule" revisited. <i>Journal of Chemical Physics</i> , 2017, 147, 161728.	1.2	12
13162	Elucidating electrolyte decomposition under electron-rich environments at the lithium-metal anode. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30861-30873.	1.3	65
13163	A quantum chemical analysis of Zn and Sb doping and co-doping in SnO <sub>2</sub> . <i>AIP Advances</i> , 2017, 7, .	0.6	11
13164	Infrared Spectra of the 1-Chloromethyl-1-methylallyl and 1-Chloromethyl-2-methylallyl Radicals Isolated in Solid <i>para</i> -Hydrogen. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8771-8784.	1.1	1
13165	Dissociative chemisorption of methane on Ni(111) using a chemically accurate fifteen dimensional potential energy surface. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30540-30550.	1.3	40
13166	Integral equation technique for scatterers with mesoscopic insertions: Application to a carbon nanotube. <i>Physical Review B</i> , 2017, 96, .	1.1	8
13167	Study on the computer-aided design of high energetic compounds based on the 1,2,3,4-tetrazine-1,3-dioxide frame. <i>Journal of Molecular Modeling</i> , 2017, 23, 340.	0.8	2
13168	On the ground state of TiO <sub>2</sub> as predicted by all electron density functional calculations in relation to experiment. <i>European Physical Journal B</i> , 2017, 90, 1.	0.6	3
13169	Probing the biotransformation of hematite nanoparticles and magnetite formation mediated by <i>Shewanella oneidensis</i> MR-1 at the molecular scale. <i>Environmental Science: Nano</i> , 2017, 4, 2395-2404.	2.2	22
13170	Vacancy defects in delafossite $\text{Cu}_2\text{NiO}_2$ : First-principles calculations. <i>Moscow University Physics Bulletin (English Translation of Vestnik Moskovskogo Universiteta, Fizika)</i> , 2017, 72, 191-195.	0.1	1
13171	Stacking fault energies of face-centered cubic concentrated solid solution alloys. <i>Acta Materialia</i> , 2017, 134, 334-345.	3.8	330
13172	New cyrhetrenyl and ferrocenyl sulfonamides: Synthesis, characterization, X-ray crystallography, theoretical study and anti- <i>Mycobacterium tuberculosis</i> activity. <i>Polyhedron</i> , 2017, 134, 166-172.	1.0	38
13173	Switching of spins and entanglement in surface-supported antiferromagnetic chains. <i>Scientific Reports</i> , 2017, 7, 2759.	1.6	8
13174	Justifying quasiparticle self-consistent schemes via gradient optimization in Baym-Kadanoff theory. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 385501.	0.7	15
13175	Precipitation of $(\text{Si}_{2-x}\text{Al}_x)\text{Hf}$ in an $\text{Al-Si-Mg-Hf}$ Alloy. <i>Microscopy and Microanalysis</i> , 2017, 23, 724-729.	0.2	2
13176	Density Functional Analysis of Fluorite-Structured $(\text{Ce}, \text{Zr})\text{O}_{2-x}/\text{CeO}_2$ Interfaces. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14678-14687.	1.5	12
13177	Water dissociation on multimetallic catalysts. <i>Applied Catalysis B: Environmental</i> , 2017, 218, 199-207.	10.8	14



#	ARTICLE	IF	CITATIONS
13178	Ab initio exploration of d0 digital magnetic heterostructures: the case of MgO and CaO $\hat{\Gamma}$ -doped with potassium. <i>European Physical Journal B</i> , 2017, 90, 1.	0.6	1
13179	Magnetism and energetics for vacancy and helium impurity in Fe-9Cr alloy: A first-principles study. <i>Computational Materials Science</i> , 2017, 138, 267-276.	1.4	10
13180	Strain effect on SnS2 nanoribbons: Robust direct bandgap of zigzag-edge and sensitive indirect semiconductor with armchair-edge states. <i>Superlattices and Microstructures</i> , 2017, 111, 480-486.	1.4	5
13181	Density Functional Theory Study on the Nucleation and Growth of Pt <sub>n</sub> Clusters on $\hat{\Gamma}$ -Al <sub>2</sub> O <sub>3</sub> (001) Surface. <i>ACS Omega</i> , 2017, 2, 3250-3259.	1.6	13
13182	Trapping of hydrogen and helium at dislocations in tungsten: an ab initio study. <i>Nuclear Fusion</i> , 2017, 57, 126040.	1.6	42
13183	Semimetallic bands derived from interlayer electrons in the quasi-two-dimensional electride $YCa_2C$ . <i>Physical Review B</i> , 2017, 96, .	1.1	17
13184	Atomic Layer Engineering of High- $\hat{\Gamma}$ Ferroelectricity in 2D Perovskites. <i>Journal of the American Chemical Society</i> , 2017, 139, 10868-10874.	6.6	55
13185	Clustering on Magnesium Surfaces – Formation and Diffusion Energies. <i>Scientific Reports</i> , 2017, 7, 5167.	1.6	7
13186	Predicted energy-structure function maps for the evaluation of small molecule organic semiconductors. <i>Journal of Materials Chemistry C</i> , 2017, 5, 7574-7584.	2.7	81
13187	Theoretical and experimental study on the optical and electrical properties of Cu <sub>2</sub> ZnTiS <sub>4</sub> and its photovoltaic applications. <i>Applied Physics Letters</i> , 2017, 111, .	1.5	7
13188	First-principles design of nanostructured hybrid photovoltaics based on layered transition metal phosphates. <i>Scientific Reports</i> , 2017, 7, 1248.	1.6	1
13189	Long-lasting phosphorescence with a tunable color in a Mn <sup>2+</sup> -doped anionic metal-organic framework. <i>Journal of Materials Chemistry C</i> , 2017, 5, 7898-7903.	2.7	56
13190	Properties of the antiferromagnetic selenite MnSeO <sub>3</sub> and its non-magnetic analogue ZnSnO <sub>3</sub> from first principles calculations. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 405501.	0.7	7
13191	First-Principle Calculation of Volta Potential of Intermetallic Particles in Aluminum Alloys and Practical Implications. <i>Journal of the Electrochemical Society</i> , 2017, 164, C465-C473.	1.3	61
13192	First-Principles Calculation of Pt Surface Energies in an Electrochemical Environment: Thermodynamic Driving Forces for Surface Faceting and Nanoparticle Reconstruction. <i>Langmuir</i> , 2017, 33, 7043-7052.	1.6	31
13193	Atomic and electronic basis for the serrations of refractory high-entropy alloys. <i>Npj Computational Materials</i> , 2017, 3, .	3.5	64
13194	Contribution to the study of structural and elastic properties of w $\hat{\Gamma}$ /4stite under pressure up to 140 GPa by pseudopotential calculations. <i>Phase Transitions</i> , 2017, , 1-12.	0.6	0
13195	Local structure of the crystalline and amorphous states of Ga <sub>2</sub> Mn <sub>2</sub> alloy without resonant bonding: A combined x-ray absorption and ab initio study. <i>Physical Review B</i> , 2017, 95, .	1.1	14

#	ARTICLE	IF	CITATIONS
13196	Facile Anhydrous Proton Transport on Hydroxyl Functionalized Graphane. <i>Physical Review Letters</i> , 2017, 118, 186101.	2.9	21
13197	Investigating the Role of Tunable Nitrogen Vacancies in Graphitic Carbon Nitride Nanosheets for Efficient Visible-Light-Driven H <sub>2</sub> Evolution and CO <sub>2</sub> Reduction. <i>ACS Sustainable Chemistry and Engineering</i> , 2017, 5, 7260-7268.	3.2	322
13198	Modeling of amorphous SiC <sub>x</sub> O <sub>6/5</sub> by classical molecular dynamics and first principles calculations. <i>Scientific Reports</i> , 2017, 7, 42705.	1.6	7
13199	Clustering of transmutation elements tantalum, rhenium and osmium in tungsten in a fusion environment. <i>Nuclear Fusion</i> , 2017, 57, 086006.	1.6	20
13200	Structures, stabilities and work functions of alkali-metal-adsorbed boron $\hat{\pm}$ 1-sheets. <i>Chemical Research in Chinese Universities</i> , 2017, 33, 631-637.	1.3	8
13201	Investigating the Role of Tunable Nitrogen Vacancies in Graphitic Carbon Nitride Nanosheets for Efficient Visible-Light-Driven H <sub>2</sub> Evolution and CO <sub>2</sub> Reduction. <i>ACS Sustainable Chemistry and Engineering</i> , 2017, 5, 7260-7268.	1.1	21
13202	Structural, thermodynamic, and mechanical properties of WCu solid solutions. <i>Journal of Physics and Chemistry of Solids</i> , 2017, 110, 401-408.	1.9	34
13203	First-principles study on electronic structure, magnetism and half-metallicity of the NbCoCrAl and NbRhCrAl compounds. <i>Results in Physics</i> , 2017, 7, 2248-2254.	2.0	37
13204	Isolated Spin Qubits in SiC with a High-Fidelity Infrared Spin-to-Photon Interface. <i>Physical Review X</i> , 2017, 7, .	2.8	125
13205	Se-Ni(OH) <sub>2</sub> -shelled vertically oriented NiSe nanowires as a superior electrocatalyst toward urea oxidation reaction of fuel cells. <i>Electrochimica Acta</i> , 2017, 248, 243-249.	2.6	77
13206	Engel-Vosko GGA calculations of the structural, electronic and optical properties of LiYO <sub>2</sub> . <i>Physica B: Condensed Matter</i> , 2017, 521, 62-68.	1.3	10
13207	Density Functional Study of Trimetallic Au <sub>x</sub> Pd <sub>y</sub> Pt <sub>z</sub> ( <i>x</i> + <i>y</i> + <i>z</i> = 7) Clusters and Their Interactions with the O <sub>2</sub> Molecule. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5226-5236.	1.1	15
13208	ORR viability of alumina-supported platinum nanocluster: exploring oxidation behaviour by DFT. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 19308-19315.	1.3	15
13209	Strain engineering of electronic and magnetic properties of Ga <sub>2</sub> S <sub>2</sub> nanoribbons. <i>Chinese Physics B</i> , 2017, 26, 057102.	0.7	1
13210	A DFT+U investigation on methylamine decomposition catalyzed by Pt <sub>4</sub> cluster supported on oxygen defective rutile(110) TiO <sub>2</sub> . <i>Chemical Research in Chinese Universities</i> , 2017, 33, 406-414.	1.3	2
13211	Graphene-supported small transition-metal clusters: A density functional theory investigation within van der Waals corrections. <i>Physical Review B</i> , 2017, 95, .	1.1	49
13212	Effects of Cr on H and He trapping and vacancy complexes in V in a fusion environment: a first-principles study. <i>European Physical Journal B</i> , 2017, 90, 1.	0.6	2
13213	Ferromagnetism and Half-Metallicity in Atomically Thin Holey Nitrogenated Graphene Based Systems. <i>ChemPhysChem</i> , 2017, 18, 2336-2346.	1.0	12

#	ARTICLE	IF	CITATIONS
13214	First-principles examination of low tolerance factor perovskites. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25420.	1.0	6
13215	Photoinduced Charge Transfer versus Fragmentation Pathways in Lanthanum Cyclopentadienyl Complexes. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4281-4296.	2.3	26
13216	The transition metal surface dependent methane decomposition in graphene chemical vapor deposition growth. <i>Nanoscale</i> , 2017, 9, 11584-11589.	2.8	76
13217	Mechanism of dicarbonyl(2,4-pentanedionato)iridium(I) decomposition on iron surface and in gas phase: Complex experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2017, 1146, 677-683.	1.8	4
13218	Quantum Monte Carlo study of the energetics of the rutile, anatase, brookite, and columbite $\text{TiO}_2$ Physical Review B, 2017, 95, .	1.1	43
13219	Relativistic coupled-cluster and density-functional studies of argon at high pressure. <i>Physical Review B</i> , 2017, 95, .	1.1	19
13220	Nitrogen-doped nanocarbon materials under electroreduction operating conditions and implications for electrocatalysis of CO <sub>2</sub> . <i>Carbon</i> , 2017, 111, 859-866.	5.4	22
13221	Benchmarking of density functionals for a soft but accurate prediction and assignment of <sup>1</sup> H and <sup>13</sup> C NMR chemical shifts in organic and biological molecules. <i>Journal of Computational Chemistry</i> , 2017, 38, 87-92.	1.5	28
13222	Selectivity of Pd-Functionalized PtNi(111) Surface: cis -3-Hexenoic Acid Adsorption. <i>Catalysis Letters</i> , 2017, 147, 58-61.	1.4	0
13223	Adsorption of As(III) and As(V) compounds on Fe <sub>3</sub> O <sub>4</sub> (0 0 1) surfaces: A first principle study. <i>Computational Materials Science</i> , 2017, 127, 110-120.	1.4	18
13224	DFT study of nitrogen monoxide adsorption and dissociation on Rh Cu nano clusters. <i>Journal of Alloys and Compounds</i> , 2017, 695, 1924-1929.	2.8	7
13225	Bubble growth from clustered hydrogen and helium atoms in tungsten under a fusion environment. <i>Nuclear Fusion</i> , 2017, 57, 016006.	1.6	23
13226	How reliable is DFT in predicting relative energies of polycyclic aromatic hydrocarbon isomers? comparison of functionals from different rungs of jacob's ladder. <i>Journal of Computational Chemistry</i> , 2017, 38, 370-382.	1.5	43
13227	Stability of the chlorinated derivatives of the DNA/RNA nucleobases, purine and pyrimidine toward radical formation via homolytic C-Cl bond dissociation. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25319.	1.0	8
13228	Strain induced polymorphism and band structure modulation in low-temperature 2,7-dioctyl[1]benzothieno[3,2-b][1]benzothiophene single crystal. <i>Science China Chemistry</i> , 2017, 60, 275-283.	4.2	4
13229	Modifying the band gap and optical properties of Germanium nanowires by surface termination. <i>Applied Surface Science</i> , 2017, 396, 1155-1163.	3.1	14
13230	A theoretical study of the effects of sp-elements on hydrogen in nickel-based alloys. <i>Computational Materials Science</i> , 2017, 128, 37-41.	1.4	3
13231	First-principles calculations of Ti <sub>3</sub> SiC <sub>2</sub> and Ti <sub>3</sub> AlC <sub>2</sub> with hydrogen interstitial. <i>Journal of Nuclear Materials</i> , 2017, 488, 261-266.	1.3	14

#	ARTICLE	IF	CITATIONS
13232	Surface Hydroxyl OH Defects of $\hat{\Gamma}$ -Al <sub>2</sub> O <sub>3</sub> and $\hat{\Gamma}$ -Al <sub>2</sub> O <sub>3</sub> by Solid State NMR, XRD, and DFT Calculations. Zeitschrift Fur Physikalische Chemie, 2017, 231, 809-825.	1.4	13
13233	Precipitation in a copper matrix modeled by <i>ab initio</i> calculations and atomistic kinetic Monte Carlo simulations. Physica Status Solidi (B): Basic Research, 2017, 254, 1600407.	0.7	7
13234	A comparative study of NbAl <sub>3</sub> and Nb <sub>3</sub> Al intermetallic compounds under pressure. Computational Materials Science, 2017, 126, 280-286.	1.4	18
13235	A spectroscopic (stopped-flow UV-Vis and <sup>1</sup> H NMR Evans method) and DFT thermodynamic study of the comproportionation reaction of [Os VIII O <sub>4</sub> (OH) <sub>n</sub> ] <sup>n-</sup> (n = 1, 2) and [Os VI O <sub>2</sub> (OH) <sub>4</sub> ] <sup>2-</sup> . Inorganica Chimica Acta, 2017, 455, 140-151.	1.2	2
13236	Sn(II)-Containing Phosphates as Optoelectronic Materials. Chemistry of Materials, 2017, 29, 2459-2465.	3.2	17
13237	Influence of ordered carbon vacancy networks on the electronic structures and elastic properties of Nb <sub>4</sub> AlC <sub>3</sub> . Journal of the American Ceramic Society, 2017, 100, 724-731.	1.9	14
13238	Computational study of the anticancer drug cisplatin. Canadian Journal of Chemistry, 2017, 95, 95-104.	0.6	3
13239	Relativistic Density Functional Theory. , 2017, , 547-578.		3
13240	Cryptic post-transition state bifurcations that reduce the efficiency of lactone-forming Rh-carbenoid C-H insertions. Chemical Science, 2017, 8, 1442-1449.	3.7	69
13241	Interfacial segregation and grain boundary embrittlement: An overview and critical assessment of experimental data and calculated results. Progress in Materials Science, 2017, 87, 83-139.	16.0	160
13242	Hydrogen dissociation and incorporation on Mg <sub>17</sub> Al <sub>12</sub> (100) surface: A density functional theory study. Applied Surface Science, 2017, 396, 851-856.	3.1	15
13243	The prospect of sensitizing organic dyes attached to the MoS <sub>2</sub> surface: Physical insights from density functional theory investigations. Chemical Physics Letters, 2017, 667, 290-295.	1.2	6
13244	Doping induced dimensionality reduction of the magnetic order in DyFe <sub>1</sub> -In O <sub>3</sub> . Journal of Alloys and Compounds, 2017, 695, 1699-1705.	2.8	2
13245	Calcium Doping of Lithium Titanium Oxide Nanospheres: A Combined First-Principles and Experimental Study. Energy Technology, 2017, 5, 539-543.	1.8	14
13246	Applications of computational chemistry to the study of the antiradical activity of carotenoids: A review. Food Chemistry, 2017, 217, 37-44.	4.2	37
13247	Study of the electronic, bonding, elastic and acoustic properties of covellite via first principles. Journal of Alloys and Compounds, 2017, 692, 440-447.	2.8	20
13248	Lithium ion adsorption and diffusion on black phosphorene nanotube: A first-principles study. Applied Surface Science, 2017, 392, 88-94.	3.1	32
13249	Optical properties of geometrically optimized graphene quantum dots. Physica E: Low-Dimensional Systems and Nanostructures, 2017, 85, 294-301.	1.3	9

#	ARTICLE	IF	CITATIONS
13250	Simulated Temperature Programmed Desorption of Acetaldehyde on CeO <sub>2</sub> (111): Evidence for the Role of Oxygen Vacancy and Hydrogen Transfer. <i>Topics in Catalysis</i> , 2017, 60, 446-458.	1.3	15
13251	Characterizing chemical stability and proton conductivity of B-site doped barium hafnate (BaHfO <sub>3</sub> ) and barium stannate (BaSnO <sub>3</sub> ) with first principles modeling. <i>Journal of Alloys and Compounds</i> , 2017, 693, 738-743.	2.8	22
13252	Stability of Ptn cluster on free/defective graphene: A first-principles study. <i>Applied Surface Science</i> , 2017, 392, 936-941.	3.1	26
13253	First-principles insights into influencing mechanisms of metalloid B on Mg-based hydrides. <i>Journal of Alloys and Compounds</i> , 2017, 693, 979-988.	2.8	21
13254	Effect of temperature on compact layer of Pt electrode in PEMFCs by first-principles molecular dynamics calculations. <i>Applied Surface Science</i> , 2017, 392, 109-116.	3.1	7
13255	Precipitate formations with self-adaptive elemental diffusion and segregation in T92 steel. <i>Journal of Alloys and Compounds</i> , 2017, 693, 264-278.	2.8	10
13256	Elastic anisotropy of novel YAIC from an ab initio study. <i>Journal of Alloys and Compounds</i> , 2017, 694, 982-988.	2.8	2
13257	A computational quest for Nd <sub>2</sub> Fe <sub>14</sub> B-type Ce and Nd phases. <i>Journal of Alloys and Compounds</i> , 2017, 693, 238-244.	2.8	15
13258	An experimental and theoretical study of glycerol oxidation to 1,3-dihydroxyacetone over bimetallic Pt-Bi catalysts. <i>AIChE Journal</i> , 2017, 63, 705-715.	1.8	60
13259	Ab initio study of optical and vibrational properties of Ni <sub>3</sub> C. <i>International Journal of Modern Physics B</i> , 2017, 31, 1750003.	1.0	3
13260	A computational study on new oxidizers as replacements for ammonium perchlorate: tetranitroacetimidic acid and tetranitroacetamide. <i>Canadian Journal of Chemistry</i> , 2017, 95, 199-206.	0.6	4
13261	Modeling the elastic anisotropies and mechanical strengths of Ir <sub>3</sub> X intermetallics. <i>Journal of Alloys and Compounds</i> , 2017, 696, 611-618.	2.8	7
13262	Iron diselenide nanoplatelets: Stable and efficient water-electrolysis catalysts. <i>Nano Energy</i> , 2017, 31, 90-95.	8.2	175
13263	X-H Bond Activation on Cr(III),O Sites (X = R, H): Key Steps in Dehydrogenation and Hydrogenation Processes. <i>Organometallics</i> , 2017, 36, 234-244.	1.1	51
13264	Theoretical insights into the sites and mechanisms for base catalyzed esterification and aldol condensation reactions over Cu. <i>Faraday Discussions</i> , 2017, 197, 59-86.	1.6	23
13265	Density functional theory-based cluster expansion to simulate thermal annealing in FeCrW alloys. <i>Philosophical Magazine</i> , 2017, 97, 299-317.	0.7	11
13266	First-principles phase diagram calculations for the rocksalt-structure quasibinary systems Ti-N, Ti-N-HfN and Zr-N-HfN. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 035401.	0.7	33
13267	Interatomic potential to study the formation of NiCr clusters in high Cr ferritic steels. <i>Journal of Nuclear Materials</i> , 2017, 484, 42-50.	1.3	20

#	ARTICLE	IF	CITATIONS
13268	Obstacles toward unity efficiency of $\text{LiNi}_{1-2x}\text{Co}_x\text{Mn}_x\text{O}_2$ ( $x=0\frac{1}{4}$ ) (NCM) cathode materials: Insights from ab initio calculations. <i>Journal of Power Sources</i> , 2017, 340, 217-228.	4.0	57
13269	Density functional theory studies on the structural and physical properties of Cu-doped anatase $\text{TiO}_2$ (101) surface. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2017, 85, 259-263.	1.3	17
13270	Layered host-guest long-afterglow ultrathin nanosheets: high-efficiency phosphorescence energy transfer at 2D confined interface. <i>Chemical Science</i> , 2017, 8, 590-599.	3.7	188
13271	Structure of graphane polymorphs. <i>Journal of Physics: Conference Series</i> , 2017, 917, 032015.	0.3	4
13272	First-principles study on the magnetic properties of ordered $\text{Nd}_6(\text{Fe,Ga})_{14}$ alloys. <i>Journal of Applied Physics</i> , 2017, 122, 243904.	1.1	8
13273	First-principles simulation on Seebeck coefficient in silicon nanowires. <i>Japanese Journal of Applied Physics</i> , 2017, 56, 06GH04.	0.8	0
13274	When water meets iron at Earth's core-mantle boundary. <i>National Science Review</i> , 2017, 4, 870-878.	4.6	75
13275	Effects of an in vacancy on local distortion of fast phase transition in Bi-doped $\text{In}_3\text{SbTe}_2$ . <i>Journal of the Korean Physical Society</i> , 2017, 71, 946-949.	0.3	1
13276	Crystallographic and optical properties and band diagrams of $\text{CuGa}_5\text{S}_8$ and $\text{Cu}_2\text{Ga}_2\text{S}_3$ phases in Cu-poor $\text{Cu}_2\text{Ga}_2\text{S}_3$ pseudo-binary system. <i>Japanese Journal of Applied Physics</i> , 2017, 56, 04CS12.	0.8	15
13277	Electronic coupling between Bi nanolines and the Si(001) substrate: An experimental and theoretical study. <i>Physical Review B</i> , 2017, 96, .	1.1	2
13278	Influence of external electric field on the electronic structure and optical properties of pyrite. <i>RSC Advances</i> , 2017, 7, 56676-56681.	1.7	11
13279	Carbon effect on the survival of vacancies in Czochralski silicon during rapid thermal anneal. <i>Journal of Applied Physics</i> , 2017, 122, 045705.	1.1	1
13280	First principles study of tunable band gap in bi layer Graphene (BLG). <i>Materials Today: Proceedings</i> , 2017, 4, 7586-7591.	0.9	1
13281	Improving Al Wettability on B 4 C by Transition Metal Doping: a Combined DFT and Experiment Study. <i>Rare Metal Materials and Engineering</i> , 2017, 46, 2345-2351.	0.8	2
13282	Structural and magnetic properties of $\text{FeGen}^+/0$ ( $n = 3-12$ ) clusters: Mass-selected anion photoelectron spectroscopy and density functional theory calculations. <i>Journal of Chemical Physics</i> , 2017, 147, 234310.	1.2	32
13283	Probing the Structural, Electronic, and Magnetic Properties of $\text{Ag}_n\text{V}$ ( $n=1-12$ ) Clusters. <i>Nanoscale Research Letters</i> , 2017, 12, 625.	3.1	15
13284	Microstructural characterization of the $\hat{\text{I}}\text{-Ni}_3(\text{Ti, Al})$ phase in a long-term-aged Ni-based superalloy. <i>Philosophical Magazine Letters</i> , 2017, 97, 442-449.	0.5	5
13285	Self-assembly 2D zinc-phthalocyanine heterojunction: An ideal platform for high efficiency solar cell. <i>Applied Physics Letters</i> , 2017, 111, 253904.	1.5	3



#	ARTICLE	IF	CITATIONS
13286	A Density Functional Theory Study of Adsorption States of Hydrogen Molecules on Ice Surfaces. Journal of the Vacuum Society of Japan, 2017, 60, 249-255.	0.3	2
13287	Energy loss and surface temperature effects in <i>ab initio</i> molecular dynamics simulations: N adsorption on Ag(111) as a case study. Physical Review B, 2017, 96, .	1.1	19
13288	First-Principle Study of the Electronic Structure and Stability of Reconstructed AgInSe <sub>2</sub> (112) Polar Surfaces. IEEE Journal of Photovoltaics, 2017, 7, 1781-1788.	1.5	4
13289	Possible effect of static surface disorder on diffractive scattering of H <sub>2</sub> from Ru(0001): Comparison between theory and experiment. Journal of Chemical Physics, 2017, 147, 244705.	1.2	10
13290	Pressure-Induced Phase Transition in Weyl Semimetallic WTe <sub>2</sub> . Small, 2017, 13, 1701887.	5.2	37
13291	Toxicity of Selected Imidazolium-based Ionic Liquids on <i>Caenorhabditis elegans</i> : a Quantitative Structure-Activity Relationship Study. Chinese Journal of Chemical Physics, 2017, 30, 423-428.	0.6	13
13292	Rare earth-based quaternary Heusler compounds <i>M</i> CoV <i>Z</i> ( <i>M</i> = Lu, Y; <i>Z</i> = Si, Ge) with tunable band characteristics for potential spintronic applications. IUCrJ, 2017, 4, 758-768.	1.0	91
13293	DFT Modelling of Cu Segregation in Al-Cu Alloys Covered by an Ultrathin Oxide Film and Possible Links with Passivity. Metals, 2017, 7, 366.	1.0	9
13294	Ruthenium-Platinum Catalysts and Direct Methanol Fuel Cells (DMFC): A Review of Theoretical and Experimental Breakthroughs. Catalysts, 2017, 7, 47.	1.6	50
13295	Effect of Substituted Mn on Electronic Characteristics of Indium Oxide and Zinc Oxide via Density Functional Theory Studying. Indian Journal of Science and Technology, 2017, 10, 1-6.	0.5	1
13296	An Ab Initio and Kinetic Monte Carlo Simulation Study of Lithium Ion Diffusion on Graphene. Materials, 2017, 10, 761.	1.3	18
13297	Insight into the Mechanism of CO Oxidation on WO <sub>3</sub> (001) Surfaces for Gas Sensing: A DFT Study. Sensors, 2017, 17, 1898.	2.1	20
13298	Protection by extra virgin olive oil against oxidative stress in vitro and in vivo. Chemical and biological studies on the health benefits due to a major component of the Mediterranean diet. PLoS ONE, 2017, 12, e0189341.	1.1	29
13299	Study of the Characteristics of Elementary Processes in a Chain Hydrogen Burning Reaction in Oxygen. Journal of Experimental and Theoretical Physics, 2017, 125, 1026-1033.	0.2	0
13300	The first principle calculation of two-dimensional Dirac materials. IOP Conference Series: Earth and Environmental Science, 2017, 100, 012053.	0.2	0
13301	Applicability of DFT model in reactive distillation. Physical Sciences Reviews, 2017, 2, .	0.8	0
13302	The vdW-DF Family of Nonlocal Exchange-Correlation Functionals. , 2017, , 241-274.		8
13303	First-principles simulation on thermoelectric properties in Bi-Sb System. Journal of Physics: Conference Series, 2017, 939, 012019.	0.3	2



#	ARTICLE	IF	CITATIONS
13304	Sensitive and selective detection of copper ions using low cost nitrogen doped carbon quantum dots as a fluorescent sensing platform. <i>ISSS Journal of Micro and Smart Systems</i> , 2017, 6, 109-117.	1.0	13
13305	A Computational Study of the Combustion of Hydrazine with Dinitrogen Tetroxide. <i>Journal of Nanotoxicology and Nanomedicine</i> , 2017, 2, 12-30.	0.7	2
13306	Theoretical and Experimental Investigations on Effects of Native Point Defects and Nitrogen Doping on the Optical Band Structure of Spinel ZnGa <sub>2</sub> O <sub>4</sub> . <i>Journal of Physical Chemistry C</i> , 2018, 122, 5509-5517.	1.5	25
13307	Cobalt adatoms on graphene: Effects of anisotropies on the correlated electronic structure. <i>Physical Review B</i> , 2018, 97, .	1.1	9
13308	Structural analysis and electrical characterization of cation-substituted lithium ion conductors Li <sub>1-x</sub> Ti <sub>x</sub> MOPO <sub>4</sub> (M=Nb, Ta, Sb). <i>Solid State Ionics</i> , 2018, 319, 170-179.	1.3	4
13309	Can Variations of <sup>1</sup> H NMR Chemical Shifts in Benzene Substituted with an Electron-Accepting (NO <sub>2</sub> )/Donating (NH <sub>2</sub> ) Group be Explained in Terms of Resonance Effects of Substituents?. <i>Chemistry - an Asian Journal</i> , 2018, 13, 877-881.	1.7	7
13310	Hapticity of asymmetric rhodium-allyl compounds in the light of real-space bonding indicators. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2018, 233, 615-626.	0.4	0
13311	Density functional theory study on the stability, electronic structure and absorption spectrum of small size g-C <sub>3</sub> N <sub>4</sub> quantum dots. <i>Computational Materials Science</i> , 2018, 148, 149-156.	1.4	14
13312	Effect of lattice structure changes caused by Al component on optical properties of AlGaN materials. <i>Optik</i> , 2018, 164, 72-77.	1.4	5
13313	Mechanical properties and point defects of MC (M=Ti, Zr) from first-principles calculation. <i>Journal of Alloys and Compounds</i> , 2018, 747, 972-977.	2.8	19
13314	Barrierless On-Surface Metal Incorporation in Phthalocyanine-Based Molecules. <i>Journal of Physical Chemistry C</i> , 2018, 122, 6678-6683.	1.5	11
13315	Shock compression of strongly correlated oxides: A liquid-regime equation of state for cerium(IV) oxide. <i>Physical Review B</i> , 2018, 97, .	1.1	17
13316	2D Chiroptical Nanostructures for High-Performance Photooxidants. <i>Advanced Functional Materials</i> , 2018, 28, 1707237.	7.8	37
13317	A meta-GGA level screened range-separated hybrid functional by employing short range Hartree-Fock with a long range semilocal functional. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8999-9005.	1.3	21
13318	Initial water adsorption on hematite (α-Fe <sub>2</sub> O <sub>3</sub> ) (0001): A DFT + U study. <i>Journal of Chemical Physics</i> , 2018, 148, .	1.2	32
13319	Removal of volatile odorous organic compounds over NiAl mixed oxides at low temperature. <i>Journal of Hazardous Materials</i> , 2018, 344, 797-810.	6.5	34
13320	Ab-initio study of structural and electronic properties of WS <sub>2</sub> /h-BN van der Waals heterostructure. <i>Surface Science</i> , 2018, 672-673, 13-18.	0.8	11
13321	Hexagonal BC <sub>2</sub> N with Remarkably High Hardness. <i>Journal of Physical Chemistry C</i> , 2018, 122, 6801-6807.	1.5	26

#	ARTICLE	IF	CITATIONS
13322	Elastic and thermodynamic properties of zirconium- and hafnium-doped $\text{Rh}_3\text{V}$ intermetallic compounds: potential aerospace material. <i>Bulletin of Materials Science</i> , 2018, 41, 1.	0.8	10
13323	Formation of reactive oxygen by $\text{N}_2\text{O}$ decomposition over binuclear cationic sites of Fe-ferrierite zeolite: Periodic DFT + U study. <i>Chemical Physics Letters</i> , 2018, 695, 222-227.	1.2	7
13324	A theoretical insight into H accumulation and bubble formation by applying isotropic strain on the $\text{W}\text{-H}$ system under a fusion environment. <i>Nuclear Fusion</i> , 2018, 58, 046014.	1.6	1
13325	Prediction of Raman spectra with DFT+ $\text{U}$ method. <i>Physical Review B</i> , 2018, 97, .	1.1	17
13326	Computational Studies on the $\text{Sc}_n\text{Ni}_m$ ( $n+m=10$ ) Clusters: Structure, Electronic and Vibrational Properties. <i>Journal of Cluster Science</i> , 2018, 29, 459-468.	1.7	3
13327	The effect of solvation and temperature on the adsorption of small organic molecules on calcite. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7140-7147.	1.3	12
13328	Detection of transient infrared absorption of $\text{SO}_3$ and 1,3,2-dioxathietane-2,2-dioxide [ $\text{cyc}-(\text{CH}_2)\text{O}(\text{SO}_2)\text{O}$ ] in the reaction $\text{CH}_2\text{OO}+\text{SO}_2$ . <i>Journal of Chemical Physics</i> , 2018, 148, 064301.	1.2	26
13329	Rotational state modification and fast ortho-para conversion of $\text{H}_2$ trapped within the highly anisotropic potential of $\text{Pd}(210)$ . <i>Physical Review B</i> , 2018, 97, .	1.1	8
13330	Active sites speciation of supported CoMoS phase probed by NO molecule: A combined IR and DFT study. <i>Journal of Catalysis</i> , 2018, 361, 62-72.	3.1	20
13331	DFT studies of thermoelectric properties of $\text{Au}$ intermetallics at 300 K. <i>Journal of Rare Earths</i> , 2018, 36, 197-202.	2.5	16
13332	Dissociation reaction of the $\frac{1}{3}\langle 110 \rangle$ edge dislocation in $\text{Al}_2\text{O}_3$ . <i>Journal of Materials Science</i> , 2018, 53, 8049-8058.	1.7	4
13333	The structure of tris(chloromethyl)amine in the gas phase using quantum chemical calculations and gas electron diffraction and as a solid and melt using Raman spectroscopy. <i>Structural Chemistry</i> , 2018, 29, 803-813.	1.0	3
13334	Experimental and Theoretical Investigations on Intermediate Band in Doped Nano- $\text{SnS}_2$ . <i>Journal of Electronic Materials</i> , 2018, 47, 2945-2953.	1.0	21
13335	Computational Study on $\text{N-N}$ Homolytic Bond Dissociation Enthalpies of Hydrazine Derivatives. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2764-2780.	1.1	10
13336	Engineering the Electronic Structure of Tin Sulfide Nanoribbons: A Computational Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 5731-5741.	1.5	18
13337	Identifying On-Surface Site-Selective Chemical Conversions by Theory-Aided NEXAFS Spectroscopy: The Case of Free-Base Corroles on $\text{Ag}(111)$ . <i>Chemistry - A European Journal</i> , 2018, 24, 6787-6797.	1.7	8
13338	Crystal Structures and Electronic Properties of Oxygen-rich Titanium Oxides at High Pressure. <i>Inorganic Chemistry</i> , 2018, 57, 3254-3260.	1.9	19
13339	Critical Role of Water and Oxygen Defects in $\text{O}$ Scission during $\text{CO}_2$ Reduction on $\text{Zn}_2\text{GeO}_4(010)$ . <i>Langmuir</i> , 2018, 34, 3742-3754.	1.6	8

#	ARTICLE	IF	CITATIONS
13340	Structural electronic and mechanical properties of YM <sub>2</sub> (M=Mn, Fe, Co) laves phase compounds: First principle calculations analyzed with datamining approach. <i>Solid State Communications</i> , 2018, 274, 9-20.	0.9	8
13341	Understanding the Improved Kinetics and Cyclability of a Li <sub>2</sub> MnSiO <sub>4</sub> Cathode with Calcium Substitution. <i>Inorganic Chemistry</i> , 2018, 57, 3223-3231.	1.9	14
13342	On the Prediction of Water Contents in Na-Saturated Dioctahedral Smectites. <i>Journal of Physical Chemistry C</i> , 2018, 122, 7484-7493.	1.5	7
13343	Iodate in calcite, aragonite and vaterite CaCO <sub>3</sub> : Insights from first-principles calculations and implications for the I/Ca geochemical proxy. <i>Geochimica Et Cosmochimica Acta</i> , 2018, 236, 351-360.	1.6	52
13344	Theoretical study of the rutile based semiconductor with visible-light responsive photocatalytic activity for water splitting. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 6131-6137.	3.8	1
13345	IR and NMR spectroscopic correlation of enterobactin by DFT. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 198, 264-277.	2.0	10
13346	Computational and Experimental Investigations of the Role of Water and Alcohols in the Desorption of Heterocyclic Aromatic Compounds from Kaolinite in Toluene. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10377-10391.	1.5	4
13347	g-C <sub>3</sub> N <sub>4</sub> /Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> (MXenes) composite with oxidized surface groups for efficient photocatalytic hydrogen evolution. <i>Journal of Materials Chemistry A</i> , 2018, 6, 9124-9131.	5.2	233
13348	Bound nuclear spin states of H <sub>2</sub> in an anisotropic potential induced by a stepped metal surface. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2018, 36, 030601.	0.9	5
13349	Oxygen reduction reaction on Pt(111), Pt(202), and Ni/Au1Pt3(202) surfaces: Probing scaling relationships of reaction energetics and interfacial composition. <i>Chemical Engineering Science</i> , 2018, 184, 239-250.	1.9	16
13350	Di-copper metallodrugs promote NCI-60 chemotherapy via singlet oxygen and superoxide production with tandem TA/TA and AT/AT oligonucleotide discrimination. <i>Nucleic Acids Research</i> , 2018, 46, 2733-2750.	6.5	41
13351	Predicting Surface Energies and Particle Morphologies of Boehmite (̳-AlOOH) from Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10400-10412.	1.5	26
13352	Application of a Coulomb energy density functional for atomic nuclei: Case studies of local density approximation and generalized gradient approximation. <i>Physical Review C</i> , 2018, 97, .	1.1	11
13353	Effect of Solvent and Substrate on the Surface Binding Mode of Carboxylate-Functionalized Aromatic Molecules. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10846-10856.	1.5	5
13354	A first-principles study of hydrogen storage capacity based on Li-Na-decorated silicene. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13903-13908.	1.3	19
13355	Effects of oxygen chemical potential on the anisotropy of the adsorption properties of Zr surfaces. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 14410-14419.	1.3	7
13356	Dual-emission MOF dye sensor for ratiometric fluorescence recognition of RDX and detection of a broad class of nitro-compounds. <i>Journal of Materials Chemistry A</i> , 2018, 6, 9183-9191.	5.2	170
13357	Experimental observation of node-line-like surface states in LaBi. <i>Physical Review B</i> , 2018, 97, .	1.1	17

#	ARTICLE	IF	CITATIONS
13358	Advances in modeling hydrocarbon cracking kinetic predictions by quantum chemical theory: A review. <i>International Journal of Energy Research</i> , 2018, 42, 3164-3181.	2.2	11
13359	Adsorption of benzene and toluene molecules on surface of pure and doped cadmium oxide nanosheets: A computational investigation. <i>Applied Surface Science</i> , 2018, 450, 509-515.	3.1	21
13360	Ab Initio Methods. , 2018, , 7-197.		2
13361	Volta Potential Evolution of Intermetallics in Aluminum Alloy Microstructure Under Thin Aqueous Adlayers: A combined DFT and Experimental Study. <i>Topics in Catalysis</i> , 2018, 61, 1169-1182.	1.3	26
13362	Adsorbing the magnetic superhalogen $MnCl_3$ to realize intriguing half-metallic and spin-gapless-semiconducting behavior in zigzag or armchair SiC nanoribbon. <i>RSC Advances</i> , 2018, 8, 13167-13177.	1.7	6
13363	Embedded atom method potential for studying mechanical properties of binary Cu-Au alloys. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2018, 26, 055006.	0.8	17
13364	Photocatalytic performance of TiO <sub>2</sub> nanocrystals with/without oxygen defects. <i>Chinese Journal of Catalysis</i> , 2018, 39, 867-875.	6.9	106
13365	Entrapped Single Tungstate Site in Zeolite for Cooperative Catalysis of Olefin Metathesis with Brønsted Acid Site. <i>Journal of the American Chemical Society</i> , 2018, 140, 6661-6667.	6.6	71
13366	Electronic structure and hydrogen storage capability of zirconium decorated graphyne. <i>AIP Conference Proceedings</i> , 2018, , .	0.3	2
13367	Inhibitory effect of three phenacyl derivatives on the oxidation of sphalerite (ZnS) in air-equilibrated acidic solution. <i>Corrosion Science</i> , 2018, 138, 154-162.	3.0	3
13368	DFT investigation on the adsorption behavior of dimethyl and trimethyl amine molecules on borophene nanotube. <i>Chemical Physics Letters</i> , 2018, 701, 34-42.	1.2	33
13369	Work function tunability of borophene via doping: A first principle study. <i>AIP Conference Proceedings</i> , 2018, , .	0.3	1
13370	Single-atom heterogeneous catalysts based on distinct carbon nitride scaffolds. <i>National Science Review</i> , 2018, 5, 642-652.	4.6	132
13371	Probing quasi-one-dimensional band structures by plasmon spectroscopy. <i>Physical Review B</i> , 2018, 97, .	1.1	19
13372	Induced Magnetic Field of Fullerenes: Role of $\pi$ - and $\sigma$ - Contributions to Spherical Aromatic, Nonaromatic, and Antiaromatic Character in $C_{60}^{+10}$ ( $q = +10, 0$ ). <i>Journal of Physical Chemistry C</i> , 2018, 122, 9688-9698.	1.5	19
13373	Water dissociating on rigid Ni(100): A quantum dynamics study on a full-dimensional potential energy surface. <i>Journal of Chemical Physics</i> , 2018, 148, 144705.	1.2	20
13374	Lithium Hexastannate: A Potential Material for Energy Storage. <i>Physica Status Solidi (B): Basic Research</i> , 2018, 255, 1700669.	0.7	16
13375	Cobalt-modified molybdenum carbide as a selective catalyst for hydrodeoxygenation of furfural. <i>Applied Catalysis B: Environmental</i> , 2018, 233, 160-166.	10.8	64

#	ARTICLE	IF	CITATIONS
13376	Applying isotropic strain on Mo to predict H solution behaviors for nuclear energy application: Temperature dependence. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 3750-3760.	3.8	7
13377	Impact of Ba to Si deposition rate ratios during molecular beam epitaxy on carrier concentration and spectral response of BaSi <sub>2</sub> epitaxial films. <i>Journal of Applied Physics</i> , 2018, 123, 045703.	1.1	55
13378	Tuning the Deoxygenation of Bulk-Dissolved Oxygen in Copper. <i>Journal of Physical Chemistry C</i> , 2018, 122, 8254-8261.	1.5	15
13379	Hydrogen Bonding Strategy to Optimize Charge Distribution of PC <sub>71</sub> BM and Enable a High Efficiency of 12.45% for Organic Solar Cells. <i>Solar Rrl</i> , 2018, 2, 1800038.	3.1	22
13380	Van der Waals graphene/g-GaSe heterostructure: Tuning the electronic properties and Schottky barrier by interlayer coupling, biaxial strain, and electric gating. <i>Journal of Alloys and Compounds</i> , 2018, 750, 765-773.	2.8	51
13381	The electronic and optical properties of amorphous silica with hydrogen defects by ab initio calculations. <i>Journal of Semiconductors</i> , 2018, 39, 042002.	2.0	5
13382	Adsorption of organic molecules on mineral surfaces studied by first-principle calculations: A review. <i>Advances in Colloid and Interface Science</i> , 2018, 256, 230-241.	7.0	52
13383	Superior twin stability and radiation resistance of nanotwinned Ag solid solution alloy. <i>Acta Materialia</i> , 2018, 151, 395-405.	3.8	27
13384	Photodissociation of CF <sub>2</sub> ICF <sub>2</sub> I in solid <i>para</i> -hydrogen: infrared spectra of <i>anti</i> - and <i>gauche</i> - $\dot{E}^{\text{TM}}$ C <sub>2</sub> F <sub>4</sub> I radicals. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12650-12658.	1.3	8
13385	Which NICS method is most consistent with ring current analysis? Assessment in simple monocycles. <i>RSC Advances</i> , 2018, 8, 13446-13453.	1.7	56
13386	Utilizing SO <sub>2</sub> as self-installing gate to regulate the separation properties of porous graphenes. <i>Carbon</i> , 2018, 134, 145-152.	5.4	3
13387	First principles study of the electronic properties and band gap modulation of two-dimensional phosphorene monolayer: Effect of strain engineering. <i>Superlattices and Microstructures</i> , 2018, 118, 289-297.	1.4	18
13388	Complex reactions on a convertible catalyst surface: A study of the S-O-Cu system. <i>Surface Science</i> , 2018, 678, 228-233.	0.8	2
13389	A theoretical investigation of structural, electronic and optical properties of bulk copper nitrides. <i>Journal of Alloys and Compounds</i> , 2018, 753, 576-585.	2.8	8
13390	Magnetic anisotropy of ultrathin Pd 4 Co(111) film by first-principles calculations. <i>Journal of Science: Advanced Materials and Devices</i> , 2018, 3, 243-253.	1.5	1
13391	What drives the H-abstraction reaction in bio-mimetic oxoiron-bTAML complexes? A computational investigation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13845-13850.	1.3	1
13392	Reconstruction of Supported Metal Nanoparticles in Reaction Conditions. <i>Angewandte Chemie</i> , 2018, 130, 6574-6579.	1.6	25
13393	Platelet precipitate in an age-hardening Mg-Zn-Gd alloy. <i>Journal of Alloys and Compounds</i> , 2018, 752, 407-411.	2.8	25

#	ARTICLE	IF	CITATIONS
13394	New design for highly durable infrared-reflective coatings. <i>Light: Science and Applications</i> , 2018, 7, 17175-17175.	7.7	37
13395	Self-powered photogalvanic phosphorene photodetectors with high polarization sensitivity and suppressed dark current. <i>Nanoscale</i> , 2018, 10, 7694-7701.	2.8	49
13396	Thermodynamic modeling of LiF-NaF-KF-CrF <sub>3</sub> system. <i>Journal of Fluorine Chemistry</i> , 2018, 209, 6-13.	0.9	15
13397	Carbon dioxide capture by nitrogen containing organic materials – A density functional theory investigation. <i>Computational and Theoretical Chemistry</i> , 2018, 1128, 1-14.	1.1	6
13398	Stability, electronic and magnetic properties of small M-doped rhodium clusters. <i>Journal of Alloys and Compounds</i> , 2018, 745, 497-504.	2.8	8
13399	First principles density functional theory study of Pb doped $\delta$ -MnO <sub>2</sub> catalytic materials. <i>Chemical Physics Letters</i> , 2018, 695, 216-221.	1.2	11
13400	Tuning the analog and digital performance of Germanene nanoribbon field effect transistors with engineering the width and geometry of source, channel and drain region in the ballistic regime. <i>Materials Science in Semiconductor Processing</i> , 2018, 80, 18-23.	1.9	11
13401	Proton Conduction and Fuel Cell Using the CuFe-Oxide Mineral Composite Based on CuFeO <sub>2</sub> Structure. <i>ACS Applied Energy Materials</i> , 2018, 1, 580-588.	2.5	28
13402	Magnetism and piezoelectricity of hexagonal boron nitride with triangular vacancy. <i>Chinese Physics B</i> , 2018, 27, 016301.	0.7	13
13403	Experimental and theoretical investigation on corrosion inhibitive properties of steel rebar by a newly designed environmentally friendly inhibitor formula. <i>RSC Advances</i> , 2018, 8, 6507-6518.	1.7	19
13404	The effect of pressure on structural, electronic, elastic, vibration and optical properties of ScXSb (X=Ni, Pd, Pt) compounds. <i>Computational Condensed Matter</i> , 2018, 14, 176-185.	0.9	16
13405	Experimental and computational investigations of LaNi <sub>5-x</sub> Al <sub>x</sub> (x=0, 0.25, 0.5, 0.75 and 1.0) tritium-storage alloys. <i>Journal of Materials Science and Technology</i> , 2018, 34, 1699-1712.	5.6	22
13406	High-pressure and high-temperature physical properties of LiF studied by density functional theory calculations and molecular dynamics simulations. <i>Journal of Physics and Chemistry of Solids</i> , 2018, 116, 209-215.	1.9	7
13407	Influence of Mo-vacancy concentration on the structural, electronic and optical properties of monolayer MoS <sub>2</sub> : A first-principles study. <i>Materials Chemistry and Physics</i> , 2018, 209, 146-151.	2.0	31
13408	Thermodynamic study of the Al-Sc-Y system. <i>Thermochimica Acta</i> , 2018, 661, 147-159.	1.2	4
13409	Facile and Efficient Decontamination of Thorium from Rare Earths Based on Selective Selenite Crystallization. <i>Inorganic Chemistry</i> , 2018, 57, 1880-1887.	1.9	32
13410	Uncovering the influence of common nonmetallic impurities on the stability and strength of a $\Sigma 5$ (310) grain boundary in Cu. <i>Acta Materialia</i> , 2018, 148, 110-122.	3.8	63
13411	DFT study on bimetallic Pt/Cu(111) as efficient catalyst for H <sub>2</sub> dissociation. <i>Applied Surface Science</i> , 2018, 441, 23-28.	3.1	9



#	ARTICLE	IF	CITATIONS
13412	Theoretical prediction of sandwiched two-dimensional phosphide binary compound sheets with tunable bandgaps and anisotropic physical properties. <i>Nanotechnology</i> , 2018, 29, 095703.	1.3	6
13413	Effect of surface Fe-S hybrid structure on the activity of the perfect and reduced $\gamma\text{-Fe}_2\text{O}_3(001)$ for chemical looping combustion. <i>Applied Surface Science</i> , 2018, 440, 29-34.	3.1	15
13414	Preparation and the superior oxygen permeability of a new CO <sub>2</sub> -resistant Ruddlesden-Popper composite oxide Pr <sub>2</sub> Ni <sub>0.9</sub> Mo <sub>0.1</sub> O <sub>4+</sub> . <i>Journal of Alloys and Compounds</i> , 2018, 742, 966-976.	2.8	13
13415	Structural investigation of chemically synthesized ferrite magnetic nanomaterials. <i>Journal of Molecular Structure</i> , 2018, 1160, 447-454.	1.8	9
13416	High-throughput theoretical optimization of the hydrogen evolution reaction on MXenes by transition metal modification. <i>Journal of Materials Chemistry A</i> , 2018, 6, 4271-4278.	5.2	198
13417	Atomic structure and electronic properties of A <sub>2</sub> B <sub>2</sub> XY (A = Si, Pb, B = Cl, I, Tl) $\text{ETQq1 1 0.784314 rgBT}$ . <i>Chemical Physics</i> , 2018, 20, 10060-10068.	1.3	4
13418	Stabilizing and Organizing Bi <sub>3</sub> Cu <sub>4</sub> and Bi <sub>7</sub> Cu <sub>12</sub> Nanoclusters in Two-Dimensional Metal-Organic Networks. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 4617-4621.	7.2	12
13419	An Aqueous Inorganic Polymer Binder for High Performance Lithium-Sulfur Batteries with Flame-Retardant Properties. <i>ACS Central Science</i> , 2018, 4, 260-267.	5.3	147
13420	Harmonizing Energy and Power Density toward 2.7 V Asymmetric Aqueous Supercapacitor. <i>Advanced Energy Materials</i> , 2018, 8, 1702630.	10.2	201
13421	Reaction of Acetylenedicarboxylic Acid Made Easy: High-Pressure Route for Polymerization. <i>Crystal Growth and Design</i> , 2018, 18, 1425-1431.	1.4	12
13422	Electronic structures and magnetic properties of Fe <sub>3</sub> Si films epitaxial on Si(001). <i>Modern Physics Letters B</i> , 2018, 32, 1750362.	1.0	1
13423	Singlet-triplet energy gaps and the degree of diradical character in binuclear copper molecular magnets characterized by spin-flip density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13127-13144.	1.3	45
13424	Honeycomb-Like Spherical Cathode Host Constructed from Hollow Metallic and Polar Co <sub>9</sub> S <sub>8</sub> Tubules for Advanced Lithium-Sulfur Batteries. <i>Advanced Functional Materials</i> , 2018, 28, 1704443.	7.8	236
13425	Proposed mechanism of HCP to FCC phase transition in titanium through first principles calculation and experiments. <i>Scientific Reports</i> , 2018, 8, 1992.	1.6	68
13426	Local atomic structure of Co B-based glassy alloys: Ab initio molecular dynamics simulations. <i>Journal of Non-Crystalline Solids</i> , 2018, 483, 118-125.	1.5	7
13427	Assessment of ten density functionals through the use of local hyper-softness to get insights about the catalytic activity. <i>Journal of Molecular Modeling</i> , 2018, 24, 42.	0.8	5
13428	Delimited Polyacenes: Edge Topology as a Tool To Modulate Carbon Nanoribbon Structure, Conjugation, and Mobility. <i>Chemistry of Materials</i> , 2018, 30, 947-957.	3.2	21
13429	Quantum Capacitance of Silicene-Based Electrodes from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 1903-1912.	1.5	39



#	ARTICLE	IF	CITATIONS
13430	Substrate engineering of graphene reactivity: towards high-performance graphene-based catalysts. Npj 2D Materials and Applications, 2018, 2, .	3.9	86
13431	Introducing DDEC6 atomic population analysis: part 4. Efficient parallel computation of net atomic charges, atomic spin moments, bond orders, and more. RSC Advances, 2018, 8, 2678-2707.	1.7	129
13432	OPE molecular junction as a hydrogen gas sensor. Current Applied Physics, 2018, 18, 273-279.	1.1	4
13433	Structure, stability, and electronic and magnetic properties of small Rh n Mn (n = 1â€“12) clusters. European Physical Journal D, 2018, 72, 1.	0.6	0
13434	First-principles studies on electronic structures and optical properties of two-dimensional Sn1âˆ“xTi(Zr)xS2 alloys. Modern Physics Letters B, 2018, 32, 1850092.	1.0	1
13435	Long-range exchange limit and dispersion in pure silica zeolites. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	3
13436	An experimental and theoretical investigation of XPS and NEXAFS of 5-halouracils. Physical Chemistry Chemical Physics, 2018, 20, 6657-6667.	1.3	8
13437	A comprehensive study of <i>g</i>-factors, elastic, structural and electronic properties of III-V semiconductors using hybrid-density functional theory. Journal of Applied Physics, 2018, 123, .	1.1	23
13438	Peierls stresses estimated via the Peierls-Nabarro model using ab-initio $\hat{\Gamma}^3$ -surface and their comparison with experiments. Acta Materialia, 2018, 148, 355-362.	3.8	51
13439	Steric and Acidity Control in Hydrogen Bonding and Proton Transfer to <i>trans</i>-W(N<sub>2</sub>)<sub>2</sub>(dppe)<sub>2</sub>. Inorganic Chemistry, 2018, 57, 1656-1664.	1.9	7
13440	Formation energies of substitutional NAs and split interstitial complexes in dilute GaAsN alloys with different growth orientations. Applied Physics A: Materials Science and Processing, 2018, 124, 1.	1.1	2
13441	Insight into the C C chain growth in Fischer-Tropsch synthesis on HCP Co(10-10) surface: The effect of crystal facets on the preferred mechanism. Computational Materials Science, 2018, 145, 263-279.	1.4	16
13442	Ti Impurity Effect on the Optical Coefficients in 2D Cu<sub>2</sub> Si: A DFT Study. Communications in Theoretical Physics, 2018, 69, 101.	1.1	3
13443	First-principles study of defect formation in a photovoltaic semiconductor Cu<sub>2</sub>ZnGeSe<sub>4</sub>. Japanese Journal of Applied Physics, 2018, 57, 02CE06.	0.8	5
13444	Silicene-terminated surface of calcium and strontium disilicides: properties and comparison with bulk structures by computational methods. Philosophical Magazine, 2018, 98, 1131-1150.	0.7	4
13445	Origin of the overpotentials for HCOO<sup>âˆ“</sup> and CO formation in the electroreduction of CO<sub>2</sub> on Cu(211): the reductive desorption processes decide. Physical Chemistry Chemical Physics, 2018, 20, 5756-5765.	1.3	19
13446	Benchmark First-Principles Calculations of Adsorbate Free Energies. ACS Catalysis, 2018, 8, 1945-1954.	5.5	43
13447	CO adsorption and oxygen activation on group 11 nanoparticles â€“ a combined DFT and high level CCSD(T) study about size effects and activation processes. Faraday Discussions, 2018, 208, 105-121.	1.6	16

#	ARTICLE	IF	CITATIONS
13448	DFT and TD-DFT calculations of the electronic structures and photophysical properties of newly designed pyrene-core arylamine derivatives as hole-transporting materials for perovskite solar cells. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	49
13449	A DFT approach for methanol synthesis via hydrogenation of CO on gallia, ceria and ZnO surfaces. <i>Applied Surface Science</i> , 2018, 436, 1003-1017.	3.1	10
13450	Activation and diffusion of ammonia borane hydrogen on gold tetramers. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25567.	1.0	5
13451	Water dissociation at the Au/±-Fe2O3(0001) interface. <i>Molecular Catalysis</i> , 2018, 446, 10-22.	1.0	6
13452	Theoretical Study of Small Iron-Oxyhydroxide Clusters and Formation of Ferrihydrite. <i>Journal of Physical Chemistry A</i> , 2018, 122, 652-661.	1.1	27
13453	Photoinduced dynamics to photoluminescence in Ln <sup>3+</sup> (Ln = Ce, Pr) doped $\beta$ -NaYF <sub>4</sub> nanocrystals computed in basis of non-collinear spin DFT with spin-orbit coupling. <i>Molecular Physics</i> , 2018, 116, 697-707.	0.8	8
13454	Catalytic role of transition metals supported on niobium oxide in O <sub>2</sub> activation. <i>Applied Surface Science</i> , 2018, 434, 1239-1247.	3.1	27
13455	First-principles energy and vibration spectrum simulations of Cr/V interacting with H in W-based alloy in a fusion reactor. <i>Journal of Nuclear Science and Technology</i> , 2018, 55, 123-137.	0.7	1
13456	Evaluation of magnesium ion migration in inorganic oxides by the bond valence site energy method. <i>Solid State Ionics</i> , 2018, 315, 111-115.	1.3	34
13457	Superposed Redox Chemistry of Fused Carbon Rings in Cyclooctatetraene-Based Organic Molecules for High-Voltage and High-Capacity Cathodes. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 2496-2503.	4.0	12
13458	DFT insight into the support effect on the adsorption and activation of key species over Co catalysts for CO <sub>2</sub> methanation. <i>Journal of CO<sub>2</sub> Utilization</i> , 2018, 24, 99-111.	3.3	36
13459	Theoretical study on the ring-opening hydrolysis reactions of N-alkylmaleimide dimers. <i>Chemical Physics Letters</i> , 2018, 692, 304-312.	1.2	1
13460	Island shape, size and interface dependency on electronic and magnetic properties of graphene hexagonal-boron nitride (h-BN) in-plane hybrids. <i>Journal of Physics and Chemistry of Solids</i> , 2018, 115, 187-198.	1.9	10
13461	Lower and Upper Bound Estimates of Material Properties of Pristine Graphene: Using Quantum Espresso. , 2018, , 253-265.		0
13462	Hydrogen storage in lithium hydride: A theoretical approach. <i>Journal of Physics and Chemistry of Solids</i> , 2018, 115, 6-17.	1.9	26
13463	How reliable are Minnesota density functionals for modeling phosphorus-hydrogen NMR spin-spin coupling constants?. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	3
13464	Investigation of Half-Heusler Compounds RhCrZ (Z = P, As, Sb, Sn): A First Principle Study. <i>Journal of Superconductivity and Novel Magnetism</i> , 2018, 31, 2637-2645.	0.8	4
13465	Ab Initio Study of Half-Heusler Compounds MnVZ (Z = P, As, Sb). <i>Journal of Superconductivity and Novel Magnetism</i> , 2018, 31, 2617-2627.	0.8	11

#	ARTICLE	IF	CITATIONS
13466	First-principles investigation on the structures, energies, electronic and defective properties of Ti <sub>2</sub> AlN surfaces. <i>Applied Surface Science</i> , 2018, 433, 1056-1066.	3.1	25
13467	First-principles study of structural phase transition, electronic, elastic and thermodynamic properties of C15-type Laves phase TiCr <sub>2</sub> under pressure. <i>Physica B: Condensed Matter</i> , 2018, 531, 79-84.	1.3	10
13468	Theoretical study of the oxygen impurity doped Ta <sub>5</sub> N <sub>6</sub> . <i>Computational Materials Science</i> , 2018, 143, 368-373.	1.4	2
13469	Theoretical Study of $\rho_{K^a}$ Values for Trivalent Rare-Earth Metal Cations in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2018, 122, 700-707.	1.1	22
13470	C-H Arylation of Phenanthrene with Trimethylphenylsilane by Pd-Chloranil Catalysis: Computational Studies on the Mechanism, Regioselectivity, and Role of Chloranil. <i>Journal of the American Chemical Society</i> , 2018, 140, 2196-2205.	6.6	29
13471	Vibrational properties of the Au-( $Tj$ ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 547 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML")	1.1	10
13472	Thermal decomposition of sol-gel derived Zn <sub>0.8</sub> Ga <sub>0.2</sub> O precursor-gel: A kinetic, thermodynamic, and DFT studies. <i>Acta Materialia</i> , 2018, 146, 152-159.	3.8	5
13473	Surface interaction of H <sub>2</sub> O and H <sub>2</sub> S onto Ca <sub>12</sub> O <sub>12</sub> nanocluster: Quantum-chemical analyses. <i>Surface and Interface Analysis</i> , 2018, 50, 411-419.	0.8	47
13474	Experimental and first principle calculation study on titanium, zirconium and aluminum oxides in promoting ferrite nucleation. <i>Journal of Alloys and Compounds</i> , 2018, 742, 112-122.	2.8	18
13475	Chemically accurate adsorption energies for methane and ethane monolayers on the MgO(001) surface. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 9760-9769.	1.3	26
13476	Transition-metal alloying of $\hat{\rho}^3$ : Effects on the ideal uniaxial compressive strength from first-principles calculations. <i>Physical Review B</i> , 2018, 97, .	1.1	21
13477	The effect of alkali metal over Mn/TiO <sub>2</sub> for low-temperature SCR of NO with NH <sub>3</sub> through DRIFT and DFT. <i>Computational Materials Science</i> , 2018, 144, 216-222.	1.4	45
13478	A Water Dimer Shift Activates a Proton Pumping Pathway in the $P_R$ $\hat{\rho}^3$ Transition of $\rho_{ba}^3$ Cytochrome $\rho_{c}$ Oxidase. <i>Inorganic Chemistry</i> , 2018, 57, 1048-1059.	1.9	11
13479	Possibility of a ferromagnetic and conducting metal-organic network. <i>Journal of Magnetism and Magnetic Materials</i> , 2018, 453, 48-52.	1.0	12
13480	Roles of sliding-induced defects and dissociated water molecules on low friction of graphene. <i>Scientific Reports</i> , 2018, 8, 121.	1.6	26
13481	Atomic scale analysis of Hf-containing precipitates in an Al-Si-Mg-Hf alloy. <i>Journal of Alloys and Compounds</i> , 2018, 741, 1070-1079.	2.8	4
13482	Molecular dynamics of reactions between (4,0) zigzag carbon nanotube and hydrogen peroxide under extreme conditions. <i>Molecular Physics</i> , 2018, 116, 708-716.	0.8	4
13483	Theoretical insight into the photodeactivation pathway of the tetradentate Pt(II) complex: The $\rho_{c}$ -conjugation effect. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4220.	1.7	7

#	ARTICLE	IF	CITATIONS
13484	Transparency enhancement for SrVO <sub>3</sub> by SrTiO <sub>3</sub> mixing: A first-principles study. Computational Materials Science, 2018, 144, 139-146.	1.4	13
13485	Tuning the indirect→direct band gap transition in the MoS <sub>2</sub> xSe <sub>x</sub> armchair nanotube by diameter modulation. Physical Chemistry Chemical Physics, 2018, 20, 3608-3613.	1.3	51
13486	Ground state geometries, UV/vis absorption spectra and charge transfer properties of triphenylamine-thiophenes based dyes for DSSCs: A TD-DFT benchmark study. Computational and Theoretical Chemistry, 2018, 1125, 39-48.	1.1	56
13487	Phase stability, magnetic, electronic, half-metallic and mechanical properties of a new equiatomic quaternary Heusler compound ZrRhTiIn: A first-principles investigation. Journal of Physics and Chemistry of Solids, 2018, 116, 72-78.	1.9	24
13488	Comparison of the Performance of van der Waals Dispersion Functionals in the Description of Water and Ethanol on Transition Metal Surfaces. Journal of Physical Chemistry C, 2018, 122, 1577-1588.	1.5	36
13489	Interactions of Oxygen and Water Molecules with Pyrite Surface: A New Insight. Langmuir, 2018, 34, 1941-1952.	1.6	39
13490	Theoretical investigations on the unsymmetrical effect of $\beta$ -link Zn→porphyrin sensitizers on the performance for dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2018, 20, 3741-3751.	1.3	24
13491	Improved Photoactivity of Pyroxene Silicates by Cation Substitutions. ChemPhysChem, 2018, 19, 943-953.	1.0	2
13492	Formic acid decomposition on Pt <sub>1</sub> /Cu (111) single platinum atom catalyst: Insights from DFT calculations and energetic span model analysis. Applied Surface Science, 2018, 436, 631-638.	3.1	30
13493	Constructing High-Dimensional Neural Network Potential Energy Surfaces for Gas→Surface Scattering and Reactions. Journal of Physical Chemistry C, 2018, 122, 1761-1769.	1.5	78
13494	Phase Transformation and Diffusion Kinetics of V <sub>2</sub> O <sub>5</sub> Electrode in Rechargeable Li and Mg Batteries: A First-Principle Study. Journal of Physical Chemistry C, 2018, 122, 1513-1521.	1.5	43
13495	Perforated N-doped monoclinic ZnWO <sub>4</sub> nanorods for efficient photocatalytic hydrogen generation and RhB degradation under natural sunlight. Catalysis Science and Technology, 2018, 8, 2909-2919.	2.1	33
13496	Reconstruction of Supported Metal Nanoparticles in Reaction Conditions. Angewandte Chemie - International Edition, 2018, 57, 6464-6469.	7.2	68
13497	Effect of Coverage on Catalytic Selectivity and Activity on Metallic and Alloy Catalysts; Vinyl Acetate Monomer Synthesis. Topics in Catalysis, 2018, 61, 722-735.	1.3	10
13498	Surface Properties of Fluorite in Presence of Water: An Atomistic Investigation. Journal of Physical Chemistry B, 2018, 122, 6829-6836.	1.2	39
13499	Electrodeposition-fabricated PtCu-alloy cathode catalysts for high-temperature proton exchange membrane fuel cells. Korean Journal of Chemical Engineering, 2018, 35, 1547-1555.	1.2	26
13500	Enhanced field-emission properties of buckled $\beta$ -borophene by means of Li decoration: a first-principles investigation. Physical Chemistry Chemical Physics, 2018, 20, 15139-15148.	1.3	8
13501	Co on the H-passivated Si(001) surface: Density-functional calculations. Physica B: Condensed Matter, 2018, 542, 44-50.	1.3	1

#	ARTICLE	IF	CITATIONS
13502	Tunable electronic coupling of cobalt sulfide/carbon composites for optimizing oxygen evolution reaction activity. <i>Journal of Materials Chemistry A</i> , 2018, 6, 10304-10312.	5.2	86
13503	Theoretical investigation of dephosphorylation of phosphate monoesters on CeO <sub>2</sub> (111). <i>Catalysis Today</i> , 2018, 312, 141-148.	2.2	16
13504	DFT+U study on the electronic structures and optical properties of pyrite and marcasite. <i>Computational Materials Science</i> , 2018, 150, 346-352.	1.4	14
13505	Effect of anti-site point defects on the mechanical and thermodynamic properties of MgZn <sub>2</sub> , MgCu <sub>2</sub> Laves phases: A first-principle study. <i>Journal of Solid State Chemistry</i> , 2018, 263, 18-23.	1.4	13
13506	Nanoindentation-induced phase transformation between SiC polymorphs. <i>Materials Letters</i> , 2018, 220, 152-155.	1.3	5
13507	Molecular and dissociative adsorption of DMMP, Sarin and Soman on dry and wet TiO <sub>2</sub> (110) using density functional theory. <i>Surface Science</i> , 2018, 675, 26-35.	0.8	28
13508	Functionalization of silicon surface by thiadiazole molecule: A DFT study. <i>Surface Science</i> , 2018, 674, 87-93.	0.8	7
13509	Chemical bonding and Cu diffusion at the Cu/Ta <sub>2</sub> N interface: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13566-13573.	1.3	10
13510	Atomistic Simulations of Metal-Al <sub>2</sub> O <sub>3</sub> Interfaces. , 2018, , 1-40.		0
13511	Insight into the effect of maleic acid on the preparation of $\hat{\pm}$ -hemihydrate gypsum from phosphogypsum in Na <sub>2</sub> SO <sub>4</sub> solution. <i>Journal of Crystal Growth</i> , 2018, 493, 34-40.	0.7	45
13512	An experimental and DFT study of the packing and structure of dithenoylmethane monocarbonylphosphine Rhodium(I) complex [Rh((C <sub>4</sub> H <sub>3</sub> S)CO)CHCO(C <sub>4</sub> H <sub>3</sub> S))(CO)(PPh <sub>3</sub> )]. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 83, 33-41.	1.3	0
13513	The Vanadium Effect on Electronic and Optical Response of MoS <sub>2</sub> Graphene-Like: Using DFT. <i>Silicon</i> , 2018, 10, 2855-2863.	1.8	13
13514	Effect of spin-orbit interactions on the structural stability, thermodynamic properties, and transport properties of lead under pressure. <i>Physical Review B</i> , 2018, 97, .	1.1	5
13515	Li conduction pathways in solid-state electrolytes: Insights from dynamics and polarizability. <i>Chemical Physics Letters</i> , 2018, 698, 234-239.	1.2	9
13516	Strongly coupling of Co <sub>9</sub> S <sub>8</sub> /Zn-Co-S heterostructures rooted in carbon nanocages towards efficient oxygen evolution reaction. <i>Journal of Catalysis</i> , 2018, 361, 322-330.	3.1	68
13517	Magnetism, optical, and thermoelectric response of CdFe <sub>2</sub> O <sub>4</sub> by using DFT scheme. <i>Chinese Physics B</i> , 2018, 27, 037103.	0.7	9
13518	Possible Martensitic Transformation in Heusler Alloy Pt <sub>2</sub> MnSn from First Principles. <i>Chinese Physics Letters</i> , 2018, 35, 038101.	1.3	2
13519	Electronic Transport Properties of Carbon-Nanotube Networks: The Effect of Nitrate Doping on Intratube and Intertube Conductances. <i>Physical Review Applied</i> , 2018, 9, .	1.5	10

#	ARTICLE	IF	CITATIONS
13520	Synthesis, crystal structure and optical absorption of NaInS <sub>2</sub> -Se. Journal of Alloys and Compounds, 2018, 750, 409-413.	2.8	8
13521	Voltammetric Determination of Serine Using Cysteine Modified Platinum Electrode and Brief Exploration from the Theoretical Perspective. Electroanalysis, 2018, 30, 1060-1065.	1.5	2
13522	Can we predict the structure and stability of molecular crystals under increased pressure? First-principles study of glycine phase transitions. Journal of Computational Chemistry, 2018, 39, 1300-1306.	1.5	19
13523	Hollow Mo-doped CoP nanoarrays for efficient overall water splitting. Nano Energy, 2018, 48, 73-80.	8.2	608
13524	The surface energy and stress of metals. Surface Science, 2018, 674, 51-68.	0.8	68
13525	Blue Phosphorus/Mg(OH) <sub>2</sub> van der Waals Heterostructures as Promising Visible-Light Photocatalysts for Water Splitting. Journal of Physical Chemistry C, 2018, 122, 7075-7080.	1.5	115
13526	Adamantane-Derived Carbon Nanothreads: High Structural Stability and Mechanical Strength. Journal of Physical Chemistry C, 2018, 122, 7945-7950.	1.5	7
13527	Effect of edge defects on band structure of zigzag graphene nanoribbons. Journal of Applied Physics, 2018, 123, .	1.1	7
13528	Theoretical insights into the minority carrier lifetime of doped Si: A computational study. Journal of Applied Physics, 2018, 123, 161420.	1.1	2
13529	Using Brønsted-Evans-Polanyi relations to predict electrode potential-dependent activation energies. Catalysis Today, 2018, 312, 82-91.	2.2	36
13530	Theoretical Investigation of CO <sub>2</sub> Adsorption and Dissociation on Low Index Surfaces of Transition Metals. Journal of Physical Chemistry C, 2018, 122, 8306-8314.	1.5	104
13531	Insight into fast Li diffusion in Li-excess spinel lithium manganese oxide. Journal of Materials Chemistry A, 2018, 6, 9893-9898.	5.2	51
13532	Semi-local machine-learned kinetic energy density functional with third-order gradients of electron density. Journal of Chemical Physics, 2018, 148, 241705.	1.2	67
13533	Two-dimensional $H_{2n}$ in Si: Raman scattering and modeling study. Physical Review B, 2018, 97, .	1.1	2
13534	Density Functional Theory: From Conceptual Level Toward Practical Functionality. , 2018, , 221-289.		0
13535	Mechanistic study of the [(dpp-bian)Re(CO) <sub>3</sub> Br] electrochemical reduction using in situ EPR spectroscopy and computational chemistry. Electrochimica Acta, 2018, 270, 526-534.	2.6	21
13536	Insight into point defects and impurities in titanium from first principles. Npj Computational Materials, 2018, 4, .	3.5	62
13537	Magnetic moment and magnetic anisotropy of Ge <sub>3</sub> Mn <sub>5</sub> thinfilms on Ge(111) substrate: A density functional study. Journal of Chemical Physics, 2018, 148, 074701.	1.2	3



#	ARTICLE	IF	CITATIONS
13538	Structural and electronic properties of PdS <sub>2</sub> nanoribbons. Journal of Magnetism and Magnetic Materials, 2018, 458, 310-316.	1.0	10
13539	High oxygen reduction activity of TM <sub>13</sub> @Pt <sub>134</sub> and TM <sub>12N</sub> @Pt <sub>134</sub> (TM=Ti, V, Mn, Fe, Co, Ni, and Cu) core-shell electrocatalysts studied by first-principles theory. Materials Chemistry and Physics, 2018, 212, 378-384.	2.0	8
13540	Calculation of Entropy of Adsorption for Small Molecules on Mineral Surfaces. Journal of Physical Chemistry C, 2018, 122, 8236-8243.	1.5	38
13541	How Accurate Is Density Functional Theory at Predicting Dipole Moments? An Assessment Using a New Database of 200 Benchmark Values. Journal of Chemical Theory and Computation, 2018, 14, 1969-1981.	2.3	180
13542	Identification of Intermediates during the Hydration of Na <sub>8</sub> [AlSiO <sub>4</sub> ] <sub>6</sub> (BH <sub>4</sub> ) <sub>2</sub> : A Combined Theoretical and Experimental Approach. Journal of Physical Chemistry A, 2018, 122, 3293-3300.	1.1	1
13543	Potential Dependence of the Buckling Structure of the Interfacial Water Bilayer on a Graphene Electrode. Journal of Physical Chemistry C, 2018, 122, 7795-7800.	1.5	4
13544	1,8-Bis(diphenylphosphino)biphenylene. A new ligand for late transition metal complexes. Zeitschrift Fur Kristallographie - Crystalline Materials, 2018, 233, 627-639.	0.4	7
13545	Dependence of H <sub>2</sub> and CO <sub>2</sub> selectivity on Cu oxidation state during partial oxidation of methanol on Cu/ZnO. Applied Catalysis A: General, 2018, 556, 64-72.	2.2	34
13546	First-principles studies on the superconductivity of aluminene. Applied Surface Science, 2018, 445, 161-166.	3.1	28
13547	Exploring the methanol decomposition mechanism on the Pt <sub>3</sub> Ni(100) surface: a periodic density functional theory study. Physical Chemistry Chemical Physics, 2018, 20, 10132-10141.	1.3	8
13548	Electronic structures and enhanced photocatalytic properties of blue phosphorene/BSe van der Waals heterostructures. Journal of Materials Chemistry A, 2018, 6, 8923-8929.	5.2	197
13549	Hindered rotation and nuclear spin isomers separation of molecularly chemisorbed H <sub>2</sub> on Pd(210). Journal of Applied Physics, 2018, 123, .	1.1	5
13550	Facile air oxidative induced dealloying of hierarchical branched PtCu nanodendrites with enhanced activity for hydrogen evolution. Applied Catalysis A: General, 2018, 557, 72-78.	2.2	22
13551	Nonequilibrium BN-ZnO: Optical properties and excitonic effects from first principles. Physical Review B, 2018, 97, .	1.1	9
13552	First-principles study of interaction between vacancies and nitrogen atoms in fcc iron. Computational Materials Science, 2018, 149, 65-72.	1.4	8
13553	Density functional theory calculations for armchair stanene nanoribbons with fluorine and sulfur functionalization. Physica E: Low-Dimensional Systems and Nanostructures, 2018, 101, 71-77.	1.3	9
13554	Observations of non-linear plasmon damping in dense plasmas. Physics of Plasmas, 2018, 25, .	0.7	29
13555	Na <sub>2</sub> MnO <sub>3</sub> as cathode materials for Na ion batteries: From first-principles investigations. Solid State Ionics, 2018, 320, 210-214.	1.3	31



#	ARTICLE	IF	CITATIONS
13556	Unveiling Adsorption Mechanisms of Elemental Mercury on Defective Boron Nitride Monolayer: A Computational Study. <i>Energy &amp; Fuels</i> , 2018, 32, 5331-5337.	2.5	27
13557	Mechanism and Kinetics of Aztreonam Hydrolysis Catalyzed by Class-C $\beta$ -Lactamase: A Temperature-Accelerated Sliced Sampling Study. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4299-4308.	1.2	18
13558	DFT study on dry reforming of methane over Ni <sub>2</sub> Fe overlayer of Ni(111) surface. <i>Applied Surface Science</i> , 2018, 443, 515-524.	3.1	42
13559	Structural, magnetic properties, and electronic structure of hexagonal FeCoSn compound. <i>Chinese Physics B</i> , 2018, 27, 026101.	0.7	5
13560	Si-Ni Alloy as Anode Materials for Lithium Ion Batteries: A First-Principles Study. <i>Materials Science Forum</i> , 2018, 913, 838-845.	0.3	0
13561	Spin Injection into Graphene from Heusler Alloy Co <sub>2</sub> MnGe (111) Surface: A First Principles Study. <i>Materials Science Forum</i> , 0, 914, 111-116.	0.3	2
13562	Adhesion, stability and electronic properties of Ti <sub>2</sub> AlN(0001)/TiAl(111) coherent interface from first-principles calculation. <i>Intermetallics</i> , 2018, 96, 49-57.	1.8	36
13563	A Benchmark Study of Electronic Couplings in Donor-Bridge-Acceptor Systems with the FMR-B Method. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2007-2016.	2.3	6
13564	Testing Electronic Friction Models: Vibrational De-excitation in Scattering of H <sub>2</sub> and D <sub>2</sub> from Cu(111). <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1803-1808.	2.1	59
13565	Stabilizing spin spirals and isolated skyrmions at low magnetic field exploiting vanishing magnetic anisotropy. <i>Nature Communications</i> , 2018, 9, 1015.	5.8	82
13566	Long-range corrected density functional through the density matrix expansion based semilocal exchange hole. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8991-8998.	1.3	21
13567	The structural, electro-optical, charge transport and nonlinear optical properties of oxazole (4 Z) Tj ETQq1 1 0.784314 rgBT /Overlock Science, 2018, 30, 75-82.	1.6	20
13568	Mechanical Properties of TiC Nanowire from DFT Calculations. <i>Iranian Journal of Science and Technology, Transaction A: Science</i> , 2018, 42, 1623-1627.	0.7	2
13569	How methoxy groups change nature of the thiophene based heterocyclic chalcones from p-channel to ambipolar transport semiconducting materials. <i>Journal of King Saud University - Science</i> , 2018, 30, 458-465.	1.6	7
13570	Metal-organic framework-derived porous shuttle-like vanadium oxides for sodium-ion battery application. <i>Nano Research</i> , 2018, 11, 449-463.	5.8	108
13571	First-Principles Investigation of Equiatomic Quaternary Heusler Alloys NbVMnAl and NbFeCrAl and a Discussion of the Generalized Electron-Filling Rule. <i>Journal of Superconductivity and Novel Magnetism</i> , 2018, 31, 189-196.	0.8	23
13572	Theoretical Investigation of Half-Metallic Ferromagnetism in Sodium-Based Fluoro-perovskite NaXF <sub>3</sub> (X = V, Co). <i>Journal of Superconductivity and Novel Magnetism</i> , 2018, 31, 285-295.	0.8	15
13573	A First Principle Study of Half-Heusler Compounds CrTiZ (Z = P, As). <i>Journal of Superconductivity and Novel Magnetism</i> , 2018, 31, 257-264.	0.8	17

#	ARTICLE	IF	CITATIONS
13574	DFT study of small aluminum and boron hydrides: isomeric composition and physical properties. <i>Structural Chemistry</i> , 2018, 29, 49-68.	1.0	14
13575	Adsorption of gaseous ethylene via induced polarization on plasmonic photocatalyst Ag/AgCl/TiO <sub>2</sub> and subsequent photodegradation. <i>Applied Catalysis B: Environmental</i> , 2018, 220, 356-361.	10.8	134
13576	Structural, Optical, and Electronic Characterization of Fe-Doped Alumina Nanoparticles. <i>Journal of Electronic Materials</i> , 2018, 47, 711-720.	1.0	25
13577	H <sub>2</sub> S adsorption and dissociation on NH-decorated graphene: A first principles study. <i>Surface Science</i> , 2018, 668, 100-106.	0.8	40
13578	Insight into the high-efficient functionalization of carbon nanotubes by advanced oxidation using peroxomonosulfate. <i>Microporous and Mesoporous Materials</i> , 2018, 260, 24-29.	2.2	7
13579	Structures, electronic properties and reaction paths from Fe(CO) <sub>5</sub> molecule to small Fe clusters. <i>Phase Transitions</i> , 2018, 91, 426-433.	0.6	24
13580	Ozone-assisted regeneration of magnetic carbon nanotubes for removing organic water pollutants. <i>Chemical Engineering Journal</i> , 2018, 335, 384-391.	6.6	37
13581	PtCoFe Nanowire Cathodes Boost Short-Circuit Currents of Ru(II)-Based Dye-Sensitized Solar Cells to a Power Conversion Efficiency of 12.29%. <i>Advanced Functional Materials</i> , 2018, 28, 1703282.	7.8	55
13582	Magneto-electronic properties and tetragonal deformation of rare-earth-element-based quaternary Heusler half-metals: A first-principles prediction. <i>Journal of Alloys and Compounds</i> , 2018, 734, 329-341.	2.8	33
13583	Antioxidant electrospun zein nanofibrous web encapsulating quercetin/cyclodextrin inclusion complex. <i>Journal of Materials Science</i> , 2018, 53, 1527-1539.	1.7	70
13584	Thermal and electrical properties of siligraphene and its derivatives. <i>Optik</i> , 2018, 157, 936-943.	1.4	13
13585	First-principles studies on electronic properties of Oligo- p -phenylene molecular device. <i>Solid State Communications</i> , 2018, 269, 50-57.	0.9	12
13586	Protomene: A new carbon allotrope. <i>Carbon</i> , 2018, 126, 574-579.	5.4	28
13587	Crystal growth, electronic structure and optical properties of Sr <sub>2</sub> Mg(BO <sub>3</sub> ) <sub>2</sub> . <i>Journal of Solid State Chemistry</i> , 2018, 258, 283-288.	1.4	9
13588	Rare earth ions doped K <sub>2</sub> Ta <sub>2</sub> O <sub>6</sub> photocatalysts with enhanced UV-vis light activity. <i>Applied Catalysis B: Environmental</i> , 2018, 224, 451-468.	10.8	46
13589	Strained noble metal di chalcogenides PtX <sub>2</sub> (X = S, Se) mono-layer: Ab initio study of electronic and lattice dynamic properties. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 95, 139-143.	1.3	16
13590	Theoretical aspect of the bonding in bis-chelate thiosemicarbazones nickel (II) complexes: A DFT study. <i>Journal of Molecular Structure</i> , 2018, 1154, 19-26.	1.8	2
13591	Adsorption and reaction of CO and H <sub>2</sub> O on WC(0001) surface: A first-principles investigation. <i>Applied Surface Science</i> , 2018, 428, 579-585.	3.1	8

#	ARTICLE	IF	CITATIONS
13592	Effect of strain engineering on 2D dichalcogenides transition metal: A DFT study. Computational Materials Science, 2018, 141, 235-242.	1.4	35
13593	Ferromagnetism and Half-Metallicity in a High-Band-Gap Hexagonal Boron Nitride System. ChemPhysChem, 2018, 19, 153-161.	1.0	10
13594	Adsorption of bentazon on CAT and CARBOPAL activated carbon: Experimental and computational study. Applied Surface Science, 2018, 433, 487-501.	3.1	9
13595	Low temperature preparation of oxygen-deficient tin dioxide nanocrystals and a role of oxygen vacancy in photocatalytic activity improvement. Journal of Colloid and Interface Science, 2018, 512, 105-114.	5.0	59
13596	Theoretical Investigations of Properties of New Half-Heusler Compounds NiFeZ (Z = Si, Ge). Journal of Superconductivity and Novel Magnetism, 2018, 31, 1751-1759.	0.8	5
13597	A Density Functional Theory Investigations of Half-Heusler Compounds RhVZ (Z = P, As, Sb). Journal of Superconductivity and Novel Magnetism, 2018, 31, 1577-1586.	0.8	21
13598	Ultrathin MoS <sub>2</sub> nanosheets tightly anchoring onto nitrogen-doped graphene for enhanced lithium storage properties. Chemical Engineering Journal, 2018, 332, 431-439.	6.6	89
13599	The effect of metal transition dopant on electronic and mechanical properties of titanium nitride: First principle method. Computational Materials Science, 2018, 141, 82-90.	1.4	10
13600	Fast formation of single-unit-cell-thick and defect-rich layered double hydroxide nanosheets with highly enhanced oxygen evolution reaction for water splitting. Nano Research, 2018, 11, 1883-1894.	5.8	165
13601	X-Ray Crystal Structure of Embelin and Its DFT Scavenging of Superoxide Radical. Journal of Computational Chemistry, 2018, 39, 1143-1148.	1.5	11
13602	Influences of Electrode Potential on Mechanism of Oxygen Reduction Reaction on Pd-Skin/Pd <sub>3</sub> Fe(111) Electrocatalyst: Insights from DFT-Based Calculations. Electroanalysis, 2018, 9, 10-21.	1.5	4
13603	Synthesis and halogenation of bis(8-methoxynaphthyl)ditelluride. Inorganica Chimica Acta, 2018, 475, 73-82.	1.2	4
13604	Elastic properties and thermal expansion of lead-free halide double perovskite Cs <sub>2</sub> AgBiBr <sub>6</sub> . Computational Materials Science, 2018, 141, 49-58.	1.4	87
13605	Hierarchical cobalt poly-phosphide hollow spheres as highly active and stable electrocatalysts for hydrogen evolution over a wide pH range. Applied Surface Science, 2018, 427, 800-806.	3.1	37
13606	Atomic and molecular adsorption on Fe(110). Surface Science, 2018, 667, 54-65.	0.8	49
13607	Atomic size and chemical effects of alloying elements Cu, Mg and Si on the structure and dynamics of molten 8090-based AlLi alloy. International Journal of Cast Metals Research, 2018, 31, 93-98.	0.5	3
13608	High Lithium Insertion Voltage Single-Crystal H <sub>2</sub> Ti <sub>12</sub> O <sub>25</sub> Nanorods as a High-Capacity and High-Rate Lithium-Ion Battery Anode Material. ChemSusChem, 2018, 11, 299-310.	3.6	18
13609	Role of the X and n factors in ion-irradiation induced phase transformations of Mn <sub>1</sub> AX <sub>n</sub> phases. Acta Materialia, 2018, 144, 432-446.	3.8	21

#	ARTICLE	IF	CITATIONS
13610	First-principles investigation on switching properties of spiropyran and merocyanine grafted graphyne nanotube device. <i>Chemical Physics Letters</i> , 2018, 691, 37-43.	1.2	33
13611	Reactivity of CO <sub>2</sub> on the surfaces of magnetite (Fe <sub>3</sub> O <sub>4</sub> ), greigite (Fe <sub>3</sub> S <sub>4</sub> ) and mackinawite (FeS). <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2018, 376, 20170065.	1.6	27
13612	Adsorption of ammonia molecules and humidity on germanane nanosheet—A density functional study. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 79, 149-156.	1.3	30
13613	Evidence for lattice softening of the Fe-Ga magnetostrictive alloy: Stress-induced local martensites. <i>Materials and Design</i> , 2018, 140, 1-6.	3.3	14
13614	High-Pressure-Induced Comminution and Recrystallization of CH <sub>3</sub> NH <sub>3</sub> PbBr <sub>3</sub> Nanocrystals as Large Thin Nanoplates. <i>Advanced Materials</i> , 2018, 30, 1705017.	11.1	89
13615	Shortfall of B3LYP in Reproducing NMR <sup>1</sup> H- <sup>13</sup> C Couplings in Some Isomeric Epoxy Structures with Strong Stereoelectronic Effects: A Benchmark Study on DFT Functionals. <i>ChemPhysChem</i> , 2018, 19, 631-642.	1.0	12
13616	Water dissociation and CO oxidation over Au/anatase catalyst. A DFT-D2 study. <i>Applied Surface Science</i> , 2018, 435, 1168-1173.	3.1	10
13617	Revisiting intrinsic brittleness and deformation behavior of B2 NiAl intermetallic compound: A first-principles study. <i>Journal of Materials Science and Technology</i> , 2018, 34, 620-626.	5.6	16
13618	DFT calculations for structural prediction and applications of intercalated lamellar compounds. <i>Dalton Transactions</i> , 2018, 47, 2852-2866.	1.6	10
13619	Confined Li ion migration in the silicon-graphene complex system: An ab initio investigation. <i>Applied Surface Science</i> , 2018, 436, 505-510.	3.1	14
13620	Adsorption and Desulfurization Mechanism of Thiophene on Layered FeS(001), (011), and (111) Surfaces: A Dispersion-Corrected Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 359-370.	1.5	24
13621	Oxygen-Vacancy-Activated CO <sub>2</sub> Splitting over Amorphous Oxide Semiconductor Photocatalyst. <i>ACS Catalysis</i> , 2018, 8, 516-525.	5.5	126
13622	First-principle study of the Nb+1C T2 systems as electrode materials for supercapacitors. <i>Computational Materials Science</i> , 2018, 143, 225-231.	1.4	26
13623	Recycling of zincite (ZnO) <i>in situ</i> uptake of hydrogen halides. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1221-1230.	1.3	26
13624	Nanoscale Pt thin film sensor for accurate detection of ppm level hydrogen in air at high humidity. <i>Sensors and Actuators B: Chemical</i> , 2018, 258, 913-919.	4.0	37
13625	Chemical Origin of Sodium Phosphate Interactions on Iron and Iron Oxide Surfaces by First Principle Calculations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 635-647.	1.5	29
13626	A DFT study of the stability of SIAs and small SIA clusters in the vicinity of solute atoms in Fe. <i>Journal of Nuclear Materials</i> , 2018, 500, 92-109.	1.3	24
13627	Exploring structural, electronic and thermo-elastic properties of metallic AMoO <sub>3</sub> (A = Pb, Ba, Sr) molybdates. <i>Applied Physics A: Materials Science and Processing</i> , 2018, 124, 1.	1.1	50

#	ARTICLE	IF	CITATIONS
13628	Potential Semiconducting and Superconducting Metastable Si <sub>3</sub> C Structures under Pressure. <i>Chemistry of Materials</i> , 2018, 30, 421-427.	3.2	5
13629	Mechanistic Studies on NaHCO <sub>3</sub> Hydrogenation and HCOOH Dehydrogenation Reactions Catalysed by a Fe <sup>II</sup> Linear Tetraphosphine Complex. <i>Chemistry - A European Journal</i> , 2018, 24, 5366-5372.	1.7	8
13630	Formation of Ag nanoparticles under electron beam irradiation: Atomistic origins from first-principles calculations. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25551.	1.0	21
13631	Zeolite Adsorption Free Energies from ab Initio Potentials of Mean Force. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 929-938.	2.3	43
13632	Pressure-induced structural phase transition in transition metal carbides TMC (TM = Ru, Rh, Pd, Os, Ir). <i>Journal of Applied Physics</i> , 2018, 123, 095101.	0.7	4
13633	Catalytic performance of Ru, Os, and Rh nanoparticles for ammonia synthesis: A density functional theory analysis. <i>Journal of Catalysis</i> , 2018, 357, 213-222.	3.1	53
13634	Comparative study on dynamical stability against strain of pristine and chemically functionalized monolayer honeycomb materials. <i>Journal of Materials Science</i> , 2018, 53, 4306-4315.	1.7	6
13635	Porous Fe <sub>2</sub> O <sub>3</sub> microcubes derived from metal organic frameworks for efficient elimination of organic pollutants and heavy metal ions. <i>Chemical Engineering Journal</i> , 2018, 336, 241-252.	6.6	179
13636	Solute-Interstitial Loop Interaction in $\delta$ -Fe: A DFT Study. <i>Journal of Nuclear Materials</i> , 2018, 499, 582-594.	1.3	34
13637	Coverage-dependent adsorption, dissociation and aggregation of H <sub>2</sub> O on the clean and pre-adsorbed oxygen Cu(111) surface: A DFT study. <i>Molecular Catalysis</i> , 2018, 445, 152-162.	1.0	18
13638	Aluminum Atom Activation of C-S Bonds: An EPR Study of the Intermediates Formed in the Reaction Between Aluminum Atoms and Dialkyl Sulfides. <i>Journal of Physical Chemistry A</i> , 2018, 122, 72-80.	1.1	2
13639	Orbital control over the metal vs. ligand reduction in a series of neutral and cationic bis(cyclopentadienyl) Ti complexes. <i>New Journal of Chemistry</i> , 2018, 42, 662-670.	1.4	8
13640	Mapping deformation mechanisms in lamellar titanium aluminide. <i>Acta Materialia</i> , 2018, 144, 835-843.	3.8	27
13641	Interaction Studies of Ammonia Gas Molecules on Borophene Nanosheet and Nanotubes: A Density Functional Study. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2018, 28, 920-931.	1.9	13
13642	The electronic, structural and magnetic properties of Heusler compounds ZrCrCoZ (Z=B, Al, Ga, In): A first-principles study. <i>Solid State Communications</i> , 2018, 270, 111-118.	0.9	10
13643	Fiber enhanced Raman sensing of levofloxacin by PCF bandgap-shifting into the visible range. <i>Analytical Methods</i> , 2018, 10, 586-592.	1.3	36
13644	Electronic and magnetic properties of monolayer $\delta$ -RuCl <sub>3</sub> : a first-principles and Monte Carlo study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 997-1004.	1.3	57
13645	Effect of alloying elements on stacking fault energy and ductility of tungsten. <i>Journal of Alloys and Compounds</i> , 2018, 737, 372-376.	2.8	42

#	ARTICLE	IF	CITATIONS
13646	Revisiting the diffusion mechanism of helium in UO <sub>2</sub> : A DFT+U study. Journal of Nuclear Materials, 2018, 498, 373-377.	1.3	15
13647	Mechanism of activity enhancement of the Ni based hydrotalcite-derived materials in carbonyl sulfide removal. Materials Chemistry and Physics, 2018, 205, 35-43.	2.0	17
13648	Electronic, magnetic, half-metallic and mechanical properties of a new quaternary Heusler compound ZrRhTiTi: Insights from first-principles studies. Solid State Communications, 2018, 269, 125-130.	0.9	14
13649	Density Functional Theoretical Studies on Chemical Enhancement of Surface-Enhanced Raman Spectroscopy in Electrochemical Interfaces. , 2018, , 455-482.		1
13650	Functional Defective Metal-Organic Coordinated Network of Mesosstructured Nanoframes for Enhanced Electrocatalysis. Advanced Functional Materials, 2018, 28, 1704177.	7.8	68
13651	First-Principles Calculations of the Structural, Electronic, Elastic and Optical Properties of LiGaS <sub>2</sub> and LiGaSe <sub>2</sub> Semiconductors Under Different Pressures. Journal of Electronic Materials, 2018, 47, 1223-1231.	1.0	10
13652	Studies of electronic, magnetic and optical properties of europium nitride EuN doped with TM (Ti, V, Tj ETQq0 0 0 rgBT/Overlock 10 Tff	0.9	0
13653	Mechanism of heterogeneous reaction between gaseous elemental mercury and H <sub>2</sub> O <sub>2</sub> on Fe <sub>3</sub> O <sub>4</sub> (1 $\hat{\text{a}}\hat{\text{e}}\hat{\text{e}}\hat{\text{0}}$ ) surface. Computational and Theoretical Chemistry, 2018, 1123, 11-19.	1.1	6
13654	Adsorption of acetylene on ordered Ni <sub>x</sub> Ag <sub>1-x</sub> /Ni (111) and effect of Ag-dopant: A DFT study. Applied Surface Science, 2018, 435, 521-528.	3.1	15
13655	Elastic, electronic structure, and optical properties of orthorhombic Na <sub>3</sub> AlF <sub>6</sub> : a first-principles study. Ionics, 2018, 24, 1377-1383.	1.2	9
13656	Selectivity tuning over monometallic and bimetallic dehydrogenation catalysts: effects of support and particle size. Catalysis Science and Technology, 2018, 8, 314-327.	2.1	23
13657	Insight into the effect of promoter Co on C <sub>2</sub> oxygenate formation from syngas on CoCu(100) and Cu(100): A comparative DFT study. Applied Surface Science, 2018, 434, 28-39.	3.1	11
13658	The behaviors of helium atoms in tantalum, rhenium and osmium. Journal of Nuclear Materials, 2018, 499, 1-8.	1.3	13
13659	Study of the Air-Tolerant 1,3 $\hat{\text{a}}\hat{\text{e}}\hat{\text{e}}$ Diphosphacyclobutane $\hat{\text{e}}\hat{\text{e}}$ 2,4 $\hat{\text{a}}\hat{\text{e}}$ diyl through the Direct Arylation. Chemical Record, 2018, 18, 445-458.	2.9	10
13660	Consecutive Oxidation of Three H <sub>2</sub> Molecules by a Gold-Vanadium Oxide Cluster Cation AuVO <sub>4</sub> +. Topics in Catalysis, 2018, 61, 28-34.	1.3	6
13661	Structural, Electronic, Magnetic and Optical Investigations of Half-Heusler Compounds YZSb (Z = Cr, Tj ETQq1 1 0,784314 rgBT/Overlock 16	0.8	16
13662	Utility of chemical computations in predicting solution free energies of metal ions. Molecular Simulation, 2018, 44, 110-116.	0.9	16
13663	First-principles calculations of orientation dependence of Si thermal oxidation based on Si emission model. Japanese Journal of Applied Physics, 2018, 57, 04FB06.	0.8	3



#	ARTICLE	IF	CITATIONS
13664	Toxicity prediction of ionic liquids based on <i>Daphnia magna</i> by using density functional theory. IOP Conference Series: Materials Science and Engineering, 2018, 344, 012017.	0.3	3
13665	Thin Film Catalysts for Proton Exchange Membrane Fuel Cells. , 2018, , 351-359.		0
13666	Multiscale Simulation of Precipitation in Copper-Alloyed Pipeline Steels and in Cu-Ni-Si Alloys. , 2018, , 1-41.		0
13667	DFT-Parameterized Object Kinetic Monte Carlo Simulations of Radiation Damage. , 2018, , 1-32.		3
13668	Valence charge distribution in homogenous silicon-aluminium thin-films. Journal of Physics Condensed Matter, 2018, 30, 335502.	0.7	2
13669	<i>Ab initio</i> study of sodium diffusion and adsorption on boron-doped graphyne as promising anode material in sodium-ion batteries. Physical Chemistry Chemical Physics, 2018, 20, 29889-29895.	1.3	36
13670	A density functional theory study of propylene epoxidation mechanism on Ag <sub>2</sub> O(001) surface. Physical Chemistry Chemical Physics, 2018, 20, 26681-26687.	1.3	13
13671	Photoinduced electron transfer and remarkable enhancement of magnetic susceptibility in bridging pyrazine complexes. Dalton Transactions, 2018, 47, 15888-15896.	1.6	18
13672	Selective synthesis of iridium( <i>iii</i> ) end-capped polyynes by oxidative addition of 1-iodopolyynes to Vaska's complex. Dalton Transactions, 2018, 47, 17046-17054.	1.6	4
13673	Theoretical investigation of conversion between different C <sub>2</sub> H <sub>x</sub> species over Pd-Ag/Pd(100) surface alloys: influence on the selectivity and transformation of carbonaceous species. New Journal of Chemistry, 2018, 42, 19827-19836.	1.4	4
13674	Discovery of zirconium dioxides for the design of better oxygen-ion conductors using efficient algorithms beyond data mining. RSC Advances, 2018, 8, 25534-25545.	1.7	18
13675	Structural and electronic properties of KY(BH <sub>4</sub> ) <sub>4</sub> : DFT+U study. RSC Advances, 2018, 8, 34374-34379.	1.7	0
13676	Structure and reducibility of yttrium-doped cerium dioxide nanoparticles and (111) surface. RSC Advances, 2018, 8, 33728-33741.	1.7	5
13677	Stability of the V and Co atomic wires: a first-principles study. RSC Advances, 2018, 8, 41552-41560.	1.7	0
13678	Simultaneous adsorption of SO <sub>2</sub> and CO <sub>2</sub> in an Ni(bdc)(ted) <sub>0.5</sub> metal-organic framework. RSC Advances, 2018, 8, 38648-38655.	1.7	10
13679	Bare versus protected tetrairidium clusters by density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 29480-29492.	1.3	4
13680	How robust is the metallicity of two dimensional gallium?. Physical Chemistry Chemical Physics, 2018, 20, 27668-27674.	1.3	14
13681	Phase transition and superconductivity in ReS <sub>2</sub> , ReSe <sub>2</sub> and ReTe <sub>2</sub> . Physical Chemistry Chemical Physics, 2018, 20, 29472-29479.	1.3	15



#	ARTICLE	IF	CITATIONS
13682	Structural and chemical analysis of second-row impurities in liquid lead–bismuth eutectic by first-principles molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 30480-30491.	1.3	6
13683	Synthesis of a novel strontium-based wide-bandgap semiconductor via X-ray photochemistry under extreme conditions. <i>Journal of Materials Chemistry C</i> , 2018, 6, 12473-12478.	2.7	11
13684	Ab-Initio Modeling of Lubricant Reactions with a Metal Al (111) Surface. , 2018, , .		0
13685	Phase transition, thermodynamic and elastic properties of ZrC. <i>Transactions of Nonferrous Metals Society of China</i> , 2018, 28, 2520-2527.	1.7	11
13686	Electronics properties of ZnSe nanotube with substitutional impurity atoms - A first-principles investigation. <i>Materials Today: Proceedings</i> , 2018, 5, 14405-14415.	0.9	0
13687	Structure of fluorographene and its polymorphous varieties. <i>Journal of Physics: Conference Series</i> , 2018, 1124, 022010.	0.3	10
13688	Intramolecular P–H–Si Dihydrogen Bonding in the 5-Dimethylsilyl-9,9-dimethylxanthen-4-yl-diphenylphosphonium Cation. <i>Organometallics</i> , 2018, 37, 4287-4296.	1.1	4
13689	Ground-state crystal structures of superconducting Nb <sub>3</sub> Al and the phase transformation under high pressures. <i>Journal of Applied Physics</i> , 2018, 124, 173902.	1.1	7
13690	Thermodynamic investigations of the uranium-molybdenum-oxygen system by a coupling of density functional theory and CALPHAD methodologies. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2018, 63, 196-211.	0.7	5
13691	Ferromagnetism of 1T–MoS <sub>2</sub> Nanoribbons Stabilized by Edge Reconstruction and Its Periodic Variation on Nanoribbons Width. <i>Journal of the American Chemical Society</i> , 2018, 140, 16206-16212.	6.6	39
13692	Computer Simulation of Cathode Materials for Lithium Ion and Lithium Batteries: A Review. <i>Energy and Environmental Materials</i> , 2018, 1, 148-173.	7.3	56
13693	Two-Dimensional, Ordered, Double Transition Metal Carbides (MXenes): A New Family of Promising Catalysts for the Hydrogen Evolution Reaction. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28113-28122.	1.5	104
13694	Synthesis and Computational Study of Semicroconaines and Nonsymmetric Croconaines. <i>Journal of Organic Chemistry</i> , 2018, 83, 14396-14405.	1.7	11
13695	Cat's-cradle-like Dirac semimetals in layer groups with multiple screw axes: Application to two-dimensional borophene and borophane. <i>Physical Review B</i> , 2018, 98, .	1.1	18
13696	Superior Compatibility of C <sub>2</sub> N with Human Red Blood Cell Membranes and the Underlying Mechanism. <i>Small</i> , 2018, 14, e1803509.	5.2	33
13697	Breaking H <sub>2</sub> with CeO <sub>2</sub> : Effect of Surface Termination. <i>ACS Omega</i> , 2018, 3, 16063-16073.	1.6	47
13698	First-principles investigation on the interlayer doping of SnSe <sub>2</sub> bilayer. <i>Journal of Nanoparticle Research</i> , 2018, 20, 1.	0.8	8
13699	Theoretical Study on PdCu/CeO <sub>2</sub> -Catalyzed Water–Gas Shift Reaction: Crucial Role of the Metal/Ceria Interface and O <sub>2</sub> Enhancement Effects. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28868-28883.	1.5	12

#	ARTICLE	IF	CITATIONS
13700	Catalytic de-halogenation of alkyl halides by copper surfaces. <i>Journal of Environmental Chemical Engineering</i> , 2018, 6, 7214-7224.	3.3	5
13701	Density functional benchmark studies on structure and energetics of 3d transition metal mononitrides. <i>Journal of Chemical Sciences</i> , 2018, 130, 1.	0.7	6
13702	Enabling Electrocatalytic N <sub>2</sub> Reduction to NH <sub>3</sub> by Y <sub>2</sub> O <sub>3</sub> Nanosheet under Ambient Conditions. <i>Industrial &amp; Engineering Chemistry Research</i> , 2018, 57, 16622-16627.	1.8	39
13703	Oxygen vacancy induced photoconductivity enhancement in Bi <sub>1-x</sub> CaxFeO <sub>3-δ</sub> nanoparticle ceramics: A combined experimental and theoretical study. <i>Journal of Applied Physics</i> , 2018, 124, 195108.	1.1	12
13704	GGA-1/2 self-energy correction for accurate band structure calculations: the case of resistive switching oxides. <i>Journal of Physics Communications</i> , 2018, 2, 105005.	0.5	70
13705	Applicability of the Strongly Constrained and Appropriately Normed Density Functional to Transition-Metal Magnetism. <i>Physical Review Letters</i> , 2018, 121, 207201.	2.9	118
13706	Dynamically self-activated catalyst for direct synthesis of hydrogen peroxide (H <sub>2</sub> O <sub>2</sub> ). <i>Materials Today Energy</i> , 2018, 10, 307-316.	2.5	7
13707	Assessing the performance of the recent meta-GGA density functionals for describing the lattice constants, bulk moduli, and cohesive energies of alkali, alkaline-earth, and transition metals. <i>Journal of Chemical Physics</i> , 2018, 149, 164703.	1.2	35
13708	Six-dimensional quantum dynamics for the dissociative chemisorption of HCl on rigid Ag(111) on three potential energy surfaces with different density functionals. <i>Journal of Chemical Physics</i> , 2018, 149, 174702.	1.2	7
13709	Halogenated Meroditerpenoids from a South Pacific Collection of the Red Alga <i>Callophycus serratus</i> . <i>Journal of Natural Products</i> , 2018, 81, 2446-2454.	1.5	16
13710	Structure and electronic properties of 5-7 graphene. <i>IOP Conference Series: Materials Science and Engineering</i> , 0, 447, 012005.	0.3	5
13712	Unified theory of direct or indirect band-gap nature of conventional semiconductors. <i>Physical Review B</i> , 2018, 98, .	1.1	60
13713	Electronic and optical properties of bilayer SnS with different stacking orders: A first principles study. <i>Journal of Applied Physics</i> , 2018, 124, .	1.1	7
13714	Stability and magnetic properties of Fe double layers on Ir (111). <i>Physical Review B</i> , 2018, 98, .	1.1	3
13715	Extrinsic doping on the atomic scale: Tuning metallicity in atomic Au chains. <i>Physical Review B</i> , 2018, 98, .	1.1	17
13716	<i>Ab initio</i> investigation of magnetic anisotropy in intermediate spin iron(III) complexes. <i>Journal of Chemical Physics</i> , 2018, 149, 234302.	1.2	10
13717	Spin-filter state of Au-Co nanowires. <i>EPJ Web of Conferences</i> , 2018, 185, 01019.	0.1	1
13718	Machine Learning a General-Purpose Interatomic Potential for Silicon. <i>Physical Review X</i> , 2018, 8, .	2.8	222

#	ARTICLE	IF	CITATIONS
13719	Efficient evaluation of electron correlation along the bond-dissociation coordinate in the ground and excited ionic states with dynamic correlation suppression and enhancement functions of the on-top pair density. <i>Physical Review A</i> , 2018, 98, .	1.0	19
13720	Silicon Oxycarbide-Derived Carbon as Potential NO <sub>2</sub> Gas Sensor: A First Principles <sup>â</sup> ™ Study. <i>IEEE Electron Device Letters</i> , 2018, 39, 1760-1763.	2.2	37
13721	Embedded-atom potential for Ni-Al alloy. <i>IOP Conference Series: Materials Science and Engineering</i> , 2018, 452, 022025.	0.3	0
13722	Ab Initio Prediction of Proton Exchange Barriers for Alkanes at Brønsted Sites of Zeolite H-MFI. <i>Journal of the American Chemical Society</i> , 2018, 140, 18151-18161.	6.6	50
13723	Remarkable negative differential resistance and perfect spin-filtering effects of the indium triphosphide (InP <sub>3</sub> ) monolayer tuned by electric and optical ways. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 29440-29445.	1.3	13
13724	Probing the M <sup>+</sup> C <sub>2</sub> NHC Bond and Its Effect on the Synthesis, Structure, and Reactivity of R <sub>2</sub> MOR(NHC) (M = Al, Ga, In) Complexes. <i>Organometallics</i> , 2018, 37, 4585-4598.	1.1	10
13725	Bandgap Tunability in a One-Dimensional System. <i>Condensed Matter</i> , 2018, 3, 34.	0.8	0
13726	An Efficient Way To Suppress the Competition between Adsorption of H <sub>2</sub> and Desorption of <i>para</i> -hydrogen of H <sub>2</sub> â€“Nb Complex from Graphene Sheet: A Promising Approach to H <sub>2</sub> Storage. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28506-28517.	1.5	45
13727	Inelastic Scattering of N <sub>2</sub> off W(001): Reconciling Experiment and Theory at Low Collision Energies. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28856-28861.	1.5	6
13728	Infrared spectra of the 1,1-dimethylallyl and 1,2-dimethylallyl radicals isolated in solid <i>para</i> -hydrogen. <i>Journal of Chemical Physics</i> , 2018, 149, 204304.	1.2	8
13729	Competing adsorption mechanisms of pyridine on Cu, Ag, Au, and Pt(110) surfaces. <i>Journal of Chemical Physics</i> , 2018, 149, 214703.	1.2	9
13730	Anharmonicity-induced first-order isostructural phase transition of zirconium under pressure. <i>Physical Review B</i> , 2018, 98, .	1.1	15
13731	Formation and structural growth of two dimensional layer of hafnene on Ir(1 <sup>11</sup> ) surface. <i>Chemical Physics Letters</i> , 2018, 712, 60-65.	1.2	3
13732	First-principles study of plutonium and cerium solubility in Gd <sub>2</sub> Sn <sub>2</sub> O <sub>7</sub> pyrochlore. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2018, 436, 211-216.	0.6	4
13733	Reversible Mechanochromic Delayed Fluorescence in 2D Metalâ€“Organic Micro/Nanosheets: Switching Singletâ€“Triplet States through Transformation between Exciplex and Excimer. <i>Advanced Science</i> , 2018, 5, 1801187.	5.6	61
13734	Transition metal-metal oxide hybrids as versatile materials for hydrogen storage. <i>Chinese Journal of Physics</i> , 2018, 56, 1917-1924.	2.0	9
13735	Efficient lattice constants and energy bandgaps for condensed systems from a meta-GGA level screened range-separated hybrid functional. <i>Journal of Chemical Physics</i> , 2018, 149, 094105.	1.2	14
13736	Odd aromatic Si <sub>4</sub> ring stabilized by V <sub>2</sub> V bond passing through it: May <sup>+</sup> bonding form without <sup>+</sup> bonding as precondition?. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25788.	1.0	1

#	ARTICLE	IF	CITATIONS
13737	Modification of $\pi$ - $\pi$ Interaction and Charge Transfer in Ratiometric Cocrystals: Amplified Spontaneous Emission and Near-Infrared Luminescence. <i>Crystal Growth and Design</i> , 2018, 18, 6470-6476.	1.4	43
13738	Active basal plane in ZT-phased MX <sub>2</sub> (M = Mo, W; X = S, Se, Te) catalysts for the hydrogen evolution reaction: A theoretical study. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 19432-19437.	3.8	15
13739	Novel Phase of AlN <sub>4</sub> as a Possible Superhard Material. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22660-22666.	1.5	17
13740	Mechanical and electromechanical properties of functionalized hexagonal boron nitride nanosheet: A density functional theory study. <i>Journal of Chemical Physics</i> , 2018, 149, 114701.	1.2	23
13741	Borderline Magnetism: How Adding $Mg$ to Paramagnetic $CeMn_3Co$ Makes a 450-K Ferromagnet with Large Magnetic Anisotropy. <i>Physical Review Applied</i> , 2018, 10, .	1.5	14
13742	Ab Initio Molecular Dynamics Simulations of Ionic Liquids. <i>Annual Reports in Computational Chemistry</i> , 2018, , 95-122.	0.9	8
13743	Strongly Enhanced Thermoelectric Performance over a Wide Temperature Range in Topological Insulator Thin Films. <i>ACS Applied Energy Materials</i> , 0, , .	2.5	4
13744	Framework of Cytochrome/Vitamin B <sub>2</sub> Linker/Graphene for Robust Microbial Electricity Generation. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 35090-35098.	4.0	22
13745	Novel bismuthene nanotubes to detect NH <sub>3</sub> , NO <sub>2</sub> and PH <sub>3</sub> gas molecules – A first-principles insight. <i>Chemical Physics Letters</i> , 2018, 712, 102-111.	1.2	41
13746	Geometry Optimizations in a Subsystem Density Functional Theory Formalism: A Benchmark Study. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5631-5644.	2.3	9
13747	InSe Monolayer: Promising Cocatalyst of $g\text{-C}_3\text{N}_4$ for Water Splitting under Visible Light. <i>ACS Applied Energy Materials</i> , 0, , .	2.5	8
13748	Structure and Vibrational Properties of Potassium-Promoted Tungsten Oxide Catalyst Monomeric Sites Supported on Alumina (K <sub>2</sub> O/WO <sub>3</sub> /Al <sub>2</sub> O <sub>3</sub> ) Characterized Using Periodic Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2018, 122, 24190-24201.	1.5	11
13749	Metal-Free Single Atom Catalyst for N <sub>2</sub> Fixation Driven by Visible Light. <i>Journal of the American Chemical Society</i> , 2018, 140, 14161-14168.	6.6	742
13750	Spectral Calculations with DFT. , 0, , .		5
13751	SnO <sub>2</sub> quantum dots @ 3D sulfur-doped reduced graphene oxides as active and durable anode for lithium ion batteries. <i>Electrochimica Acta</i> , 2018, 291, 24-30.	2.6	37
13752	Transition metal modification and carbon vacancy promoted Cr <sub>2</sub> CO <sub>2</sub> (MXenes): a new opportunity for a highly active catalyst for the hydrogen evolution reaction. <i>Journal of Materials Chemistry A</i> , 2018, 6, 20956-20965.	5.2	74
13753	Computation-Aided Design of Single-Atom Catalysts for One-Pot CO <sub>2</sub> Capture, Activation, and Conversion. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 36866-36872.	4.0	70
13754	Hidden order in URu <sub>2</sub> Si <sub>2</sub> : Symmetry-induced antitoroidal vortices. <i>Physical Review B</i> , 2018, 98, .	1.1	1

#	ARTICLE	IF	CITATIONS
13755	Recent Developments in Density Functional Approximations. , 2018, , 1-14.		2
13756	Adsorption of CO <sub>2</sub> on Heterostructures of Bi <sub>2</sub> O <sub>3</sub> Nanocluster-Modified TiO <sub>2</sub> and the Role of Reduction in Promoting CO <sub>2</sub> Activation. ACS Omega, 2018, 3, 13117-13128.	1.6	20
13757	High-energy-density dual-ion battery for stationary storage of electricity using concentrated potassium fluorosulfonylimide. Nature Communications, 2018, 9, 4469.	5.8	213
13758	Davydov-type excitonic effects on the absorption spectra of parallel-stacked and herringbone aggregates of pentacene: Time-dependent density-functional theory and time-dependent density-functional tight binding. Journal of Chemical Physics, 2018, 149, 134111.	1.2	17
13759	Moiré Valleytronics: Realizing Dense Arrays of Topological Helical Channels. Physical Review Letters, 2018, 121, 186403.	2.9	19
13760	Numerical investigation for lithium isotope effect in ionic superconductor. Fusion Engineering and Design, 2018, 136, 205-209.	1.0	8
13761	First-Principles Study on the Stabilities, Electronic and Optical Properties of GexSn1-xSe Alloys. Nanomaterials, 2018, 8, 876.	1.9	1
13762	Mechanical and Thermal Conductivity Properties of Enhanced Phases in Mg-Zn-Zr System from First Principles. Materials, 2018, 11, 2010.	1.3	8
13763	Wet Chemical Modification of H-Terminated Si Surfaces as a First Step in Atomic Layer Deposition. , 2018, , 886-900.		0
13764	Theoretical Study of Moisture-Pretreated Lithium as Potential Material for Natural Gas Upgrading. Industrial & Engineering Chemistry Research, 2018, , .	1.8	3
13765	Adsorption and removal of phenoxy acetic herbicides from water by using commercial activated carbons: experimental and computational studies. Journal of Contaminant Hydrology, 2018, 218, 84-93.	1.6	39
13766	Vibrational Spectroscopy of Sodalite: Theory and Experiments. Journal of Physical Chemistry C, 2018, 122, 24765-24779.	1.5	26
13767	Simultaneous Control over Lattice Doping and Nanocluster Modification of a Hybrid CuO <sub>x</sub> /TiO <sub>2</sub> Photocatalyst during Flame Synthesis for Enhancing Hydrogen Evolution. Solar Rrl, 2018, 2, 1800215.	3.1	17
13768	Chemical shift reference scale for Li solid state NMR derived by first-principles DFT calculations. Journal of Magnetic Resonance, 2018, 297, 33-41.	1.2	14
13769	Mesoscale modeling of irradiation damage evolution in bcc iron and vanadium: A comparative study. Fusion Engineering and Design, 2018, 137, 303-311.	1.0	8
13770	Grain-Boundary Shear-Migration Coupling in Al Bicrystals. Atomistic Modeling. Physics of the Solid State, 2018, 60, 1916-1923.	0.2	5
13771	CHD3 dissociation on Pt(111): A comparison of the reaction dynamics based on the PBE functional and on a specific reaction parameter functional. Journal of Chemical Physics, 2018, 149, 044701.	1.2	16
13772	Additional Insights between Fermi Level in Orbital SIC and the Localization Equation Constraints in SIC-DFT. Journal of Physical Chemistry Letters, 2018, 9, 6456-6462.	2.1	13

#	ARTICLE	IF	CITATIONS
13773	Paths to Stabilizing Electronically Aberrant Compounds: A Defect-Stabilized Polymorph and Constrained Atomic Motion in PtGa <sub>2</sub> . <i>Inorganic Chemistry</i> , 2018, 57, 13880-13894.	1.9	7
13774	A Density Functional Theory Study on the Diffusion of Fission Gas Atoms in Uranium Dioxide. <i>Journal of Nuclear Engineering and Radiation Science</i> , 2018, 4, .	0.2	1
13775	Theoretical Descriptors of Electrdes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9371-9391.	1.1	63
13776	How One-Dimensional Are Atomic Gold Chains on a Substrate?. <i>Journal of Physical Chemistry C</i> , 2018, 122, 25580-25588.	1.5	22
13777	Temperature-Sensitive Structure Evolution of Lithium-Manganese-Rich Layered Oxides for Lithium-Ion Batteries. <i>Journal of the American Chemical Society</i> , 2018, 140, 15279-15289.	6.6	163
13778	A rhombohedral ferroelectric phase in epitaxially strained Hf <sub>0.5</sub> Zr <sub>0.5</sub> O <sub>2</sub> thin films. <i>Nature Materials</i> , 2018, 17, 1095-1100.	13.3	324
13779	DFT simulation on hydrogen storage property over Sc decorated B38 fullerene. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 19540-19546.	3.8	33
13780	Single atom alloy catalyst for SO <sub>3</sub> decomposition: enhancement of platinum catalyst's performance by Ag atom embedding. <i>Nanoscale</i> , 2018, 10, 20599-20610.	2.8	24
13781	A first-principles study of pristine and Al-doped activated carbon interacting with 5-Fluorouracil anticancer drug. <i>European Physical Journal E</i> , 2018, 41, 107.	0.7	10
13782	Realizing Shallow Acceptor Levels in Delafossite CuAlO <sub>2</sub> () Surfaces by Chalcogen Doping. <i>Physica Status Solidi - Rapid Research Letters</i> , 2018, 12, 1800381.	1.2	2
13783	Two-Dimensional MoxW1-xS2 Graded Alloys: Growth and Optical Properties. <i>Scientific Reports</i> , 2018, 8, 12889.	1.6	24
13784	Removal Process of Structural Oxygen from Tetrahedrons in Muscovite during Acid Leaching of Vanadium-Bearing Shale. <i>Minerals (Basel, Switzerland)</i> , 2018, 8, 208.	0.8	19
13785	Effects of Li on hydrogen absorption properties of Mg <sub>17</sub> Al <sub>12</sub> (110) surface: A density functional theory study. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 18330-18338.	3.8	7
13786	Alternative forms and transferability of electron-proton correlation functionals in nuclear-electronic orbital density functional theory. <i>Journal of Chemical Physics</i> , 2018, 149, 044110.	1.2	28
13787	First-principles study of the nanotubes from the TiO <sub>2</sub> hexagonal sheet. <i>Journal of Materials Science</i> , 2018, 53, 15530-15540.	1.7	4
13788	Accurate Description of Low-Lying Excited States in a Series of Photoreactive Clusters [Os <sub>3</sub> (CO) <sub>10</sub> ( $\pm$ -diimine)] by DFT Calculations. <i>Inorganic Chemistry</i> , 2018, 57, 11704-11716.	1.9	3
13789	Activating Aromatic Rings as Na-Ion Storage Sites to Achieve High Capacity. <i>CheM</i> , 2018, 4, 2463-2478.	5.8	82
13790	Suppressing heating rate-dependent martensitic stabilization in ductile Cu-Al-Mn shape memory alloys by Ni addition: An experimental and first-principles study. <i>Materials Characterization</i> , 2018, 145, 381-388.	1.9	9



#	ARTICLE	IF	CITATIONS
13791	Structures and Superconducting Properties of Ultra-Hydrogen-Rich Selenium Hydride H <sub>6</sub> Se. <i>Physica Status Solidi (B): Basic Research</i> , 2018, 255, 1800224.	0.7	3
13792	Boosted Electrocatalytic N <sub>2</sub> Reduction to NH <sub>3</sub> by Defect-Rich MoS <sub>2</sub> Nanoflower. <i>Advanced Energy Materials</i> , 2018, 8, 1801357.	10.2	482
13793	SAMPL6 host-guest challenge: binding free energies via a multistep approach. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 1097-1115.	1.3	16
13794	Accurate lattice geometrical parameters and bulk moduli from a semilocal density functional. <i>AIP Advances</i> , 2018, 8, .	0.6	15
13795	Efficient design principle for interfacial charge separation in hydrogen-intercalated nonstoichiometric oxides. <i>Nano Energy</i> , 2018, 53, 887-897.	8.2	27
13796	Strain-Enhanced Li Storage and Diffusion on the Graphyne as the Anode Material in the Li-Ion Battery. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22838-22848.	1.5	58
13797	First principle investigation of electronic transport properties of the edge shaped graphene-porphine molecular junction device. <i>AIP Advances</i> , 2018, 8, .	0.6	5
13798	Activity and Selectivity Control in CO <sub>2</sub> Electroreduction to Multicarbon Products over CuO Catalysts via Electrolyte Design. <i>ACS Catalysis</i> , 2018, 8, 10012-10020.	5.5	173
13799	Investigation of electronic structure and optical properties of thallium lead halides: First principle calculations. <i>Journal of Applied Physics</i> , 2018, 124, 093102.	1.1	1
13800	Dry Reforming of Methane on Single-Site Ni/MgO Catalysts: Importance of Site Confinement. <i>ACS Catalysis</i> , 2018, 8, 9821-9835.	5.5	156
13801	Towards rational design of metal-organic framework-based drug delivery systems. <i>Russian Chemical Reviews</i> , 2018, 87, 831-858.	2.5	26
13802	Assessing the SCAN functional for itinerant electron ferromagnets. <i>Physical Review B</i> , 2018, 98, .	1.1	64
13803	Do Semilocal Density-Functional Approximations Recover Dispersion Energies at Small Intermonomer Separations?. <i>Physical Review Letters</i> , 2018, 121, 113402.	2.9	33
13804	Engineering of the resistive switching properties in V <sub>2</sub> O <sub>5</sub> thin film by atomic structural transition: Experiment and theory. <i>Journal of Applied Physics</i> , 2018, 124, .	1.1	3
13805	Assessing Density-Functional Theory for Equation-Of-State. <i>Computation</i> , 2018, 6, 13.	1.0	16
13806	Proposed mechanism of twin formation during hexagonal-close-packed structure to face-centered-cubic phase transition. <i>Solid State Communications</i> , 2018, 284-286, 40-44.	0.9	8
13807	Rapidly probing the interaction between sulfamethazine antibiotics and fulvic acids. <i>Environmental Pollution</i> , 2018, 243, 752-757.	3.7	21
13809	Molecularly thin two-dimensional hybrid perovskites with tunable optoelectronic properties due to reversible surface relaxation. <i>Nature Materials</i> , 2018, 17, 908-914.	13.3	295



#	ARTICLE	IF	CITATIONS
13810	Frequency-dependent polarizabilities of diatomic molecules: Density functional theory and ab initio methods compared with quantum-defect Green function technique. <i>Chemical Physics Letters</i> , 2018, 711, 42-47.	1.2	5
13811	Intermetallic Growth and Interfacial Properties of the Grain Refiners in Al Alloys. <i>Materials</i> , 2018, 11, 636.	1.3	14
13812	In-situ investigation of pressure effect on structural evolution and conductivity of Na <sub>3</sub> SbS <sub>4</sub> superionic conductor. <i>Journal of Power Sources</i> , 2018, 401, 111-116.	4.0	26
13813	Development of a semi-empirical potential for simulation of Ni solute segregation into grain boundaries in Ag. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2018, 26, 075004.	0.8	25
13814	Mixed-valence Compounds: AuO <sub>2</sub> and AuS. <i>ChemPhysChem</i> , 2018, 19, 2989-2994.	1.0	7
13815	Alkyl-Modified Gold Surfaces: Characterization of the Au-C Bond. <i>Langmuir</i> , 2018, 34, 11264-11271.	1.6	26
13816	Surface Adsorption Affects the Performance of Alkaline Anion-Exchange Membrane Fuel Cells. <i>ACS Catalysis</i> , 2018, 8, 9429-9439.	5.5	55
13817	A tungsten-rhenium interatomic potential for point defect studies. <i>Journal of Applied Physics</i> , 2018, 123, .	1.1	22
13818	First-principles calculations of nitrogen-doped antimony triselenide: A prospective material for solar cells and infrared optoelectronic devices. <i>Frontiers of Physics</i> , 2018, 13, 1.	2.4	9
13819	Segregation induced order-disorder transition in Cu(Au) surface alloys. <i>Acta Materialia</i> , 2018, 154, 220-227.	3.8	11
13820	Identification of the Nearby Hydroxyls' Role in Promoting HCHO Oxidation over a Pt Catalyst. <i>Industrial &amp; Engineering Chemistry Research</i> , 2018, 57, 8183-8189.	1.8	20
13821	Synthetic and Postsynthetic Chemistry of M <sub>4</sub> Au <sub>x</sub> Ag <sub>44</sub> -(MBA) <sub>30</sub> Alloy Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2018, 122, 13166-13174.	1.5	22
13822	Characterization and Modeling of Deformation Mechanisms in Ni-Base Superalloy 718. <i>Minerals, Metals and Materials Series</i> , 2018, , 319-338.	0.3	3
13823	Exploring the Limitation of Molecular Water Oxidation Catalysts. <i>Journal of Physical Chemistry C</i> , 2018, 122, 12404-12412.	1.5	37
13824	Tuning electronic and magnetic properties of Mn-mullite oxide sub-nanoclusters <i>via</i> MnO <sub>n</sub> polyhedron units. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 16151-16158.	1.3	4
13825	Probing the structural, electronic and magnetic properties of Ag <sub>n</sub> Sc (n = 1-16) clusters. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 15824-15834.	1.3	20
13826	Crystal-defect-induced facet-dependent electrocatalytic activity of 3D gold nanoflowers for the selective nanomolar detection of ascorbic acid. <i>Nanoscale</i> , 2018, 10, 11091-11102.	2.8	17
13827	Two dimensional self-assembly zinc porphyrin and zinc phthalocyanine heterojunctions with record high power conversion efficiencies. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 25LT02.	0.7	3

#	ARTICLE	IF	CITATIONS
13828	First principle calculations with SIC correction of Fe-doped CuO compound. Computational Condensed Matter, 2018, 16, e00304.	0.9	14
13829	Influences of vacancies on the structural, electronic and optical properties of monoclinic BiVO <sub>4</sub> . Journal of Physics and Chemistry of Solids, 2018, 121, 85-92.	1.9	19
13830	High-pressure-assisted X-ray-induced damage as a new route for chemical and structural synthesis. Physical Chemistry Chemical Physics, 2018, 20, 18949-18956.	1.3	14
13831	New strategy for designing promising mid-infrared nonlinear optical materials: narrowing the band gap for large nonlinear optical efficiencies and reducing the thermal effect for a high laser-induced damage threshold. Chemical Science, 2018, 9, 5700-5708.	3.7	104
13832	Stable dye-encapsulated indium-organic framework as dual-emitting sensor for the detection of Hg <sup>2+</sup> /Cr <sup>2+</sup> /O <sup>2-</sup> and a wide range of nitro-compounds. Journal of Materials Chemistry C, 2018, 6, 6440-6448.	2.7	126
13833	A systematic evaluation of the role of lanthanide elements in functional complex oxides; implications for energy conversion devices. Journal of Materials Chemistry A, 2018, 6, 11819-11829.	5.2	21
13834	Structural, elastic, electronic, phonon, dielectric and optical properties of Bi <sub>3</sub> TeBO <sub>9</sub> from first-principles calculations. Journal of Physics and Chemistry of Solids, 2018, 121, 139-144.	1.9	17
13835	Interfacial Properties of Monolayer SnS-Metal Contacts. Journal of Physical Chemistry C, 2018, 122, 12322-12331.	1.5	15
13836	Structural details of Al <sub>2</sub> O <sub>3</sub> /SiO <sub>2</sub> junctions and their role in the formation of electron tunnel barriers. Physical Review B, 2018, 97, .		
13837	Barium in High Oxidation States in Pressure-Stabilized Barium Fluorides. Journal of Physical Chemistry C, 2018, 122, 12448-12453.	1.5	22
13838	Catalytic Transformations of 1-Butene over Palladium. A Combined Experimental and Theoretical Study. ACS Catalysis, 2018, 8, 5675-5685.	5.5	14
13839	Atomic and Molecular Adsorption on Cu(111). Topics in Catalysis, 2018, 61, 736-750.	1.3	45
13840	Tuning the electronic property of two dimensional SiSe monolayer by in-plane strain. Chemical Physics Letters, 2018, 705, 12-18.	1.2	13
13841	Influence of surface relaxation on solute atoms positioning within atom probe tomography reconstructions. Materials Characterization, 2018, 146, 324-335.	1.9	21
13842	Chemical Bond Energies of 3d Transition Metals Studied by Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 3479-3492.	2.3	64
13843	Interaction energy profile for diphenyl diselenide in complex with Î-aminolevulinic acid dehydratase enzyme using quantum calculations and a molecular fragmentation method. Computational Toxicology, 2018, 7, 9-19.	1.8	5
13844	Structural Diversity in a New Series of Halogenated Quinoly Salicylaldimides-Based Fe <sup>III</sup> Complexes Showing Solid-State Halogen-Bonding/Halogen-Halogen Interactions. Crystal Growth and Design, 2018, 18, 4187-4199.	1.4	10
13845	Distinguishing between Charge-Transfer Mechanisms at Organic/Inorganic Interfaces Employing Hybrid Functionals. Journal of Physical Chemistry C, 2018, 122, 14640-14653.	1.5	12

#	ARTICLE	IF	CITATIONS
13846	High photoluminescence quantum yield of 18.7% by using nitrogen-doped Ti <sub>3</sub> C <sub>2</sub> MXene quantum dots. Journal of Materials Chemistry C, 2018, 6, 6360-6369.	2.7	159
13847	Universal link of magnetic exchange and structural behavior under pressure in chromium spinels. Physical Review B, 2018, 97, .	1.1	24
13848	Au <sub>147</sub> nanoparticles: Ordered or amorphous?. Journal of Chemical Physics, 2018, 148, 204308.	1.2	22
13849	The effect of vacancies on the optical properties and plasmonic states of zinc oxide: A first-principle study. Materials Research Express, 2018, 5, 066303.	0.8	8
13850	Species formed during NO adsorption and NO <sup>-</sup> + <sup>-</sup> O <sub>2</sub> co-adsorption on ceria: A combined FTIR and DFT study. Molecular Catalysis, 2018, 451, 114-124.	1.0	30
13852	Effect of tensile strain on the band structure and carrier transport of germanium monosulphide monolayer: a first-principles study. Micro and Nano Letters, 2018, 13, 600-605.	0.6	14
13853	A DFT study of pure and lithium doped gold clusters. AIP Conference Proceedings, 2018, , .	0.3	0
13854	Benchmarking DFT methods on linear and nonlinear electric properties of spatially confined molecules. International Journal of Quantum Chemistry, 2018, 118, e25666.	1.0	14
13855	Mechanistic Insights into Iridium Catalyzed Disproportionation of Formic Acid to CO <sub>2</sub> and Methanol: A DFT Study. Organometallics, 2018, 37, 1519-1525.	1.1	17
13856	Performance of exchange-correlation functionals in density functional theory calculations for liquid metal: A benchmark test for sodium. Journal of Chemical Physics, 2018, 148, 144501.	1.2	5
13857	A new molecular pathway allows the chemoselective reduction of nitroaromatics on non-noble metal catalysts. Journal of Catalysis, 2018, 364, 19-30.	3.1	57
13858	Strain tuned InSe/MoS <sub>2</sub> bilayer van der Waals heterostructures for photovoltaics or photocatalysis. Physical Chemistry Chemical Physics, 2018, 20, 17574-17582.	1.3	48
13859	First-principle study on the oxidative leaching mechanism of sphalerite in Ammoniacal solution. Hydrometallurgy, 2018, 179, 198-206.	1.8	7
13860	Electronic structure and fermiology of LaFe <sub>2</sub> Ge <sub>2</sub> . Solid State Communications, 2018, 281, 12-16.	0.9	1
13861	Unveiling the multifunctional roles of hitherto known capping ligand oleic acid as blue emitter and sensitizer in tuning the emission colour to white in red-emitting phosphors. Physical Chemistry Chemical Physics, 2018, 20, 19087-19097.	1.3	4
13862	Quasiparticle band structures of CuCl, CuBr, AgCl, and AgBr: The extreme case. Physical Review B, 2018, 98, .	1.1	30
13863	Geometric symmetry modulated spin polarization of electron transport in graphene-like zigzag FeB <sub>2</sub> nanoribbons. European Physical Journal B, 2018, 91, 1.	0.6	2
13864	Keto-enol tautomerism in micro-hydrated acetylacetone: an atoms-in-molecules study. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	6

#	ARTICLE	IF	CITATIONS
13865	Modeling Hydrocarbon Oxidation Mechanisms Catalyzed by Microporous Materials. , 2018, , 265-295.		0
13866	Interaction trends between single metal atoms and oxide supports identified with density functional theory and statistical learning. <i>Nature Catalysis</i> , 2018, 1, 531-539.	16.1	269
13867	Density functional theory calculations for magnetic properties of Co <sub>3</sub> W systems. <i>Journal of Chemical Physics</i> , 2018, 149, 014303.	1.2	2
13868	Mechanism of NO <sup>+</sup> CO reaction over highly dispersed cuprous oxide on $\gamma$ -alumina catalyst using a metal <sup>+</sup> support interfacial site in the presence of oxygen: similarities to and differences from biological systems. <i>Catalysis Science and Technology</i> , 2018, 8, 3833-3845.	2.1	16
13869	Gradient-level and nonlocal density functional descriptions of Cu-Au intermetallic compounds. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	5
13870	Implementation of Magnetic Dipole Interaction in the Planewave-Basis Approach for Slab Systems. <i>Journal of the Physical Society of Japan</i> , 2018, 87, 064803.	0.7	5
13871	EPAW-1.0 code for evolutionary optimization of PAW datasets especially for high-pressure applications. <i>Computer Physics Communications</i> , 2018, 233, 110-122.	3.0	2
13872	A comparative study of the dissolubility of pure and silicon substituted hydroxyapatite from density functional theory calculations. <i>Journal of Molecular Modeling</i> , 2018, 24, 168.	0.8	3
13873	Biohybridization of Supported Gold Nanoassemblies on Silicon. <i>Journal of Physical Chemistry C</i> , 2018, 122, 16113-16121.	1.5	4
13874	A heterogeneous single-atom palladium catalyst surpassing homogeneous systems for Suzuki coupling. <i>Nature Nanotechnology</i> , 2018, 13, 702-707.	15.6	471
13875	First principles calculation of boron diffusion in fcc-Fe. <i>Current Applied Physics</i> , 2018, 18, 1108-1112.	1.1	17
13876	Adsorption of Li <sub>2</sub> O <sub>2</sub> , Na <sub>2</sub> O <sub>2</sub> , and NaO <sub>2</sub> on TiC(111) Surface for Metal <sup>+</sup> Air Rechargeable Batteries: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 16473-16480.	1.5	12
13877	Effect of Step Density and Orientation on the Apparent pH Dependence of Hydrogen and Hydroxide Adsorption on Stepped Platinum Surfaces. <i>Journal of Physical Chemistry C</i> , 2018, 122, 16756-16764.	1.5	50
13878	Dynamics of N <sub>2</sub> sticking on W(100): the decisive role of van der Waals interactions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19326-19331.	1.3	10
13879	A Comparison of Pd <sub>0</sub> Nanoparticles and Pd <sup>2+</sup> Modified Bi <sub>2</sub> O <sub>2</sub> CO <sub>3</sub> for Visible Light-Driven Photocatalysis. <i>Journal of Nanomaterials</i> , 2018, 2018, 1-9.	1.5	14
13880	Strain Effect on the Superconductivity in Borophenes. <i>Journal of Physical Chemistry C</i> , 2018, 122, 16916-16924.	1.5	38
13881	Two-Dimensional-Layered Perovskite AlTa <sub>2</sub> O <sub>7</sub> :Bi <sup>3+</sup> (A = K and Na) Phosphors with Versatile Structures and Tunable Photoluminescence. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 24648-24655.	4.0	91
13882	Experimental and computational investigations of the photosensitive Schottky barrier diode property of an azobenzene based small organic molecule. <i>New Journal of Chemistry</i> , 2018, 42, 13430-13441.	1.4	8

#	ARTICLE	IF	CITATIONS
13883	Atomic diffusion in liquid nickel: First-principles modeling. <i>Journal of Chemical Physics</i> , 2018, 148, 244503.	1.2	10
13884	Crystal structure and elasticity of Al-bearing phase H under high pressure. <i>AIP Advances</i> , 2018, 8, .	0.6	2
13885	First-principles study on the electrical and thermal properties of the semiconducting Sc <sub>3</sub> (CN)F <sub>2</sub> MXene. <i>RSC Advances</i> , 2018, 8, 22452-22459.	1.7	24
13886	Defect physics in complex energy materials. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 293001.	0.7	29
13887	DFT modelling of ethanol on BaTiO <sub>3</sub> (0001) surface. <i>Applied Surface Science</i> , 2018, 456, 276-289.	3.1	18
13888	Nickel(II) based homo- vs heterometallic 1D coordination polymers derived from a novel 6-aminouracil building block: Structures, topologies, non-covalent interactions, magnetism, and antibacterial activity. <i>Inorganica Chimica Acta</i> , 2018, 482, 384-394.	1.2	10
13889	The reassessment of the structural transition regions along the liquidus of Fe-Si alloys and a possible liquid-liquid structural transition in FeSi <sub>2</sub> alloy. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2018, 382, 2655-2661.	0.9	8
13890	Frozen-density embedding as a quasi-diabatization tool: Charge-localized states for spin-density calculations. <i>Journal of Chemical Physics</i> , 2018, 148, 214104.	1.2	13
13891	Realization of N-Type Semiconducting of Phosphorene through Surface Metal Doping and Work Function Study. <i>Journal of Nanomaterials</i> , 2018, 2018, 1-9.	1.5	9
13892	Effect of Ag Doping on Electronic Structure of Cluster Compounds Ag <sub>x</sub> Mo <sub>9</sub> Se <sub>11</sub> ( <i>x</i> = 3.4, 3.9). <i>ACS Applied Energy Materials</i> , 2018, 1, 4032-4039.	2.5	8
13893	Edge States Caused by Shift of Dirac Points at the Armchair Edge of Distorted Nanographene. <i>Journal of the Physical Society of Japan</i> , 2018, 87, 084706.	0.7	2
13894	Surface terminations of hematite ( $\alpha$ -Fe <sub>2</sub> O <sub>3</sub> ) exposed to oxygen, hydrogen, or water: dependence on the density functional theory methodology. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 275002.	0.7	16
13895	Hydrogen bubble nucleation by self-clustering: density functional theory and statistical model studies using tungsten as a model system. <i>Nuclear Fusion</i> , 2018, 58, 096021.	1.6	34
13896	Nodal-chain network, intersecting nodal rings and triple points coexisting in nonsymmorphic Ba <sub>3</sub> Si <sub>4</sub> . <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21177-21183.	1.3	22
13897	Theoretical study of acetate decomposition on Au(111) surface: Oxygen-assisted $\hat{\nu}$ -CH activation mechanism. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 17048-17056.	3.8	2
13898	Structural Origin of the Midgap Electronic States and the Urbach Tail in Pnictogen-Chalcogenide Glasses. <i>Journal of Physical Chemistry B</i> , 2018, 122, 8082-8097.	1.2	6
13899	Hydrogen Spillover to Copper Clusters on Hydroxylated $\hat{\nu}$ -Al <sub>2</sub> O <sub>3</sub> . <i>Journal of Physical Chemistry C</i> , 2018, 122, 18445-18455.	1.5	44
13900	Electronic Structure of Two-Dimensional Lead(II) Iodide Perovskites: An Experimental and Theoretical Study. <i>Chemistry of Materials</i> , 2018, 30, 4959-4967.	3.2	29

#	ARTICLE	IF	CITATIONS
13901	Reverse-martensitic hcp-to-fcc transformation in technetium under shock compression. Journal of Applied Physics, 2018, 124, .	1.1	5
13902	A study of the hydrogen adsorption mechanism of W18O49 using first-principles calculations. Computational Materials Science, 2018, 154, 53-59.	1.4	15
13903	First principles study of the electronic properties and Schottky barrier in vertically stacked graphene on the Janus MoSeS under electric field. Computational Materials Science, 2018, 153, 438-444.	1.4	56
13904	Water dissociation on K <sub>2</sub> O-pre-adsorbed transition metals: a systematic theoretical study. Physical Chemistry Chemical Physics, 2018, 20, 19850-19859.	1.3	7
13905	First-principles studies on the interface between light-absorbing layer and Mo back electrode in Cu(In,Ga)Se <sub>2</sub> , Cu <sub>2</sub> ZnSn(S,Se) <sub>4</sub> , and Cu <sub>2</sub> SnS <sub>3</sub> solar cells. Japanese Journal of Applied Physics, 2018, 57, 08RC17.	0.8	7
13906	Structural, Electronic, Magnetic, and Optical Properties of Half-Heusler Alloys RuMnZ (Z = P, As): a First-Principle Study. Journal of Superconductivity and Novel Magnetism, 2018, 31, 233-239.	0.8	31
13907	Current progress and future challenges in rare-earth-free permanent magnets. Acta Materialia, 2018, 158, 118-137.	3.8	351
13908	Can Popular DFT Approximations and Truncated Coupled Cluster Theory Describe the Potential Energy Surface of the Beryllium Dimer?. Australian Journal of Chemistry, 2018, 71, 804.	0.5	6
13909	Phase Exploration and Identification of Multinary Transition-Metal Selenides as High-Efficiency Oxygen Evolution Electrocatalysts through Combinatorial Electrodeposition. ACS Catalysis, 2018, 8, 8273-8289.	5.5	76
13910	Improved LDA-1/2 method for band structure calculations in covalent semiconductors. Computational Materials Science, 2018, 153, 493-505.	1.4	63
13911	Insight into lithium-ion mobility in Li <sub>2</sub> La(TaTi)O <sub>7</sub> . Journal of Materials Chemistry A, 2018, 6, 22152-22160.	5.2	16
13912	Improving the catalytic activity for hydrogen evolution of monolayered SnSe <sub>2</sub> (1 $\bar{1}$ <sub>0</sub> ) <sub>x</sub> /i>S <sub>2</sub> <sub>x</sub> /i> by mechanical strain. Beilstein Journal of Nanotechnology, 2018, 9, 1820-1827.	1.5	14
13913	An experimental and theoretical study of the hydrogen resistance of Ti <sub>3</sub> SiC <sub>2</sub> and Ti <sub>3</sub> AlC <sub>2</sub> . Corrosion Science, 2018, 142, 295-304.	3.0	10
13914	How does the electric current propagate through fully-hydrogenated borophene?. Physical Chemistry Chemical Physics, 2018, 20, 21552-21556.	1.3	32
13915	Assessing the performance of the Tao-Mo semilocal density functional in the projector-augmented-wave method. Journal of Chemical Physics, 2018, 149, 044120.	1.2	50
13916	Bipolar Resistive Switching Characteristics of Thermally Evaporated V <sub>2</sub> O <sub>5</sub> Thin Films. IEEE Electron Device Letters, 2018, 39, 1290-1293.	2.2	4
13917	Nucleobases adsorption studies on silicane layer: A first-principles investigation. Journal of Molecular Graphics and Modelling, 2018, 85, 48-55.	1.3	16
13918	DFT Study on Intermetallic Pd-Cu Alloy with Cover Layer Pd as Efficient Catalyst for Oxygen Reduction Reaction. Materials, 2018, 11, 33.	1.3	24



#	ARTICLE	IF	CITATIONS
13919	Structural and Electronic Properties of Different Terminations for Quartz (001) Surfaces as Well as Water Molecule Adsorption on It: A First-Principles Study. <i>Minerals (Basel, Switzerland)</i> , 2018, 8, 58.	0.8	27
13920	Interfacial stability, electronic property, and surface reactivity of $\hat{1}\pm$ -MoO <sub>3</sub> / $\hat{1}^3$ -Al <sub>2</sub> O <sub>3</sub> composites: DFT and DFT+ $\hat{u}$ calculations. <i>Computational Materials Science</i> , 2018, 153, 217-227.	1.4	8
13921	The Electronic Structures of CoGe <sub><i>n</i></sub> ( <i>n</i> = 1–3) Clusters from Multiconfigurational CASSCF/CASPT2 and RASSCF/RASPT2 Calculations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6407-6415.	1.1	13
13922	CO <sub>2</sub> interaction with violarite (FeNi <sub>2</sub> S <sub>4</sub> ) surfaces: a dispersion-corrected DFT study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 20439-20446.	1.3	15
13923	Precipitation strengthening in Cu–Ni–Si alloys modeled with ab initio based interatomic potentials. <i>Journal of Chemical Physics</i> , 2018, 149, 024701.	1.2	5
13924	Effects of Scandium Addition on the Structural Stability and Ideal Strengths of Magnesium-Lithium Alloys. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2018, 73, 947-956.	0.7	1
13925	Multilayered Platinum Nanotube for Oxygen Reduction in a Fuel Cell Cathode: Origin of Activity and Product Selectivity. <i>ACS Applied Energy Materials</i> , 2018, 1, 3890-3899.	2.5	10
13926	How Does Palladium–Amino Acid Cooperative Catalysis Enable Regio- and Stereoselective C(sp <sup>3</sup> )–H Functionalization in Aldehydes and Ketones? A DFT Mechanistic Study. <i>ACS Catalysis</i> , 2018, 8, 7698-7709.	5.5	38
13927	Interaction between interstitial carbon atoms and a $\frac{1}{2}$ $\hat{c}$ self-interstitial atoms loop in an iron matrix: a combined DFT, off lattice KMC and MD study. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 335901.	0.7	2
13928	A model study on the photodecarbonyl reaction of ( $\hat{1}$ -5-C <sub>5</sub> H <sub>5</sub> )M(CO) <sub>2</sub> (M = Co, Rh, Ir). <i>RSC Advances</i> , 2018, 8, 24641-24653.	1.7	0
13929	Single Molybdenum Atom Anchored on N-Doped Carbon as a Promising Electrocatalyst for Nitrogen Reduction into Ammonia at Ambient Conditions. <i>Journal of Physical Chemistry C</i> , 2018, 122, 16842-16847.	1.5	223
13930	Insight into the enhanced photocatalytic activity of SrTiO <sub>3</sub> in the presence of a (Ni, V/Nb/Ta/Sb) pair. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 20078-20087.	1.3	23
13931	Resolving the excited state relaxation dynamics of guanosine monomers and hydrogen-bonded homodimers in chloroform solution. <i>Chemical Physics</i> , 2018, 515, 480-492.	0.9	2
13932	Theoretical and experimental investigation on ligands-CdS clusters interactions: Influence of solvent. <i>Journal of Molecular Structure</i> , 2018, 1173, 894-902.	1.8	5
13933	C <sub>2</sub> N-graphene supported single-atom catalysts for CO <sub>2</sub> electrochemical reduction reaction: mechanistic insight and catalyst screening. <i>Nanoscale</i> , 2018, 10, 15262-15272.	2.8	156
13934	Mechanistic insights into hydrodeoxygenation of phenol on bimetallic phosphide catalysts. <i>Catalysis Science and Technology</i> , 2018, 8, 4083-4096.	2.1	31
13935	Cobalt-iron (oxides) water oxidation catalysts: Tracking catalyst redox states and reaction dynamic mechanism. <i>Journal of Catalysis</i> , 2018, 365, 227-237.	3.1	28
13936	Three-dimensional phase field simulation of intragranular void formation and thermal conductivity in irradiated $\hat{1}\pm$ -Fe. <i>Journal of Materials Science</i> , 2018, 53, 11002-11014.	1.7	15



#	ARTICLE	IF	CITATIONS
13937	Theoretical study of ZrCoH <sub>3</sub> and the anti-disproportionation ability of alloying elements. International Journal of Hydrogen Energy, 2018, 43, 10410-10419.	3.8	25
13938	First-principles calculations on interface structure and fracture characteristic of TiC/TiZrC nano-multilayer film based on virtual crystal approximation. Journal of Alloys and Compounds, 2018, 755, 211-223.	2.8	32
13939	CH <sub>3</sub> Cl/Cu(410): Interaction and Adsorption Geometry. Journal of Physical Chemistry C, 2018, 122, 11825-11831.	1.5	8
13940	Structure of Copper-Cobalt Surface Alloys in Equilibrium with Carbon Monoxide Gas. Journal of the American Chemical Society, 2018, 140, 6575-6581.	6.6	23
13941	Insight into the role of the promoters Pt, Ru and B in inhibiting the deactivation of Co catalysts in Fischer-Tropsch synthesis. Applied Surface Science, 2018, 453, 309-319.	3.1	16
13942	The structure and elasticity of phase B silicates under high pressure by first principles simulation. Chinese Physics B, 2018, 27, 047402.	0.7	2
13943	Structural, phase transition, mechanical and thermodynamic properties of TMNs under external pressures: A first-principles study. International Journal of Modern Physics B, 2018, 32, 1850181.	1.0	4
13944	Structural, Electronic, and Optical Properties of Cubic Y <sub>2</sub> O <sub>3</sub> : First-Principles Calculations. Moscow University Physics Bulletin (English Translation of Vestnik Moskovskogo Universiteta, Fizika), 2018, 73, 95-100.	0.1	3
13945	First-principles simulation on thermoelectric properties of transition metal dichalcogenide monolayers. Japanese Journal of Applied Physics, 2018, 57, 06HE04.	0.8	4
13946	3D-Graphene/Boron Nitride-stacking Material: a Fundamental van der Waals Heterostructure. Chemical Research in Chinese Universities, 2018, 34, 434-439.	1.3	7
13947	Influence mechanism of supports on the reactivity of Ni-based oxygen carriers for chemical looping reforming: A DFT study. Fuel, 2018, 229, 88-94.	3.4	36
13948	Molecular dynamics simulation of the size-dependent morphological stability of cubic shape silver nanoparticles. Molecular Simulation, 2018, 44, 981-991.	0.9	26
13949	Study on the reaction mechanism between Pb <sub>3</sub> O <sub>4</sub> and Si in stored silicon delay composition. Journal of Thermal Analysis and Calorimetry, 2018, 132, 327-336.	2.0	7
13950	Double Kagome Bands in a Two-Dimensional Phosphorus Carbide P <sub>2</sub> C <sub>3</sub> . Journal of Physical Chemistry Letters, 2018, 9, 2751-2756.	2.1	29
13951	Exfoliation of a non-van der Waals material from iron ore hematite. Nature Nanotechnology, 2018, 13, 602-609.	15.6	295
13952	Molecular insights into avibactam mediated class C $\beta$ -lactamase inhibition: competition between reverse acylation and hydrolysis through desulfation. Physical Chemistry Chemical Physics, 2018, 20, 1111-1121.	1.3	8
13953	Density functional theory study of twin boundaries of Zn under high pressure. Journal of Physical Chemistry C, 2018, 122, 11825-11831.	1.4	5
13954	Deconstructing collagen piezoelectricity using alanine-hydroxyproline-glycine building blocks. Nanoscale, 2018, 10, 9653-9663.	2.8	36

#	ARTICLE	IF	CITATIONS
13955	DFT insight into the effect of potassium on the adsorption, activation and dissociation of CO <sub>2</sub> over Fe-based catalysts. Physical Chemistry Chemical Physics, 2018, 20, 14694-14707.	1.3	40
13956	Room-temperature ferromagnetism in carbon-doped Y <sub>2</sub> O <sub>3</sub> for	1.1	22
13957	Insight into destabilization mechanism of Mg-based hydrides interstitially co-doped with nonmetals: a DFT study. European Physical Journal B, 2018, 91, 1.	0.6	1
13958	Hydration of Atmospheric Molecular Clusters: A New Method for Systematic Configurational Sampling. Journal of Physical Chemistry A, 2018, 122, 5026-5036.	1.1	53
13959	Properties of BiMnO <sub>3</sub> and BiMn <sub>0.5</sub> Nb <sub>0.5</sub> O <sub>3</sub> from ab initio simulations. Materials Chemistry and Physics, 2018, 218, 160-165.	2.0	1
13960	Enhanced Photosensitive Schottky Diode Behavior of Pyrazine over 2-Aminopyrimidine Ligand in Copper(II)-Phthalate MOFs: Experimental and Theoretical Rationalization. ACS Omega, 2018, 3, 9160-9171.	1.6	26
13961	Thermodynamic modeling of the Mo-Ni system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 62, 215-222.	0.7	6
13962	Antimonene nanosheet device for detection of explosive vapors – A first-principles inspection. Chemical Physics Letters, 2018, 708, 130-137.	1.2	39
13963	Improving the activity of gold nanoparticles for the water-gas shift reaction using TiO <sub>2</sub> -Y <sub>2</sub> O <sub>3</sub> : an example of catalyst design. Physical Chemistry Chemical Physics, 2018, 20, 22076-22083.	1.3	8
13964	Benchmarking of GGA density functionals for modeling structures of nanoporous, rigid and flexible MOFs. Journal of Chemical Physics, 2018, 149, 064110.	1.2	23
13965	Molecular Orientations Change Reaction Kinetics and Mechanism: A Review on Catalytic Alcohol Oxidation in Gas Phase and Liquid Phase on Size-Controlled Pt Nanoparticles. Catalysts, 2018, 8, 226.	1.6	16
13966	Atomic engineering of high-density isolated Co atoms on graphene with proximal-atom controlled reaction selectivity. Nature Communications, 2018, 9, 3197.	5.8	146
13967	Interaction of Hydrogen with Graphitic Surfaces, Clean and Doped with Metal Clusters. , 2018, , 1-22.		0
13968	Single atom detachment from Cu clusters, and diffusion and trapping on CeO <sub>2</sub> (111): implications in Ostwald ripening and atomic redispersion. Nanoscale, 2018, 10, 17893-17901.	2.8	47
13969	Six-dimensional potential energy surfaces of the dissociative chemisorption of HCl on Ag(111) with three density functionals. Journal of Chemical Physics, 2018, 149, 054702.	1.2	15
13970	A DFT Study on the Adsorption of H <sub>2</sub> S and SO <sub>2</sub> on Ni Doped MoS <sub>2</sub> Monolayer. Nanomaterials, 2018, 8, 646.	1.9	120
13971	Terahertz spectroscopy and vibrational analysis of sulfur mustard by quantum chemical calculations. Computational and Theoretical Chemistry, 2018, 1142, 21-27.	1.1	1
13972	Activity Trends for Catalytic CO and NO Co-Oxidation at Low Temperature Diesel Emission Conditions. Industrial & Engineering Chemistry Research, 2018, 57, 12715-12725.	1.8	13

#	ARTICLE	IF	CITATIONS
13973	Long triple carbon chains formation by heat treatment of graphene nanoribbon: Molecular dynamics study with revised Brenner potential. Carbon, 2018, 140, 543-556.	5.4	13
13974	High Curie temperature and half-metallicity in an atomically thin main group-based boron phosphide system: long range ferromagnetism. Physical Chemistry Chemical Physics, 2018, 20, 22877-22889.	1.3	26
13975	Unravelling the electrochemical mechanisms for nitrogen fixation on single transition metal atoms embedded in defective graphitic carbon nitride. Journal of Materials Chemistry A, 2018, 6, 21941-21948.	5.2	161
13976	DFT study of [BH <sub>4</sub> ] <sup>-</sup> rotation in pressure-driven phase transition of MBH <sub>4</sub> . Computational Materials Science, 2018, 154, 143-146.	1.4	1
13977	Magneto-electronic properties of GaN codoped with (V, Mn) impurities for spintronic devices: Ab-initio and Monte Carlo studies. Physica A: Statistical Mechanics and Its Applications, 2018, 512, 1249-1259.	1.2	15
13978	First-principles study of the (Cu x Ni <sub>1-x</sub> ) <sub>3</sub> Sn precipitations with different structures in Cu-Ni-Sn alloys. Chinese Physics B, 2018, 27, 086302.	0.7	7
13979	Transition metals adsorption and conductivity modification in carbon nanotubes: analytical modeling and DFT study. Adsorption, 2018, 24, 575-583.	1.4	7
13980	Theoretical Insights into 1D Transition-Metal Nanoalloys Grown on the NiAl(110) Surface. ACS Omega, 2018, 3, 8819-8828.	1.6	3
13981	Theoretical Aspects of Hydrogen Dynamics at Metal Surfaces. , 2018, , 281-291.		0
13982	Understanding the facet-dependent catalytic performance of hematite microcrystals in a CO oxidation reaction. Inorganic Chemistry Frontiers, 2018, 5, 2332-2339.	3.0	27
13983	First-Principles Study of the Adsorption and Depolymerization Mechanisms of Sodium Silicate on Iron Surfaces at High Temperature. Journal of Physical Chemistry C, 2018, 122, 20827-20840.	1.5	18
13984	Tetraphenylethene-Induced Free Volumes for the Isomerization of Spiropyran toward Multifunctional Materials in the Solid State. ACS Applied Materials & Interfaces, 2018, 10, 30879-30886.	4.0	62
13985	The adsorption of alcohols on strained Pt <sub>3</sub> Ni(111) substrates: a density functional investigation within the D3 van der Waals correction. Physical Chemistry Chemical Physics, 2018, 20, 24210-24221.	1.3	14
13986	Unexpected Ground-State Structure and Mechanical Properties of Ir <sub>2</sub> Zr Intermetallic Compound. Materials, 2018, 11, 103.	1.3	2
13987	Strain dependent electronic and optical properties of PtS <sub>2</sub> monolayer. Chemical Physics Letters, 2018, 709, 65-70.	1.2	53
13988	Strain effect on the electronic properties of Ce-doped SnS <sub>2</sub> monolayer. Physica B: Condensed Matter, 2018, 547, 1-5.	1.3	11
13989	The Utility of Calculated Proton Affinities in Drug Design: A DFT Study. Australian Journal of Chemistry, 2018, 71, 580.	0.5	1
13990	First principles study of the structural, electronic and optical properties of epitaxial GaSb <sub>1-x</sub> N <sub>x</sub> Bi <sub>x</sub> , lattice matched to GaSb. Materials Research Express, 2018, 5, 115901.	0.8	3

#	ARTICLE	IF	CITATIONS
13991	Tuning the Electronic Structures and Transport Properties of Zigzag Blue Phosphorene Nanoribbons. IEEE Transactions on Electron Devices, 2018, 65, 4646-4651.	1.6	38
13992	High throughput screening for two-dimensional topological insulators. 2D Materials, 2018, 5, 045023.	2.0	25
13993	Strength evaluation on the interface of precipitates with segregated hydrogen in Al-Mg-Zn alloys by ab initio calculation. Keikinzoku/Journal of Japan Institute of Light Metals, 2018, 68, 189-193.	0.1	0
13994	Suppressing Voltage Decay of a Lithium-Rich Cathode Material by Surface Enrichment with Atomic Ruthenium. ACS Applied Materials & Interfaces, 2018, 10, 21349-21355.	4.0	36
13995	Structures and Stability of Iron Halides at the Earth's Mantle and Core Pressures: Implications for the Missing Halogen Paradox. ACS Earth and Space Chemistry, 2018, 2, 711-719.	1.2	8
13996	First-principles study of bandgap tuning in Ge <sub>1-x</sub> PbxSe. International Journal of Modern Physics B, 2018, 32, 1850076.	1.0	0
13997	The Nature of Chemical Bonding in Lewis Adducts as Reflected by <sup>27</sup> Al NMR Quadrupolar Coupling Constant: Combined Solid-State NMR and Quantum Chemical Approach. Inorganic Chemistry, 2018, 57, 7428-7437.	1.9	7
13998	Structure of 4-(Dimethylamino)benzotrile Using Gas Electron Diffraction: A New Lease of Life for the Only Gas Electron Diffractometer in the U.K. Journal of Physical Chemistry A, 2018, 122, 5656-5665.	1.1	6
13999	Synthesis and Electronic Phosphorescence of Dicyanoocatetrayne (NC <sub>10</sub> N) in Cryogenic Matrixes. Journal of Physical Chemistry A, 2018, 122, 5580-5588.	1.1	3
14000	Strategy to modulate the ĩ€-bridged units in bis(4-methoxyphenyl)amine-based hole-transporting materials for improvement of perovskite solar cell performance. Journal of Materials Chemistry C, 2018, 6, 6816-6822.	2.7	20
14001	Effects of external magnetic field and out-of-plane strain on magneto-optical Kerr spectra in CrI <sub>3</sub> monolayer. Journal of Physics Condensed Matter, 2018, 30, 285303.	0.7	16
14002	Molecular Treatment of Nano-Kaolinite Generations. Inorganic Chemistry, 2018, 57, 7151-7167.	1.9	16
14003	Water Dissociation on Clean and Potassium Preadsorbed Transition Metals: A Systematic Theoretical Study. Journal of Physical Chemistry C, 2018, 122, 15474-15484.	1.5	16
14004	Structural, elastic, electronic and thermodynamic properties of Zr <sub>2</sub> under high-pressure: First-principle study. International Journal of Modern Physics B, 2018, 32, 1850200.	1.0	3
14005	Amine group induced high activity of highly torn amine functionalized nitrogen-doped graphene as the metal-free catalyst for hydrogen evolution reaction. Carbon, 2018, 138, 169-178.	5.4	46
14006	On-Surface Synthesis of Spin Crossover Polymeric Chains. Journal of Physical Chemistry C, 2018, 122, 15033-15040.	1.5	17
14007	Nature of Localized Excitons in $CsMgX$ ( $X = Cl, Br, I$ ) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 102 Td (display="inline") <math>T_j ETQq_0 0 0 rgBT /Overlock 10 Tf 50 102 Td</math>	1.5	8
14008	Review Applied, 2018, 9. Investigation of the initial reactions of lithium oxides on the graphitic carbon nitrides (g-C <sub>3</sub> N <sub>4</sub> ) for catalyst in non-aqueous lithium - air batteries: A first-principles calculations. Thin Solid Films, 2018, 660, 186-190.	0.8	6

#	ARTICLE	IF	CITATIONS
14009	Strontium and barium in aqueous solution and a potassium channel binding site. <i>Journal of Chemical Physics</i> , 2018, 148, 222831.	1.2	18
14010	Effect of illumination and Se vacancies on fast oxidation of ultrathin gallium selenide. <i>Nanoscale</i> , 2018, 10, 12180-12186.	2.8	37
14011	Stabilizing and Organizing Bi <sub>3</sub> Cu <sub>4</sub> and Bi <sub>7</sub> Cu <sub>12</sub> Nanoclusters in Two-Dimensional Metal-Organic Networks. <i>Angewandte Chemie</i> , 2018, 130, 4707-4711.	1.6	5
14012	Utilizing a metal as a sulfur host for high performance Li-S batteries. <i>Nano Energy</i> , 2018, 50, 685-690.	8.2	40
14013	Interlayer coupling and electric field tunable electronic properties and Schottky barrier in a graphene/bilayer-GaSe van der Waals heterostructure. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17899-17908.	1.3	99
14014	Optical Properties of Cu <sub>2</sub> ZnSn(S <sub>x</sub> ) <sub>4</sub> by First-Principles Calculations. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2018, 215, 1700945.	0.8	4
14015	Comprehensive Phase Diagrams of MoS <sub>2</sub> Edge Sites Using Dispersion-Corrected DFT Free Energy Calculations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 15318-15329.	1.5	18
14016	Effects of trigonal deformation on electronic structure and thermoelectric properties of bismuth. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 285504.	0.7	17
14017	Origin of efficient oxygen reduction reaction on Pd monolayer supported on Pd-M (M=Ni, Fe) intermetallic alloy. <i>Electrochimica Acta</i> , 2018, 282, 680-686.	2.6	26
14018	From semilocal density functionals to random phase approximation renormalized perturbation theory: A methodological assessment of structural phase transitions. <i>Physical Review B</i> , 2018, 97, .	1.1	68
14019	Atomistic simulations of interaction between basal & dislocations and three-dimensional twins in magnesium. <i>Acta Materialia</i> , 2018, 155, 187-198.	3.8	63
14020	Interfacial properties of high-order aggregation of organic dyes: A combination of static and dynamic properties. <i>Energy</i> , 2018, 158, 537-545.	4.5	15
14021	On the role of water in selective hydrogenation of cinnamaldehyde to cinnamyl alcohol on PtFe catalysts. <i>Journal of Catalysis</i> , 2018, 364, 192-203.	3.1	87
14022	Dioxygen activation routes in Mars-van Krevelen redox cycles catalyzed by metal oxides. <i>Journal of Catalysis</i> , 2018, 364, 228-247.	3.1	36
14023	Thickness-Dependent Reactivity of O <sub>2</sub> on Cu Layers Grown on Ru(0001) Surfaces. <i>Journal of Physical Chemistry C</i> , 2018, 122, 15529-15538.	1.5	8
14024	Hydrogen-free defects in hydrogenated black TiO <sub>2</sub> . <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19871-19876.	1.3	6
14025	Sulfur/nickel ferrite composite as cathode with high-volumetric-capacity for lithium-sulfur battery. <i>Science China Materials</i> , 2019, 62, 74-86.	3.5	86
14026	Screening for the selective inhibitors of MMP-9 from natural products based on pharmacophore modeling and molecular docking in combination with bioassay experiment, hybrid QM/MM calculation, and MD simulation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 3135-3149.	2.0	13

#	ARTICLE	IF	CITATIONS
14027	Graphene intercalated Ni-SiO <sub>2</sub> /GO-Ni-foam catalyst with enhanced reactivity and heat-transfer for CO <sub>2</sub> methanation. <i>Chemical Engineering Science</i> , 2019, 194, 10-21.	1.9	43
14028	Understanding the Spin Transport in H <sub>2</sub> O-Adsorbed CNT-Based Magnetic Tunnel Junction. <i>Journal of Superconductivity and Novel Magnetism</i> , 2019, 32, 925-929.	0.8	1
14029	Ab initio phase stabilities and mechanical properties of multicomponent alloys: A comprehensive review for high entropy alloys and compositionally complex alloys. <i>Materials Characterization</i> , 2019, 147, 464-511.	1.9	231
14030	Structural and optical evolution in Pb <sub>100</sub> -Ag <sub>Se</sub> ( $x = 3, 6, 9$ and $12$ ) thin films by chemical bath deposition. <i>Journal of Alloys and Compounds</i> , 2019, 770, 649-654.	2.8	9
14031	Mechanism and kinetics of Cu <sub>2</sub> O oxidation in chemical looping with oxygen uncoupling. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 4371-4378.	2.4	24
14032	Density-functional study of the La <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> low-index surfaces. <i>Surface Science</i> , 2019, 689, 121235.	0.8	2
14033	Arsenene monolayer as an outstanding anode material for (Li/Na/Mg)-ion batteries: density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19951-19962.	1.3	66
14034	Monitoring the electronic, thermal and optical properties of two-dimensional MoO <sub>2</sub> under strain <i>via</i> vibrational spectroscopies: a first-principles investigation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19904-19914.	1.3	24
14035	A charge optimized many-body potential for iron/iron-fluoride systems. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20118-20131.	1.3	4
14036	Microscopic Nature of Magnetic Ground State in CeAuSb <sub>2</sub> . <i>Physica Status Solidi - Rapid Research Letters</i> , 2019, 13, 1900304.	1.2	3
14037	Electronic, magnetic, and optical properties of Mn-doped GaSb: A first-principles study. <i>Physica B: Condensed Matter</i> , 2019, 572, 225-229.	1.3	5
14038	Optimizing electron-rich arylamine derivatives in thiophene-fused derivatives as $\pi$ -bridge-based hole transporting materials for perovskite solar cells. <i>RSC Advances</i> , 2019, 9, 24733-24741.	1.7	12
14039	Three-dimensional graphene networks modified with acetylenic linkages for high-performance optoelectronics and Li-ion battery anode material. <i>Carbon</i> , 2019, 154, 478-484.	5.4	10
14040	Assessing the Accuracy of Density Functional Theory through Structure and Dynamics of the Water-Air Interface. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4914-4919.	2.1	43
14041	Elevated temperature microstructural stability in cast AlCuMnZr alloys through solute segregation. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2019, 765, 138279.	2.6	89
14042	Adsorption of Formic Acid on CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Lead-Halide Organic-Inorganic Perovskites. <i>Journal of Physical Chemistry C</i> , 2019, 123, 22873-22886.	1.5	5
14043	Strain-tunable CO <sub>2</sub> storage by black phosphorene and $\hat{I}$ -PC from combined first principles and molecular dynamics studies. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20107-20117.	1.3	11
14044	X-ray diffraction, Mössbauer spectroscopy, neutron diffraction, optical absorption and ab-initio calculation of magnetic process in orthorhombic YFe <sub>x</sub> Cr <sub>(1-x)</sub> O <sub>3</sub> ( $0 \leq x \leq 1$ ) compounds. <i>Hyperfine Interactions</i> , 2019, 240, 1.		8



#	ARTICLE	IF	CITATIONS
14045	Mechanistic understanding of catalysis by combining mass spectrometry and computation. <i>Chemical Communications</i> , 2019, 55, 12749-12764.	2.2	25
14046	Strong Electronic Interaction of Amorphous Fe <sub>2</sub> O <sub>3</sub> Nanosheets with Single-Atom Pt toward Enhanced Carbon Monoxide Oxidation. <i>Advanced Functional Materials</i> , 2019, 29, 1904278.	7.8	51
14047	Statistically representative databases for density functional theory <i>via</i> data science. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19092-19103.	1.3	20
14048	p-Type Conductivity of Hydrated Amorphous V <sub>2</sub> O <sub>5</sub> and Its Enhanced Photocatalytic Performance in ZnO/V <sub>2</sub> O <sub>5</sub> /rGO. <i>ACS Applied Electronic Materials</i> , 2019, 1, 1881-1889.	2.0	13
14049	Number of Reactive Charge Carriers—A Hidden Linker between Band Structure and Catalytic Performance in Photocatalysts. <i>ACS Catalysis</i> , 2019, 9, 8852-8861.	5.5	31
14050	Organometallic compound as an efficient catalyst toward oxygen reduction reaction. <i>Inorganic Chemistry Communication</i> , 2019, 108, 107520.	1.8	8
14051	DFT + <i>U</i> and Low-Temperature XPS Studies of Fe-Depleted Chalcopyrite (CuFeS <sub>2</sub> ) Surfaces: A Focus on Polysulfide Species. <i>Journal of Physical Chemistry C</i> , 2019, 123, 21031-21041.	1.5	29
14052	First-principles study of lithium and chlorine co-decorated graphene. <i>Materials Research Express</i> , 2019, 6, 105603.	0.8	2
14053	Sulfur-functionalized vanadium carbide MXene (V <sub>2</sub> CS <sub>2</sub> ) as a promising anchoring material for lithium-sulfur batteries. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 18559-18568.	1.3	96
14054	Synthesis and DFT calculations of new ruthenium(II) nitrosyl complexes using <i>cis-fac</i> -dichlorotetrakis(dimethylsulfoxide)ruthenium(II) precursor and different oximes as sources of nitrosyl ligand. <i>Journal of Coordination Chemistry</i> , 2019, 72, 2200-2214.	0.8	2
14055	Ultrafine Defective RuO <sub>2</sub> Electrocatayst Integrated on Carbon Cloth for Robust Water Oxidation in Acidic Media. <i>Advanced Energy Materials</i> , 2019, 9, 1901313.	10.2	182
14056	First-principles calculations on half-metal ferromagnetic results of VZrAs and VZrSb half-heusler compounds and Al <sub>1-x</sub> M <sub>x</sub> As (M= Co, Fe and x= 0.0625, 0.125, 0.25) diluted magnetic semiconductors. <i>Journal of Alloys and Compounds</i> , 2019, 807, 151656.	2.8	17
14057	Effects of thiol ligands on the growth and stability of CdS nanoclusters. <i>Journal of Molecular Structure</i> , 2019, 1198, 126832.	1.8	6
14058	Stable InSe transistors with high-field effect mobility for reliable nerve signal sensing. <i>Npj 2D Materials and Applications</i> , 2019, 3, .	3.9	31
14059	Vibration signatures of the structural phase transition of Sn/Ge(111) compared to Sn/Si(111). <i>Physical Review B</i> , 2019, 100, .	1.1	3
14060	Efficient band gap prediction of semiconductors and insulators from a semilocal exchange-correlation functional. <i>Physical Review B</i> , 2019, 100, .	1.1	35
14061	Lithiation-Induced Structural Rearrangement and Stress Change in SiCO-Derived Porous Carbon: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 19315-19321.	1.5	2
14062	Confinement-Enhanced Rapid Interlayer Diffusion within Graphene-Supported Anisotropic ReSe <sub>2</sub> Electrodes. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 31147-31154.	4.0	13



#	ARTICLE	IF	CITATIONS
14063	Improving the Quantum Capacitance of Graphene-Based Supercapacitors by the Doping and Co-Doping: First-Principles Calculations. ACS Omega, 2019, 4, 13209-13217.	1.6	73
14064	Large nonvolatile control of interfacial magnetic anisotropy in CoPt by a ferroelectric ZnO-based tunneling barrier. Physical Review B, 2019, 100, .	1.1	3
14065	The role of isotropic and anisotropic Hubbard corrections for the magnetic ordering and absolute band alignment of hematite $\pm$ -Fe <sub>2</sub> O <sub>3</sub> (0001) surfaces. Progress in Natural Science: Materials International, 2019, 29, 349-355.	1.8	5
14066	Metal-Free B@<i>g</i>-CN: Visible/Infrared Light-Driven Single Atom Photocatalyst Enables Spontaneous Dinitrogen Reduction to Ammonia. Nano Letters, 2019, 19, 6391-6399.	4.5	236
14067	First principle predictions on half-metallic results of MnZrX (X = In, Tl, C, Si, Ge, Sn, Pb, N, P, As, Sb, O, S). Tj ETQg0 0 0 rgBT /Overlo	1.0	19
14068	Implicit solvent effects in the determination of Brønsted-Årnsen-Evans-Polanyi relationships for heterogeneously catalyzed reactions. Physical Chemistry Chemical Physics, 2019, 21, 17687-17695.	1.3	4
14069	Superior triethylamine detection at room temperature by {-112} faceted WO <sub>3</sub> gas sensor. Journal of Hazardous Materials, 2019, 380, 120876.	6.5	95
14070	Design of a Highly Active Pd Catalyst with P,N Hemilabile Ligands for Alkoxy carbonylation of Alkynes and Allenes: A Density Functional Theory Study. Chemistry - A European Journal, 2019, 25, 11625-11629.	1.7	11
14071	Cost-effective density functional theory (DFT) calculations of equilibrium isotopic fractionation in large organic molecules. Physical Chemistry Chemical Physics, 2019, 21, 17555-17570.	1.3	11
14072	NiSe <sub>2</sub> as Co Catalyst with CdS: Nanocomposites for High Performance Photodriven Hydrogen Evolution under Visible Light Irradiation. ChemPlusChem, 2019, 84, 999-1010.	1.3	12
14073	A computational study of structural, electronic and carrier mobility of boron and phosphorus/nitrogen co-doped graphene. Physica B: Condensed Matter, 2019, 571, 291-295.	1.3	19
14074	Analysis of over-magnetization of elemental transition metal solids from the SCAN density functional. Physical Review B, 2019, 100, .	1.1	37
14075	A study on magnetic, electronic, elastic and vibrational properties of Ir <sub>2</sub> MnAl Heusler alloy for spintronic applications. Materials Research Express, 2019, 6, 096571.	0.8	6
14076	Unveiling the Electric-Current-Limiting and Photodetection Effect in Two-Dimensional Hydrogenated Borophene. Physical Review Applied, 2019, 11, .	1.5	45
14077	Comparative study of electronic-structure methods for platinum-containing molecules: bond lengths and bond dissociation energies. European Physical Journal D, 2019, 73, 1.	0.6	3
14078	Theoretical and experimental spectroscopic studies, XPS analysis, dimer interaction energies and molecular docking study of 5-(adamantan-1-yl)-N-methyl-1,3,4-thiadiazol-2-amine. Journal of Physics and Chemistry of Solids, 2019, 135, 109091.	1.9	11
14079	Mitigating Voltage Decay of Li-Rich Layered Oxide by Incorporation of 5d Metal Rhenium. Journal of Physical Chemistry C, 2019, 123, 18870-18876.	1.5	23
14080	Hole doped $\pm$ -MgAgSb as potential low temperature thermoelectric materials. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 125833.	0.9	3

#	ARTICLE	IF	CITATIONS
14081	Novel synergistic in situ synthesis of lithium-ion poly(ethylene citrate)-TiO <sub>2</sub> nanocomposites as promising fluorine-free solid polymer electrolytes for lithium batteries. <i>Journal of Physics and Chemistry of Solids</i> , 2019, 135, 109082.	1.9	17
14082	Theoretical and experimental investigation of geometry and stability of small potassium iodide K <sub>n</sub> I <sub>(n)</sub> . <i>Tj ETQq1</i> , 2019, 1.0, 14	1.0	2
14083	Predictive model of hydrogen trapping and bubbling in nanovoids in bcc metals. <i>Nature Materials</i> , 2019, 18, 833-839.	13.3	83
14084	Tuning of Schottky barriers in borophene/MoS <sub>2</sub> van der Waals heterostructure by external electric field. <i>AIP Conference Proceedings</i> , 2019, , .	0.3	0
14085	Aluminium segregation profiles in the (110), (100) and (111) surface regions of the Fe <sub>0.85</sub> Al <sub>0.15</sub> random body-centered cubic alloy. <i>Applied Surface Science</i> , 2019, 492, 886-895.	3.1	7
14086	Properties of spin polarization and spin transport for zigzag antimonene nanoribbons with single vacancies. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019, 114, 113622.	1.3	1
14087	DFT insights into the formation of sulfur vacancies over corner/edge site of Co/Ni-promoted MoS <sub>2</sub> and WS <sub>2</sub> under the hydrodesulfurization conditions. <i>Applied Catalysis B: Environmental</i> , 2019, 257, 117937.	10.8	44
14088	X-ray crystal structures, density functional theory and docking on deacetylase enzyme for antiproliferative activity of hispolon derivatives on HCT116 colon cancer. <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 3805-3812.	1.4	7
14089	Modulating the electronic properties of pure, B-doped and N-doped <i>h</i> <sup>3</sup> -graphdiyne via electric field. <i>Materials Research Express</i> , 2019, 6, 095610.	0.8	2
14090	First principles study of structural stability against the distribution of Mg and Al atoms and adsorption behaviors of heavy metals of attapulgite. <i>Computational Materials Science</i> , 2019, 169, 109106.	1.4	20
14091	A new reflowing strategy based on lithiophilic substrates towards smooth and stable lithium metal anodes. <i>Journal of Materials Chemistry A</i> , 2019, 7, 18126-18134.	5.2	32
14092	Li <sub>4</sub> V <sub>2</sub> Mn(PO <sub>4</sub> ) <sub>4</sub> -stabilized Li[Li <sub>0.2</sub> Mn <sub>0.54</sub> Ni <sub>0.13</sub> Co <sub>0.13</sub> ]O <sub>2</sub> cathode materials for lithium ion batteries. <i>Nano Energy</i> , 2019, 63, 103889.	8.2	138
14093	Ion-selectivity of iron sulfides and their effect on H <sub>2</sub> S corrosion. <i>Corrosion Science</i> , 2019, 158, 108085.	3.0	15
14094	Inactivation of HeLa cells on nanoporous gold. <i>Materialia</i> , 2019, 7, 100370.	1.3	3
14095	The origin of the conductivity maximum in molten salts. III. Zinc halides. <i>Journal of Chemical Physics</i> , 2019, 151, 034507.	1.2	3
14096	Experimental and simulation studies of strontium/fluoride-codoped hydroxyapatite nanoparticles with osteogenic and antibacterial activities. <i>Colloids and Surfaces B: Biointerfaces</i> , 2019, 182, 110359.	2.5	43
14097	Interface intrinsic strengthening mechanism on the tensile properties of Al <sub>2</sub> O <sub>3</sub> /Al composites. <i>Computational Materials Science</i> , 2019, 169, 109131.	1.4	18
14098	Syntheses, crystal structures, and characterizations of three new pyrophosphates CsNaZnP <sub>2</sub> O <sub>7</sub> , RbNaZnP <sub>2</sub> O <sub>7</sub> , and RbLiMgP <sub>2</sub> O <sub>7</sub> . <i>Solid State Sciences</i> , 2019, 95, 105940.	1.5	4

#	ARTICLE	IF	CITATIONS
14099	Single-Atom-Thick Active Layers Realized in Nanolaminated $\text{Ti}_3\text{(Al}_x\text{Cu}_{1-x}\text{)}\text{C}_2$ and Its Artificial Enzyme Behavior. <i>ACS Nano</i> , 2019, 13, 9198-9205.	7.3	59
14100	A semiconducting layered metal-organic framework magnet. <i>Nature Communications</i> , 2019, 10, 3260.	5.8	119
14101	The reaction of phenoxatellurine with single-electron oxidizers revisited. <i>New Journal of Chemistry</i> , 2019, 43, 12754-12766.	1.4	13
14102	Improving Electrochemical $\text{Pb}^{2+}$ Detection Using a Vertically Aligned 2D $\text{MoS}_2$ Nanofilm. <i>Analytical Chemistry</i> , 2019, 91, 11770-11777.	3.2	73
14103	Atomic scale study of stress-induced misaligned subsurface layers in KDP crystals. <i>Scientific Reports</i> , 2019, 9, 10399.	1.6	5
14104	Systematic exploration of N, C configurational effects on the ORR performance of Fe-N doped graphene catalysts based on DFT calculations. <i>RSC Advances</i> , 2019, 9, 22656-22667.	1.7	40
14105	Fabrication of large-scale graphene/2D-germanium heterostructure by intercalation. <i>Chinese Physics B</i> , 2019, 28, 078103.	0.7	6
14106	First-principles insight into Li and Na ion storage in graphene oxide*. <i>Chinese Physics B</i> , 2019, 28, 078201.	0.7	3
14107	First-principles study of the atomic structures, electronic properties, and surface stability of $\text{BaTiO}_3(001)$ and $(011)$ surfaces. <i>Surface and Interface Analysis</i> , 2019, 51, 1021-1032.	0.8	16
14108	Overwhelming the Performance of Single Atoms with Atomic Clusters for Platinum-Catalyzed Hydrogen Evolution. <i>ACS Catalysis</i> , 2019, 9, 8213-8223.	5.5	68
14109	Acrylonitrile vapor adsorption studies on armchair arsenene nanoribbon based on DFT study. <i>Applied Surface Science</i> , 2019, 494, 1148-1155.	3.1	23
14110	Cationic gold clusters with eight valence electrons: possible spherical aromatic systems with Sigma holes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17779-17785.	1.3	4
14111	High intrinsic $zT$ in $\text{InP}_3$ monolayer at room temperature. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 365501.	0.7	6
14112	Novel Insights into the Hydroxylation Behaviors of $\alpha$ -Quartz (101) Surface and its Effects on the Adsorption of Sodium Oleate. <i>Minerals (Basel, Switzerland)</i> , 2019, 9, 450.	0.8	50
14113	DFT calculations in periodic boundary conditions of gas-phase acidities and of transition-metal anionic clusters: case study with carboxylate-stabilized ruthenium clusters. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	4
14114	A DFT study on effects of W solution on cemented carbides Co phase pressurized properties. <i>Journal of Alloys and Compounds</i> , 2019, 806, 1242-1249.	2.8	0
14115	Toward a Specific Reaction Parameter Density Functional for $\text{H}_2 + \text{Ni}(111)$ : Comparison of Theory with Molecular Beam Sticking Experiments. <i>Journal of Physical Chemistry C</i> , 2019, 123, 20420-20433.	1.5	12
14116	A comprehensive assessment of the low-temperature thermal properties and thermodynamic functions of $\text{CeO}_2$ . <i>Journal of Chemical Physics</i> , 2019, 151, 044202.	1.2	5

#	ARTICLE	IF	CITATIONS
14117	Noncovalent Close Contacts in Fluorinated Thiophene-Phenylene-Thiophene Conjugated Units: Understanding the Nature and Dominance of O-H versus S-H and O-F Interactions with Respect to the Control of Polymer Conformation. <i>Chemistry of Materials</i> , 2019, 31, 7070-7079.	3.2	23
14118	Accurate Band Gap Predictions of Semiconductors in the Framework of the Similarity Transformed Equation of Motion Coupled Cluster Theory. <i>Inorganic Chemistry</i> , 2019, 58, 9303-9315.	1.9	58
14119	Electrochemical Synthesis of Cation Vacancy-Enriched Ultrathin Bimetallic Oxyhydroxide Nanoplatelets for Enhanced Water Oxidation. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 25958-25966.	4.0	25
14120	Hydrogen Isotope Separation via Ion Penetration through Group-IV Monolayer Materials in Electrochemical Environment. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4618-4624.	2.1	5
14121	Single molybdenum center supported on N-doped black phosphorus as an efficient electrocatalyst for nitrogen fixation. <i>Nanoscale</i> , 2019, 11, 13600-13611.	2.8	102
14122	Research on the Effect of Carbon Defects on the Hydrophilicity of Coal Pyrite Surface from the Insight of Quantum Chemistry. <i>Molecules</i> , 2019, 24, 2285.	1.7	7
14123	Fast and Accurate Artificial Neural Network Potential Model for MAPbI <sub>3</sub> Perovskite Materials. <i>ACS Omega</i> , 2019, 4, 10950-10959.	1.6	31
14124	Magnetic Signatures of Hydroxyl- and Water-Terminated Neutral and Tetra-Anionic Mn <sub>12</sub> -Acetate. <i>Journal of Computational Chemistry</i> , 2019, 40, 2301-2308.	1.5	8
14125	Surface charge-induced activation of Ni-loaded CdS for efficient and robust photocatalytic dehydrogenation of methanol. <i>Applied Catalysis B: Environmental</i> , 2019, 257, 117869.	10.8	41
14126	H permeation in molybdenum: temperature dependence and compensation effect from first-principles simulation. <i>Journal of Nuclear Science and Technology</i> , 2019, 56, 1014-1028.	0.7	2
14127	Comparative study of density functionals for the description of lithium-graphite intercalation compounds. <i>Journal of Computational Chemistry</i> , 2019, 40, 2400-2412.	1.5	21
14128	Multiple superionic states in helium-water compounds. <i>Nature Physics</i> , 2019, 15, 1065-1070.	6.5	69
14129	A dual approach to study the synthesis, crystal structure, thermal, optical and nonlinear optical properties of copper (II) malonate complex {(C <sub>7</sub> H <sub>8</sub> O <sub>2</sub> N) <sub>2</sub> [Cu(C <sub>3</sub> H <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ]}. <i>Inorganic Chemistry Communication</i> , 2019, 107, 107450.	1.8	5
14130	Chalcogenide glasses as a playground for the application of first-principles molecular dynamics to disordered materials. <i>Solid State Sciences</i> , 2019, 95, 105925.	1.5	4
14131	An interfacial electron transfer relay center for accelerating the hydrogen evolution reaction. <i>Journal of Materials Chemistry A</i> , 2019, 7, 18304-18310.	5.2	19
14132	Scaling of intrinsic domain wall magnetoresistance with confinement in electromigrated nanocontacts. <i>Physical Review B</i> , 2019, 99, .	1.1	7
14133	Revealing Atomic Structure and Oxidation States of Dopants in Charge-Ordered Nanoparticles for Migration-Promoted Oxygen-Exchange Capacity. <i>Chemistry of Materials</i> , 2019, 31, 5769-5777.	3.2	10
14134	Structural Evolutions of Vertically Aligned Two-Dimensional MoS <sub>2</sub> Layers Revealed by in Situ Heating Transmission Electron Microscopy. <i>Journal of Physical Chemistry C</i> , 2019, 123, 27843-27853.	1.5	13

#	ARTICLE	IF	CITATIONS
14135	Surface Functionalization of Reconstructed Si(111) with Methionine. Journal of Physical Chemistry C, 2019, 123, 26980-26988.	1.5	2
14136	Study on Crystal Growth Kinetics and Preferred Orientation for LiF Crystal in Dimethyl Sulfoxide/1,3-Dioxolane-based Electrolyte. Journal of Physical Chemistry C, 2019, 123, 28048-28057.	1.5	12
14137	The structures, stability, mechanical properties and electronic properties of X (X=Nb, Ge, Ni) doped Al <sub>2</sub> Cu: a first-principle study. Materials Research Express, 2019, 6, 1165b5.	0.8	6
14138	QCM based enantioselective discrimination of enantiomers by a pair of serine derived homochiral coordination polymers. Biosensors and Bioelectronics, 2019, 144, 111667.	5.3	13
14139	Benchmark study of the linear and nonlinear optical polarizabilities in proto-type NLO molecule of <i>p</i> -nitroaniline. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950030.	1.8	74
14140	Strong and Tunable Electrical Anisotropy in Type-II Weyl Semimetal Candidate WP <sub>2</sub> with Broken Inversion Symmetry. Advanced Materials, 2019, 31, e1903498.	11.1	13
14141	Temperature-dependent nucleation kinetics of Guinier-Preston zones in Al-Cu alloys: An atomistic kinetic Monte Carlo and classical nucleation theory approach. Acta Materialia, 2019, 179, 262-272.	3.8	31
14142	Mutualistic decomposition pathway of formaldehyde on O-predosed $\gamma$ -MnO <sub>2</sub> . Applied Surface Science, 2019, 498, 143784.	3.1	12
14143	Insight in the properties of WO <sub>3</sub>  Y: A first-principle study. Results in Physics, 2019, 15, 102670.	2.0	3
14144	A Theoretical Study on the Electronic Structure and Floatability of Rare Earth Elements (La, Ce, Nd) Tj ETQq1 1 0.784314 rgBT /Overlock	0.8	11
14145	Modified embedded-atom method potential for cadmium. Hyperfine Interactions, 2019, 240, 1.	0.2	0
14146	Numerical approach to evaluate performance of porous SiC <sub>5</sub> /4O <sub>3</sub> /2 as potential high temperature hydrogen gas sensor. International Journal of Hydrogen Energy, 2019, 44, 26679-26684.	3.8	17
14147	Tomographic layer-by-layer analysis of epitaxial iron-silicide nanostructures by DFT-assisted STS. Applied Surface Science, 2019, 496, 143583.	3.1	4
14148	DFT Study into the Influence of Carbon Material on the Hydrophobicity of a Coal Pyrite Surface. Molecules, 2019, 24, 3534.	1.7	4
14149	Chitosan encapsulated water-soluble silver bionanocomposite for size-dependent antibacterial activity. Nano Structures Nano Objects, 2019, 20, 100393.	1.9	44
14150	Tuning electronic and magnetic properties of armchair InSe nanoribbons by hydrogenation. Superlattices and Microstructures, 2019, 135, 106282.	1.4	1
14151	Coverage and Stability of NH <sub>x</sub> -Terminated Cobalt and Ruthenium Surfaces: A First-Principles Investigation. Journal of Physical Chemistry C, 2019, 123, 25166-25175.	1.5	10
14152	Influence of Oxygen-Sulfur Exchange on the Structural, Electronic, and Stability Properties of Alkali Hexastannates. Journal of Physical Chemistry C, 2019, 123, 24375-24382.	1.5	6

#	ARTICLE	IF	CITATIONS
14153	FeP/MoS <sub>2</sub> Enriched with Dense Catalytic Sites and High Electrical Conductivity for the Hydrogen Evolution Reaction. ACS Sustainable Chemistry and Engineering, 2019, 7, 17671-17681.	3.2	24
14154	Settling the Long-Standing Debate on the Proton Storage Site of the Prototype Light-Driven Proton Pump Bacteriorhodopsin. Journal of Physical Chemistry B, 2019, 123, 9598-9608.	1.2	18
14155	Effect of Cu, N co-doping on conductive properties of AgSnO <sub>2</sub> contact. Materials Research Express, 2019, 6, 106311.	0.8	5
14156	The Reliability of the Density-Functional Theory in Actinide Endohedral Systems. Advanced Theory and Simulations, 2019, 2, 1900138.	1.3	8
14157	Interpretation and Automatic Generation of Fermi-Orbital Descriptors. Journal of Computational Chemistry, 2019, 40, 2843-2857.	1.5	21
14158	Implementation of magnesium doping in SrTiO <sub>3</sub> for correlating electronic, structural and optical properties: A DFT study. Chinese Journal of Physics, 2019, 62, 388-394.	2.0	11
14159	Semiconductor-Microbial Mechanism of Selective Dissolution of Chalcocite in Bioleaching. ACS Omega, 2019, 4, 18279-18288.	1.6	7
14160	Stabilities, and electronic and piezoelectric properties of two-dimensional tin dichalcogenide derived Janus monolayers. Journal of Materials Chemistry C, 2019, 7, 13203-13210.	2.7	72
14161	Structure and electronic properties of graphyne polymorphs formed from 4-8 graphene. IOP Conference Series: Materials Science and Engineering, 2019, 537, 022070.	0.3	2
14162	Doping sp-hybridized B atoms in graphyne supported single cobalt atoms for hydrogen evolution electrocatalysis. International Journal of Hydrogen Energy, 2019, 44, 27421-27428.	3.8	23
14163	A multiferroic molecular magnetic qubit. Journal of Chemical Physics, 2019, 151, 174105.	1.2	9
14164	Using Pd-Doped <sup>13</sup> C-Graphyne to Detect Dissolved Gases in Transformer Oil: A Density Functional Theory Investigation. Nanomaterials, 2019, 9, 1490.	1.9	37
14165	Insight into the Oxidation Mechanism of Furanic Compounds on Pt(111). ACS Catalysis, 2019, 9, 11360-11370.	5.5	10
14166	Tools for Prescreening the Most Active Sites on Ir and Rh Clusters toward C-H Bond Cleavage of Ethane: NBO Charges and Wiberg Bond Indexes. ACS Omega, 2019, 4, 18809-18819.	1.6	10
14167	Reproducing benchmark potential energy curves of molecular bond dissociation with small complete active space aided with density and density-matrix functional corrections. Journal of Chemical Physics, 2019, 151, 164122.	1.2	7
14168	On the calculation of the bandgap of periodic solids with MGGA functionals using the total energy. Journal of Chemical Physics, 2019, 151, 161102.	1.2	10
14169	Dissociating stable nitrogen molecules under mild conditions by cyclic strain engineering. Science Advances, 2019, 5, eaax8275.	4.7	9
14171	Boron-Doped g-C <sub>6</sub> N <sub>6</sub> Layer as a Metal-Free Photoelectrocatalyst for N <sub>2</sub> Reduction Reaction. Journal of Physical Chemistry C, 2019, 123, 28739-28743.	1.5	35



#	ARTICLE	IF	CITATIONS
14172	First-principles study of crystal structures and superconductivity of ternary $\text{YSH}_6$ and $\text{LaSH}_6$ at high pressures. <i>Physical Review B</i> , 2019, 100, .	1.1	33
14173	Frustrated and Allowed Structural Transitions: The Theory-Guided Discovery of the Modulated Structure of IrSi. <i>Journal of the American Chemical Society</i> , 2019, 141, 19424-19435.	6.6	12
14174	Relevance of the Pauli kinetic energy density for semilocal functionals. <i>Physical Review B</i> , 2019, 100, .	1.1	38
14175	Contrasting Oxygen Reduction Reactions on Zero- and One-Dimensional Defects of $\text{MoS}_2$ for Versatile Applications. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 46327-46336.	4.0	22
14176	Modulation of Inverse Spinel $\text{Fe}_3\text{O}_4$ by Phosphorus Doping as an Industrially Promising Electrocatalyst for Hydrogen Evolution. <i>Advanced Materials</i> , 2019, 31, e1905107.	11.1	225
14177	Picosecond to Nanosecond Manipulation of Excited-State Lifetimes in Complexes with an $\text{Fe}^{\text{II}}$ to $\text{Ti}^{\text{IV}}$ Metal-to-Metal Charge Transfer: The Role of Ferrocene Centered Excited States. <i>Inorganic Chemistry</i> , 2019, 58, 15320-15329.	1.9	7
14178	Synergy of a Metallic NiCo Dimer Anchored on a $\text{C}_2\text{N}_4$ Graphene Matrix Promotes the Electrochemical $\text{CO}_2$ Reduction Reaction. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 19113-19121.	3.2	91
14179	First-Principles Investigation on the Fully Compensated Ferrimagnetic Behavior in $\text{Ti}_2\text{NbSb}$ and $\text{TiZrNbSb}$ . <i>Chinese Physics Letters</i> , 2019, 36, 067101.	1.3	0
14180	Electron-phonon coupling and Kohn anomaly due to floating two-dimensional electronic bands on the surface of $\text{ZrSiS}$ . <i>Physical Review B</i> , 2019, 100, .	1.1	5
14181	Boosting Cell Performance of $\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ via Surface Structure Design. <i>Small</i> , 2019, 15, e1904854.	5.2	92
14182	Quantitative Multilayer $\text{Cu}(410)$ Structure and Relaxation Determined by QLEED. <i>Scientific Reports</i> , 2019, 9, 16882.	1.6	1
14183	Improved optoelectronic properties in $\text{Cd}_{\text{Sex}}\text{Te}_{1-x}$ through controlled composition and short-range order. <i>Solar Energy</i> , 2019, 194, 742-750.	2.9	19
14184	Interface Effects on Epilayer Surface Density of States by Scanning Tunneling Spectroscopy and Density Functional Theory. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900140.	1.3	2
14185	DFT Quantum Chemical Studies on Structural, Nonlinear Optical, Reactivity and Thermodynamic Properties of 4-(Methoxy- $\{(E)\text{-}[(\text{thiophen-}2\text{-yl)ethylimino]methyl\}$ phenol. <i>ChemistrySelect</i> , 2019, 4, 10876-10883.	0.7	9
14186	High-Performance Inverted Planar Perovskite Solar Cells Enhanced by Thickness Tuning of New Dopant-Free Hole Transporting Layer. <i>Small</i> , 2019, 15, e1904715.	5.2	47
14187	Photoactive Earth-Abundant Iron Pyrite Catalysts for Electrocatalytic Nitrogen Reduction Reaction. <i>Small</i> , 2019, 15, e1904723.	5.2	33
14188	Ab initio studies of $\text{Ti}_2\text{S}_3$ as a new cathode material for magnesium secondary batteries. <i>Materials Today Communications</i> , 2019, 20, 100598.	0.9	4
14189	First-principles studies on carbon diffusion in tungsten*. <i>Chinese Physics B</i> , 2019, 28, 116106.	0.7	4



#	ARTICLE	IF	CITATIONS
14190	Charge nonconservation of molecular devices in the presence of a nonlocal potential. <i>Physical Review B</i> , 2019, 100, .	1.1	3
14191	Phase diagrams and electronic properties of B-S and H-B-S systems under high pressure. <i>Physical Review B</i> , 2019, 100, .	1.1	14
14192	Crystal and Electronic Structures of MgCo <sub>2</sub> xMnxO <sub>4</sub> as Cathode Material for Magnesium Secondary Batteries Using First-Principles Calculations and Quantum Beam Measurements. <i>Bulletin of the Chemical Society of Japan</i> , 2019, 92, 1950-1959.	2.0	15
14193	DFT Fe <sub>3</sub> –O–O Vibrational Frequency Calculations over Catalytic Reaction Cycle States in the Dinuclear Center of Cytochrome <i>c</i> Oxidase. <i>Inorganic Chemistry</i> , 2019, 58, 13933-13944.	1.9	11
14194	Pristine–Graphene–Supported Nitrogen–Doped Carbon Self–Assembled from Glucaminium–Based Ionic Liquids as Metal–Free Catalyst for Oxygen Evolution. <i>ChemSusChem</i> , 2019, 12, 5041-5050.	3.6	25
14195	Adsorption Characteristics of Gas Molecules (H <sub>2</sub> O, CO <sub>2</sub> , CO, CH <sub>4</sub> , and H <sub>2</sub> ) on CaO-Based Catalysts during Biomass Thermal Conversion with in Situ CO <sub>2</sub> Capture. <i>Catalysts</i> , 2019, 9, 757.	1.6	13
14196	First-Principles Study of the Impact of Grain Boundary Formation in the Cathode Material LiFePO <sub>4</sub> . <i>Condensed Matter</i> , 2019, 4, 80.	0.8	8
14197	Correlations of Equilibrium Properties and Electronic Structure of Pure Metals. <i>Materials</i> , 2019, 12, 2932.	1.3	2
14198	First-principles study of electronic and optical properties of sulfur doped tin monoxide: A potential applicant for optoelectronic devices. <i>Ceramics International</i> , 2019, 45, 7495-7503.	2.3	7
14199	O <sub>2</sub> Adsorption Associated with Sulfur Vacancies on MoS <sub>2</sub> Microspheres. <i>Inorganic Chemistry</i> , 2019, 58, 2169-2176.	1.9	40
14200	Theoretical Study on Fe–Se–H Hydrides under High Pressure. <i>Journal of Physical Chemistry C</i> , 2019, 123, 28008-28014.	1.5	5
14201	Novel Synthesis of Red Phosphorus Nanodot/Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> MXenes from Low-Cost Ti <sub>3</sub> SiC <sub>2</sub> MAX Phases for Superior Lithium- and Sodium-Ion Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 42086-42093.	4.0	45
14202	Crystalline phase transitions and vibrational spectra of silicon up to multiterapascal pressures. <i>Physical Review B</i> , 2019, 100, .	1.1	9
14203	Magnetic Properties of Trimers of Heavy p-Elements of Groups IV–VI. <i>JETP Letters</i> , 2019, 110, 211-216.	0.4	1
14204	Vibrational Circular Dichroism of Thiolate-Protected Au <sub>25</sub> Clusters: Accurate Prediction of Spectra and Chirality Transfer within the Mixed Ligand Shell. <i>Journal of Physical Chemistry C</i> , 2019, 123, 22586-22594.	1.5	9
14205	New insights into the origin of unstable sodium graphite intercalation compounds. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19378-19390.	1.3	68
14206	Unusually strong heteroatomic bonding in the complex polyanion of intermetallic Ba <sub>6</sub> Pt <sub>22</sub> Al <sub>53</sub> . <i>Dalton Transactions</i> , 2019, 48, 14103-14114.	1.6	3
14207	Nanostructure of Cr <sub>2</sub> CO <sub>2</sub> MXene Supported Single Metal Atom as an Efficient Bifunctional Electrocatalyst for Overall Water Splitting. <i>ACS Applied Energy Materials</i> , 2019, 2, 6851-6859.	2.5	81

#	ARTICLE	IF	CITATIONS
14208	Cytotoxicity of C <sub>2</sub> N Originating from Oxidative Stress Instead of Membrane Stress. ACS Applied Materials & Interfaces, 2019, 11, 34575-34585.	4.0	13
14209	Cu <sub>x</sub> O <sub>y</sub> @COF: An efficient heterogeneous catalyst system for CO <sub>2</sub> cycloadditions under ambient conditions. Journal of CO <sub>2</sub> Utilization, 2019, 34, 533-542.	3.3	42
14210	Complete active space and corrected density functional theories helping each other to describe vertical electronic $\hat{a}^*_{\text{exc}}$ excitations in prototype multiple-bonded molecules. Journal of Chemical Physics, 2019, 151, 024111.	1.2	8
14211	Rh nanoroses for isopropanol oxidation reaction. Applied Catalysis B: Environmental, 2019, 259, 118082.	10.8	44
14212	Mechanistic Insights into Selective CO <sub>2</sub> Conversion via RWGS on Transition Metal Phosphides: A DFT Study. Journal of Physical Chemistry C, 2019, 123, 22918-22931.	1.5	25
14213	Magnetic Anisotropy of Graphene-Coated Thin Iron Films. Physics of the Solid State, 2019, 61, 1310-1315.	0.2	3
14214	Effect of anionic and cationic substitutions on the magnetic property of hydrated $\hat{a}^*_{\text{exc}}$ -MnO <sub>2</sub> . AIP Conference Proceedings, 2019, , .	0.3	0
14215	Computational assessment on the Tolman cone angles for P-ligands. Dalton Transactions, 2019, 48, 15036-15048.	1.6	62
14216	Nickel Hydrides under High Pressure. Journal of Physical Chemistry C, 2019, 123, 24243-24247.	1.5	3
14217	Unveiling the Role of Oxygen Vacancy in Li <sub>2</sub> MnO <sub>3</sub> upon Delithiation. Journal of Physical Chemistry C, 2019, 123, 23403-23409.	1.5	14
14218	Efficient Vibrational Energy Redistribution between Stretching Modes: State-to-State Quantum Scattering of $H_2$ $H_2$ $O_2$ from Cu(111). Physical Review Letters, 2019, 123, 106001.	2.9	16
14219	Density functional theory study of the effect of Vanadium doping on electronic and optical properties of NiO. International Journal of Computational Materials Science and Engineering, 2019, 08, 1950007.	0.5	1
14220	Density Functional Theory Study of Defect Induced Ferromagnetism and Half-Metallicity in Ca <sub>2</sub> Based Monolayer for Spintronics Applications. ACS Applied Nano Materials, 2019, 2, 6152-6161.	2.4	15
14221	Anticorrosion mechanism of Cr-doped nickel-base alloy in Br/O environment: a DFT study. Molecular Simulation, 2019, 45, 1506-1514.	0.9	2
14222	Band structures, effective masses and exciton binding energies of perovskite polymorphs of CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> . Solar Energy, 2019, 190, 617-621.	2.9	19
14223	Reactivity and selectivity descriptors of dioxygen activation routes on metal oxides. Journal of Catalysis, 2019, 377, 692-710.	3.1	9
14224	Triggered reversible phase transformation between layered and spinel structure in manganese-based layered compounds. Nature Communications, 2019, 10, 3385.	5.8	42
14225	Zn-Doped Cu(100) facet with efficient catalytic ability for the CO <sub>2</sub> electroreduction to ethylene. Physical Chemistry Chemical Physics, 2019, 21, 21341-21348.	1.3	25

#	ARTICLE	IF	CITATIONS
14226	Linking capacity loss and retention of nickel hexacyanoferrate to a two-site intercalation mechanism for aqueous Mg <sup>2+</sup> and Ca <sup>2+</sup> ions. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20177-20188.	1.3	24
14227	Monoclinic gallium selenide: an AgGaS <sub>2</sub> -type structure variant with balanced infrared nonlinear optical performance. <i>Journal of Materials Chemistry C</i> , 2019, 7, 11752-11756.	2.7	30
14228	Geometries, electronic and magnetic properties of Aun and Aun-1Li (n=2-6) clusters using density functional theory. <i>AIP Conference Proceedings</i> , 2019, , .	0.3	0
14229	<i>Ab-Initio</i> Study of (111) to (001) Texture Transformation in Ag Thin Films. <i>Materials Transactions</i> , 2019, 60, 437-440.	0.4	1
14230	TiO <sub>2</sub> â€“SrTiO <sub>3</sub> Biphase Nanoceramics as Advanced Thermoelectric Materials. <i>Materials</i> , 2019, 12, 2895.	1.3	11
14231	Single molybdenum atom anchored on 2D Ti <sub>2</sub> NO <sub>2</sub> MXene as a promising electrocatalyst for N <sub>2</sub> fixation. <i>Nanoscale</i> , 2019, 11, 18132-18141.	2.8	55
14232	Theoretical Investigation on the Single Transition-Metal Atom-Decorated Defective MoS <sub>2</sub> for Electrocatalytic Ammonia Synthesis. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 36506-36514.	4.0	88
14233	Theoretical Investigation of the Electrochemical Performance of Transition Metal Nitrides for Lithiumâ€“Sulfur Batteries. <i>Journal of Physical Chemistry C</i> , 2019, 123, 25025-25030.	1.5	35
14234	Strong Vibrational Relaxation of NO Scattered from Au(111): Importance of the Adiabatic Potential Energy Surface. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5969-5974.	2.1	35
14235	Structural stability of SrZrO <sub>3</sub> perovskite and improvement in electronic and optical properties by Ca and Ba doping for optoelectronic applications: a DFT approach. <i>Philosophical Magazine</i> , 2019, 99, 3133-3145.	0.7	14
14236	Topological insulator nanoribbons â€“ A new paradigm for high thermoelectric performance. <i>Nano Energy</i> , 2019, 66, 104092.	8.2	6
14237	Influence of trigonal deformation on band structure and Seebeck coefficient of tellurium. <i>Journal of Physics and Chemistry of Solids</i> , 2019, 135, 109114.	1.9	17
14238	The role of Mn and Fe transition metal atoms mediation on the aniline adsorption by B40 fullerene: A computational investigation. <i>Journal of Molecular Liquids</i> , 2019, 294, 111638.	2.3	17
14239	Adsorption, Absorption, Diffusion, and Permeation of Hydrogen and Its Isotopes in bcc Bulk Fe and Fe(100) Surface: Plane Wave-Based Density Functional Theoretical Investigations. <i>Journal of Physical Chemistry C</i> , 2019, 123, 23951-23966.	1.5	11
14240	Mn promotes the rate of nucleation and growth of precipitates by increasing Frenkel pairs in Feâ€“Cu based alloys. <i>RSC Advances</i> , 2019, 9, 19620-19629.	1.7	1
14241	Vanadium occupation and its leachability differences in trioctahedral and dioctahedral mica. <i>RSC Advances</i> , 2019, 9, 27615-27624.	1.7	10
14242	Structural, electronic and magnetic properties of MxPt1-X, (M= Co, Ni and V) binary alloys. <i>Heliyon</i> , 2019, 5, e02433.	1.4	6
14243	Co-segregation behavior of Sc and Zr solutes and their effect on the Al $\epsilon$ 5 (210) [110] symmetrical tilt grain boundary: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19437-19446.	1.3	14

#	ARTICLE	IF	CITATIONS
14244	Magnetic, Electronic, Mechanic, Anisotropic Elastic and Vibrational Properties of Antiferromagnetic Ru <sub>2</sub> TGa (T = Cr, Mn, and Co) Heusler Alloys. <i>Journal of Electronic Materials</i> , 2019, 48, 7608-7622.	1.0	10
14245	Effect of Cu/Al doping on electronic structure and optical properties of ZnO. <i>Results in Physics</i> , 2019, 15, 102649.	2.0	32
14246	Semilocal exchange-correlation potentials for solid-state calculations: Current status and future directions. <i>Journal of Applied Physics</i> , 2019, 126, .	1.1	41
14247	Theoretical investigation of structural, magnetic and elastic properties of half Heusler LiCrZ (Z = P, Tj ETQq1 1 0.784314 rgBJ /Overlo	1.3	41
14248	Carotenoid Nuclear Reorganization and Interplay of Bright and Dark Excited States. <i>Journal of Physical Chemistry B</i> , 2019, 123, 8628-8643.	1.2	27
14249	Electronic and structural properties of low-index Li <sub>2</sub> Al <sub>3</sub> Zr surfaces by first-principle calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019, 66, 101645.	0.7	16
14250	Bifunctional Electrocatalytic Activity of Bis(iminothiolato)nickel Monolayer for Overall Water Splitting. <i>Journal of Physical Chemistry C</i> , 2019, 123, 25651-25656.	1.5	17
14251	First-principles study of bubble formation and cohesion properties of hydrogen at Fe/W interfaces. <i>International Journal of Hydrogen Energy</i> , 2019, 44, 26469-26476.	3.8	10
14252	Stabilizing Low-Coordinated O Ions To Operate Cationic and Anionic Redox Chemistry of Li-Ion Battery Materials. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 37768-37778.	4.0	13
14253	Active Sites in Single-Layer BiOX (X = Cl, Br, and I) Catalysts for the Hydrogen Evolution Reaction. <i>Inorganic Chemistry</i> , 2019, 58, 13195-13202.	1.9	29
14254	The top-down crystallisation of Mercury's core. <i>Earth and Planetary Science Letters</i> , 2019, 528, 115838.	1.8	11
14255	Theoretical prediction and experimental study on catalytic mechanism of incorporated Ni for hydrogen absorption of Mg. <i>International Journal of Hydrogen Energy</i> , 2019, 44, 27885-27895.	3.8	23
14256	Structural and electronic properties of VSb <sub>2</sub> and FeSb <sub>2</sub> . <i>Materials Today: Proceedings</i> , 2019, 13, 991-997.	0.9	7
14257	Ab Initio/Transition-State Theory Study of the Reactions of $\dot{S}_{5H_{9}}$ Species of Relevance to 1,3-Pentadiene, Part I: Potential Energy Surfaces, Thermochemistry, and High-Pressure Limiting Rate Constants. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9019-9052.	1.1	19
14258	Tailoring a Molecule's Optical Absorbance Using Surface Plasmonics. <i>Journal of Physical Chemistry C</i> , 2019, 123, 26498-26508.	1.5	4
14259	Ab Initio Study of Ternary W <sub>5</sub> Si <sub>3</sub> Type TM <sub>5</sub> Sn <sub>2</sub> X Compounds (TM = Nb, Ti and X = Al, Si). <i>Materials</i> , 2019, 12, 3217.	1.3	5
14260	The Cr impurity effect on the optical properties of the Ti <sub>2</sub> N graphene-like materials: a DFT study. <i>International Nano Letters</i> , 2019, 9, 289-298.	2.3	1
14261	A detailed physical analysis on the interaction between transition elements (3d, 4d and 5d) and point defects in molybdenum for nuclear material application. <i>Journal of Nuclear Materials</i> , 2019, 527, 151805.	1.3	6

#	ARTICLE	IF	CITATIONS
14262	Geometric and Electronic Structures of $VB_4^{+0}$ Clusters and Reactivity of the Cationic Cluster with Methane from Quantum Chemical Calculations. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9223-9233.	1.1	3
14263	Temperature-dependent gas sensing properties of porous silicon oxycarbide: Insight from first principles. <i>Applied Surface Science</i> , 2019, 493, 1286-1290.	3.1	10
14264	Solvation effect on binding modes of model lignin dimer compounds on MWW 2D-zeolite. <i>Journal of Chemical Physics</i> , 2019, 151, 114708.	1.2	2
14265	First principles study of structural, electronic and mechanical properties of metal carbides $M_2C$ and $MC_2$ (M= Os, Ir, Pt). <i>Solid State Communications</i> , 2019, 291, 43-50.	0.9	8
14266	Electronic structure and magnetic properties of $XMgC$ (X=Li, Na, K, Rb). <i>Solid State Communications</i> , 2019, 291, 36-42.	0.9	2
14267	Screened hybrid meta-GGA exchange-correlation functionals for extended systems. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3002-3015.	1.3	16
14268	Theoretical study on the influence of electric field direction on the photovoltaic performance of aryl amine organic dyes for dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2019, 43, 651-661.	1.4	7
14269	A hypervalent and cubically coordinated molecular phase of $IF_8$ predicted at high pressure. <i>Chemical Science</i> , 2019, 10, 2543-2550.	3.7	36
14270	Effect of V and Y doping on the structural, optical and electronic properties of CdS (hexagonal and) $Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5$	1.1	32
14271	Insight into the Discharge Products and Mechanism of Room-Temperature Sodium Sulfur Batteries: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 3988-3995.	1.5	30
14272	Metal-free electrocatalyst for reducing nitrogen to ammonia using a Lewis acid pair. <i>Journal of Materials Chemistry A</i> , 2019, 7, 4865-4871.	5.2	115
14273	Effect of Silica on Reduction Behaviors of Hematite-carbon Composite Compact at 1223-1373 K. <i>ISIJ International</i> , 2019, 59, 227-234.	0.6	11
14274	Enhancing the efficiency of density functionals with an improved iso-orbital indicator. <i>Physical Review B</i> , 2019, 99, .	1.1	37
14275	Role of Mineral Surfaces in Prebiotic Chemical Evolution. In <i>Silico Quantum Mechanical Studies</i> . <i>Life</i> , 2019, 9, 10.	1.1	44
14276	Two-dimensional honeycomb borophene oxide: strong anisotropy and nodal loop transformation. <i>Nanoscale</i> , 2019, 11, 2468-2475.	2.8	84
14277	Single-Metal Atom Anchored on Boron Monolayer ( $B_{12}$ ) as an Electrocatalyst for Nitrogen Reduction into Ammonia at Ambient Conditions: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4274-4281.	1.5	86
14278	Prediction of phonon-mediated superconductivity in two-dimensional $Mo_2B_2$ . <i>Journal of Materials Chemistry C</i> , 2019, 7, 2589-2595.	2.7	39
14279	Adsorption of metal atoms on silicene: stability and quantum capacitance of silicene-based electrode materials. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4276-4285.	1.3	29

#	ARTICLE	IF	CITATIONS
14280	Bis(6-diphenylphosphinoacenaphth-5-yl)telluride as a ligand toward coinage metal chlorides. Dalton Transactions, 2019, 48, 2635-2645.	1.6	3
14281	Effect of Defects on the Properties of ZnGa <sub>2</sub> O <sub>4</sub> Thin-Film Transistors. ACS Applied Electronic Materials, 2019, 1, 253-259.	2.0	18
14282	A Systematic Theoretical Study of Water Gas Shift Reaction on Cu(111) and Cu(110): Potassium Effect. ACS Catalysis, 2019, 9, 2261-2274.	5.5	77
14283	Hydrogen Chemisorption Isotherms on Platinum Particles at Catalytic Temperatures: Langmuir and Two-Dimensional Gas Models Revisited. Journal of Physical Chemistry C, 2019, 123, 8447-8462.	1.5	28
14284	DFT Simulation on Interaction of H <sub>2</sub> O Molecules with ZnS and Cu-Activated Surfaces. Journal of Physical Chemistry C, 2019, 123, 3048-3057.	1.5	36
14285	Insight of the thermal conductivity of $\mu$ -iron at Earth's core conditions from the newly developed direct <i>ab initio</i> methodology. Journal of Applied Physics, 2019, 125, .	1.1	5
14286	Solid emission color tuning of organic charge transfer cocrystals based on planar $\pi$ -conjugated donors and TCNB. Journal of Solid State Chemistry, 2019, 272, 96-101.	1.4	14
14287	First-principles investigation on detection of phosgene gas molecules using phosphorene nanosheet device. Chemical Physics Letters, 2019, 717, 99-106.	1.2	52
14288	Energy Dissipation Effects on the Adsorption Dynamics of N <sub>2</sub> on W(100). Journal of Physical Chemistry C, 2019, 123, 2900-2910.	1.5	5
14289	Engineering the magnetic properties of PtSe <sub>2</sub> monolayer through transition metal doping. Journal of Physics Condensed Matter, 2019, 31, 145502.	0.7	36
14290	Half-metallic properties of transition metals adsorbed on WS <sub>2</sub> monolayer: A first-principles study. Journal of Magnetism and Magnetic Materials, 2019, 481, 129-135.	1.0	17
14291	Investigation on two new antimony-based quaternary chalcogenides: Na <sub>6</sub> CdSb <sub>4</sub> S <sub>10</sub> and Na <sub>3</sub> CdSbSe <sub>4</sub> . New Journal of Chemistry, 2019, 43, 3350-3356.	1.4	0
14292	Uniform Pd <sub>0.33</sub> Ir <sub>0.67</sub> nanoparticles supported on nitrogen-doped carbon with remarkable activity toward the alkaline hydrogen oxidation reaction. Journal of Materials Chemistry A, 2019, 7, 3161-3169.	5.2	50
14293	Structural Change Analysis of Cerianite in Weathered Residual Rare Earth Ore by Mechanochemical Reduction Using X-Ray Absorption Fine Structure. Minerals (Basel, Switzerland), 2019, 9, 267.	0.8	10
14294	sp <sup>3</sup> C-H Borylation Catalyzed by Iridium(III) Triboryl Complex: Comprehensive Theoretical Study of Reactivity, Regioselectivity, and Prediction of Excellent Ligand. Journal of the American Chemical Society, 2019, 141, 9854-9866.	6.6	44
14295	Reassessment of the Mechanisms of Thermal C-H Bond Activation of Methane by Cationic Magnesium Oxides: A Critical Evaluation of the Suitability of Different Density Functionals. ChemPhysChem, 2019, 20, 1812-1821.	1.0	5
14296	Organic Semiconductors Derived from Dinaphtho-Fused <i>s</i> -Indacenes: How Molecular Structure and Film Morphology Influence Thin-Film Transistor Performance. Chemistry of Materials, 2019, 31, 6962-6970.	3.2	41
14297	Molecular Modeling of Interactions between N-(Carboxymethyl)-N-tetradecylglycine and Fluorapatite. Minerals (Basel, Switzerland), 2019, 9, 278.	0.8	7



#	ARTICLE	IF	CITATIONS
14298	Understanding of relationship between dopant and substitutional site to develop novel phase-change materials based on $\text{In}_3\text{SbTe}_2$ . Japanese Journal of Applied Physics, 2019, 58, SBBB02.	0.8	15
14299	Interface reaction of high-strength low-alloy steel with $\text{Al-43.4Zn-1.6Si}$ (wt.%) metallic coating. Journal of Iron and Steel Research International, 2019, 26, 1304-1314.	1.4	2
14300	Theoretical Screening of Single-Atom-Embedded MoSSe Nanosheets for Electrocatalytic $\text{N}_2$ Fixation. Journal of Physical Chemistry C, 2019, 123, 14501-14507.	1.5	72
14301	Hydrogen-enhanced decohesion mechanism of the special $\langle 5(012)[100] \rangle$ grain boundary in Ni with Mo and C solutes. Computational Materials Science, 2019, 167, 100-110.	1.4	37
14302	Silicene nanosheet device with nanopore to identify the nucleobases – A first-principles perspective. Chemical Physics Letters, 2019, 730, 70-75.	1.2	28
14303	The selective hydrogenation of furfural over intermetallic compounds with outstanding catalytic performance. Green Chemistry, 2019, 21, 5352-5362.	4.6	92
14304	Mechanism of the Palladium-Catalyzed $\text{C}(\text{sp}^3)\text{-H}$ Arylation of Aliphatic Amines: Unraveling the Crucial Role of Silver(I) Additives. ACS Catalysis, 2019, 9, 6672-6680.	5.5	38
14305	$\text{Cs}_2\text{CdVO}_6\text{Cl}_2$ and $\text{Cs}_3\text{CdVO}_{12}\text{Br}$ : two new non-centrosymmetric oxyhalides containing $d^{0}$ and $d^{10}$ cations and exhibiting second harmonic generation activity. Dalton Transactions, 2019, 48, 10642-10651.	1.6	9
14306	DFT study on electronic and optical properties of graphene modified by phosphorus. Materials Research Express, 2019, 6, 085635.	0.8	17
14307	High Electron Mobility in [1]Benzothieno[3,2- <i>b</i> ]benzothiophene-Based Field-Effect Transistors: Toward n-Type BTBTs. Chemistry of Materials, 2019, 31, 5254-5263.	3.2	55
14308	Route to achieving enhanced quantum capacitance in functionalized graphene based supercapacitor electrodes. Journal of Physics Condensed Matter, 2019, 31, 475502.	0.7	26
14309	Comparison of first-principles methods to extract magnetic parameters in ultrathin films: Co/Pt(111). Physical Review B, 2019, 99, .	1.1	39
14310	Benchmark of Density Functionals for the Calculation of the Redox Potential of $\text{Fe}^{3+}/\text{Fe}^{2+}$ Within Protein Coordination Shells. Frontiers in Chemistry, 2019, 7, 391.	1.8	14
14311	Hexagonal CuCl Monolayer for Water Splitting: A DFT Study. ACS Applied Nano Materials, 2019, 2, 4238-4246.	2.4	25
14312	Thickness dependent thermal stability of 2D gallene. Chemical Communications, 2019, 55, 8872-8875.	2.2	19
14313	New Members of SHG Active Dugganite Family, $\text{A}_3\text{BC}_3\text{D}_2\text{O}_{14}$ (A = Ba, Pb; B = Te, Sb; C = Al, Ga, Fe, Zn; D) $\text{J. Eur. Ceram. Soc.}$ 2019, 39, 1743-1748.	1.7	4
14314	$\text{As}$ Monolayer: Vibrational Properties and Raman Spectra. ACS Omega, 2019, 4, 10171-10175.	1.6	13
14315	Effects of Mo alloying on stability and diffusion of hydrogen in the Nb <sub>16</sub> H phase: a first-principles investigation. RSC Advances, 2019, 9, 19495-19500.	1.7	5



#	ARTICLE	IF	CITATIONS
14316	Insight into void formation near grain boundary from phase-field simulations. Nuclear Instruments & Methods in Physics Research B, 2019, 453, 50-55.	0.6	1
14317	Structure and Electrical Performance of Na <sub>2</sub> C <sub>6</sub> O <sub>6</sub> under High Pressure. Journal of Physical Chemistry C, 2019, 123, 17163-17169.	1.5	3
14318	Stability predictions of magnetic M <sub>2</sub> AX compounds. Journal of Physics Condensed Matter, 2019, 31, 405902.	0.7	17
14319	Theoretical Screening of Single Transition Metal Atoms Embedded in MXene Defects as Superior Electrocatalyst of Nitrogen Reduction Reaction. Small Methods, 2019, 3, 1900337.	4.6	213
14320	Configurational Sampling of Noncovalent (Atmospheric) Molecular Clusters: Sulfuric Acid and Guanidine. Journal of Physical Chemistry A, 2019, 123, 6022-6033.	1.1	54
14321	Quantum density functional theory studies of structural, elastic, and opto-electronic properties of ZMoO <sub>3</sub> (Z = Ba and Sr) under pressure. Chinese Physics B, 2019, 28, 066101.	0.7	18
14322	Theoretical study of electronic properties and spin density in Pt-Co alloys. Materials Research Express, 2019, 6, 096514.	0.8	4
14323	Shock compression of niobium from first-principles. Journal of Applied Physics, 2019, 125, .	1.1	11
14324	Improving the Performance of Tao's Mo Non-empirical Density Functional with Broader Applicability in Quantum Chemistry and Materials Science. Journal of Physical Chemistry A, 2019, 123, 6356-6369.	1.1	29
14325	Whether Corrugated or Planar Vacancy Graphene-like Carbon Nitride (g-C <sub>3</sub> N <sub>4</sub> ) Is More Effective for Nitrogen Reduction Reaction?. Journal of Physical Chemistry C, 2019, 123, 17296-17305.	1.5	46
14326	Effect of non-hydrostatic stress on the structure and elasticity of NaCl by first-principles calculation. AIP Advances, 2019, 9, 055014.	0.6	4
14327	Characterization of Ni <sub>3</sub> Sn intermetallic nanoparticles fabricated by thermal plasma process and catalytic properties for methanol decomposition. Science and Technology of Advanced Materials, 2019, 20, 622-631.	2.8	13
14328	Control of the Reaction Mechanism of Alkylaromatics Transalkylation by Means of Molecular Confinement Effects Associated to Zeolite Channel Architecture. ACS Catalysis, 2019, 9, 5935-5946.	5.5	29
14329	Theoretical prediction of germanium selenium nanosheet as a potential anode material for high-performance alkali-metal based battery. Journal of Solid State Chemistry, 2019, 277, 17-24.	1.4	7
14330	First-principles investigations of a new trigonal boron nitride. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 114, 113573.	1.3	3
14331	Cobalt-catalyzed nitrile hydrogenation: Insights into the reaction mechanism and product selectivity from DFT analysis. Surface Science, 2019, 688, 31-44.	0.8	15
14332	Specific Reaction Parameter Density Functional Based on the Meta-Generalized Gradient Approximation: Application to H <sub>2</sub> + Cu(111) and H <sub>2</sub> + Ag(111). Journal of Physical Chemistry A, 2019, 123, 5395-5406.	1.1	28
14333	Low viscosity of the Earth's inner core. Nature Communications, 2019, 10, 2483.	5.8	32

#	ARTICLE	IF	CITATIONS
14334	Interface dipoles of Ir(ppy) <sub>3</sub> on Cu(111). <i>Nanoscale</i> , 2019, 11, 12695-12703.	2.8	3
14335	Monolayer triphosphates MP <sub>3</sub> (M = Sn, Ge) with excellent basal catalytic activity for hydrogen evolution reaction. <i>Nanoscale</i> , 2019, 11, 12210-12219.	2.8	76
14336	Graphyne doped with transition-metal single atoms as effective bifunctional electrocatalysts for water splitting. <i>Applied Surface Science</i> , 2019, 492, 8-15.	3.1	74
14337	CO adsorption on Fe-doped vacancy-defected CNTs – A DFT study. <i>Chemical Physics Letters</i> , 2019, 730, 316-320.	1.2	21
14338	Nanoparticle Linker-Controlled Molecular Wire Devices Based on Double Molecular Monolayers. <i>Small</i> , 2019, 15, 1901183.	5.2	9
14339	Catalytic performance of ionic liquid for dehydrochlorination reaction: Excellent activity and unparalleled stability. <i>Applied Catalysis B: Environmental</i> , 2019, 255, 117757.	10.8	19
14340	The role of strong electron correlations in determination of band structure and charge distribution of transition metal dihalide monolayers. <i>Journal of Physics and Chemistry of Solids</i> , 2019, 134, 324-332.	1.9	23
14341	A New Class of Bifunctional Perovskites BaMX <sub>4</sub> (M = Co, Ni, Fe, Mn; X = F, Cl, Br, I): An n-Type Semiconductor with Combined Multiferroic and Photovoltaic Properties. <i>Journal of Physical Chemistry C</i> , 2019, 123, 14303-14311.	1.5	1
14342	Physically-Informed artificial neural networks for atomistic modeling of materials. <i>Nature Communications</i> , 2019, 10, 2339.	5.8	177
14343	DFT insights into the direct desulfurization pathways of DBT and 4,6-DMDBT catalyzed by Co-promoted and Ni-promoted MoS <sub>2</sub> corner sites. <i>Chemical Engineering Science</i> , 2019, 206, 249-260.	1.9	28
14344	Dimension engineering of single-layer PtN <sub>2</sub> with the Cairo tessellation. <i>Journal of Applied Physics</i> , 2019, 125, 204302.	1.1	4
14345	Structural, Elastic, Mechanical and Electronic Properties of NbW-Based Intermetallic Compounds: First-Principles Calculations. <i>Physica Status Solidi (B): Basic Research</i> , 2019, 256, 1800570.	0.7	1
14346	Effect of hydrogen atom and hydrogen filled vacancies on stacking fault energy in $\bar{1}^3$ -Fe by first-principles calculations. <i>International Journal of Hydrogen Energy</i> , 2019, 44, 17136-17145.	3.8	20
14347	Cooperative transport enabling fast Li-ion diffusion in Thio-LISICON Li <sub>10</sub> SiP <sub>2</sub> S <sub>12</sub> solid electrolyte. <i>Nano Energy</i> , 2019, 62, 844-852.	8.2	42
14348	Adsorption of Polyaromatic Backbone Impacts the Performance of Anion Exchange Membrane Fuel Cells. <i>Chemistry of Materials</i> , 2019, 31, 4195-4204.	3.2	91
14349	Dynamics of Cluster Isomerization Induced by Hydrogen Adsorption. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15236-15243.	1.5	12
14350	Etching and Exfoliation Properties of Cr <sub>2</sub> AlC into Cr <sub>2</sub> CO <sub>2</sub> and the Electrocatalytic Performances of 2D Cr <sub>2</sub> CO <sub>2</sub> MXene. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15629-15636.	1.5	29
14351	Material design for Ge <sub>2</sub> Sb <sub>2</sub> Te <sub>5</sub> phase-change material with thermal stability and lattice distortion. <i>Scripta Materialia</i> , 2019, 170, 16-19.	2.6	7

#	ARTICLE	IF	CITATIONS
14352	The behavior of helium atoms in He <sup>+</sup> ion implanted W/Ni bilayer nanocomposite. Applied Surface Science, 2019, 486, 274-280.	3.1	7
14353	Dynamics of dissociative chemisorption of O <sub>2</sub> on Cu(100) surface: A theoretical study. Surface Science, 2019, 688, 45-50.	0.8	7
14354	Electronic structures and thermoelectric properties of polytype phases of bismuth. Journal of Physics and Chemistry of Solids, 2019, 134, 52-57.	1.9	13
14355	Deep insights into the exfoliation properties of MAX to MXenes and the hydrogen evolution performances of 2D MXenes. Journal of Materials Chemistry A, 2019, 7, 15862-15870.	5.2	58
14356	Using Pauli energy to appraise the quality of approximate semilocal non-interacting kinetic energy density functionals. Journal of Chemical Physics, 2019, 150, 204106.	1.2	26
14357	Understanding the effects of metal particle size on the NO <sub>2</sub> reduction from a DFT study. Applied Surface Science, 2019, 489, 1019-1029.	3.1	10
14358	Connecting Solution-Phase to Single-Molecule Properties of Ni(Salophen). Journal of Physical Chemistry Letters, 2019, 10, 3525-3530.	2.1	8
14359	Tuning the electronic and magnetic properties of MoS <sub>2</sub> nanotubes with vacancy defects. RSC Advances, 2019, 9, 17203-17210.	1.7	12
14360	A DFT study about the effects of exchange-correlation functional on the structural and electronic properties of Anatase. Journal of Physics: Conference Series, 2019, 1219, 012019.	0.3	6
14361	First-principles study of molecule adsorption on Ni-decorated monolayer MoS <sub>2</sub> . Journal of Computational Electronics, 2019, 18, 826-835.	1.3	12
14362	Properties of Isolated and TiO <sub>2</sub> (110) Supported Pt <sub>13</sub> Clusters: A Theoretical Study. Topics in Catalysis, 2019, 62, 989-1003.	1.3	11
14363	Phase diagrams, electronic and magnetic properties of the quaternary Heusler alloy NbRhCrAl. Chinese Journal of Physics, 2019, 60, 549-563.	2.0	35
14364	Vanadium extraction from black shale: Enhanced leaching due to fluoride addition. Hydrometallurgy, 2019, 187, 141-148.	1.8	33
14365	Effect of magnesium doping on band gap and optical properties of SrZrO <sub>3</sub> perovskite: A first-principles study. Optik, 2019, 191, 132-138.	1.4	31
14366	Activating peroxydisulfate by morphology-dependent NiO catalysts: Structural origin of different catalytic properties. Applied Catalysis B: Environmental, 2019, 256, 117806.	10.8	44
14367	A DFT study of H <sub>2</sub> O adsorption on the V <sub>2</sub> O <sub>5</sub> (0 0 1) surface including van der Waals interactions. Chemical Physics Letters, 2019, 730, 171-178.	1.2	7
14368	Pressure-Induced Polymorphism of Caprolactam: A Neutron Diffraction Study. Molecules, 2019, 24, 2174.	1.7	4
14369	Short-range ordered structure and phase stability of supersaturated nitrided layer on austenitic stainless steel. Acta Materialia, 2019, 175, 314-323.	3.8	16

#	ARTICLE	IF	CITATIONS
14370	The effect of GGA functionals on the oxygen reduction reaction catalyzed by Pt(111) and FeN <sub>4</sub> doped graphene. <i>Journal of Molecular Modeling</i> , 2019, 25, 180.	0.8	6
14371	Interfacial graphene modulated energetic behavior of the point-defect at the Au/HfO <sub>2</sub> interface. <i>Applied Surface Science</i> , 2019, 489, 608-613.	3.1	4
14372	Synthesis, structure and characterization of a new triphosphate: CsMg <sub>2</sub> P <sub>3</sub> O <sub>10</sub> . <i>Solid State Sciences</i> , 2019, 94, 133-137.	1.5	0
14373	Seeking large Seebeck effects in LaX(X = Mn and Co)O <sub>3</sub> /SrTiO <sub>3</sub> superlattices by exploiting high spin-polarized effects. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14973-14983.	1.3	7
14374	Phonon origin and lattice evolution in charge density wave states. <i>Physical Review B</i> , 2019, 99, .	1.1	27
14375	Strain Effect on the Magnetism of N-Doped Molybdenum Disulfide. <i>Physica Status Solidi (B): Basic Research</i> , 2019, 256, 1900110.	0.7	2
14376	Adsorption and Photodegradation of Acetaldehyde and Ethylene on TiO <sub>2</sub> (001) Surface: Experimental and First Principle Studies. <i>Catalysis Letters</i> , 2019, 149, 2728-2738.	1.4	9
14377	Gold(sulfide) sulfide: unusual bonding and an unexpected computational challenge in a simple solid. <i>Chemical Science</i> , 2019, 10, 6467-6475.	3.7	12
14378	Hydrogen-rich syngas production from chemical looping steam reforming of bio-oil model compound: Effect of bimetal on LaNi <sub>0.8</sub> M <sub>0.2</sub> O <sub>3</sub> (M = Fe, Co, Cu, and Mn). <i>International Journal of Energy Research</i> , 2019, 43, 4534-4545.	2.2	18
14379	DFT Study on the Interaction Properties of V-Series Nerve Agent Molecules on Novel Bismuthene Nanotubes. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2019, 29, 2226-2236.	1.9	19
14380	Interfacial interaction and effects of GaAs/Graphene hetero-structures studied by First-principle calculations. <i>Journal of Alloys and Compounds</i> , 2019, 795, 351-360.	2.8	3
14381	High-Temperature Ferromagnetism in an Fe <sub>3</sub> P Monolayer with a Large Magnetic Anisotropy. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2733-2738.	2.1	79
14382	Halogen bonds in N-bromosuccinimide and other N-halosuccinimides. <i>Structural Chemistry</i> , 2019, 30, 2205-2215.	1.0	6
14383	Study of the adsorption of NH <sub>3</sub> and NO <sub>x</sub> on the nano- $\gamma$ -Fe <sub>2</sub> O <sub>3</sub> (001) surface with density functional theory. <i>Applied Surface Science</i> , 2019, 487, 171-179.	3.1	39
14384	Topological analysis of CeMn <sub>5</sub> (M = Co, Rh) electron charge densities. <i>Computational Materials Science</i> , 2019, 164, 205-217.	1.4	3
14385	Computational Screening of Electrocatalytic Activity of Transition Metal-Doped CdS Nanotubes for Water Splitting. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13419-13427.	1.5	10
14386	Phase stability, mechanical and electronic properties of Hf-Te alloys from first-principles calculations. <i>Chinese Journal of Physics</i> , 2019, 60, 122-132.	2.0	6
14387	Effect on Schottky Barrier of Graphene/WSe <sub>2</sub> Heterostructure With Vertical Electric Field and Biaxial Strain. <i>Physica Status Solidi (B): Basic Research</i> , 2019, 256, 1900161.	0.7	14

#	ARTICLE	IF	CITATIONS
14388	Thermal stability of aluminum oxide nanoparticles: role of oxygen concentration. <i>Inorganic Chemistry Frontiers</i> , 2019, 6, 1701-1706.	3.0	6
14389	Structural, Magnetic and Electronic Properties of 3d Transition-Metal Atoms Adsorbed Monolayer BC2N: A First-principles Study. <i>Materials</i> , 2019, 12, 1601.	1.3	8
14390	An investigation of thin Zn films on 4H-SiC(0001) graphene. <i>Applied Surface Science</i> , 2019, 487, 1348-1355.	3.1	8
14391	Pressure-induced structure, vibrational properties, and initial decomposition mechanisms of $\hat{\Gamma}$ -HMX crystal: A periodic DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 90, 144-152.	1.3	5
14392	Energy framework approach to the supramolecular reactions: interplay of the secondary bonding interaction in $\text{Ph}_2\text{E}_2$ ( $\text{E} = \text{Se}, \text{Te}$ )/ $\text{I-C}_6\text{F}_4\text{-I}$ co-crystals. <i>New Journal of Chemistry</i> , 2019, 43, 7941-7949.	1.4	22
14393	Nonlinear elasticity of $\hat{\Gamma}$ -Fe: The pressure effect. <i>Physical Review B</i> , 2019, 99, .	1.1	2
14394	Theoretical Study of the Water-Gas Shift Reaction on a Au/Hematite Model Catalyst. <i>Topics in Catalysis</i> , 2019, 62, 908-917.	1.3	6
14395	Single Mo atoms supported on N-Doped carbon with N/C edge-site for enhanced electrochemical hydrogen evolution. <i>International Journal of Hydrogen Energy</i> , 2019, 44, 14861-14868.	3.8	26
14396	Porous size dependent g-C <sub>3</sub> N <sub>4</sub> for efficient photocatalysts: Regulation synthesizes and physical mechanism. <i>Materials Today Energy</i> , 2019, 13, 11-21.	2.5	41
14397	Green synthesis of zinc doped cobalt ferrite nanoparticles: Structural, optical, photocatalytic and antibacterial studies. <i>Nano Structures Nano Objects</i> , 2019, 19, 100322.	1.9	98
14398	Selenium Edge as a Selective Anchoring Site for Lithium-Sulfur Batteries with $\text{MoSe}_2$ /Graphene-Based Cathodes. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 19986-19993.	4.0	67
14399	Structural, vibrational and electronic properties of $\text{SnMBO}_4$ ( $\text{M} = \text{Al}, \text{Ga}$ ): a predictive hybrid DFT study. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 345701.	0.7	6
14400	Structure and Dynamics of Water at the Water-Air Interface Using First-Principles Molecular Dynamics Simulations. II. NonLocal vs Empirical van der Waals Corrections. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3836-3843.	2.3	12
14401	Crystal structure prediction of ReN at high pressure: a new incompressible phase. <i>Phase Transitions</i> , 2019, 92, 595-602.	0.6	1
14402	DFT Study on the Interaction of Subnanometer Cobalt Clusters with Pristine/Defective Graphene. <i>Bulletin of the Korean Chemical Society</i> , 2019, 40, 446-452.	1.0	6
14403	Competition between formation of $\text{Al}_2\text{O}_3$ and $\text{Cr}_2\text{O}_3$ in oxidation of $\text{Al}_0.3\text{CoCrCuFeNi}$ high entropy alloy: A first-principles study. <i>Scripta Materialia</i> , 2019, 168, 139-143.	2.6	28
14404	DFT modelling of the edge dislocation in 4H-SiC. <i>Journal of Materials Science</i> , 2019, 54, 10737-10745.	1.7	13
14405	Insight into delithiation process on the $\text{LiFePO}_4$ (010) surface from a novel viewpoint of the work function. <i>Solid State Ionics</i> , 2019, 338, 25-30.	1.3	10

#	ARTICLE	IF	CITATIONS
14406	NO gas sensor based on ZnGa <sub>2</sub> O <sub>4</sub> epilayer grown by metalorganic chemical vapor deposition. <i>Scientific Reports</i> , 2019, 9, 7459.	1.6	50
14407	The performance of adsorption, dissociation and diffusion mechanism of hydrogen on the Ti-doped ZrCo(110) surface. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12597-12605.	1.3	14
14408	Stabilizing the metastable superhard material wurtzite boron nitride by three-dimensional networks of planar defects. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 11181-11186.	3.3	19
14409	Alloy structure of rare earth Ce with Pt base metal, and the adsorption of CO. <i>Materials Research Express</i> , 2019, 6, 046538.	0.8	0
14410	Perceptions on the adsorption of COPD biomarker vapors on violet phosphorene nanosheet - A first-principles study. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 91, 22-29.	1.3	27
14411	Implications of Oxygen-Sulfur Exchange on Structural, Electronic Properties, and Stability of Alkali-Metal Hexatitanates. <i>Physica Status Solidi (B): Basic Research</i> , 2019, 256, 1800568.	0.7	7
14412	Foam-like Co <sub>9</sub> S <sub>8</sub> /Ni <sub>3</sub> S <sub>2</sub> heterostructure nanowire arrays for efficient bifunctional overall water-splitting. <i>Applied Catalysis B: Environmental</i> , 2019, 253, 246-252.	10.8	138
14413	General adsorption model for H <sub>2</sub> S, H <sub>2</sub> Se, H <sub>2</sub> Te, NH <sub>3</sub> , PH <sub>3</sub> , AsH <sub>3</sub> and SbH <sub>3</sub> on the V <sub>2</sub> O <sub>5</sub> (0 0 1) surface including the van der Waals interaction. <i>Chemical Physics Letters</i> , 2019, 720, 58-63.	1.2	30
14414	First principle study of the adsorption of formaldehyde molecule on intrinsic and doped BN sheet. <i>Chemical Physics Letters</i> , 2019, 726, 77-82.	1.2	14
14415	Chemical optimization towards superior electrocatalysis of Janus 1T-MoSX (X = O, Se, Te) for hydrogen evolution: Small composition tuning makes big difference. <i>Electrochimica Acta</i> , 2019, 310, 153-161.	2.6	9
14416	Density functional theory study of furfural electrochemical oxidation on the Pt (111) surface. <i>Journal of Catalysis</i> , 2019, 373, 322-335.	3.1	37
14417	Ammonia borane dehydrogenation tendencies using Pt <sub>4</sub> , Au <sub>4</sub> , and Pt <sub>2</sub> Au <sub>2</sub> clusters as catalysts. <i>Molecular Catalysis</i> , 2019, 471, 9-20.	1.0	8
14418	First-Principles Kinetic and Spectroscopic Insights into Single-Atom Catalysis. <i>ACS Catalysis</i> , 2019, 9, 5002-5010.	5.5	37
14419	Electronic structures and magnetic properties of (Al, Cr) co-doped 4H-SiC: a first-principles study. <i>Materials Research Express</i> , 2019, 6, 096316.	0.8	2
14420	Long-range screened hybrid-functional theory satisfying the local-density linear response. <i>Physical Review A</i> , 2019, 99, .	1.0	16
14421	Renormalized interactions in truncated cluster expansions. <i>Physical Review B</i> , 2019, 99, .	1.1	9
14422	Broken symmetry states of metallacrowns: Distribution of spins and the $\langle \mathbf{m}_i \mathbf{g} \mathbf{m}_i \rangle$ tensor. <i>Physical Review B</i> , 2019, 99, .	1.1	5
14423	Molecular structure and electron accepting-donating capacity of hydroxylated La@C <sub>82</sub> endohedral metallofullerene. <i>Chemical Physics</i> , 2019, 523, 114-123.	0.9	7



#	ARTICLE	IF	CITATIONS
14424	Optical properties of oxygen vacancy in gamma-LiAlO <sub>2</sub> : A computational study. Chemical Physics Letters, 2019, 727, 85-89.	1.2	5
14425	Transferability of the SRP32-vdW specific reaction parameter functional to CHD <sub>3</sub> dissociation on Pt(110)-(2 Å <sup>-1</sup> ). Journal of Chemical Physics, 2019, 150, 124702.	1.2	17
14426	Theoretical calculations on half-metallic results properties of FeZrX (X = P, As, Sb and Bi) half-Heusler compounds: density functional theory. Materials Research Express, 2019, 6, 086102.	0.8	17
14427	Large Second Harmonic Generation (SHG) Effect and High Laser-Induced Damage Threshold (LIDT) Observed Coexisting in Gallium Selenide. Angewandte Chemie, 2019, 131, 8171-8175.	1.6	37
14428	Large Second Harmonic Generation (SHG) Effect and High Laser-Induced Damage Threshold (LIDT) Observed Coexisting in Gallium Selenide. Angewandte Chemie - International Edition, 2019, 58, 8087-8091.	7.2	145
14429	{Zn <sub>6</sub> } Cluster Based Metal-Organic Framework with Enhanced Room-Temperature Phosphorescence and Optoelectronic Performances. Inorganic Chemistry, 2019, 58, 6215-6221.	1.9	231
14430	Analysis of the Interaction Between Classical and Quantum Plasmons via FDTD-TDDFT Method. IEEE Journal on Multiscale and Multiphysics Computational Techniques, 2019, 4, 111-118.	1.4	9
14431	The mixing state of mineral dusts with typical anthropogenic pollutants: A mechanism study. Atmospheric Environment, 2019, 209, 192-200.	1.9	7
14432	Segregation of Sc and its effects on the strength of Al 5 (210) [100] symmetrical tilt grain boundary. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2019, 756, 389-395.	2.6	16
14433	From the Terrace Contraction to the Hexameric Sulfur Phase in the Au(100) Surface: A Combined Density Functional Theory and Scanning Tunneling Microscopy Study. Journal of Physical Chemistry C, 2019, 123, 12183-12194.	1.5	0
14434	Corrosion Behavior of a Pyrite and Arsenopyrite Galvanic Pair in the Presence of Sulfuric Acid, Ferric Ions and HQ0211 Bacterial Strain. Minerals (Basel, Switzerland), 2019, 9, 169.	0.8	7
14435	Understanding the Photocatalytic Properties of Pt/CeO <sub>x</sub> /TiO <sub>2</sub> : Structural Effects on Electronic and Optical Properties. ChemPhysChem, 2019, 20, 1624-1629.	1.0	8
14436	Electronically-Coupled Phase Boundaries in $\text{Fe}_2\text{O}_3/\text{Fe}_3\text{O}_4$ Nanocomposite Photoanodes for Enhanced Water Oxidation. ACS Applied Nano Materials, 2019, 2, 334-342.	2.4	32
14437	Catalytic upgrading of ethanol to <i>n</i> -butanol using an aliphatic Mn-PNP complex: theoretical insights into reaction mechanisms and product selectivity. Catalysis Science and Technology, 2019, 9, 2794-2805.	2.1	19
14438	Enhancing the Catalytic Activity of Tri-iodide Reduction by Tuning the Surface Electronic Structure of PtPd Alloy Nanocrystals. Journal of Physical Chemistry C, 2019, 123, 12722-12729.	1.5	7
14439	All-electron fully relativistic Kohn-Sham theory for solids based on the Dirac-Coulomb Hamiltonian and Gaussian-type functions. Physical Review B, 2019, 99, .	1.1	24
14440	Towards an integrated modeling of the plasma-solid interface. Frontiers of Chemical Science and Engineering, 2019, 13, 201-237.	2.3	34
14441	Nonradical activation of peroxydisulfate promoted by oxygen vacancy-laden NiO for catalytic phenol oxidative polymerization. Applied Catalysis B: Environmental, 2019, 254, 166-173.	10.8	107



#	ARTICLE	IF	CITATIONS
14442	Enhanced photovoltaic performance of dye-sensitized solar cells by the adsorption of Zn-porphyrin dye molecule on TiO <sub>2</sub> surfaces. <i>Journal of Alloys and Compounds</i> , 2019, 794, 35-44.	2.8	4
14443	Energetics and kinetics of hydrogen at the grain boundary of the Ni alloys: A first-principles study. <i>Journal of Alloys and Compounds</i> , 2019, 795, 343-350.	2.8	8
14444	Non-intuitive concomitant enhancement of dielectric permittivity, breakdown strength and energy density in percolative polymer nanocomposites by trace Ag nanodots. <i>Journal of Materials Chemistry A</i> , 2019, 7, 15198-15206.	5.2	61
14445	FeN <sub>3</sub> -embedded carbon as an efficient sorbent for mercury adsorption: A theoretical study. <i>Chemical Engineering Journal</i> , 2019, 374, 1337-1343.	6.6	19
14446	A phosphorescent iridium probe for sensing polarity in the endoplasmic reticulum and <i>in vivo</i> . <i>Dalton Transactions</i> , 2019, 48, 7728-7734.	1.6	11
14447	Hopf-chain networks evolved from triple points. <i>Physical Review B</i> , 2019, 99, .	1.1	17
14448	Tuning electron density of metal nickel by support defects in Ni/ZrO <sub>2</sub> for selective hydrogenation of fatty acids to alkanes and alcohols. <i>Applied Catalysis B: Environmental</i> , 2019, 253, 170-178.	10.8	133
14449	Effects of O <sub>2</sub> and H <sub>2</sub> O in the Oxidative Steam-Reforming Reaction of Ethanol on Rh Catalysts. <i>Journal of Physical Chemistry C</i> , 2019, 123, 11649-11661.	1.5	10
14450	A reactive force field molecular dynamics study of molecular nitrogen and water mixtures under high temperature and high pressure. <i>Journal of Molecular Modeling</i> , 2019, 25, 120.	0.8	3
14451	Synthesis, Crystal Structure Analysis, and Electrochemical Properties of Rock-Salt Type Mg <sub>x</sub> Ni <sub>y</sub> Co <sub>z</sub> O <sub>2</sub> as a Cathode Material for Mg Rechargeable Batteries. <i>Inorganic Chemistry</i> , 2019, 58, 5664-5670.	1.9	16
14452	Approaching the Quantitative Description of Enantioselective Adsorption by the Density Functional Theory Means. <i>Journal of Physical Chemistry C</i> , 2019, 123, 11714-11722.	1.5	5
14453	Nitrogen-Doped Cobalt Phosphide for Enhanced Hydrogen Evolution Activity. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 17359-17367.	4.0	40
14454	Global Isomeric Survey of Elusive Cyclopropanetrione: Unknown but Viable Isomers. <i>Frontiers in Chemistry</i> , 2019, 7, 193.	1.8	4
14455	DFT Analysis of the Adsorption of Phenol on the Nonpolar (101̄...0) ZnO Surface. <i>Journal of Physical Chemistry C</i> , 2019, 123, 12296-12304.	1.5	26
14456	BTEX adsorption on TiO <sub>2</sub> anatase and rutile surfaces: DFT functionals. <i>Journal of Molecular Modeling</i> , 2019, 25, 137.	0.8	8
14457	Effect of Al solute concentration on mechanical properties of Al <sub>x</sub> FeCuCrNi high-entropy alloys: A first-principles study. <i>Physica B: Condensed Matter</i> , 2019, 566, 30-37.	1.3	30
14458	Plasmon-Enhanced Hydrogen Evolution on Specific Facet of Silver Nanocrystals. <i>Chemistry of Materials</i> , 2019, 31, 3722-3728.	3.2	33
14459	Unexpected Xe Cations and Superconductivity in Yâ€“Xe Intermediate Compounds under Pressure. <i>Journal of Physical Chemistry C</i> , 2019, 123, 9323-9330.	1.5	6

#	ARTICLE	IF	CITATIONS
14460	DFT-GIPAW 27Al NMR Simulations for Intermetallics: Accuracy Issues and Magnetic Screening Mechanisms. <i>Journal of Physical Chemistry C</i> , 2019, 123, 9371-9381.	1.5	5
14461	Extensive deep neural networks for transferring small scale learning to large scale systems. <i>Chemical Science</i> , 2019, 10, 4129-4140.	3.7	32
14462	Electronic structure of cobalt/iron carbide from <i>ab-initio</i> calculations. <i>Materials Research Express</i> , 2019, 6, 076302.	0.8	1
14463	Intercalated Cation Disorder in Prussian Blue Analogues: First-Principles and Grand Canonical Analyses. <i>Journal of Physical Chemistry C</i> , 2019, 123, 10191-10204.	1.5	13
14464	Artificial neural network assisted by first-principles calculations for predicting transformation temperatures in shape memory alloys. <i>International Journal of Modern Physics B</i> , 2019, 33, 1950055.	1.0	7
14465	Electronics of Ba adsorbed on Ge(001). <i>Applied Surface Science</i> , 2019, 481, 1474-1482.	3.1	1
14466	HO selective cleavage Fe S bond for FeS <sub>2</sub> electrolysis in alkaline solution. <i>Electrochimica Acta</i> , 2019, 306, 327-338.	2.6	20
14467	Oriented attachment growth of monocrystalline cuprous oxide nanowires in pure water. <i>Nanoscale Advances</i> , 2019, 1, 2174-2179.	2.2	3
14468	Uptake, accumulation and metabolization of 1-butyl-3-methylimidazolium bromide by ryegrass from water: Prospects for phytoremediation. <i>Water Research</i> , 2019, 156, 82-91.	5.3	29
14469	Sonogashira Cross-Coupling of Aryltrimethylammonium Salts. <i>ACS Catalysis</i> , 2019, 9, 3730-3736.	5.5	43
14470	Synergistic Regulation of Polysulfides Conversion and Deposition by MOF-Derived Hierarchically Ordered Carbonaceous Composite for High-Energy Lithium-Sulfur Batteries. <i>Advanced Functional Materials</i> , 2019, 29, 1900875.	7.8	104
14471	2D-3D transformation of palladium and gold nanoparticles on functionalized Mo <sub>2</sub> C by multiscale simulation. <i>Applied Surface Science</i> , 2019, 481, 554-563.	3.1	10
14472	First-principles analysis of vibrational modes of calcite, magnesite and dolomite. <i>Journal of Physics and Chemistry of Solids</i> , 2019, 131, 1-9.	1.9	13
14473	Molecular engineering of anchoring groups for designing efficient triazatruxene-based organic dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2019, 43, 6480-6491.	1.4	15
14474	Facile synthesis of a bismuth nanostructure with enhanced selectivity for electrochemical conversion of CO <sub>2</sub> to formate. <i>Nanoscale</i> , 2019, 11, 7805-7812.	2.8	80
14475	Hierarchical Ni <sub>2</sub> P/Cr <sub>2</sub> CT <sub>x</sub> (MXene) composites with oxidized surface groups as efficient bifunctional electrocatalysts for overall water splitting. <i>Journal of Materials Chemistry A</i> , 2019, 7, 9324-9334.	5.2	54
14476	A Bifunctional Saddle-Shaped Small Molecule as a Dopant-Free Hole Transporting Material and Interfacial Layer for Efficient and Stable Perovskite Solar Cells. <i>Solar Rrl</i> , 2019, 3, 1900011.	3.1	34
14477	First principle studies on structure, magneto-electronic and elastic properties of photovoltaic semiconductor halide (RbGeI <sub>3</sub> ) and ferromagnetic half metal oxide (RbDyO <sub>3</sub> ). <i>Computational Condensed Matter</i> , 2019, 19, e00381.	0.9	14

#	ARTICLE	IF	CITATIONS
14478	Hydrogenation properties of five-component Mg <sub>60</sub> Ce <sub>10</sub> Ni <sub>20</sub> Cu <sub>5</sub> X <sub>5</sub> (X= Co, Zn) metallic glasses. <i>Intermetallics</i> , 2019, 108, 94-99.	1.8	21
14479	New insights on the nature of impurity levels in V-doped In <sub>2</sub> S <sub>3</sub> : why is it impossible to obtain a metallic intermediate band?. <i>Journal of Materials Chemistry A</i> , 2019, 7, 7745-7751.	5.2	12
14480	Theoretical Investigations on the Mechanical, Magneto-Electronic Properties and Half-Metallic Characteristics of ZrRhTiZ (Z = Al, Ga) Quaternary Heusler Compounds. <i>Applied Sciences (Switzerland)</i> , 2019, 9, 883.	1.3	17
14481	Self-Assembly Evolution of Metal-Free Naphthalocyanine Molecules on Ag(111) at the Submonolayer Coverage. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7202-7208.	1.5	5
14482	Structural Dependence of Non-Linear Optical Properties of Molecules Containing Naphthalene Linked to Nitrophenyl Group—A DFT Study. <i>Asian Journal of Chemistry</i> , 2019, 31, 505-509.	0.1	0
14483	Interaction of Ethylene with Irn (n = 1–10): From Bare Clusters to $\gamma$ -Al <sub>2</sub> O <sub>3</sub> -Supported Nanoparticles. <i>Nanomaterials</i> , 2019, 9, 331.	1.9	6
14484	Neural network force fields for simple metals and semiconductors: construction and application to the calculation of phonons and melting temperatures. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 6506-6516.	1.3	25
14485	Molecular mechanisms of atomic layer etching of cobalt with sequential exposure to molecular chlorine and diketones. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2019, 37, 021004.	0.9	41
14486	Pt/CeO <sub>2</sub> and Pt/CeSnO <sub>x</sub> Catalysts for Low-Temperature CO Oxidation Prepared by Plasma-Arc Technique. <i>Frontiers in Chemistry</i> , 2019, 7, 114.	1.8	24
14487	Hexagonal boron nitride nanosheet for effective ambient N <sub>2</sub> fixation to NH <sub>3</sub> . <i>Nano Research</i> , 2019, 12, 919-924.	5.8	120
14488	A metal-semiconductor transition triggered by atomically flat zigzag edge in monolayer transition-metal dichalcogenides. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019, 383, 1636-1641.	0.9	2
14489	Effects of Dimethyl Disulfide Cosolvent on Li–S Battery Chemistry and Performance. <i>Chemistry of Materials</i> , 2019, 31, 2377-2389.	3.2	11
14490	Ultrathin Two-Dimensional Metal–Organic Framework Nanosheets with the Inherent Open Active Sites as Electrocatalysts in Aprotic Li–O <sub>2</sub> Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 11403-11413.	4.0	108
14491	Martensitic transformation of Ti <sub>50</sub> (Ni <sub>50-x</sub> Cu <sub>x</sub> ) and Ni <sub>50</sub> (Ti <sub>50-x</sub> Zr <sub>x</sub> ) shape-memory alloys. <i>Scientific Reports</i> , 2019, 9, 3221.	1.6	13
14492	<sup>1</sup> H and <sup>93</sup> Nb Solid-State NMR and IR Study of Acidity of Nanodisperse Nb <sub>2</sub> O <sub>5</sub> ·nH <sub>2</sub> O. <i>Applied Magnetic Resonance</i> , 2019, 50, 589-597.	0.6	4
14493	A study of the basis set dependence of the bifunctional expression of the non-interacting kinetic energy for atomic systems. <i>Computational and Theoretical Chemistry</i> , 2019, 1155, 56-60.	1.1	4
14494	Mechanistic understanding of enhanced photocatalytic activity of N-doped BiVO <sub>4</sub> towards degradation of ibuprofen: An experimental and theoretical approach. <i>Molecular Catalysis</i> , 2019, 470, 8-18.	1.0	27
14495	Fluorinated perovskite as magnetic spin-polarised semiconductor. <i>Solid State Communications</i> , 2019, 294, 39-42.	0.9	0

#	ARTICLE	IF	CITATIONS
14496	Modeling of $M_{12}$ Keggin Heteroatom Reactivity by Anion Adsorption. <i>Crystal Growth and Design</i> , 2019, 19, 2820-2829.	1.4	10
14497	Transmetallation of bis(6-diphenylphosphinoxy-acenaph-5-yl)mercury with tin tetrachloride, antimony trichloride and bismuth trichloride. <i>Dalton Transactions</i> , 2019, 48, 5585-5594.	1.6	11
14498	Palladium-catalysed alkyne alkoxy carbonylation with P,N-chelating ligands revisited: a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8543-8552.	1.3	14
14499	The diverse electronic properties of C/BN heteronanotubes with polar discontinuity. <i>Journal Physics D: Applied Physics</i> , 2019, 52, 215302.	1.3	2
14500	Quantum anomalous Hall effects and various topological mechanisms in functionalized Sn monolayers. <i>New Journal of Physics</i> , 2019, 21, 023010.	1.2	2
14501	Potential high- $T_c$ superconductivity in $CaYH_{12}$ under pressure. <i>Physical Review B</i> , 2019, 99, ...	1.1	109
14502	Anharmonic and Anomalous Trends in the High-Pressure Phase Diagram of Silicon. <i>Physical Review Letters</i> , 2019, 122, 125701.	2.9	15
14503	Oriented Transformation of CoLDH into 2D/3D ZIF67 to Achieve Co-N-C Hybrids for Efficient Overall Water Splitting. <i>Advanced Energy Materials</i> , 2019, 9, 1803918.	10.2	260
14504	C-H versus O-H bond scission in methanol decomposition on Pt(111): Role of the dispersion interaction. <i>Applied Surface Science</i> , 2019, 481, 1327-1334.	3.1	17
14505	Innovating e-waste recycling: From waste multi-layer ceramic capacitors to Nb-Pb codoped and Ag-Pd-Sn-Ni loaded BaTiO <sub>3</sub> nano-photocatalyst through one-step ball milling process. <i>Sustainable Materials and Technologies</i> , 2019, 21, e00101.	1.7	14
14506	Thermochemical analysis of Mo-C-H system for synthesis of molybdenum carbides. <i>Thermochimica Acta</i> , 2019, 676, 27-32.	1.2	4
14507	Martensitic transformation and magnetic properties in Pd <sub>2</sub> MnGa Heusler alloy by DFT study. <i>Modern Physics Letters B</i> , 2019, 33, 1950074.	1.0	1
14508	Electronic structure of gadolinium-doped ceria system: A DFT study. <i>Modern Physics Letters B</i> , 2019, 33, 1950095.	1.0	2
14509	Adsorption and desorption of hydrogen on/from single-vacancy and double-vacancy graphenes. <i>Nuclear Science and Techniques/Hewuli</i> , 2019, 30, 1.	1.3	14
14510	The effect of protons on the Mg <sup>2+</sup> migration in an $\sqrt{2} \times \sqrt{2} \times \sqrt{5}$ cathode for magnesium batteries: a first-principles investigation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7406-7411.	1.3	18
14511	Coadsorption of CO and O over strained metal surfaces. <i>Chemical Physics Letters</i> , 2019, 722, 18-25.	1.2	8
14512	Origin of ferromagnetism in Cu-doped ZnO. <i>Scientific Reports</i> , 2019, 9, 2461.	1.6	63
14513	Defect-assisted surface modification enhances the visible light photocatalytic performance of g-C <sub>3</sub> N <sub>4</sub> @C-TiO <sub>2</sub> direct Z-scheme heterojunctions. <i>Chinese Journal of Catalysis</i> , 2019, 40, 424-433.	6.9	228

#	ARTICLE	IF	CITATIONS
14514	Mn <sub>3</sub> O <sub>4</sub> nanoparticles@reduced graphene oxide composite: An efficient electrocatalyst for artificial N <sub>2</sub> fixation to NH <sub>3</sub> at ambient conditions. Nano Research, 2019, 12, 1093-1098.	5.8	93
14515	IrF <sub>8</sub> Molecular Crystal under High Pressure. Journal of the American Chemical Society, 2019, 141, 5409-5414.	6.6	40
14516	G-Quadruplex binding optimization by gold(III) insertion into the center of a porphyrin. Dalton Transactions, 2019, 48, 6091-6099.	1.6	14
14517	DFT Computed Dielectric Response and THz Spectra of Organic Co-Crystals and Their Constituent Components. Molecules, 2019, 24, 959.	1.7	2
14518	Electron-phonon coupling, superconductivity, and nontrivial band topology in NbN polytypes. Physical Review B, 2019, 99, .	1.1	31
14519	Extent of Spin Contamination Errors in DFT/Plane-wave Calculation of Surfaces: A Case of Au Atom Aggregation on a MgO Surface. Molecules, 2019, 24, 505.	1.7	26
14520	Two-dimensional dual carbon-coupled defective nickel quantum dots towards highly efficient overall water splitting. Applied Catalysis B: Environmental, 2019, 250, 213-223.	10.8	101
14521	SrCdSnQ <sub>4</sub> (Q = S and Se): infrared nonlinear optical chalcogenides with mixed NLO-active and synergetic distorted motifs. Journal of Materials Chemistry C, 2019, 7, 4459-4465.	2.7	52
14522	Local Lattice Strains Around Alloying Elements in Metals. , 2019, , 221-260.		1
14523	Magnetic MFe <sub>2</sub> O <sub>4</sub> -Ag <sub>2</sub> O (M = Zn, Co, & Ni) composite photocatalysts and their application for dye wastewater treatment. Journal of Environmental Chemical Engineering, 2019, 7, 103011.	3.3	11
14524	Physical mechanism on edge-dependent electrons transfer in graphene in mid infrared region. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 216, 136-145.	2.0	7
14525	Bilayer phosphorene under high pressure: <i>in situ</i> Raman spectroscopy. Physical Chemistry Chemical Physics, 2019, 21, 7298-7304.	1.3	19
14526	Amino Acid Immobilization of Copper Surface Diffusion on Cu(111). Advanced Materials Interfaces, 2019, 6, 1900021.	1.9	7
14527	Lyophobicity and slagging resistance mechanism of h-BN based coating for coal-fired boilers. Fuel Processing Technology, 2019, 188, 43-50.	3.7	8
14528	Preparation of bulk metallic glasses by modifying local structure of icosahedral quasicrystals. Intermetallics, 2019, 109, 97-104.	1.8	9
14529	Suppression of the thermal embrittlement induced by sulfur segregation to grain boundary in Ni-based electrodeposits. Materialia, 2019, 6, 100312.	1.3	8
14530	The adsorption properties of Fe, Co, and Ni atoms on $\hat{\Gamma}$ -WC(0001) surface: a first principles study. Materials Research Express, 2019, 6, 075609.	0.8	3
14531	Formation of an $\hat{\Gamma}$ -Diimine from Isocyanide Coupling Using Thorium(IV) and Uranium(IV) Phosphido-Methyl Complexes. Organometallics, 2019, 38, 1733-1740.	1.1	11

#	ARTICLE	IF	CITATIONS
14532	Increased electrode activity during geosmin oxidation provided by Pt nanoparticle-embedded nanocarbon film. <i>Nanoscale</i> , 2019, 11, 8845-8854.	2.8	4
14533	B-terminated (111) polar surfaces of BP and BAs: promising metal-free electrocatalysts with large reaction regions for nitrogen fixation. <i>Journal of Materials Chemistry A</i> , 2019, 7, 13284-13292.	5.2	87
14534	<i>In situ</i> exsolved FeNi <sub>3</sub> nanoparticles on nickel doped Sr <sub>2</sub> Fe <sub>1.5</sub> Mo <sub>0.5</sub> O <sub>6</sub> perovskite for efficient electrochemical CO <sub>2</sub> reduction reaction. <i>Journal of Materials Chemistry A</i> , 2019, 7, 11967-11975.	5.2	159
14535	Reaction energy benchmarks of hydrocarbon combustion by Gaussian basis and plane wave basis approaches. <i>Journal of Computational Chemistry</i> , 2019, 40, 1866-1873.	1.5	3
14536	Atomic investigation on reversible and irreversible lithium storage in silicon incorporated with multi-layered graphene. <i>Materials Letters</i> , 2019, 244, 108-110.	1.3	4
14537	Band structure and thermoelectric performances of antimony under trigonal transformation. <i>Journal of Applied Physics</i> , 2019, 125, .	1.1	20
14538	Broken cubic symmetry driven co-emergence of type-I and type-II Dirac points in topological crystalline insulator ThTaN <sub>3</sub> . <i>Journal of Physics Condensed Matter</i> , 2019, 31, 295501.	0.7	3
14539	Precipitation, planar defects and dislocations in alloys: Simulations on Ni <sub>3</sub> Si and Ni <sub>3</sub> Al precipitates. <i>European Physical Journal: Special Topics</i> , 2019, 227, 1559-1574.	1.2	6
14540	First-principle study of metal-organic frameworks of the 4d and 5d transition metal series with phthalocyanine and tetracyanobenzene. <i>Superlattices and Microstructures</i> , 2019, 130, 122-126.	1.4	3
14541	Structural, electronic and optical properties of pulsed laser deposited Cu <sub>2</sub> SnS <sub>3</sub> photo absorber thin films: A combined experimental and computational study. <i>Thin Solid Films</i> , 2019, 677, 62-67.	0.8	9
14542	First-Principles Molecular Dynamics of Monomethylhydrazine and Nitrogen Dioxide. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2394-2399.	2.1	8
14543	Shedding Light on Pseudocapacitive Active Edges of Single-Layer Graphene Nanoribbons as High-Capacitance Supercapacitors. <i>ACS Applied Energy Materials</i> , 2019, 2, 3665-3675.	2.5	18
14544	Diethanolamine and quaternium-15 interaction studies on antimonene nanosheet based on first-principles studies. <i>Computational and Theoretical Chemistry</i> , 2019, 1157, 19-27.	1.1	25
14545	Properties of group III-V semiconductor: BAs. <i>Bulletin of Materials Science</i> , 2019, 42, 1.	0.8	11
14546	Two-dimensional graphyne-like carbon nitrides: Moderate band gaps, high carrier mobility, high flexibility and type-II band alignment. <i>Carbon</i> , 2019, 149, 234-241.	5.4	38
14547	Evaluating Transition Metal Barrier Heights with the Latest Density Functional Theory Exchange-Correlation Functionals: The MOBH35 Benchmark Database. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3761-3781.	1.1	104
14548	Optical Stability of 1,1'-Binaphthyl Derivatives. <i>ACS Omega</i> , 2019, 4, 6044-6049.	1.6	11
14549	Experimental and computational study of Tm-doped TiO <sub>2</sub> : The effect of Li <sup>+</sup> on Vis-response photocatalysis and luminescence. <i>Applied Catalysis B: Environmental</i> , 2019, 252, 138-151.	10.8	25



#	ARTICLE	IF	CITATIONS
14550	High pressure behavior of mercury difluoride (HgF <sub>2</sub> ). Chemical Physics Letters, 2019, 724, 35-41.	1.2	7
14551	Structural and electronic properties of the $\hat{\pm}$ -GeSe surface. Surface Science, 2019, 686, 17-21.	0.8	4
14552	Lithiation of the Two-Dimensional Silicon Carbideâ€“Graphene van der Waals Heterostructure: A First Principles Study. Journal of Physical Chemistry C, 2019, 123, 10738-10745.	1.5	19
14553	On the involvement of d-electrons in superatomic shells: the group 3 and 4 transition metals. Physical Chemistry Chemical Physics, 2019, 21, 8035-8045.	1.3	11
14554	Effect of stretching on the initial oxidation of 3C-SiC nanowire by first-principle simulation. Applied Surface Science, 2019, 483, 170-177.	3.1	5
14555	A quantum chemical study of the effect of substituents in governing the strength of the Sâ€“F bonds of sulfenyl-type fluorides toward homolytic dissociation and fluorine atom transfer. Chemical Data Collections, 2019, 20, 100186.	1.1	5
14556	Defect energy levels and persistent luminescence in Cu-doped ZnS. Computational Materials Science, 2019, 163, 63-67.	1.4	25
14557	Dynamical stability and vibrational properties of Pt clusters. Journal of Physics and Chemistry of Solids, 2019, 131, 131-138.	1.9	7
14558	Catalytically Active Au Layers Grown on Pd Nanoparticles for Direct Synthesis of H <sub>2</sub> O <sub>2</sub> : Lattice Strain and Charge-Transfer Perspective Analyses. ACS Nano, 2019, 13, 4761-4770.	7.3	42
14559	A complete catalytic reaction scheme for HgO oxidation by HCl over RuO <sub>2</sub> /TiO <sub>2</sub> catalyst. Journal of Hazardous Materials, 2019, 373, 660-670.	6.5	17
14560	The structuralâ€“magnetic properties relationship of amorphous pure Fe revealed by the minimum coordination polyhedron. Journal of Non-Crystalline Solids, 2019, 513, 70-75.	1.5	5
14561	Synergic effect of adsorbed gas and charging on surface flashover. Scientific Reports, 2019, 9, 5464.	1.6	35
14562	First-principles study of He behavior in a NiCoFeCr concentrated solidâ€“solution alloy. Materials Research Letters, 2019, 7, 188-193.	4.1	21
14563	Adsorption and ultrafast diffusion of lithium in bilayer graphene: <i>ab initio</i> and kinetic Monte Carlo simulation study. Physical Review B, 2019, 99, .	1.1	28
14564	Structures, photoresponse properties and DNA binding abilities of 4-(4-pyridinyl)-2-pyridone salts. RSC Advances, 2019, 9, 9663-9677.	1.7	24
14565	Stability of graphite-like ZnO film with Cu doping: First principle study. European Physical Journal Plus, 2019, 134, 1.	1.2	3
14566	Band Gap Modulation of Tantalum(V) Perovskite Semiconductors by Anion Control. Catalysts, 2019, 9, 161.	1.6	8
14567	The electronic and optical properties of MgO mono-layer: Based on GGA-mBJ. Results in Physics, 2019, 12, 2038-2043.	2.0	51



#	ARTICLE	IF	CITATIONS
14568	Modeling the effect of surface CO coverage on the electrocatalytic reduction of CO <sub>2</sub> to CO on Pd surfaces. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9876-9882.	1.3	34
14569	Highly sensitive and room temperature detection of ultra-low concentrations of O <sub>3</sub> using self-powered sensing elements of Cu <sub>2</sub> O nanocubes. <i>Nanoscale Advances</i> , 2019, 1, 2009-2017.	2.2	15
14570	Mechanism of hardening and damage initiation in oxygen embrittlement of body-centred-cubic niobium. <i>Acta Materialia</i> , 2019, 168, 331-342.	3.8	60
14571	Self-regeneration of Au/CeO <sub>2</sub> based catalysts with enhanced activity and ultra-stability for acetylene hydrochlorination. <i>Nature Communications</i> , 2019, 10, 914.	5.8	86
14572	Self-Suppression of Lithium Dendrite in All-Solid-State Lithium Metal Batteries with Poly(vinylidene fluoride) Electrolyte. <i>ACS Energy Letters</i> , 2019, 4, 2983-2988.	11.1	298
14573	Determination of Reaction Rate Coefficients in Free-Radical Polymerization Using Density Functional Theory. <i>Journal of Polymer Science: Part B: Polymer Physics</i> , 2019, 57, 47-98.		6
14574	Investigation of humidity sensor based on Au modified ZnO nanosheets via hydrothermal method and first principle. <i>Sensors and Actuators B: Chemical</i> , 2019, 287, 526-534.	4.0	109
14575	Acceleration of material R&D process through rational design. <i>Computational Materials Science</i> , 2019, 160, 397-402.	1.4	2
14576	Recent advances in computational photocatalysis: A review. <i>Canadian Journal of Chemical Engineering</i> , 2019, 97, 1982-1998.	0.9	45
14577	From Waste to Nb-doped and Pd-loaded TiO <sub>2</sub> /BaTiO <sub>3</sub> Heterostructure: Highly Efficient Photocatalytic Performance. <i>ChemSusChem</i> , 2019, 12, 2819-2828.	3.6	13
14578	Effects of different phases, compositional change, and doping on ductility improvement of NbAl <sub>3</sub> phases. <i>Journal of Alloys and Compounds</i> , 2019, 788, 172-182.	2.8	5
14579	First-principles calculations of structural, elastic and thermodynamic properties of (h, r)-TiAl <sub>2</sub> . <i>Physica B: Condensed Matter</i> , 2019, 561, 29-36.	1.3	13
14580	Mechanism of Nitric Oxide Reduction by Hydrogen on Ni(110) and Ir/Ni(110): First Principles and Microkinetic Modeling. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4825-4836.	1.5	12
14581	Uncertainty Quantification in First-Principles Predictions of Harmonic Vibrational Frequencies of Molecules and Molecular Complexes. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4072-4084.	1.5	16
14582	Magnetic Polymer Chains of Transition Metal Atoms and Zwitterionic Quinone. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4582-4589.	1.5	13
14583	Asymmetric MXene/monolayer transition metal dichalcogenide heterostructures for functional applications. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	23
14584	Close Relationships between NMR <i>J</i> -Coupling Alternation (JCA) and Molecular Properties of Carbon Chains. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1605-1615.	2.3	4
14585	Theoretical Study of NO Dissociation on an Open Flat Ru(101̄...1) Surface. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5488-5494.	1.5	0

#	ARTICLE	IF	CITATIONS
14586	Electronic origin of antimicrobial activity owing to surface effect. <i>Scientific Reports</i> , 2019, 9, 1091.	1.6	6
14587	Interaction between Bi Dopants and Intrinsic Defects in LiNbO <sub>3</sub> from Local and Hybrid Density Functional Theory Calculations. <i>Inorganic Chemistry</i> , 2019, 58, 3661-3669.	1.9	8
14588	Trends and Descriptors of Metal-Modified Transition Metal Carbides for Hydrogen Evolution in Alkaline Electrolyte. <i>ACS Catalysis</i> , 2019, 9, 2415-2422.	5.5	74
14589	A Combined Study of TEM-EDS/XPS and Molecular Modeling on the Aging of THPP, ZPP, and BKNO <sub>3</sub> Explosive Charges in PMDs under Accelerated Aging Conditions. <i>Energies</i> , 2019, 12, 151.	1.6	2
14590	Highly dispersed Pt nanoparticles on hierarchical titania nanoflowers with {010} facets for gas sensing and photocatalysis. <i>Journal of Materials Science</i> , 2019, 54, 6826-6840.	1.7	12
14591	Mechanochemical reactions and hydrogen storage capacities in MBH <sub>4</sub> –Si <sub>2</sub> systems (M Li or Na). <i>International Journal of Hydrogen Energy</i> , 2019, 44, 7381-7391.	3.8	13
14592	A stable Ta <sub>3</sub> N <sub>5</sub> @PANI core-shell photocatalyst: Shell thickness effect, high-efficient photocatalytic performance and enhanced mechanism. <i>Journal of Catalysis</i> , 2019, 371, 175-184.	3.1	47
14593	Restructuring of MFI Framework Zeolite Models and Their Associated Artifacts in Density Functional Theory Calculations. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6572-6585.	1.5	21
14594	Stabilizing High Metal Loadings of Thermally Stable Platinum Single Atoms on an Industrial Catalyst Support. <i>ACS Catalysis</i> , 2019, 9, 3978-3990.	5.5	233
14595	The Influence of Boron Dopant on the Structural and Mechanical Properties of Silicon: First Principles Study. <i>Minerals, Metals and Materials Series</i> , 2019, , 191-199.	0.3	1
14596	Interface-Driven Phase Transition of Phase-Change Material. <i>Crystal Growth and Design</i> , 2019, 19, 2123-2130.	1.4	5
14597	Magneto-Seebeck effect in Co <sub>2</sub> FeAl/MgO/Co <sub>2</sub> FeAl: first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5803-5812.	1.3	12
14598	The Influence of Phosphorus Dopant on the Structural and Mechanical Properties of Silicon. <i>Minerals, Metals and Materials Series</i> , 2019, , 201-211.	0.3	0
14599	Modeling solution hardening in BCC refractory complex concentrated alloys: NbTiZr, Nb <sub>1.5</sub> TiZr <sub>0.5</sub> and Nb <sub>0.5</sub> TiZr <sub>1.5</sub> . <i>Acta Materialia</i> , 2019, 168, 222-236.	3.8	103
14600	Adsorption of SO <sub>2</sub> molecules on Fe-doped carbon nanotubes: the first principles study. <i>Adsorption</i> , 2019, 25, 217-224.	1.4	21
14601	On the possibility of severe corrosion of a Ni-W-Cr alloy in fluoride molten salts at high temperature. <i>Corrosion Science</i> , 2019, 149, 218-225.	3.0	42
14602	Enhanced Lewis acid-base adducts in doped stanene: Sensing and photocatalysis. <i>Applied Surface Science</i> , 2019, 478, 946-958.	3.1	10
14603	The medium-range orders transition in liquid Fe–Al alloys. <i>Computational Materials Science</i> , 2019, 161, 199-208.	1.4	6

#	ARTICLE	IF	CITATIONS
14604	Ambiguous Role of N $\hat{+}$ Sn Coordinated Stannylene: Lewis Base or Acid?. <i>Organometallics</i> , 2019, 38, 816-828.	1.1	15
14605	Theoretical Surface Science Beyond Gradient-Corrected Density Functional Theory: Water at $\hat{+}$ -Al <sub>2</sub> O <sub>3</sub> (0001) as a Case Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6675-6684.	1.5	15
14606	Chemical Durability and Dissolution Kinetics of Iodoapatite in Aqueous Solutions. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 452-462.	1.2	16
14607	From DFT to machine learning: recent approaches to materials science—a review. <i>JPhys Materials</i> , 2019, 2, 032001.	1.8	385
14608	Quantum-mechanical modeling of divalent cation incorporation into uranium dioxide. <i>Journal of Nuclear Materials</i> , 2019, 517, 362-370.	1.3	3
14609	Computational Approach To Reveal the Structural Stability and Electronic Properties of Lithiated M/CNT (M = Si, Ge) Nanocomposites as Anodes for Lithium-Ion Batteries. <i>ACS Omega</i> , 2019, 4, 4153-4160.	1.6	2
14610	Subnanometer cobalt oxide clusters as selective low temperature oxidative dehydrogenation catalysts. <i>Nature Communications</i> , 2019, 10, 954.	5.8	38
14611	Landau—Devonshire thermodynamic potentials for displacive perovskite ferroelectrics from first principles. <i>Journal of Materials Science</i> , 2019, 54, 8381-8400.	1.7	10
14612	Influence of Spin State and Cation Distribution on Stability and Electronic Properties of Ternary Transition-Metal Oxides. <i>ACS Omega</i> , 2019, 4, 4138-4146.	1.6	22
14613	Element Replacement Approach by Reaction with Lewis Acidic Molten Salts to Synthesize Nanolaminated MAX Phases and MXenes. <i>Journal of the American Chemical Society</i> , 2019, 141, 4730-4737.	6.6	811
14614	Thermoelasticity of Iron—and Aluminum—bearing MgSiO <sub>3</sub> Postperovskite. <i>Journal of Geophysical Research: Solid Earth</i> , 2019, 124, 2417-2427.	1.4	5
14615	Density functional theory description of random Cu-Au alloys. <i>Physical Review B</i> , 2019, 99, .	1.1	5
14616	The impact of alloying elements on the precipitation stability and kinetics in iron based alloys: An atomistic study. <i>Computational Materials Science</i> , 2019, 161, 309-320.	1.4	27
14617	Water Splitting Reaction at Polar Lithium Niobate Surfaces. <i>ACS Omega</i> , 2019, 4, 3850-3859.	1.6	16
14618	Structural, phonon, elastic, thermodynamic and electronic properties of Mg—X (X = La, Nd, Sm) intermetallics: The first principles study. <i>Journal of Magnesium and Alloys</i> , 2019, 7, 166-185.	5.5	31
14619	Solution effect on improved structural compatibility of NiTi-based alloys by systematic first-principles calculations. <i>Journal of Applied Physics</i> , 2019, 125, .	1.1	4
14620	Correlation energy functionals from adiabatic connection formalism. <i>Physical Review B</i> , 2019, 99, .	1.1	19
14621	Coulomb exchange functional with generalized gradient approximation for self-consistent Skyrme Hartree-Fock calculations. <i>Physical Review C</i> , 2019, 99, .	1.1	11

#	ARTICLE	IF	CITATIONS
14622	Jahn–Teller type small polaron assisted Na diffusion in NaMnO <sub>2</sub> as a cathode material for Na-ion batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 6053-6061.	5.2	27
14623	Transition metal complexes of antimony centered ligands based upon acenaphthyl scaffolds. Coordination non-innocent or not?. <i>Dalton Transactions</i> , 2019, 48, 4504-4513.	1.6	18
14624	Density Functional Theory Study of Aspirin Adsorption on BCN Sheets and their Hydrogen Evolution Reaction Activity: a Comparative Study with Graphene and Hexagonal Boron Nitride. <i>ChemPhysChem</i> , 2019, 20, 687-694.	1.0	16
14625	Spectroscopic Evidence and Density Functional Theory (DFT) Analysis of Low-Temperature Oxidation of Cu <sup>+</sup> to Cu <sup>2+</sup> NO <sub>x</sub> in Cu-CHA Catalysts: Implications for the SCR-NO <sub>x</sub> Reaction Mechanism. <i>ACS Catalysis</i> , 2019, 9, 2725-2738.	5.5	55
14626	Lithium insertion in Si electrodes studied by first principles method. <i>IOP Conference Series: Materials Science and Engineering</i> , 2019, 688, 033041.	0.3	0
14627	Thickness-dependent Strengthening Effect of Grain Refiner Al <sub>3</sub> Zr and Al <sub>3</sub> (Zr,Sc) in Al Alloys. <i>IOP Conference Series: Materials Science and Engineering</i> , 2019, 585, 012027.	0.3	0
14628	Plasmonic performance of Au <sub>x</sub> Ag <sub>y</sub> Cu <sub>1-x-y</sub> alloys from many-body perturbation theory. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 315901.	0.7	5
14629	Impact of single atomic defects and vacancies on the magnetic anisotropy energy of CoPt thin films. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 435803.	0.7	0
14630	Effect of a small amount of Fe-addition on intergranular fracture of Al–7.3%mass%Mg alloys. <i>Keikinzoku/Journal of Japan Institute of Light Metals</i> , 2019, 69, 457-464.	0.1	5
14631	Improvement of functionals in density functional theory by the inverse Kohn–Sham method and density functional perturbation theory. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2019, 52, 245003.	0.6	11
14632	Heat of fusion of rhenium from first-principle simulations and the Richards–Tammann relation. <i>Journal of Physics: Conference Series</i> , 2019, 1385, 012027.	0.3	0
14633	Comparative study of the effect of the exchange-correlation functional on the structural and electronic properties of rutile. <i>Journal of Physics: Conference Series</i> , 2019, 1386, 012074.	0.3	1
14634	Theoretical calculation of elastic properties and electronic structure of B2 iron aluminides and ternary iron–aluminum alloys. <i>Materials Research Express</i> , 2019, 6, 1265f4.	0.8	5
14635	Multifunctional 2D CuSe monolayer nanodevice. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 355301.	0.7	8
14636	Quantum mechanical study of chemical reactivity of graphene doped with iron in aqueous medium for applications in biomedicine. <i>Journal of Nanoparticle Research</i> , 2019, 21, 1.	0.8	2
14637	First-Principles Calculation of Physical Tensors of $\hat{\pm}$ -Diisopropylammonium Bromide ( $\hat{\pm}$ -DIPAB) Molecular Ferroelectric Crystal. <i>Frontiers in Physics</i> , 2019, 7, .	1.0	6
14638	Near-infrared phosphorescence emission of Zn(II) coordination polymer based on 3,5-bis(1-imidazolyl)pyridine: Syntheses, structure and photoelectron performance. <i>Journal of Solid State Chemistry</i> , 2019, 279, 120958.	1.4	15
14639	Minimized lithium trapping by isovalent isomorphism for high initial Coulombic efficiency of silicon anodes. <i>Science Advances</i> , 2019, 5, eaax0651.	4.7	122

#	ARTICLE	IF	CITATIONS
14640	Density functional theory calculated data of different electronic states and bond stretch isomers of tris(trifluoroacetylacetonato)-manganese(III). Data in Brief, 2019, 27, 104758.	0.5	6
14641	Blue phosphorene nanoribbon for detection of chloroform vapours – a first-principles study. International Journal of Environmental Analytical Chemistry, 2019, , 1-13.	1.8	13
14642	Metastable intermetallic phases in the Al-Sm system. Materials Today Communications, 2019, 21, 100673.	0.9	4
14643	Effect of rare earth (Sc, Y, La, Sm and Gd) doping on mechanical and thermodynamic properties of Al <sub>12</sub> Mg <sub>17</sub> intermetallic compounds. Modern Physics Letters B, 2019, 33, 1950442.	1.0	1
14644	Water interaction and dissociation on stoichiometric and defective Mn- and Fe-doped CeO <sub>2</sub> surfaces. Materials Today Communications, 2019, 21, 100703.	0.9	2
14645	Structure–thermodynamics relationship of schoepite from first-principles. Physical Chemistry Chemical Physics, 2019, 21, 25569-25576.	1.3	4
14646	Effect of anion substitution on the structural and transport properties of argyrodites Cu <sub>7</sub> PSe <sub>6</sub> xS <sub>x</sub> . Dalton Transactions, 2019, 48, 15822-15829.	1.6	17
14647	Protonation and electrochemical properties of a bisphosphide diiron hexacarbonyl complex bearing amino groups on the phosphide bridge. Dalton Transactions, 2019, 48, 16595-16603.	1.6	7
14648	FeP <sub>3</sub> monolayer as a high-efficiency catalyst for hydrogen evolution reaction. Journal of Materials Chemistry A, 2019, 7, 25665-25671.	5.2	43
14649	Ti <sub>2</sub> VGe Heuslerene: theoretical prediction of a novel 2D material. Journal of Materials Chemistry C, 2019, 7, 13559-13572.	2.7	36
14650	Effect of S-vacancy on the oxidation state of Ce in monolayer SnS <sub>2</sub> . International Journal of Modern Physics B, 2019, 33, 1950308.	1.0	3
14651	Helicity-dependent terahertz photocurrent and phonon dynamics in hybrid metal halide perovskites. Journal of Chemical Physics, 2019, 151, 244706.	1.2	16
14652	Electronic Structure and Excited State Dynamics of TiO <sub>2</sub> Nanowires. ACS Symposium Series, 2019, , 23-46.	0.5	0
14653	Ferromagnetism from non-magnetic ions: Ag-doped ZnO. Scientific Reports, 2019, 9, 20039.	1.6	42
14654	Partial substitution induced centrosymmetric to noncentrosymmetric structure transformation and promising second-order nonlinear optical properties of (K <sub>0.38</sub> Ba <sub>0.81</sub> )Ga <sub>2</sub> Se <sub>4</sub> . Chemical Communications, 2019, 55, 13701-13704.	2.2	73
14655	Dependence of electron transfer dynamics on the number of graphene layers in ĩ-stacked 2D materials: insights from ab initio nonadiabatic molecular dynamics. Physical Chemistry Chemical Physics, 2019, 21, 23198-23208.	1.3	10
14656	Kinetic-energy-based error quantification in Kohn–Sham density functional theory. Physical Chemistry Chemical Physics, 2019, 21, 26492-26501.	1.3	4
14657	Experimental and theoretical investigation of lithium-ion conductivity in Li <sub>2</sub> LaNbTiO <sub>7</sub> . Dalton Transactions, 2019, 48, 17281-17290.	1.6	6

#	ARTICLE	IF	CITATIONS
14658	Laser-engineered oxygen vacancies for improving the NO <sub>2</sub> sensing performance of SnO <sub>2</sub> nanowires. <i>Journal of Materials Chemistry A</i> , 2019, 7, 27205-27211.	5.2	33
14659	Photo-sensitizing thin-film ferroelectric oxides using materials databases and high-throughput calculations. <i>Journal of Materials Chemistry A</i> , 2019, 7, 27323-27333.	5.2	12
14660	Probing Structural Reconstruction of Metal Nanoparticles under Annealing and Water Vapor Conditions: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 29783-29793.	1.5	7
14661	Enhanced Photocatalytic Activity of SiC-Based Ternary Graphene Materials: A DFT Study and the Photocatalytic Mechanism. <i>ACS Omega</i> , 2019, 4, 20142-20151.	1.6	20
14662	Six-dimensional potential energy surfaces for the dissociative chemisorption of HCl on rigid Ag(100) and Ag(110) surfaces. <i>Journal of Chemical Physics</i> , 2019, 151, 144707.	1.2	10
14663	Optical injection of spin current into a zigzag nanoribbon of monolayer $\text{MoS}_2$ with antiferromagnetic Kekule distortion. <i>Physical Review B</i> , 2019, 100, .		
14664	Computation of formation enthalpies and molar volumes of halides. <i>Solid State Ionics</i> , 2019, 343, 115081.	1.3	0
14665	Boron-Decorated Graphitic Carbon Nitride (g-C <sub>3</sub> N <sub>4</sub> ): An Efficient Sensor for H <sub>2</sub> S, SO <sub>2</sub> , and NH <sub>3</sub> Capture. <i>Journal of Physical Chemistry C</i> , 2019, 123, 29513-29523.	1.5	39
14666	Mössbauer Spectroscopy of Triphylite (LiFePO <sub>4</sub> ) at Low Temperatures. <i>Condensed Matter</i> , 2019, 4, 86.	0.8	7
14667	Carbon nanotube array as a van der Waals two-dimensional hyperbolic material. <i>Physical Review B</i> , 2019, 100, .	1.1	7
14668	Dynamic Polarizabilities of Diatomic Molecules: A Comparison of the ab initio and Density Functional Theory Methods with the Reduced-Added Green Function Method of the Quantum Defect Theory. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2019, 127, 798-807.	0.2	2
14669	Experimental and Theoretical Studies on the Structural and Vibrational Spectra of Schiff Base and Their Complex. <i>International Journal of Chemoinformatics and Chemical Engineering</i> , 2019, 8, 47-55.	0.1	1
14670	Alloying Element Segregation and Grain Boundary Reconstruction, Atomistic Modeling. <i>Metals</i> , 2019, 9, 1319.	1.0	7
14671	DFT Modeling of Organocatalytic Ring-Opening Polymerization of Cyclic Esters: A Crucial Role of Proton Exchange and Hydrogen Bonding. <i>Polymers</i> , 2019, 11, 2078.	2.0	23
14672	Distinct dependence on size of Pt and Rh nanoclusters on graphene/Pt(111) in the decomposition of methanol-d <sub>4</sub> . <i>Journal of Chemical Physics</i> , 2019, 151, 224707.	1.2	19
14673	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. <i>Journal of Chemical Physics</i> , 2019, 151, 214108.	1.2	56
14674	Coherent charge-phonon correlations and exciton dynamics in orthorhombic CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> measured by ultrafast multi-THz spectroscopy. <i>Journal of Chemical Physics</i> , 2019, 151, 214201.	1.2	6
14675	Coexistence of two different atomic structures in the $\sqrt{3}\times\sqrt{3}$ pyramidal twin boundary in $\text{Al}_2\text{O}_3$ . <i>Philosophical Magazine Letters</i> , 2019, 99, 435-443.	0.5	4



#	ARTICLE	IF	CITATIONS
14676	Short- and Intermediate-Range Structure and Dynamics of Fe-Ni-C Liquid Under Compression. <i>Frontiers in Earth Science</i> , 2019, 7, .	0.8	8
14677	On the linear geometry of lanthanide hydroxide (Ln-OH, Ln = La–Lu). <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21890-21897.	1.3	1
14678	The doping and oxidation of 2D black and blue phosphorene: a new photocatalyst for nitrogen reduction driven by visible light. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 24449-24457.	1.3	18
14679	Isomeric Ir(III) complexes for tracking mitochondrial pH fluctuations and inducing mitochondrial dysfunction during photodynamic therapy. <i>Dalton Transactions</i> , 2019, 48, 17200-17209.	1.6	16
14680	Fluorine-enriched mesoporous carbon as efficient oxygen reduction catalyst: understanding the defects in porous matrix and fuel cell applications. <i>Nanoscale Advances</i> , 2019, 1, 4926-4937.	2.2	30
14681	Topological semi-metal Na3Bi as efficient spin injector in current driven magnetic tunnel junction. <i>Journal of Applied Physics</i> , 2019, 126, .	1.1	5
14682	Atomic Co/Ni dual sites and Co/Ni alloy nanoparticles in N-doped porous Janus-like carbon frameworks for bifunctional oxygen electrocatalysis. <i>Applied Catalysis B: Environmental</i> , 2019, 240, 112-121.	10.8	334
14683	<sup>57</sup> Fe Mössbauer study of epitaxial TiN thin film grown on MgO (100) by magnetron sputtering. <i>Applied Surface Science</i> , 2019, 464, 682-691.	3.1	5
14684	A DFT+u study, including the van der waals interaction, on the adsorption of XO <sub>2</sub> molecules on the v2o5(001) surface (x= S, N, O, C). <i>Surface Science</i> , 2019, 679, 110-116.	0.8	1
14685	Insight into the effect of co-doped to the photocatalytic performance and electronic structure of g-C <sub>3</sub> N <sub>4</sub> by first principle. <i>Applied Catalysis B: Environmental</i> , 2019, 241, 319-328.	10.8	122
14686	Piezoelectricity and dipolar polarization of group V-IV-III-VI sheets: A first-principles study. <i>Applied Surface Science</i> , 2019, 463, 918-922.	3.1	15
14687	Exploring adsorption behavior and oxidation mechanism of mercury on monolayer Ti <sub>2</sub> CO <sub>2</sub> (MXenes) from first principles. <i>Applied Surface Science</i> , 2019, 464, 53-60.	3.1	31
14688	Prediction of a flexible anode material for Li/Na ion batteries: Phosphorous carbide monolayer (±-PC). <i>Carbon</i> , 2019, 141, 444-450.	5.4	70
14689	Improving the electrical conductivity of Siligraphene SiC <sub>7</sub> by strain. <i>Optik</i> , 2019, 177, 118-122.	1.4	13
14690	First-principles analysis of acetonitrile reaction pathways to primary, secondary, and tertiary amines on Pd(111). <i>Surface Science</i> , 2019, 682, 84-98.	0.8	14
14691	First-principles study of structural, mechanical, and electronic properties of typical iron-containing phases in Al-Cu alloys under different pressures. <i>Physica B: Condensed Matter</i> , 2019, 555, 112-117.	1.3	4
14692	Exploring the electronic and magnetic properties of new metal halides from bulk to two-dimensional monolayer: RuX <sub>3</sub> (X = Br, I). <i>Journal of Magnetism and Magnetic Materials</i> , 2019, 476, 111-119.	1.0	48
14693	Theoretical study on UH <sub>4</sub> , UH <sub>8</sub> and UH <sub>10</sub> at high pressure. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019, 383, 774-780.	0.9	4



#	ARTICLE	IF	CITATIONS
14694	How does the NMR thermometer work? Application of combined quantum molecular dynamics and GIPAW calculations into the study of lead nitrate. <i>Journal of Computational Chemistry</i> , 2019, 40, 811-819.	1.5	1
14695	Mo isolated single atoms on S, N-codoped carbon as efficient catalyst for hydrogen evolution reaction: A theoretical evaluation. <i>Applied Surface Science</i> , 2019, 473, 770-776.	3.1	38
14696	Mitigating Metal Dendrite Formation in Lithium-Sulfur Batteries via Morphology-Tunable Graphene Oxide Interfaces. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 2060-2070.	4.0	19
14697	Negative differential conductance effect and electrical anisotropy of 2D ZrB <sub>2</sub> monolayers. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 065301.	0.7	33
14698	A systematic study on the crystal facets-dependent gas sensing properties of anatase TiO <sub>2</sub> with designed {010}, {101} and {001} facets. <i>Ceramics International</i> , 2019, 45, 6282-6290.	2.3	28
14699	Reduction of NO with CO on the Co <sub>3</sub> O <sub>4</sub> (110)-B and CoO(110) Surfaces: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1770-1778.	1.5	15
14700	Visible-Light-Triggered Release of Sulfonamides in MOF/Ag-Based Nanoparticle Composites: Performance, Mechanism, and DFT Calculations. <i>ACS Applied Nano Materials</i> , 2019, 2, 418-428.	2.4	23
14701	Promoting effect of Ni on the structure and electronic properties of Ni <sub>x</sub> Mo(1-x)S <sub>2</sub> catalyst and benzene adsorption: A periodic DFT study. <i>Applied Surface Science</i> , 2019, 471, 607-614.	3.1	5
14702	Adsorption and decomposition of metal decorated phosphorene toward H <sub>2</sub> S, HCN and NH <sub>3</sub> molecules. <i>Applied Surface Science</i> , 2019, 473, 242-250.	3.1	34
14703	Activation of CO <sub>2</sub> at chromia-nanocluster-modified rutile and anatase TiO <sub>2</sub> . <i>Catalysis Today</i> , 2019, 326, 68-74.	2.2	5
14704	Electronic structures and optical properties of Fe/Co-doped cubic BaTiO <sub>3</sub> ceramics. <i>Ceramics International</i> , 2019, 45, 6303-6311.	2.3	18
14705	Electronic and electrical properties of siligraphene (g-SiC <sub>3</sub> ) in the presence of several strains. <i>Journal of Physics and Chemistry of Solids</i> , 2019, 127, 231-237.	1.9	19
14706	The DFT study on Rh-C bond dissociation enthalpies of (iminoacyl)rhodium(III)hydride and (iminoacyl)rhodium(III)alkyl. <i>Tetrahedron Letters</i> , 2019, 60, 310-321.	0.7	4
14707	Theoretical Insights into Heterogeneous (Photo)electrochemical CO <sub>2</sub> Reduction. <i>Chemical Reviews</i> , 2019, 119, 6631-6669.	23.0	431
14708	Exploration of high-pressure structural transition and electronic properties of BaFe <sub>2</sub> S <sub>3</sub> . <i>Journal of Physics Condensed Matter</i> , 2019, 31, 115401.	0.7	2
14709	Benchmark study of popular density functionals for calculating binding energies of three-center two-electron bonds. <i>Journal of Computational Chemistry</i> , 2019, 40, 657-670.	1.5	11
14710	Density functional theory-based investigations of solute kinetics and precipitate formation in binary magnesium-rare earth alloys: A review. <i>Computational Materials Science</i> , 2019, 159, 235-256.	1.4	18
14711	First-Principles Modeling of Interface Effects in Oxides. , 2019, , 1-30.		0

#	ARTICLE	IF	CITATIONS
14712	Ferromagnetism in Mn and Fe doped ZrO <sub>2</sub> by ab-initio calculations. Computational Condensed Matter, 2019, 19, e00361.	0.9	9
14713	Electron correlation energy with a combined complete active space and corrected density-functional approach in a small basis versus the reference complete basis set limit: A close agreement. Chemical Physics Letters, 2019, 716, 227-230.	1.2	8
14714	Electronic Structure and Properties of Lithium-Rich Complex Oxides. ACS Applied Electronic Materials, 2019, 1, 75-81.	2.0	10
14715	Theoretical Study of Formation of Secondary Arsenic Minerals: Scorodite and Pharmacosiderite. ACS Earth and Space Chemistry, 2019, 3, 192-201.	1.2	17
14716	Atomistic study of an ideal metal/thermoelectric contact: The full-Heusler/half-Heusler interface. APL Materials, 2019, 7, 013202.	2.2	7
14717	Phonon properties and thermal conductivity from first principles, lattice dynamics, and the Boltzmann transport equation. Journal of Applied Physics, 2019, 125, .	1.1	141
14718	Mechanism of the catalytic oxidation of methane on Pt(111) surfaces in moist environment: A density functional theory study. Applied Surface Science, 2019, 471, 566-586.	3.1	15
14719	High-Magnetization Tetragonal Ferrite-Based Films Induced by Carbon and Oxygen Vacancy Pairs. ACS Applied Materials & Interfaces, 2019, 11, 1049-1056.	4.0	5
14720	Elastic and acoustical properties of Cr <sub>3</sub> AlB <sub>4</sub> under pressure. Journal of Physics and Chemistry of Solids, 2019, 126, 65-71.	1.9	9
14721	1T-MoS <sub>2</sub> monolayer doped with isolated Ni atoms as highly active hydrogen evolution catalysts: A density functional study. Applied Surface Science, 2019, 469, 292-297.	3.1	41
14722	Electronic, Optical and Elastic Properties of Cu <sub>2</sub> CdGeSe <sub>4</sub> : A First-Principles Study. Journal of Electronic Materials, 2019, 48, 705-715.	1.0	15
14723	Potassium-Promoted Reduction of Cu <sub>2</sub> O/Cu(111) by CO. Journal of Physical Chemistry C, 2019, 123, 8057-8066.	1.5	20
14724	Interplay of solute-mixed self-interstitial atoms and substitutional solutes with interstitial and substitutional helium atoms in tungsten-transition metal alloys. Nuclear Fusion, 2019, 59, 026002.	1.6	8
14725	Charge compensation doping to improve the photocatalytic and photoelectrochemical activities of Ta <sub>3</sub> N <sub>5</sub> : A theoretical study. Applied Catalysis B: Environmental, 2019, 244, 502-510.	10.8	24
14726	Simulation of the crystal structure formation from the small lithium clusters. Molecular Physics, 2019, 117, 1833-1837.	0.8	3
14727	First-principles predictions on structural, electronic, magnetic and elastic properties of Mn <sub>2</sub> IrAl Heusler alloy. Materials Research Express, 2019, 6, 036101.	0.8	9
14728	Role of Dimensionality for Photocatalytic Water Splitting: CdS Nanotube versus Bulk Structure. ChemPhysChem, 2019, 20, 383-391.	1.0	20
14729	Electrocatalytic Hydrogenation of N <sub>2</sub> to NH <sub>3</sub> by MnO: Experimental and Theoretical Investigations. Advanced Science, 2019, 6, 1801182.	5.6	117

#	ARTICLE	IF	CITATIONS
14730	Nanopyramid boron-doped diamond electrode realizing nanomolar detection limit of 4-nonylphenol. <i>Sensors and Actuators B: Chemical</i> , 2019, 281, 830-836.	4.0	24
14731	Pure and M-doped (M=Zn, Cu, Ni, Co) cadmium oxide nanosheets, novel adsorbents for the adsorption of ethyl benzene and ortho, meta, para xylene: a theoretical study. <i>Adsorption</i> , 2019, 25, 51-62.	1.4	0
14732	Study of the Geometric Structures, Electronic and Magnetic Properties of Aluminium-Antimony Alloy Clusters. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2019, 74, 109-120.	0.7	1
14733	Silver atom, trimer and tetramer species supported on a ceria nanoparticle: A density functional study. <i>Surface Science</i> , 2019, 681, 38-46.	0.8	8
14734	Formation and temporal evolution of modulated structure in high Nb-containing lamellar $\hat{1}^3$ -TiAl alloy. <i>Acta Materialia</i> , 2019, 165, 215-227.	3.8	35
14735	CO <sub>2</sub> reduction by H <sub>2</sub> to CHO on Ru(0001): DFT evaluation of three pathways. <i>Surface Science</i> , 2019, 681, 54-58.	0.8	11
14736	Hydrogen storage in MIL-88 series. <i>Journal of Materials Science</i> , 2019, 54, 3994-4010.	1.7	27
14737	Phase stability and weak metallic bonding within ternary layered borides CrAlB, Cr <sub>2</sub> AlB <sub>2</sub> , Cr <sub>3</sub> AlB <sub>4</sub> , and Cr <sub>4</sub> AlB <sub>6</sub> . <i>Journal of the American Ceramic Society</i> , 2019, 102, 3715-3727.	1.9	55
14738	DFT study on the influence of sulfur on the hydrophobicity of pyrite surfaces in the process of oxidation. <i>Applied Surface Science</i> , 2019, 466, 964-969.	3.1	19
14739	Effects of a vacancy, Cr and Mo on the electronic structure of FeAl <sub>3</sub> (100) [111] grain boundaries. <i>Materials Research Express</i> , 2019, 6, 026514.	0.8	0
14740	The Effect of Donor Additives on the Stability and Structure of 5- <i>l</i> -Diphenylphosphinoacenaphth <sup>6</sup> -yllithium. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 712-720.	1.0	8
14741	Evaluation of methods for obtaining dispersion energies used in density functional calculations of intermolecular interactions. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	18
14742	A Eu <sup>3+</sup> -Eu <sup>2+</sup> ion redox shuttle imparts operational durability to Pb-I perovskite solar cells. <i>Science</i> , 2019, 363, 265-270.	6.0	793
14743	Transport properties of doped zigzag graphene nanoribbons. <i>Chinese Journal of Physics</i> , 2019, 57, 47-52.	2.0	7
14744	Triplet Tuning: A Novel Family of Non-Empirical Exchange-Correlation Functionals. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1226-1241.	2.3	34
14745	Interaction Behavior of Cyanogen Fluoride and Chloride Gas Molecules on Red Phosphorene Nanosheet: A DFT Study. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2019, 29, 954-963.	1.9	30
14746	Surface thermodynamic stability of Li-rich Li <sub>2</sub> MnO <sub>3</sub> : Effect of defective graphene. <i>Energy Storage Materials</i> , 2019, 22, 113-119.	9.5	45
14747	Reduction of impurity contents in aluminum plates electrodeposited from a dimethylsulfone-aluminum chloride bath. <i>Journal of Alloys and Compounds</i> , 2019, 783, 919-926.	2.8	8

#	ARTICLE	IF	CITATIONS
14748	Reactive and Nonreactive Scattering of HCl from Au(111): An Ab Initio Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 2287-2299.	1.5	30
14749	Phase transition in two-dimensional tellurene under mechanical strain modulation. <i>Nano Energy</i> , 2019, 58, 202-210.	8.2	43
14750	Computational Screening for ORR Activity of 3d Transition Metal Based M@Pt Core-Shell Clusters. <i>Journal of Physical Chemistry C</i> , 2019, 123, 3634-3644.	1.5	48
14751	Catalytic oxidation of ethyl acetate over Ru-Cu bimetallic catalysts: Further insights into reaction mechanism via in situ FTIR and DFT studies. <i>Journal of Catalysis</i> , 2019, 369, 482-492.	3.1	52
14752	Interfacial engineering of OD/2D SnS <sub>2</sub> heterostructure onto nitrogen-doped graphene for boosted lithium storage capability. <i>Journal of Colloid and Interface Science</i> , 2019, 538, 116-124.	5.0	23
14753	Origins and Control of Optical Absorption in a Nondilute Oxide Solid Solution: Sr(Ti,Fe)O <sub>3</sub> Perovskite Case Study. <i>Chemistry of Materials</i> , 2019, 31, 1030-1041.	3.2	17
14754	Density Functional Theory Study of Arsenic Adsorption on the Fe <sub>2</sub> O <sub>3</sub> (001) Surface. <i>Energy &amp; Fuels</i> , 2019, 33, 1414-1421.	2.5	49
14755	Understanding Carrier Transport in Organic Semiconductors: Computation of Charge Mobility Considering Quantum Nuclear Tunneling and Delocalization Effects. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1477-1491.	2.3	33
14756	Relationship between Energetic Performance and Clustering Effects on Incremental Nitramine Groups: A Theoretical Perspective. <i>Journal of Physical Chemistry A</i> , 2019, 123, 742-749.	1.1	6
14757	Effect of magnesium on structural and optical properties of CaTiO <sub>3</sub> : A DFT study. <i>Physica B: Condensed Matter</i> , 2019, 568, 88-91.	1.3	19
14758	Effect of Surface Ni on Oxygen Reduction Reaction in Dealloyed Nanoporous Pt-Ni. <i>Industrial &amp; Engineering Chemistry Research</i> , 2019, 58, 7438-7447.	1.8	9
14759	Thickness dependent electronic properties of Pt dichalcogenides. <i>Npj 2D Materials and Applications</i> , 2019, 3, .	3.9	138
14760	Effective and Novel Application of Hydrodynamic Voltammetry to the Study of Superoxide Radical Scavenging by Natural Phenolic Antioxidants. <i>Antioxidants</i> , 2019, 8, 14.	2.2	30
14761	Mechanical and electronic properties under high pressure on ternary AlGaN and InGaN compounds: a first-principles perspective. <i>Materials Research Express</i> , 2019, 6, 015052.	0.8	14
14762	Shape Magnetic Anisotropy From Spin Density in Nanoscale Slab Systems. <i>IEEE Transactions on Magnetics</i> , 2019, 55, 1-4.	1.2	1
14763	Atomistic Simulation: A Unique and Powerful Computational Tool for Corrosion Inhibition Research. <i>Arabian Journal for Science and Engineering</i> , 2019, 44, 1-32.	1.7	158
14764	Energetics of helium-vacancy complexes in Fe-9Cr alloys from first-principles calculations. <i>Journal of Nuclear Materials</i> , 2019, 513, 143-151.	1.3	26
14765	Decohesion Energy of $\Sigma 5(012)$ Grain Boundaries in Ni as Function of Hydrogen Content. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2019, 50, 451-456.	1.1	3

#	ARTICLE	IF	CITATIONS
14766	A hybrid density functional study of optical and electronic properties of AlGa-codoped ZnO. <i>Optik</i> , 2019, 179, 566-573.	1.4	8
14767	Coupling of Acetaldehyde to Crotonaldehyde on CeO <sub>2</sub> (111): Bifunctional Mechanism and Role of Oxygen Vacancies. <i>Journal of Physical Chemistry C</i> , 2019, 123, 8273-8286.	1.5	23
14768	Surface characterization of face-centered cubic crystals. <i>Mechanics of Materials</i> , 2019, 129, 15-22.	1.7	13
14769	The effect of anti-site disorder and tetragonal distortion on the electronic structure of Ti <sub>2</sub> VSb. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019, 383, 243-247.	0.9	2
14770	Electronic processes in NO dimerization on Ag and Cu clusters: DFT and MRMP2 studies. <i>Journal of Computational Chemistry</i> , 2019, 40, 181-190.	1.5	9
14771	Dislocation pile-ups at $\hat{\Gamma}^{21}$ precipitate interfaces in Mg-rare earth (RE) alloys. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2019, 742, 278-286.	2.6	32
14772	Arsenene nanoribbons for sensing NH <sub>3</sub> and PH <sub>3</sub> gas molecules – A first-principles perspective. <i>Applied Surface Science</i> , 2019, 469, 173-180.	3.1	77
14773	Intramolecular Cyclization of 3,3-Diarylpropenylamides of Electron-Deficient Alkenes: Stereoselective Synthesis of Functionalized Hexahydrobenzo[ <i>f</i> ]isoindoles. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 204-220.	1.2	2
14774	Hydrogen induced changes of optical and magnetic properties of nanocrystalline Zn <sub>0.95</sub> Gd <sub>0.03</sub> M <sub>0.02</sub> O (M=Al,Mg): Experimental and DFT studies. <i>Journal of Alloys and Compounds</i> , 2019, 776, 575-585.	2.8	3
14775	Computational Methods in Spectroscopy. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019, , 1-48.	0.6	0
14776	Investigating Raman spectra and density functional theory calculations on SrAl <sub>2</sub> O <sub>4</sub> polymorphs. <i>Journal of Raman Spectroscopy</i> , 2019, 50, 91-101.	1.2	9
14777	First-principles study of CN point defects on sidewall surface of [0001]-oriented GaN nanowires. <i>Applied Surface Science</i> , 2019, 467-468, 293-297.	3.1	7
14778	The influence of spatial limits on the modeling chemical reactivity: The example of CO <sub>2</sub> hydration in MeX zeolites (Me = K, Rb, Cs). <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25820.	1.0	1
14779	Aurophilicity and Photoluminescence of (6-Diphenylpicogenoacene)gold Compounds. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 647-659.	1.0	12
14780	Ceramic phases with one-dimensional long-range order. <i>Nature Materials</i> , 2019, 18, 19-23.	13.3	18
14781	Band gap modulation of ZrX <sub>2</sub> (X = S, Se, Te) mono-layers under biaxial strain and transverse electric field and its lattice dynamic properties: a first principles study. <i>Materials Research Express</i> , 2019, 6, 036308.	0.8	10
14782	Performance of DFT for C <sub>60</sub> Isomerization Energies: A Noticeable Exception to Jacob's Ladder. <i>Journal of Physical Chemistry A</i> , 2019, 123, 257-266.	1.1	19
14783	Electrocatalytic N <sub>2</sub> Fixation over Hollow VO <sub>2</sub> Microspheres at Ambient Conditions. <i>ChemElectroChem</i> , 2019, 6, 1014-1018.	1.7	59

#	ARTICLE	IF	CITATIONS
14784	A General Two-Step Strategy-Based High-Throughput Screening of Single Atom Catalysts for Nitrogen Fixation. <i>Small Methods</i> , 2019, 3, 1800376.	4.6	303
14785	Dipole controlled Schottky barrier in the blue-phosphorene-phase of GeSe based van der Waals heterostructures. <i>Nanoscale Horizons</i> , 2019, 4, 480-489.	4.1	32
14786	Data-Driven Materials Exploration for Li-Ion Conductive Ceramics by Exhaustive and Informatics-Aided Computations. <i>Chemical Record</i> , 2019, 19, 771-778.	2.9	37
14787	Computational assessment on the interaction of amantadine drug with B <sub>12</sub> N <sub>12</sub> and Zn <sub>12</sub> O <sub>12</sub> nanocages and improvement in adsorption behaviors by impurity Al doping. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	27
14788	Integration of phenylammoniumiodide (PAI) as a surface coating molecule towards ambient stable MAPbI <sub>3</sub> perovskite for solar cell application. <i>Solar Energy Materials and Solar Cells</i> , 2019, 191, 316-328.	3.0	17
14789	Investigation on electronic structures and mechanical properties of Nb-doped TiAl <sub>2</sub> intermetallic compound. <i>Journal of Alloys and Compounds</i> , 2019, 780, 41-48.	2.8	19
14790	Atomic Modeling and Electronic Structure of Mixed Ionic-Electronic Conductor SrTi <sub>1-x</sub> Fe <sub>x</sub> O <sub>3</sub> Considered as a Mixture of SrTiO <sub>3</sub> and Sr <sub>2</sub> Fe <sub>2</sub> O <sub>5</sub> . <i>Chemistry of Materials</i> , 2019, 31, 233-243.	3.2	13
14791	1,2-H Atom Rearrangements in Benzyloxyl Radicals. <i>Journal of Physical Chemistry A</i> , 2019, 123, 492-504.	1.1	5
14792	Elementary kinetics of nitrogen electroreduction on Fe surfaces. <i>Journal of Chemical Physics</i> , 2019, 150, 041708.	1.2	32
14793	Germanene nanotube electroresistive molecular device for detection of NO <sub>2</sub> and SO <sub>2</sub> gas molecules: a first-principles investigation. <i>Journal of Computational Electronics</i> , 2019, 18, 308-318.	1.3	27
14794	Generalized Gradient Approximation Exchange Energy Functional with Near-Best Semilocal Performance. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 303-310.	2.3	24
14795	Density functional theory. , 2019, , 119-159.		7
14796	Insight into phosphate doped BiVO <sub>4</sub> heterostructure for multifunctional photocatalytic performances: A combined experimental and DFT study. <i>Applied Surface Science</i> , 2019, 466, 787-800.	3.1	36
14797	Development of a pair potential for Ta-He system. <i>Computational Materials Science</i> , 2019, 156, 268-272.	1.4	4
14798	Electronic structure and photoluminescence properties of a novel single-phased color tunable phosphor KAlGeO <sub>4</sub> :Bi <sup>3+</sup> ,Eu <sup>3+</sup> for WLEDs. <i>Journal of Alloys and Compounds</i> , 2019, 774, 477-486.	2.8	69
14799	Single-molecule tunnel magnetoresistance of azulene. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019, 105, 219-223.	1.3	3
14800	Reversible hydrogen storage behaviors of Ti <sub>2</sub> N MXenes predicted by first-principles calculations. <i>Journal of Materials Science</i> , 2019, 54, 493-505.	1.7	38
14801	Study of active surface centers of Pt/CeO <sub>2</sub> catalysts prepared using radio-frequency plasma sputtering technique. <i>Surface Science</i> , 2019, 679, 273-283.	0.8	37



#	ARTICLE	IF	CITATIONS
14802	A comparative first-principles study of point defect properties in the layered MX <sub>2</sub> (M = Mo, W; X = S, Te); Substitution by the groups III, V and VII elements. <i>Computational Materials Science</i> , 2019, 156, 280-285.	1.4	3
14803	Prediction of HfB <sub>3</sub> from first-principles calculations: crystal structures, stabilities, electronic properties and hardnesses. <i>Molecular Physics</i> , 2019, 117, 547-556.	0.8	6
14804	Thermodynamic description for the NaF-KF-RbF-ZnF <sub>2</sub> system. <i>Journal of Fluorine Chemistry</i> , 2019, 217, 90-96.	0.9	2
14805	First-principles investigation of water adsorption on FeCrAl (111) surfaces. <i>Applied Surface Science</i> , 2019, 465, 259-266.	3.1	8
14806	Surface modification vs sorption strength: Study of nedaplatin drug supported on silica. <i>Applied Surface Science</i> , 2019, 465, 693-699.	3.1	7
14807	Structural, electronic and optical properties of copper-doped SrTiO <sub>3</sub> perovskite: A DFT study. <i>Physica B: Condensed Matter</i> , 2019, 552, 52-57.	1.3	69
14808	Density functional theory study on improved reactivity of alkali-doped Fe <sub>2</sub> O <sub>3</sub> oxygen carriers for chemical looping hydrogen production. <i>Fuel</i> , 2019, 236, 1057-1064.	3.4	38
14809	A combined experimental and density functional theory investigation of the hydrogen bonding of 2-cyclohexen-1-one and 3-methyl-2-cyclohexen-1-one in solvents. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 208, 32-39.	2.0	6
14810	Theoretical Treatment for Properties of Surfaces and Their Interplay with Bulk Properties of Crystals. <i>Advanced Theory and Simulations</i> , 2019, 2, 1800117.	1.3	2
14811	Effect of substrate relaxation on adsorption energies: The example of Fe <sub>2</sub> O <sub>3</sub> (0001) and Fe <sub>3</sub> O <sub>4</sub> (111). <i>Surface Science</i> , 2019, 679, 225-229.	0.8	10
14812	Density Functional Theory Study of Mn <sub>n</sub> +1AX <sub>n</sub> Phases: A Review. <i>Critical Reviews in Solid State and Materials Sciences</i> , 2019, 44, 56-107.	6.8	46
14813	Understanding the multifunctionality in Cu-doped BiVO <sub>4</sub> semiconductor photocatalyst. <i>Journal of Environmental Sciences</i> , 2019, 75, 84-97.	3.2	56
14814	Combining Theory and Experiment for Multitechnique Characterization of Activated CO <sub>2</sub> on Transition Metal Carbide (001) Surfaces. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7567-7576.	1.5	22
14815	Ab initio study of mono-layer 2-D insulators (X-(OH) <sub>2</sub> and h-BN) and their use in MTJ memory device. <i>Microsystem Technologies</i> , 2019, 25, 1909-1917.	1.2	8
14816	First-principles kinetics study of carbon monoxide promoted Ostwald ripening of Au particles on FeO/Pt(111). <i>Journal of Energy Chemistry</i> , 2019, 30, 108-113.	7.1	12
14817	DFT STUDY OF METHYL (CH <sub>3</sub> ) AND HYDROXYL (OH) ADSORPTION ON A GOLD (001) SURFACE. <i>Surface Review and Letters</i> , 2019, 26, 1850198.	0.5	4
14818	Unraveling the Stable Phase, High Absorption Coefficient, Optical and Mechanical Properties of Hybrid Perovskite CH <sub>3</sub> NH <sub>3</sub> Pb <sub>x</sub> Mg <sub>1-x</sub> I <sub>3</sub> : Density Functional Approach. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2020, 30, 299-309.	1.9	16
14819	Reshaping of Rh nanoparticles in operando conditions. <i>Catalysis Today</i> , 2020, 350, 184-191.	2.2	3



#	ARTICLE	IF	CITATIONS
14820	Thiadiazole-2-Thiol-5-Thione and 2,5-Dimercapto-1,3,4-Thiadiazol Tautomerism, Conformational Stability, Vibrational Assignments, Inhibitor Efficiency and Quantum Chemical Calculations. Zeitschrift Fur Physikalische Chemie, 2020, 234, 415-440.	1.4	8
14821	The structural, electronic and magnetic properties of Ag <sub>4</sub> M and Ag <sub>4</sub> MCO (M=Sc, Zn) clusters. Molecular Physics, 2020, 118, 1622051.	0.8	4
14822	Effect of functionalization of iron oxide nanoparticles on the physical properties of poly (aniline-co-pyrrole) based nanocomposites: Experimental and theoretical studies. Arabian Journal of Chemistry, 2020, 13, 2331-2339.	2.3	17
14823	Isocyanic acid (HNCO) adsorption on the flat and defective Rh(001) surfaces: Pure DFT and DFT+vdW calculations. Journal of Physics and Chemistry of Solids, 2020, 138, 109162.	1.9	4
14824	Tunable terahertz reflection spectrum based on zinc-blende structure crystals excited by ultrasonic. Optik, 2020, 200, 163392.	1.4	0
14825	First-principles calculations on interface stability and migration of H and He in W-ZrC interfaces. Applied Surface Science, 2020, 499, 143995.	3.1	34
14826	A DFT study on corrosion mechanism of steel bar under water-oxygen interaction. Computational Materials Science, 2020, 171, 109265.	1.4	22
14827	Thermoelectric transport properties of magnetic carbon-based organic chains. Chemical Physics, 2020, 528, 110524.	0.9	2
14828	A flexible non-enzymatic glucose sensor based on copper nanoparticles anchored on laser-induced graphene. Carbon, 2020, 156, 506-513.	5.4	235
14829	First principle study of feasibility of dinitrogen reduction to ammonia on two-dimensional transition metal phthalocyanine monolayer. Applied Surface Science, 2020, 500, 144032.	3.1	34
14830	Theoretical study on structural properties of silicon-doped benzothiazole/SnO <sub>2</sub> (110): A novel molecular design for solar cells. Applied Surface Science, 2020, 501, 144054.	3.1	4
14831	First-principles investigation of structural, electronic, optical and thermal properties of Zinc doped SrTiO <sub>3</sub> . Optik, 2020, 201, 163481.	1.4	26
14832	Pseudopotential for plane-wave density functional theory studies of metallic uranium. Computational Materials Science, 2020, 171, 109221.	1.4	11
14833	Charge-neutral epitaxial graphene on 6H-SiC(0001) via FeSi intercalation. Carbon, 2020, 156, 187-193.	5.4	12
14834	TM-CmHm organometallics (TM=Fe, Co, Ni, Cu, Zn and m=4, 5, 6) for highly efficient Pt-free catalytic activation of O <sub>2</sub> molecule. Journal of Molecular Structure, 2020, 1200, 127008.	1.8	5
14835	New LaMnO <sub>3</sub> surface energy results obtained from density-functional theory. Surface Science, 2020, 695, 121500.	0.8	6
14836	Facile Green Synthesis of Silver Bionanocomposite with Size Dependent Antibacterial and Synergistic Effects: A Combined Experimental and Theoretical Studies. Journal of Inorganic and Organometallic Polymers and Materials, 2020, 30, 1839-1851.	1.9	16
14837	Boron trifluoride interaction studies on graphdiyne nanotubes – A first-principles insight. Chemical Physics Letters, 2020, 738, 136841.	1.2	41

#	ARTICLE	IF	CITATIONS
14838	Crystal structure and mechanical properties of nickel–cobalt alloys with different compositions: A first-principles study. <i>Journal of Physics and Chemistry of Solids</i> , 2020, 137, 109194.	1.9	25
14839	Formation of phenoxy-type Environmental Persistent Free Radicals (EPFRs) from dissociative adsorption of phenol on Cu/Fe and their partial oxides. <i>Chemosphere</i> , 2020, 240, 124921.	4.2	17
14840	Predicting excellent anisotropic thermoelectric performance of the layered oxychalcogenides BiAgOCh (Ch = S, Se, and Te). <i>Computational Materials Science</i> , 2020, 171, 109273.	1.4	12
14841	Towards photoferroic materials by design: recent progress and perspectives. <i>JPhys Energy</i> , 2020, 2, 011001.	2.3	13
14842	Single cobalt atom anchored on N-doped graphyne for boosting the overall water splitting. <i>Applied Surface Science</i> , 2020, 502, 144155.	3.1	50
14843	Modifying effects and mechanisms of graphene on dehydrogenation properties of sodium borohydride. <i>Journal of Materials Science</i> , 2020, 55, 1959-1972.	1.7	12
14844	Structural and electronic properties of bastnaesite and implications for surface reactions in flotation. <i>Journal of Rare Earths</i> , 2020, 38, 332-338.	2.5	14
14845	Carbon chain growth mechanism of higher alcohols synthesis from syngas on CoCu(100): A combined DFT and kMC study. <i>Surface Science</i> , 2020, 691, 121513.	0.8	4
14846	<i>Ab initio</i> modeling and design of vanadia-based electrode materials for post-lithium batteries. <i>Journal Physics D: Applied Physics</i> , 2020, 53, 083001.	1.3	9
14847	Surface-scale affinity and adsorption selectivity of alkaline earth metal oxides to H <sub>2</sub> O and CO <sub>2</sub> : Insight into SOFC anode modification. <i>Applied Surface Science</i> , 2020, 503, 144333.	3.1	10
14848	Enhancement of corrosion resistance of a high Zn-yttrium aluminum alloy. <i>Journal of Alloys and Compounds</i> , 2020, 817, 152744.	2.8	5
14849	An overview of the first principles studies of doped RE-TM5 systems for the development of hard magnetic properties. <i>Journal of Magnetism and Magnetic Materials</i> , 2020, 496, 165902.	1.0	13
14850	Mechanistic Insight of the Catalytic Role of WOX/SiO <sub>2</sub> Catalyst in 2,5-Dimethylfuran to Para-xylene Conversion by DFT Calculation. <i>Catalysis Letters</i> , 2020, 150, 794-801.	1.4	7
14851	Uncovering the electrochemical mechanisms for hydrogen evolution reaction of heteroatom doped M <sub>2</sub> C MXene (M = Ti, Mo). <i>Applied Surface Science</i> , 2020, 500, 143987.	3.1	93
14852	DFT study of ethanol adsorption on CaO(001) surface. <i>Applied Surface Science</i> , 2020, 500, 144254.	3.1	25
14853	Understanding the structural and chemical evolution of layered potassium titanates for sodium ion batteries. <i>Energy Storage Materials</i> , 2020, 25, 502-509.	9.5	17
14854	Two-dimensional carbon nitride (C <sub>3</sub> N) nanosheets as promising materials for H <sub>2</sub> S and NH <sub>3</sub> elimination: A computational approach. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 117, 113794.	1.3	31
14855	Electron transport properties of silicene: Intrinsic and dirty cases with screening effects. <i>Journal of Molecular Structure</i> , 2020, 1199, 126878.	1.8	3

#	ARTICLE	IF	CITATIONS
14856	Enhanced photovoltaic performances of C219-based dye sensitizers by introducing electron-withdrawing substituents: a density functional theory study. <i>Molecular Physics</i> , 2020, 118, e1636151.	0.8	2
14857	A giant enhancement of magnetic moment in a ternary three-shell icosahedral cluster: Fe@Mn <sub>12</sub> @Au <sub>20</sub> . <i>Molecular Physics</i> , 2020, 118, e1659434.	0.8	2
14858	Unraveling the stacking effect and stability in nanocrystalline antimony through DFT. <i>Journal of Physics and Chemistry of Solids</i> , 2020, 136, 109156.	1.9	5
14859	Crystal structure prediction of ReN <sub>2</sub> under high pressure. <i>Indian Journal of Physics</i> , 2020, 94, 1711-1716.	0.9	1
14860	Oxysulfide Li <sub>2</sub> BeSO: A potential new material for solid electrolyte predicted from first principles. <i>Journal of Alloys and Compounds</i> , 2020, 818, 152844.	2.8	1
14861	Dopant screening of modified Fe <sub>2</sub> O <sub>3</sub> oxygen carriers in chemical looping hydrogen production. <i>Fuel</i> , 2020, 262, 116489.	3.4	52
14862	Beyond the Vegard's law: solid mixing excess volume and thermodynamic potentials prediction, from end-members. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126059.	0.9	2
14863	Photoisomerization and Mesophase Formation in Azo-Ionic Liquids. <i>Crystal Growth and Design</i> , 2020, 20, 214-225.	1.4	9
14864	Enhanced electrochemical properties of iron oxalate with more stable Li <sup>+</sup> ions diffusion channels by controlling polymorphic structure. <i>Chemical Engineering Journal</i> , 2020, 384, 123281.	6.6	42
14865	External electric field effect on electronic properties and charge transfer in Co <sub>2</sub> /Ni <sub>2</sub> spinterface. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26092.	1.0	3
14866	Iron-nitrogen doped carbon with exclusive presence of Fe <sub>x</sub> N active sites as an efficient ORR electrocatalyst for Zn-air battery. <i>Applied Catalysis B: Environmental</i> , 2020, 268, 118405.	10.8	80
14867	First-principles investigation on the atomic structure, stability and electronic property of O(001)/B <sub>2</sub> (110) interface in Ti <sub>2</sub> AlNb alloys. <i>Journal of Alloys and Compounds</i> , 2020, 817, 152734.	2.8	12
14868	A coverage dependent study of the adsorption of pyridine on the (111) coinage metal surfaces. <i>Surface Science</i> , 2020, 693, 121525.	0.8	12
14869	A theoretical investigation on the nucleophilic behavior of Meldrum's acid linked to experimental evidences. <i>Chemical Physics Letters</i> , 2020, 738, 136908.	1.2	3
14870	Consequences of Curvature on Induced Magnetic Field: The Case of Helicenes. <i>Chemistry - A European Journal</i> , 2020, 26, 326-330.	1.7	21
14871	Comparisons of half-metallic results of Al <sub>0.75</sub> Co <sub>0.25</sub> Sb diluted magnetic semiconductor with generalized gradient approximation (GGA) and Tran Blaha modified Becke-Johnson (TB_mBJ) potential methods. <i>Physica B: Condensed Matter</i> , 2020, 581, 411841.	1.3	14
14872	Atomic-Scale Mechanism of Unidirectional Oxide Growth. <i>Advanced Functional Materials</i> , 2020, 30, 1906504.	7.8	30
14873	Promising hole-transporting materials for perovskite solar cells: Modulation of the electron-deficient units in triphenylamine derivative-based molecules. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26070.	1.0	7

#	ARTICLE	IF	CITATIONS
14874	The Synergy of Dilute Pd and Surface Oxygen Species for Methane Upgrading on Au <sub>3</sub> Pd(111). Energy Technology, 2020, 8, 1900732.	1.8	3
14875	Time-resolved in-situ IR and DFT study: NH <sub>3</sub> adsorption and redox cycle of acid site on vanadium-based catalysts for NO abatement via selective catalytic reduction. Chemical Engineering Journal, 2020, 382, 122756.	6.6	24
14876	Probing the active sites of site-specific nitrogen doping in metal-free graphdiyne for electrochemical oxygen reduction reactions. Science Bulletin, 2020, 65, 45-54.	4.3	52
14877	Calculating nuclear magnetic resonance chemical shifts in solvated systems. Magnetic Resonance in Chemistry, 2020, 58, 611-624.	1.1	17
14878	Shape change of submicron nickel particles under hydrogen and nickel chloride vapor. Applied Surface Science, 2020, 509, 145274.	3.1	4
14879	Theoretical Insight into the Role of Defects and Facets in the Selectivity of Products in Water Oxidation over Bismuth Vanadate (BiVO <sub>4</sub> ). ACS Sustainable Chemistry and Engineering, 2020, 8, 1980-1988.	3.2	15
14880	Magnetic ground state of face-centered-cubic structure of iron. Journal of Physics Condensed Matter, 2020, 32, 165806.	0.7	12
14881	Promoted CO <sub>2</sub> electroreduction over indium-doped SnP <sub>3</sub> : A computational study. Journal of Energy Chemistry, 2020, 48, 1-6.	7.1	19
14882	Designing rare-earth free permanent magnets in heusler alloys via interstitial doping. Acta Materialia, 2020, 186, 355-362.	3.8	20
14883	An integrated experimental and computational study of diffusion and atomic mobility of the aluminum-magnesium system. Acta Materialia, 2020, 189, 214-231.	3.8	29
14884	Anatomy of large perpendicular magnetic anisotropy in free-standing Co/Ni (1 1 1) multilayer. Journal of Magnetism and Magnetic Materials, 2020, 500, 166357.	1.0	5
14885	Single-atom transition metals supported on black phosphorene for electrochemical nitrogen reduction. Nanoscale, 2020, 12, 4903-4908.	2.8	107
14886	Investigation of the Mn dopant-enhanced photoluminescence performance of lead-free Cs <sub>2</sub> AgInCl <sub>6</sub> double perovskite crystals. Physical Chemistry Chemical Physics, 2020, 22, 1815-1819.	1.3	25
14887	Strain effects on Co,N co-decorated graphyne catalysts for overall water splitting electrocatalysis. Physical Chemistry Chemical Physics, 2020, 22, 2457-2465.	1.3	32
14888	High throughput study on magnetic ground states with Hubbard <i>U</i> corrections in transition metal dihalide monolayers. Nanoscale Advances, 2020, 2, 495-501.	2.2	25
14889	Monoaurated <i>vs.</i> diaurated intermediates: causality or independence?. Chemical Science, 2020, 11, 980-988.	3.7	10
14890	Tuning the surface segregation composition of a PdCo alloy by the atmosphere for increasing electrocatalytic activity. Sustainable Energy and Fuels, 2020, 4, 380-386.	2.5	13
14891	Atomically dispersed asymmetric Cu-B pair on 2D carbon nitride synergistically boosts the conversion of CO into C <sub>2</sub> products. Journal of Materials Chemistry A, 2020, 8, 599-606.	5.2	58

#	ARTICLE	IF	CITATIONS
14892	Theoretical dopant screening and processing optimization for vanadium disulfide as cathode material for Li-air batteries: A density functional theory study. <i>Applied Surface Science</i> , 2020, 508, 145276.	3.1	8
14893	Tripyridinophane Platform Containing Three Acetate Pendant Arms: An Attractive Structural Entry for the Development of Neutral Eu(III) and Tb(III) Complexes in Aqueous Solution. <i>Inorganic Chemistry</i> , 2020, 59, 1496-1512.	1.9	8
14894	Accurate Water Properties from an Efficient ab Initio Method. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 974-987.	2.3	15
14895	First-principles investigation of the electronic properties of the Bi <sub>2</sub> O <sub>4</sub> (101)/BiVO <sub>4</sub> (010) heterojunction towards more efficient solar water splitting. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 2449-2456.	1.3	18
14896	Effect of Hydrotalcites Interlayer Water on Pt-Catalyzed Aqueous-Phase Selective Hydrogenation of Cinnamaldehyde. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 2516-2524.	4.0	28
14897	High-throughput HSE study on the doping effect in anatase TiO <sub>2</sub> . <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 39-53.	1.3	30
14898	C <sub>2</sub> N/BlueP van der Waals hetero-structure: an efficient photocatalytic water splitting 2D material. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1485-1492.	1.3	34
14899	Catalytic mechanisms of oxygen-containing groups over vanadium active sites in an Al-MCM-41 framework for production of 2,5-diformylfuran from 5-hydroxymethylfurfural. <i>Catalysis Science and Technology</i> , 2020, 10, 278-290.	2.1	15
14900	Mechanistic insight into the organocalcium-mediated nucleophilic alkylation of benzene and further rational design. <i>Catalysis Science and Technology</i> , 2020, 10, 950-958.	2.1	4
14901	Catalytic formation of N3-substituted quinazoline-2,4(1 <i>H</i> ),3 <i>H</i> -diones by Pd( <i>scpd</i> )EN@GO composite and its mechanistic investigations through DFT calculations. <i>New Journal of Chemistry</i> , 2020, 44, 141-151.	1.4	26
14902	Ultra stable superatomic structure of doubly magic Ga <sub>13</sub> and Ga <sub>13</sub> Li electrolyte. <i>Nanoscale</i> , 2020, 12, 289-295.	2.8	3
14903	Metal single-atom coordinated graphitic carbon nitride as an efficient catalyst for CO oxidation. <i>Nanoscale</i> , 2020, 12, 364-371.	2.8	59
14904	Metal-free highly efficient photocatalysts for overall water splitting: C <sub>3</sub> N <sub>5</sub> multilayers. <i>Nanoscale</i> , 2020, 12, 306-315.	2.8	57
14905	Revealing cooperative Li-ion migration in Li <sub>1+x</sub> Al <sub>x</sub> Ti <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> solid state electrolytes with high Al doping. <i>Journal of Materials Chemistry A</i> , 2020, 8, 342-348.	5.2	41
14906	Cu <sub>2</sub> MgO <sub>3</sub> Electronic and Magnetic Properties – a DFT Study. <i>Israel Journal of Chemistry</i> , 2020, 60, 863-869.	1.0	2
14907	Methanol synthesis from CO <sub>2</sub> : a DFT investigation on Zn-promoted Cu catalyst. <i>Research on Chemical Intermediates</i> , 2020, 46, 1749-1769.	1.3	14
14908	Environmentally benign synthesis of a PGM-free catalyst for low temperature CO oxidation. <i>Applied Catalysis B: Environmental</i> , 2020, 264, 118547.	10.8	20
14909	Germanium and iron double-substituted ZnGa <sub>2</sub> O <sub>4</sub> solid-solution photocatalysts with modulated band structure for boosting photocatalytic CO <sub>2</sub> reduction with H <sub>2</sub> O. <i>Applied Catalysis B: Environmental</i> , 2020, 265, 118551.	10.8	31

#	ARTICLE	IF	CITATIONS
14910	An experimental and theoretical approach to investigate correlation between electromagnetic properties of doped ferrites & its interfacial reactivity with dopamine. Applied Surface Science, 2020, 506, 144945.	3.1	3
14911	Benchmark study of DFT and composite methods for bond dissociation energies in argon compounds. Chemical Physics, 2020, 531, 110676.	0.9	8
14912	$\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"} \rangle \langle \text{mml:msup} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi mathvariant="normal"} \rangle \text{C} \langle \text{mml:mi} \rangle \langle \text{mml:mi mathvariant="normal"} \rangle \text{u} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \hat{\text{I}} \langle \text{mml:mi} \rangle \langle \text{mml:mo} \rangle + \langle \text{mml:mo} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msup} \rangle$ active sites stabilization through Mott-Schottky effect for promoting highly efficient conversion of carbon monoxide into n-propanol. Journal of Catalysis, 2020, 382, 49-56.	3.1	27
14913	Intrinsic carrier mobility of monolayer GeS and GeSe: First-principles calculation. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 118, 113877.	1.3	40
14914	Isomeric Thiolate Monolayer Protected Au <sub>92</sub> and Au <sub>102</sub> Nanomolecules. Journal of Physical Chemistry C, 2020, 124, 1655-1666.	1.5	9
14915	Two-Dimensional Transition Metal Porphyrin Sheets as a Promising Single-Atom-Catalyst for Dinitrogen Electrochemical Reduction to Ammonia: A Theoretical Study. Journal of Physical Chemistry C, 2020, 124, 1492-1499.	1.5	30
14916	Revealing Grain-Boundary-Induced Degradation Mechanisms in Li-Rich Cathode Materials. Nano Letters, 2020, 20, 1208-1217.	4.5	62
14917	Bioinspired Electrocatalyst for Electrochemical Reduction of N <sub>2</sub> to NH <sub>3</sub> in Ambient Conditions. ACS Applied Materials & Interfaces, 2020, 12, 2445-2451.	4.0	39
14918	A TDDFT study of some dinuclear compounds containing CpM(CO) <sub>3</sub> or CpM(CO) <sub>2</sub> groups. Molecular Physics, 2020, 118, e1692153.	0.8	0
14919	Electronic structure of hydroxylated La@C <sub>82</sub> endohedral metallofullerene: implications on photovoltaic cells. Molecular Physics, 2020, 118, e1705411.	0.8	3
14920	Adsorption of antimonite and antimonate from aqueous solution using modified polyacrylonitrile with an ultrahigh percentage of amidoxime groups. Journal of Hazardous Materials, 2020, 388, 121997.	6.5	37
14921	Experimental and theoretical substantiation of differences of geometric isomers of copper(II) $\hat{\text{I}}$ -amino acid chelates in ATR-FTIR spectra. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 229, 117950.	2.0	14
14922	The physical structure and surface reactivity of graphene oxide. Diamond and Related Materials, 2020, 101, 107613.	1.8	7
14923	Humidity impact on photo-catalytic degradation: Adsorption behavior simulations and catalytic reaction mechanisms for main gaseous pollutants in papermaking industry. Journal of Cleaner Production, 2020, 244, 118863.	4.6	14
14924	Ab initio study on physical and chemical interactions at borates and iron oxide interface at high temperature. Chemical Physics, 2020, 529, 110548.	0.9	8
14925	Site preference of V and its influence on the elastic properties in the boride series V <sub>x</sub> Mo <sub>5</sub> SiB <sub>2</sub> as studied by first principles density functional theory. Journal of Alloys and Compounds, 2020, 819, 153041.	2.8	3
14926	DFT calculation for stability and quantum capacitance of MoS <sub>2</sub> monolayer-based electrode materials. Materials Today Communications, 2020, 22, 100772.	0.9	15
14927	Structural and electronic properties of tungsten oxides under high pressures. Journal of Physics Condensed Matter, 2020, 32, 085403.	0.7	2



#	ARTICLE	IF	CITATIONS
14928	The Effects of Fe and Si Elements on Structural, Mechanical, and Electronic Properties of an Fe <sup>2+</sup> /Si <sup>4+</sup> /Ti System by First-Principles Calculations. <i>Physica Status Solidi (B): Basic Research</i> , 2020, 257, 1900479.	0.7	1
14929	Theoretical study on group III elements and F co-doped ZnO. <i>Journal of Alloys and Compounds</i> , 2020, 819, 153012.	2.8	12
14930	Structural, magnetic properties and diagram phases of the quaternary Heusler compound MnNiCuSb. <i>Journal of Magnetism and Magnetic Materials</i> , 2020, 497, 166059.	1.0	4
14931	Surface-generated copper ions induce multilayer growth of small peptides. <i>Applied Surface Science</i> , 2020, 507, 145105.	3.1	2
14932	Surface chemistry dictates stability and oxidation state of supported single metal catalyst atoms. <i>Chemical Science</i> , 2020, 11, 1469-1477.	3.7	16
14933	Copper-based redox shuttles supported by preorganized tetradentate ligands for dye-sensitized solar cells. <i>Dalton Transactions</i> , 2020, 49, 343-355.	1.6	19
14934	A theoretical indicator of transition-metal nanoclusters applied in the carbon nanotube nucleation process: a DFT study. <i>Dalton Transactions</i> , 2020, 49, 492-503.	1.6	10
14935	Lithium intercalation drives mechanical properties deterioration in bulk and single-layered black phosphorus: a first-principles study. <i>2D Materials</i> , 2020, 7, 025028.	2.0	10
14936	Mechanism of the reaction of VB <sub>5</sub> <sup>+</sup> cluster with methane from density functional theory calculations. <i>Computational and Theoretical Chemistry</i> , 2020, 1173, 112701.	1.1	3
14937	Layered Cathode Materials for Lithium-Ion Batteries: Review of Computational Studies on LiNi <sub>1-x</sub> Co <sub>x</sub> Mn <sub>y</sub> O <sub>2</sub> and LiNi <sub>1-x</sub> Co <sub>x</sub> Al <sub>y</sub> O <sub>2</sub> . <i>Chemistry of Materials</i> , 2020, 32, 915-952.	3.2	196
14938	Tris(Î <sup>2</sup> -ketoiminato)ruthenium(III) - Structural and electronic data of the neutral, oxidized and reduced forms. <i>Data in Brief</i> , 2020, 28, 104833.	0.5	1
14939	Photo-catalytic degradation of mixed gaseous HCHO and C <sub>6</sub> H <sub>6</sub> in paper mills: Experimental and theoretical study on the adsorption behavior simulation and catalytic reaction mechanism. <i>Journal of Hazardous Materials</i> , 2020, 388, 121779.	6.5	16
14940	An efficient materials genome method to predict heterostructure interfaces. <i>Materials Today Communications</i> , 2020, 23, 100866.	0.9	1
14941	Ab Initio Study on the Lower Mantle Minerals. <i>Annual Review of Earth and Planetary Sciences</i> , 2020, 48, 99-119.	4.6	5
14942	Anisotropic Elastic, Electronic and Vibrational Properties of the Semiconductor AgScX (X = Ge, C) Compounds. <i>Journal of Electronic Materials</i> , 2020, 49, 1849-1856.	1.0	5
14943	Electronic structure and thermoelectric properties of PbTe <sub>1-x</sub> Sex from first-principles calculations. <i>Computational Materials Science</i> , 2020, 173, 109404.	1.4	3
14944	Ultrathin Prussian blue analogue nanosheet arrays with open bimetal centers for efficient overall water splitting. <i>Nano Energy</i> , 2020, 68, 104371.	8.2	123
14945	Phase transition of nanoscale Au atom chains on NiAl(110). <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126183.	0.9	0



#	ARTICLE	IF	CITATIONS
14946	Mechanisms of Pressure-Induced Structural Transformation in Confined Sodium Borate Glasses. <i>Journal of Physical Chemistry B</i> , 2020, 124, 277-287.	1.2	5
14947	Enhanced N <sub>2</sub> Electroreduction over LaCoO <sub>3</sub> by Introducing Oxygen Vacancies. <i>ACS Catalysis</i> , 2020, 10, 1077-1085.	5.5	98
14948	Stability and superconductivity of TiPHn (n = 1~8) under high pressure. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126189.	0.9	11
14949	Charge reordering of MgO (100) surface by Sn cluster deposition: Implications for heterogeneous catalysis. <i>Applied Surface Science</i> , 2020, 506, 144963.	3.1	3
14950	Holey graphitic carbon nitride (g-CN) supported bifunctional single atom electrocatalysts for highly efficient overall water splitting. <i>Applied Catalysis B: Environmental</i> , 2020, 264, 118521.	10.8	137
14951	Vacancy concentration of films and nanoparticles. <i>Computational Materials Science</i> , 2020, 173, 109416.	1.4	8
14952	Density functional theory calculations of iron - vanadium carbide interfaces and the effect of hydrogen. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 2382-2389.	3.8	33
14953	Mechanistic evaluation of Li2O2 adsorption on carbon nanotube electrodes: A theoretical study. <i>Applied Surface Science</i> , 2020, 506, 145050.	3.1	9
14954	Recycling waste tantalum capacitors to synthesize high value-added Ta2O5 and polyaniline-decorated Ta2O5 photocatalyst by an integrated chlorination-sintering-chemisorption process. <i>Journal of Cleaner Production</i> , 2020, 252, 117206.	4.6	24
14955	Phase stability and magnetic properties in Co2Cr(Al,Si) shape memory alloys. <i>Journal of Magnetism and Magnetic Materials</i> , 2020, 500, 166311.	1.0	3
14956	Effect of Cu Preferential Orientation on the Microstructure and Properties of Anodized Cu <sub>x</sub> O Films. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 261-268.	1.0	10
14957	Insight into highly selective dimethyl trisulfide detection based on WO3 nanorod bundles with exposed (002) facets. <i>Sensors and Actuators B: Chemical</i> , 2020, 305, 127538.	4.0	19
14958	Half-metallic behavior and magnetic properties of the quaternary Heusler alloys YFeCrZ (Z=Al, Sb and) Tj ETQq0 0 0 rgBT /Overlock 10 T	2.8	42
14959	Energy Band Engineering of Polymeric Carbon Nitride with Indium Doping for High Enhancement in Charge Separation and Photocatalytic Performance. <i>ACS Applied Energy Materials</i> , 2020, 3, 377-386.	2.5	26
14960	The single-Mo-atom-embedded-graphdiyne monolayer with ultra-low onset potential as high efficient electrocatalyst for N2 reduction reaction. <i>Applied Surface Science</i> , 2020, 506, 144941.	3.1	48
14961	A Flexible Potassium-Ion Hybrid Capacitor with Superior Rate Performance and Long Cycling Life. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 2424-2431.	4.0	59
14962	Study of the nitric oxide reduction of SCR-NH3 on Î³Fe2O3 catalyst surface with quantum chemistry. <i>Applied Surface Science</i> , 2020, 509, 144659.	3.1	24
14963	Porous Ni <sub>1-x</sub> Cu <sub>x</sub> O Nanowire Arrays as Noble-Metal-Free High-Performance Catalysts for Ammonia-Borane Electrooxidation. <i>ACS Catalysis</i> , 2020, 10, 721-735.	5.5	25

#	ARTICLE	IF	CITATIONS
14964	Predicting gases sensing performance of $\hat{I}\pm$ -MoO <sub>3</sub> from nano-structural and electronic properties. <i>Applied Surface Science</i> , 2020, 509, 144913.	3.1	18
14965	Development and application of EAM potentials for Ti, Al and Nb with enhanced planar fault energy of Ti. <i>Computational Materials Science</i> , 2020, 173, 109432.	1.4	7
14966	Growth and structure of Cu, Ag and Au clusters on $\hat{I}\pm$ -Fe <sub>2</sub> O <sub>3</sub> (0001): A comparative density functional study. <i>Computational Materials Science</i> , 2020, 173, 109392.	1.4	4
14967	Kinetics and Thermodynamics of Reactions Involving Criegee Intermediates: An Assessment of Density Functional Theory and Ab Initio Methods Through Comparison with CCSDT(Q)/CBS Data. <i>Journal of Computational Chemistry</i> , 2020, 41, 328-339.	1.5	13
14968	High energy-storage density under low electric field in lead-free relaxor ferroelectric film based on synergistic effect of multiple polar structures. <i>Journal of Power Sources</i> , 2020, 448, 227457.	4.0	56
14969	d-orbital-frustration-induced ferromagnetic monolayer Cu <sub>3</sub> O <sub>2</sub> . <i>Physica B: Condensed Matter</i> , 2020, 577, 411826.	1.3	3
14970	Strong Jahn-Teller effect at NiO <sub>4</sub> tetrahedron in NiCo <sub>2</sub> O <sub>4</sub> spinel. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126114.	0.9	4
14971	Non-covalent interactions between epinephrine and nitroaromatic compounds: A DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 228, 117827.	2.0	22
14972	A minimal Tersoff potential for diamond silicon with improved descriptions of elastic and phonon transport properties. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 135901.	0.7	9
14973	ALD-assisted synthesis of V <sub>2</sub> O <sub>5</sub> nanoislands on SnO <sub>2</sub> nanowires for improving NO <sub>2</sub> sensing performance. <i>Applied Surface Science</i> , 2020, 509, 144821.	3.1	18
14974	DFT performance in the IQA energy partition of small water clusters. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	2
14975	Thickness effect on the structural, electronic and energetic properties of the cubic KMgF <sub>3</sub> (0 $\hat{A}$ 0 $\hat{A}$ 1) surfaces: A first-principles study. <i>Applied Surface Science</i> , 2020, 506, 144678.	3.1	4
14976	The ground-state structure, optical-absorption and photoelectron spectrum of silver clusters. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 117, 113805.	1.3	27
14977	Adsorption and dissociation of the methanethiol (CH <sub>3</sub> SH) molecule on the Fe(100) surface. <i>Surface and Interface Analysis</i> , 2020, 52, 156-166.	0.8	5
14978	Density functional studies of the adsorption of OCN and coadsorption of O and CN on Ag(001) surface. <i>Computational Condensed Matter</i> , 2020, 22, e00446.	0.9	7
14979	Viscosity, undercoolability and short-range order in quasicrystal-forming Al-Cu-Fe melts. <i>Journal of Molecular Liquids</i> , 2020, 299, 112207.	2.3	30
14980	Explosive vapor detection using novel graphdiyne nanoribbonsâ€™ a first-principles investigation. <i>Structural Chemistry</i> , 2020, 31, 709-717.	1.0	22
14981	Solar-driven efficient methane catalytic oxidation over epitaxial ZnO/La <sub>0.8</sub> Sr <sub>0.2</sub> CoO <sub>3</sub> heterojunctions. <i>Applied Catalysis B: Environmental</i> , 2020, 265, 118469.	10.8	44

#	ARTICLE	IF	CITATIONS
14982	Fast synthesis of large-scale single-crystal graphene with well-defined edges upon sodium chloride addition. <i>Carbon</i> , 2020, 158, 904-911.	5.4	3
14983	Friction and Wear Behavior of CrN Coating on 316L Stainless Steel in Liquid Sodium at Elevated Temperature. <i>Tribology International</i> , 2020, 143, 106079.	3.0	33
14984	Effect of pre-adsorbed sulfur on CH <sub>x</sub> (x=1-3) formation from synthesis gas reaction over Cu(111) surface. <i>Applied Surface Science</i> , 2020, 509, 145246.	3.1	5
14985	Calculation of the EPR g-tensor from auxiliary density functional theory. <i>Journal of Chemical Physics</i> , 2020, 152, 014105.	1.2	0
14986	First Principles Density Functional Theory Prediction of the Crystal Structure and the Elastic Properties of Mo <sub>2</sub> ZrB <sub>2</sub> and Mo <sub>2</sub> HfB <sub>2</sub> . <i>Crystals</i> , 2020, 10, 865.	1.0	4
14987	Hydrogen clustering in bcc metals: Atomic origin and strong stress anisotropy. <i>Acta Materialia</i> , 2020, 201, 23-35.	3.8	20
14988	Effect of Mg and Cu doping on structural, optical, electronic, and thermal properties of ZnS quantum dots. <i>Journal of Materials Science: Materials in Electronics</i> , 2020, 31, 21342-21354.	1.1	13
14989	First-principles study of FeNi <sub>1-x</sub> Cr <sub>x</sub> (0 ≤ x ≤ 1) disordered alloys from special quasirandom structures. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2020, 71, 102007.	0.7	7
14990	Investigating structural, electronic and optical properties of CdS:Cr (A GGA and GGA+U study). <i>Solid State Sciences</i> , 2020, 108, 106437.	1.5	3
14991	Physisorbed State Regulates the Dissociation Mechanism of H <sub>2</sub> O on Ni(100). <i>Journal of Physical Chemistry A</i> , 2020, 124, 8724-8732.	1.1	5
14992	Effective Descriptor for Designing High-Performance Catalysts for the Hydrogen Evolution Reaction. <i>Journal of Physical Chemistry C</i> , 2020, 124, 23134-23142.	1.5	20
14993	The role of adsorbed hydroxide in hydrogen evolution reaction kinetics on modified platinum. <i>Nature Energy</i> , 2020, 5, 891-899.	19.8	400
14994	Water-gas shift reaction co-catalyzed by polyoxometalate (POM)-gold composites: the "magic" role of POMs. <i>Catalysis Science and Technology</i> , 2020, 10, 8219-8229.	2.1	8
14995	Localization and steric effect of the lone electron pair of the tellurium Te <sup>4+</sup> cation and other cations of the p-block elements. A systematic study. <i>Journal of Applied Crystallography</i> , 2020, 53, 1243-1251.	1.9	9
14996	Half-metallicity in M <sub>n</sub> and V doped tin-carbide SnC. <i>Computational Condensed Matter</i> , 2020, 25, e00504.	0.9	5
14997	Boosting nitrogen-doping and controlling interlayer spacing in pre-reduced graphene oxides. <i>Nano Energy</i> , 2020, 78, 105286.	8.2	24
14998	Heterogeneous interface of Se@Sb@C boosting potassium storage. <i>Nano Energy</i> , 2020, 78, 105345.	8.2	51
14999	Computation of NMR Shielding Constants for Solids Using an Embedded Cluster Approach with DFT, Double-Hybrid DFT, and MP2. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6950-6967.	2.3	21

#	ARTICLE	IF	CITATIONS
15000	Research Progress on the Anti-Disproportionation of the ZrCo Alloy by Element Substitution. <i>Materials</i> , 2020, 13, 3977.	1.3	9
15001	Graphene nano-flakes on Cu low-index surfaces by density functional theory and molecular dynamics simulations. <i>Frontiers of Nanoscience</i> , 2020, 17, 141-159.	0.3	2
15002	Understanding solute effect on grain boundary strength based on atomic size and electronic interaction. <i>Scientific Reports</i> , 2020, 10, 16856.	1.6	10
15003	Method for the accurate prediction of electron transfer potentials using an effective absolute potential. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25833-25840.	1.3	15
15004	Quantum Algorithms for Quantum Chemistry and Quantum Materials Science. <i>Chemical Reviews</i> , 2020, 120, 12685-12717.	23.0	311
15005	Reproducibility of potential energy surfaces of organic/metal interfaces on the example of PTCDA on Ag(111). <i>Journal of Chemical Physics</i> , 2020, 153, 104701.	1.2	12
15006	Quantum size effect in conductive properties of silver nanofilms. <i>Thin Solid Films</i> , 2020, 710, 138263.	0.8	9
15007	First-principles investigation on the transport properties of quaternary CoFeRGa (R = Ti, V, Cr, Mn, Cu). <i>Tj ETQq1 1 0.784314, rgBT /Over</i>	1.3	10
15008	A revised mechanism for (p)ppGpp synthesis by Rel proteins: The critical role of the 2â€²-OH of GTP. <i>Journal of Biological Chemistry</i> , 2020, 295, 12851-12867.	1.6	8
15009	A novel layered birnessite-type sodium molybdate as dual-ion electrodes for high capacity battery. <i>Electrochimica Acta</i> , 2020, 363, 137229.	2.6	10
15010	Computational study of the effect of functionalization on natural gas components separation and adsorption in NUM-3a MOF. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 101, 107731.	1.3	8
15011	Crystal structures and elastic properties of Ti(Cu,Pt) <sub>2</sub> and Ti(Cu,Pt) <sub>3</sub> phases. <i>Transactions of Nonferrous Metals Society of China</i> , 2020, 30, 1839-1848.	1.7	9
15012	Silyl Cations Stabilized by Pincer Type Ligands with Adjustable Donor Atoms. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 4093-4110.	1.0	7
15013	Electromagnetic control of spin ordered Mn<sub>3</sub> qubits: a density functional study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27547-27553.	1.3	5
15014	Pressure-Induced Metallization of Diamond at Room Temperature. <i>Journal of Superhard Materials</i> , 2020, 42, 177-189.	0.5	1
15015	Black Phosphorus Nanosheets Modified with Au Nanoparticles as High Conductivity and High Activity Electrocatalyst for Oxygen Evolution Reaction. <i>Advanced Energy Materials</i> , 2020, 10, 2002424.	10.2	79
15016	Theoretical and Experimental Overview of Structural, Dielectric, Crystallographic, Electronic, Optical, and Physical Tensors of Î±-DIPAB and Iodine-Doped Î±-DIPAB Molecular Ferroelectric Crystals. <i>Journal of Electronic Materials</i> , 2020, 49, 7112-7132.	1.0	0
15017	Accelerating 2D MXene catalyst discovery for the hydrogen evolution reaction by computer-driven workflow and an ensemble learning strategy. <i>Journal of Materials Chemistry A</i> , 2020, 8, 23488-23497.	5.2	71

#	ARTICLE	IF	CITATIONS
15018	Effect of Magnetic Field Annealing on Magnetic Properties of Iron-Gallium Alloys. <i>Physics of the Solid State</i> , 2020, 62, 1746-1754.	0.2	5
15019	Coordination Flexibility of the Rh(PXP) Complex to NH <sub>3</sub> , CO, and C <sub>2</sub> H <sub>4</sub> (PXP = Diphosphine-Based Pincer Ligand; X = B, Al, and Ga): Theoretical Insight. <i>Inorganic Chemistry</i> , 2020, 59, 15862-15876.	1.9	9
15020	Palladium-catalysed methoxycarbonylation of ethene with bidentate diphosphine ligands: a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 24330-24336.	1.3	11
15021	Combining phonon accuracy with high transferability in Gaussian approximation potential models. <i>Journal of Chemical Physics</i> , 2020, 153, 044104.	1.2	29
15022	Charge transfer and hydrogen adsorption in the Pd/Ag bimetallic nano system: an experimental and theoretical DFT cluster approach. <i>Molecular Physics</i> , 2020, 118, e1820090.	0.8	1
15023	Computational and experimental studies on the efficiency of Rosmarinus officinalis polyphenols as green corrosion inhibitors for XC48 steel in acidic medium. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 606, 125458.	2.3	51
15024	Optical, electronic, and mechanical properties of p-type conductive oxide BaBiO <sub>3</sub> : A density functional theory study. <i>Chemical Physics Letters</i> , 2020, 761, 138054.	1.2	8
15025	Interatomic potentials and defect properties of Fe-Cr-Al alloys. <i>Journal of Nuclear Materials</i> , 2020, 541, 152421.	1.3	18
15026	Investigation of the mono vacancy effects on the structural, electronic and magnetic properties of graphene hexagonal-boron nitride in-plane hybrid embracing diamond shaped graphene island. <i>Solid State Sciences</i> , 2020, 108, 106395.	1.5	2
15027	DFT Study on the Hydrogenation of CO <sub>2</sub> to Methanol on Ho-Doped Cu(211) Surface. <i>Journal of Physical Chemistry C</i> , 2020, 124, 22426-22434.	1.5	13
15028	Understanding and Improving the Kinetics of Bulk Carbonation on Sodium Carbonate. <i>Journal of Physical Chemistry C</i> , 2020, 124, 23106-23115.	1.5	5
15029	Subsystem density-functional theory for interacting open-shell systems: spin densities and magnetic exchange couplings. <i>Faraday Discussions</i> , 2020, 224, 201-226.	1.6	8
15030	On-surface synthesis of size- and shape-controlled two-dimensional Aun nanoclusters using a flexible fullerene molecular template. <i>Nanoscale</i> , 2020, 12, 21657-21664.	2.8	1
15031	Metathetic synthesis of lead cyanamide as a p-type semiconductor. <i>Dalton Transactions</i> , 2020, 49, 14061-14067.	1.6	16
15032	Phase-controlled synthesis of Ni nanocrystals with high catalytic activity in 4-nitrophenol reduction. <i>Journal of Materials Chemistry A</i> , 2020, 8, 22143-22154.	5.2	22
15033	Formaldehyde oxidation on Co-doped reduced CeO <sub>2</sub> (111): First-principles calculations. <i>Surface Science</i> , 2020, 701, 121693.	0.8	11
15034	Theoretical investigation of amino-acid adsorption on hydroxylated quartz surfaces: dispersion can determine enantioselectivity. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16571-16578.	1.3	7
15035	Correlation between Nonlinear Optical Properties and Electronic Band Modification in Cobalt-Doped ZnO Nanorods. <i>Physical Review Applied</i> , 2020, 14, .	1.5	5

#	ARTICLE	IF	CITATIONS
15036	Single Mn atom anchored on N-doped porous carbon as highly efficient Fenton-like catalyst for the degradation of organic contaminants. <i>Applied Catalysis B: Environmental</i> , 2020, 279, 119363.	10.8	182
15037	Enhanced Shift Currents in Monolayer 2D GeS and SnS by Strain-Induced Band Gap Engineering. <i>ACS Omega</i> , 2020, 5, 17207-17214.	1.6	32
15038	Cobalt vacancies assisted ion diffusion in Co <sub>2</sub> AlO <sub>4</sub> carbon nanofibers for enhancing lithium battery performance. <i>Dalton Transactions</i> , 2020, 49, 10127-10137.	1.6	2
15039	The geometry, electronic and magnetic properties of VLi <sub>n</sub> (n=1-13) clusters using the first-principles and PSO method. <i>Molecular Physics</i> , 2020, 118, .	0.8	2
15040	Hydrogen Transport in Tungsten for Nuclear Energy Application: Temperature Dependence and Compensation Effect. <i>Fusion Science and Technology</i> , 2020, 76, 616-631.	0.6	3
15041	First-principles study of the structure, elastic constants, electronic and thermodynamic properties of C15 laves phase ZrMo <sub>2</sub> . <i>International Journal of Modern Physics B</i> , 2020, 34, 2050170.	1.0	0
15042	Understanding the Ionic Diffusivity in the (Meta)Stable (Un)doped Solid-State Electrolyte from First-Principles: A Case Study of LISICON. <i>Journal of Physical Chemistry C</i> , 2020, 124, 17485-17493.	1.5	6
15043	Giant momentum-dependent spin splitting in centrosymmetric low- $Z$ antiferromagnets. <i>Physical Review B</i> , 2020, 102, .	1.1	101
15044	Identification of Active Sites on High-Performance Pt/Al <sub>2</sub> O <sub>3</sub> Catalyst for Cryogenic CO Oxidation. <i>ACS Catalysis</i> , 2020, 10, 8815-8824.	5.5	54
15045	Mechanism of Nucleotidyltransfer Reaction and Role of Mg <sup>2+</sup> Ion in Sugar Nucleotidyltransferases. <i>Biophysical Journal</i> , 2020, 119, 619-627.	0.2	2
15046	Energetics of heterogeneous Mg {101 $\bar{1}$ } deformation twinning migration using an atomistically informed phase-field model. <i>Computational Materials Science</i> , 2020, 183, 109907.	1.4	5
15047	Exploration of novel High-Pressure Structures of Hf <sub>2</sub> O <sub>3</sub> . <i>Materials Chemistry and Physics</i> , 2020, 254, 123532.	2.0	0
15048	New direction's piezoelectricity and new applications of two-dimensional group V-IV-III-VI films: A theoretical study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 124, 114214.	1.3	9
15049	DFT-Based Cu(111)   Cu <sub>2</sub> O(111) Model for Copper Metal Covered by Ultrathin Copper Oxide: Structure, Electronic Properties, and Reactivity. <i>Journal of Physical Chemistry C</i> , 2020, 124, 17048-17057.	1.5	27
15050	Plasma-Made Graphene Nanostructures with Molecularly Dispersed F and Na Sites for Solar Desalination of Oil-Contaminated Seawater with Complete In-Water and In-Air Oil Rejection. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 38512-38521.	4.0	32
15051	Electronic Structure Modeling of Metal-Organic Frameworks. <i>Chemical Reviews</i> , 2020, 120, 8641-8715.	23.0	149
15052	Synthesis, Structure and Bonding Analysis of the Zwitterionic PPP-Pincer Complex (6-Ph <sub>2</sub> P-Ace-5-) <sub>2</sub> P(O)AuCl <sub>2</sub> . <i>Crystals</i> , 2020, 10, 564.	1.0	1
15053	Frustrated and Allowed Structural Transitions at the Limits of the BaAl <sub>4</sub> Type: The (3 +) Tj ETQq1 1 0.784314 rgBT /Overloc <i>Chemistry</i> , 2020, 59, 10208-10222.	1.9	5



#	ARTICLE	IF	CITATIONS
15054	High-precision equation of state data for $\text{TiO}_2$ : A structural analog of $\text{SiO}_2$ . Physical Review B, 2020, 102, .	1.1	12
15055	Correlated morphological and chemical mechanisms for the superior corrosion resistance of alumina-deposited 2D nanofilms on copper. Materialia, 2020, 11, 100697.	1.3	5
15056	Theoretical study of the effects of alloying elements on Cu nanotwins. Science China: Physics, Mechanics and Astronomy, 2020, 63, 1.	2.0	15
15057	Structural, electronic properties and boron stability of (001) surface of Nb <sub>5</sub> Si <sub>3</sub> intermetallic by first-principles calculations. Vacuum, 2020, 179, 109558.	1.6	5
15058	The Grapefruit Effect: Interaction between Cytochrome P450 and Coumarin Food Components, Bergamottin, Fraxidin and Osthole. X-ray Crystal Structure and DFT Studies. Molecules, 2020, 25, 3158.	1.7	9
15059	Determining the crystal and electronic structures of the magnesium secondary battery cathode material $\text{MgCo}_{2-x}\text{Mn}_x\text{O}_4$ using first-principles calculations and a quantum beam during discharge. Journal of Materials Science, 2020, 55, 13852-13870.	1.7	6
15060	Adsorption structure of adenine on cerium oxide. Applied Surface Science, 2020, 530, 147257.	3.1	8
15061	Transmetallation of Bis(diphenylphosphinoacene)Mercury and Tributyltin with Precious Metal Chlorides. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2020, 646, 856-865.	0.6	4
15062	Interaction of propylthiouracil, an anti-thyroid drug with boron nitride nanotube: a DFT study. Adsorption, 2020, 26, 1385-1396.	1.4	11
15063	First-Principle Study of Structural, Elastic, Electronic and Magnetic Properties of the Quaternary Heusler CoZrFeP. Journal of Superconductivity and Novel Magnetism, 2020, 33, 2899-2905.	0.8	6
15064	Computational Screening of Atomically Thin Two-Dimensional Nanomaterial-Coated Cs <sub>3</sub> Sb Heterostructures for High-Performance Photocathodes. Journal of Physical Chemistry C, 2020, 124, 26396-26403.	1.5	3
15065	Overlap-Driven Splitting of Triplet Pairs in Singlet Fission. Journal of the American Chemical Society, 2020, 142, 20040-20047.	6.6	26
15066	Band gap and magnetic engineering of penta-graphene <i>via</i> adsorption of small transition clusters. Physical Chemistry Chemical Physics, 2020, 22, 26155-26166.	1.3	5
15067	First-principles study on the type-II g-C <sub>6</sub> N <sub>6</sub> /GaS heterojunction: A promising photocatalyst for water splitting. Diamond and Related Materials, 2020, 110, 108157.	1.8	21
15068	2D Octagon-Structure Carbon and Its Polarization Resolved Raman Spectra. Nanomaterials, 2020, 10, 2252.	1.9	6
15069	Reaction mechanism of Ca <sub>2</sub> Fe <sub>2</sub> O <sub>5</sub> oxygen carrier with CO in chemical looping hydrogen production. Applied Surface Science, 2020, 534, 147583.	3.1	18
15070	Polynitro-acetone, dimethyl ether, and dimethylamine: a series of potential green and powerful oxidants for propellants. Journal of Molecular Modeling, 2020, 26, 347.	0.8	1
15071	First-principles study of binary and ternary alloys based on PdCu as oxygen reduction catalysts. Chemical Physics Letters, 2020, 758, 137932.	1.2	0



#	ARTICLE	IF	CITATIONS
15072	The geometric and electronic structures of a $\text{Ag}_{13}\text{Cu}_{10}(\text{SAdm})_{12}\text{X}_3$ nanocluster. Dalton Transactions, 2020, 49, 17164-17168.	1.6	7
15073	Confirmation of the PPLB Derivative Discontinuity: Exact Chemical Potential at Finite Temperatures of a Model System. Journal of Chemical Theory and Computation, 2020, 16, 7225-7231.	2.3	5
15074	Structural, mechanical and thermodynamic properties study on Mg–Y alloys from first-principles calculations. International Journal of Modern Physics B, 2020, 34, 2050220.	1.0	3
15075	Unraveling the effect of Al doping on CO adsorption at $\text{ZnO}(101\bar{1},0)$ . RSC Advances, 2020, 10, 40663-40672.	1.7	10
15076	First principles study on copper and iridium co-doped $\text{SrTiO}_3$ for shifting the optical absorption into visible region. SN Applied Sciences, 2020, 2, 1.	1.5	3
15077	Ground and excited state geometrical and optical properties of $\text{Au}(n=13)$ nanoclusters: A first-principles study. Computational and Theoretical Chemistry, 2020, 1190, 113007.	1.1	4
15078	Computational Investigations of Dispersion Interactions between Small Molecules and Graphene-like Flakes. Journal of Physical Chemistry A, 2020, 124, 9552-9561.	1.1	7
15079	Advanced superhard composite materials with extremely improved mechanical strength by interfacial segregation of dilute dopants. Scientific Reports, 2020, 10, 21008.	1.6	4
15080	First-principles investigation of the structure and electronic properties of graphene toward Li adsorption. Molecular Simulation, 2020, 46, 1522-1529.	0.9	5
15081	Ground and Excited State Electronic Structures of d8-Squared Planar Platinum(II) and Gold(III) Complexes Bearing Cyclometallated 2,6-Diphenylpyridine and Pyrene-Derived N-Heterocyclic Carbene. Russian Journal of Inorganic Chemistry, 2020, 65, 1695-1702.	0.3	0
15082	Photocatalytic $\text{CO}_2$ Reduction: A Review of Ab Initio Mechanism, Kinetics, and Multiscale Modeling Simulations. ACS Catalysis, 2020, 10, 14984-15007.	5.5	199
15083	Single Atoms on a Nitrogen-Doped Boron Phosphide Monolayer: A New Promising Bifunctional Electrocatalyst for ORR and OER. ACS Applied Materials & Interfaces, 2020, 12, 52549-52559.	4.0	95
15084	Nonradiative Relaxation Dynamics of a Cesium Lead Halide Perovskite Photovoltaic Architecture: Effect of External Electric Fields. Journal of Physical Chemistry Letters, 2020, 11, 9983-9989.	2.1	11
15085	Diffusion, permeation and solubility of hydrogen, deuterium and tritium in crystalline tungsten: First principles DFT simulations. International Journal of Hydrogen Energy, 2020, 45, 29095-29109.	3.8	27
15086	Self-Elimination of Intrinsic Defects Improves the Low-Temperature Performance of Perovskite Photovoltaics. Joule, 2020, 4, 1961-1976.	11.7	152
15087	Oxygen defect chemistry for the reversible transformation of titanates for sizeable potassium storage. Journal of Materials Chemistry A, 2020, 8, 17550-17557.	5.2	5
15088	Relativistic Structure-Activity Relationship of Cisplatin(II) Complexes. Journal of Structural Chemistry, 2020, 61, 688-693.	0.3	3
15089	Bis(6-diphenylphosphinoacenaphth(5a)yl)sulfoxide: A New Ligand for Late Transition Metal Complexes. European Journal of Inorganic Chemistry, 2020, 2020, 3829-3836.	1.0	2

#	ARTICLE	IF	CITATIONS
15090	First-principles investigation of structural modification, fine band gap engineering, and optical response of $\text{La}_{1-x}\text{Ba}_x\text{GaO}_3$ for optoelectronic applications. <i>Applied Physics A: Materials Science and Processing</i> , 2020, 126, 1.	1.1	8
15091	A review of recent progress in thermoelectric materials through computational methods. <i>Materials for Renewable and Sustainable Energy</i> , 2020, 9, 1.	1.5	37
15092	DFT study of the oxidation of HgO by O <sub>2</sub> on an Mn-doped buckled g-C <sub>3</sub> N <sub>4</sub> catalyst. <i>Current Applied Physics</i> , 2022, 40, 83-89.	1.1	10
15093	Atomic-scale phase separation induced clustering of solute atoms. <i>Nature Communications</i> , 2020, 11, 3934.	5.8	11
15094	Origin of the abnormal reduction of the dielectric response for ReCOB crystals and its mechanism: theoretical and experimental exploration. <i>Journal of Materials Chemistry C</i> , 2020, 8, 10109-10120.	2.7	1
15095	Oscillating stationary distributions of nanoclusters in an open system. <i>Mathematical and Computer Modelling of Dynamical Systems</i> , 2020, 26, 562-575.	1.4	2
15096	Graphene Oxide-BiOCl Nanoparticle Composites as Catalysts for Oxidation of Volatile Organic Compounds in Nonthermal Plasmas. <i>ACS Applied Nano Materials</i> , 2020, 3, 9363-9374.	2.4	13
15097	Construction of Highly Active and Selective Polydopamine Modified Hollow ZnO/Co <sub>3</sub> O <sub>4</sub> p-n Heterojunction Catalyst for Photocatalytic CO <sub>2</sub> Reduction. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 11465-11476.	3.2	84
15098	Shortcomings of meta-GGA functionals when describing magnetism. <i>Physical Review B</i> , 2020, 102, .	1.1	27
15099	Realizing white emission in Sc <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub> :Eu <sup>3+</sup> /Dy <sup>3+</sup> /Ce <sup>3+</sup> phosphors through computation and experiment. <i>Journal of Solid State Chemistry</i> , 2020, 290, 121592.	1.4	11
15100	Unveiling the adsorption properties of 3d, 4d, and 5d metal adatoms on the MoS <sub>2</sub> monolayer: A DFT-D3 investigation. <i>Surface Science</i> , 2020, 701, 121700.	0.8	19
15101	Dual-ion battery with MoS <sub>2</sub> cathode. <i>Energy Storage Materials</i> , 2020, 32, 159-166.	9.5	18
15102	CO oxidation through the formation of carboxyl intermediate on Pt(111) surface: A first principles study. <i>Journal of Physics: Conference Series</i> , 2020, 1494, 012040.	0.3	0
15103	First Principle Calculation of Electronic Structure and Stabilities of TiC/Mg Composites Interfaces. <i>IOP Conference Series: Materials Science and Engineering</i> , 2020, 774, 012096.	0.3	2
15104	Magnetocrystalline anisotropy of small CoPt binary alloy metal clusters: interplay between structure, chemical composition, and spin-orbit coupling. <i>Journal of Nanoparticle Research</i> , 2020, 22, 1.	0.8	4
15105	Exchange-correlation functionals for band gaps of solids: benchmark, reparametrization and machine learning. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	156
15106	Rationalizing the Reactivity of Mixed Allyl Rare-Earth Borohydride Complexes with DFT Studies. <i>Catalysts</i> , 2020, 10, 820.	1.6	7
15107	Arenium cation or radical cation? An insight into the cyclodehydrogenation reaction of 2-substituted binaphthyls mediated by Lewis acids. <i>RSC Advances</i> , 2020, 10, 21974-21985.	1.7	7

#	ARTICLE	IF	CITATIONS
15108	A superior electronic conducting tellurium electrode enabled high rate capability rechargeable Mg batteries. <i>Materials Today Energy</i> , 2020, 17, 100450.	2.5	15
15109	Boosting the cyclic stability and supercapacitive performance of graphene hydrogels via excessive nitrogen doping: Experimental and DFT insights. <i>Sustainable Materials and Technologies</i> , 2020, 25, e00206.	1.7	11
15110	Next-Generation Nonlocal van der Waals Density Functional. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5893-5911.	2.3	57
15111	Significant hydrogen isotopes permeation resistance via nitride nano-multilayer coating. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 19583-19589.	3.8	13
15112	An effective method to screen carbon (boron, nitrogen) based two-dimensional hydrogen storage materials. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 25054-25064.	3.8	13
15113	Formation, evolution and characteristics of copper sulfide nanoparticles in the reactions of aqueous cupric and sulfide ions. <i>Materials Chemistry and Physics</i> , 2020, 255, 123600.	2.0	14
15114	Why do RuO <sub>2</sub> electrodes catalyze electrochemical CO <sub>2</sub> reduction to methanol rather than methane or perhaps neither of those?. <i>Chemical Science</i> , 2020, 11, 9542-9553.	3.7	17
15115	First-Principles Study of the Geometric and Electronic Structures and Optical Properties of Vacancy Magnesium Ferrite. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2020, 51, 5432-5443.	1.1	7
15116	Structural response of alkali metal borates at Fe <sub>2</sub> O <sub>3</sub> sliding interface: The effect of alkali cations. <i>Computational Materials Science</i> , 2020, 184, 109930.	1.4	4
15117	qvasp: A flexible toolkit for VASP users in materials simulations. <i>Computer Physics Communications</i> , 2020, 257, 107535.	3.0	88
15118	Exploring electrocatalytic stability and activity of unmodified and platinum-modified tungsten and niobium nitrides. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 22883-22892.	3.8	17
15119	Noncollinear frustrated antiferromagnetic Mn <sub>3</sub> P monolayer and its tunability via a spin degree of freedom. <i>Journal of Materials Chemistry C</i> , 2020, 8, 11369-11375.	2.7	3
15120	Electrocatalytic N <sub>2</sub> reduction to NH <sub>3</sub> with high Faradaic efficiency enabled by vanadium phosphide nanoparticle on V foil. <i>Nano Research</i> , 2020, 13, 2967-2972.	5.8	45
15121	Quantum Simulations of Preferable H <sub>2</sub> O Dissociation Pathway on the Ru-Alloyed Pt(111) Surface Based on Density Functional Theory. <i>Key Engineering Materials</i> , 0, 840, 495-500.	0.4	3
15122	Enhancement of the quantum capacitances of group-14 elemental two-dimensional materials by Ti-doping: A first principles study. <i>Applied Surface Science</i> , 2020, 530, 147301.	3.1	8
15123	CNC-pincer iron complexes containing a bis(N-heterocyclic carbene)Amido ligand: Synthesis and application to catalytic hydrogenation of alkenes. <i>Journal of Organometallic Chemistry</i> , 2020, 923, 121436.	0.8	8
15124	First-principles study of C <sub>3</sub> N nanoribbons as anode materials for Li-ion batteries. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126741.	0.9	7
15125	Redox behaviour of [Ru(η <sup>2</sup> -diketonato) <sub>3</sub> ] compounds. <i>Electrochimica Acta</i> , 2020, 337, 135801.	2.6	11

#	ARTICLE	IF	CITATIONS
15126	Adsorption of NO <sub>2</sub> and NO <sub>3</sub> on Cobalt Spinel Nanocubes and Interfacial Dynamics of the Resultant NO <sub>x</sub> Adspecies (x = 1, 2, and 3): DFT, Atomistic Thermodynamic, IR, and Isotopic Exchange Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 19681-19697.	1.5	9
15127	Three Reversible Redox States of Thiolate-Bridged Dirhodium Complexes without Metal-Metal Bonds. <i>Journal of the American Chemical Society</i> , 2020, 142, 16313-16323.	6.6	2
15128	Visible-Light-Activated C-C Bond Cleavage and Aerobic Oxidation of Benzyl Alcohols Employing BiMXO <sub>5</sub> (M=Mg, Cd, Ni, Co, Pb, Ca and X=V, P). <i>Chemistry - an Asian Journal</i> , 2020, 15, 3104-3115.	1.7	10
15129	Yttrium-decorated C48B12 as hydrogen storage media: A DFT study. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 24895-24901.	3.8	23
15130	DFT Studies on Thermal and Oxidative Degradation of Monoethanolamine. <i>Industrial &amp; Engineering Chemistry Research</i> , 2020, 59, 15214-15225.	1.8	12
15131	Ultrafast photoinduced band splitting and carrier dynamics in chiral tellurium nanosheets. <i>Nature Communications</i> , 2020, 11, 3991.	5.8	39
15132	Atomic structure of Co <sub>92</sub> B <sub>x</sub> Ta <sub>8</sub> glassy alloys studied by ab initio molecular dynamics simulations. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26406.	1.0	1
15133	Theoretical exploration on the vibrational and mechanical properties of M <sub>3</sub> C <sub>2</sub> /M <sub>3</sub> C <sub>2</sub> T <sub>2</sub> MXenes. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26409.	1.0	10
15134	Oxidation of chalcopyrite in air-equilibrated acidic solution: Inhibition with phenacyl derivatives. <i>Transactions of Nonferrous Metals Society of China</i> , 2020, 30, 1928-1942.	1.7	2
15135	Benchmark study of density functionals for the insertions of olefin and polar monomers catalyzed by $\hat{\pm}$ -diimine palladium complexes. <i>Computational and Theoretical Chemistry</i> , 2020, 1187, 112942.	1.1	3
15136	New Pressure Stabilization Structure in Two-Dimensional PtSe <sub>2</sub> . <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 7342-7349.	2.1	15
15137	Thermoelectric and optical properties of the SrS graphene by DFT. <i>Philosophical Magazine</i> , 2020, 100, 3108-3124.	0.7	8
15138	Computational studies on triphenyldiyne as a two-dimensional visible-light-driven photocatalyst for overall water splitting. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20061-20068.	1.3	4
15139	Mechanistic insight into H <sub>2</sub> -mediated Ni surface diffusion and deposition to form branched Ni nanocrystals: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 23869-23877.	1.3	1
15140	Non-compact oxide-island growth induced by surface phase transition of the intermetallic NiAl during vacuum annealing. <i>Acta Materialia</i> , 2020, 201, 244-253.	3.8	5
15141	Computational Design of Two-Dimensional Boron-Containing Compounds as Efficient Metal-free Electrocatalysts toward Nitrogen Reduction Independent of Heteroatom Doping. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 50505-50515.	4.0	20
15142	Non-precious-metal catalysts for alkaline water electrolysis: <i>operando</i> characterizations, theoretical calculations, and recent advances. <i>Chemical Society Reviews</i> , 2020, 49, 9154-9196.	18.7	448
15143	Anisotropic behavior of excitons in single-crystal $\hat{\pm}$ -SnS. <i>AIP Advances</i> , 2020, 10, .	0.6	9

#	ARTICLE	IF	CITATIONS
15144	Hydrogenation of pyrrole: Infrared spectra of the 2,3-dihydropyrrol-2-yl and 2,3-dihydropyrrol-3-yl radicals isolated in solid <i>para</i> -hydrogen. <i>Journal of Chemical Physics</i> , 2020, 153, 164302.	1.2	6
15145	Electronic, optical and thermoelectric properties of the WS <sub>2</sub> /GaN interfaces: a DFT study. <i>International Nano Letters</i> , 2020, 10, 249-261.	2.3	2
15146	Ab initio study of the stability of H-He clusters at lattice defects in tungsten. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2020, 478, 269-273.	0.6	6
15147	First-principles simulation of h interacting with transition elements in molybdenum for nuclear material application. <i>Journal of Nuclear Materials</i> , 2020, 541, 152437.	1.3	4
15148	Phase stability, brittle-ductile transition, and electronic structures of the TiAl alloying with Fe, Ru, Ge, and Sn: a first-principle investigation. <i>Journal of Molecular Modeling</i> , 2020, 26, 320.	0.8	6
15149	Atomic relaxation around defects in magnetically disordered materials computed by atomic spin constraints within an efficient Lagrange formalism. <i>Physical Review B</i> , 2020, 102, .	1.1	15
15150	Pauli energy and information-theoretic approach for evaluating dynamic and nondynamic electron correlation. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	2
15151	Computational studies reveal mechanism by which quinone derivatives can inhibit SARS-CoV-2. Study of embelin and two therapeutic compounds of interest, methyl prednisolone and dexamethasone. <i>Journal of Infection and Public Health</i> , 2020, 13, 1868-1877.	1.9	34
15152	Rationally Designed Semiconducting 2D Surface-Confined Metal-Organic Network. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 51122-51132.	4.0	3
15153	Fast site-to-site electron transfer of high-entropy alloy nanocatalyst driving redox electrocatalysis. <i>Nature Communications</i> , 2020, 11, 5437.	5.8	288
15154	Critical Magnetic Behavior of the Rare Earth-Based Alloy GdN: Monte Carlo Simulations and Density Functional Theory Method. <i>Journal of Materials Engineering and Performance</i> , 2020, 29, 7361-7368.	1.2	37
15155	Near Degeneracy of Magnetic Phases in Two-Dimensional Chromium Telluride with Enhanced Perpendicular Magnetic Anisotropy. <i>ACS Nano</i> , 2020, 14, 15256-15266.	7.3	35
15156	Stepwise construction of silica-supported tantalum/iridium heteropolymetallic catalysts using surface organometallic chemistry. <i>Journal of Catalysis</i> , 2020, 392, 287-301.	3.1	11
15157	First principles study of magnetization and magnetic anisotropy energy of small Co-Pt clusters. <i>Results in Physics</i> , 2020, 19, 103394.	2.0	2
15158	Density functional theory calculation of helium segregation and decohesion effect in W110/Ni111 interphase boundary. <i>Journal of Applied Physics</i> , 2020, 128, .	1.1	7
15159	Computational study about the thermal stability and the detonation performance of nitro-substituted thymine. <i>Journal of Molecular Modeling</i> , 2020, 26, 253.	0.8	0
15160	First-principles study on the mechanical and thermodynamic properties of MoNbTaTiW. <i>International Journal of Minerals, Metallurgy and Materials</i> , 2020, 27, 1398-1404.	2.4	19
15161	The structural properties of silicon-doped DBrTBT/ZnSe solar cell materials: a theoretical study. <i>New Journal of Chemistry</i> , 2020, 44, 15289-15296.	1.4	0

#	ARTICLE	IF	CITATIONS
15162	Atomically-precise dopant-controlled single cluster catalysis for electrochemical nitrogen reduction. <i>Nature Communications</i> , 2020, 11, 4389.	5.8	110
15163	The InSe/SiH type-II van der Waals heterostructure as a promising water splitting photocatalyst: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 21436-21444.	1.3	30
15164	First-principles study of electronic and magnetic properties of nickel doped hexagonal boron nitride (h-BN). <i>European Physical Journal B</i> , 2020, 93, 1.	0.6	4
15165	Theoretical Analysis on Heteroleptic Cu(I)-Based Complexes for Dye-Sensitized Solar Cells: Effect of Anchors on Electronic Structure, Spectrum, Excitation, and Intramolecular and Interfacial Electron Transfer. <i>Molecules</i> , 2020, 25, 3681.	1.7	16
15166	Assessing the validity of <math>\langle \text{DLPNO-CCSD} \rangle \text{(T)}</math> in the calculation of activation and reaction energies of ubiquitous enzymatic reactions. <i>Journal of Computational Chemistry</i> , 2020, 41, 2459-2468.	1.5	16
15167	Cubic to pseudo-cubic tetragonal phase transformation with lithium and beryllium doping in CaTiO <sub>3</sub> and its impact on electronic and optical properties: a DFT approach. <i>Bulletin of Materials Science</i> , 2020, 43, 1.	0.8	9
15168	Nitrogen-free TMS <sub>4</sub> -centers in metal-organic frameworks for ammonia synthesis. <i>Journal of Materials Chemistry A</i> , 2020, 8, 20047-20053.	5.2	45
15169	An Extended Benchmark of Density Functionals for Calculating the Standard Reduction Potentials of Vanadium Compounds. <i>Russian Journal of Physical Chemistry A</i> , 2020, 94, 1616-1622.	0.1	2
15170	DFT study of electronic and electrical properties of stana-silicene as a novel 2D nanomaterial. <i>Optical and Quantum Electronics</i> , 2020, 52, 1.	1.5	3
15171	Elucidating Mechanistic Origin of the Catalytic Activity of the Fe(111) Surface and Nanoclusters toward the Electrochemical Nitrogen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2020, 124, 20193-20202.	1.5	15
15172	Design of superatomic systems: exploiting favourable conditions for the delocalisation of d-electron density in transition metal doped clusters. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 18585-18594.	1.3	5
15173	Gas adsorption properties (N <sub>2</sub> , H <sub>2</sub> , O <sub>2</sub> , NO, NO <sub>2</sub> , CO) Tj ETQq1 1 0.784314 rgB // first-principles study. <i>New Journal of Chemistry</i> , 2020, 44, 18763-18769.	1.4	30
15174	Magnetotransport properties and topological phase transition in NaCd <sub>4</sub> As <sub>3</sub> . <i>Physical Review B</i> , 2020, 102, .	1.1	1
15175	Atomistic Structures and Energetics of Perovskite Nucleation Pathway During Sequential Deposition Process. <i>Multiscale Science and Engineering</i> , 2020, 2, 227-234.	0.9	1
15176	Density Functional Theory Study of Single Metal Atoms Embedded into MBene for Electrocatalytic Conversion of N <sub>2</sub> to NH <sub>3</sub> . <i>ACS Applied Nano Materials</i> , 2020, 3, 9870-9879.	2.4	35
15177	Triple Interface Passivation Strategy-Enabled Efficient and Stable Inverted Perovskite Solar Cells. <i>Small Methods</i> , 2020, 4, 2000478.	4.6	44
15178	Deterministic control of an antiferromagnetic spin arrangement using ultrafast optical excitation. <i>Communications Physics</i> , 2020, 3, .	2.0	10
15179	Atomic dynamics of stress-induced lattice misalignment structures in a KDP subsurface. <i>RSC Advances</i> , 2020, 10, 23944-23952.	1.7	4



#	ARTICLE	IF	CITATIONS
15180	Photoinduced charge transfer in quasi-one-dimensional polymers in two-photon absorption. RSC Advances, 2020, 10, 33288-33298.	1.7	3
15181	Catalytic activity of water molecules in gas-phase glycine dimerization. International Journal of Quantum Chemistry, 2020, 120, e26469.	1.0	11
15182	Highly Efficient Photo-/Electrocatalytic Reduction of Nitrogen into Ammonia by Dual-Metal Sites. ACS Central Science, 2020, 6, 1762-1771.	5.3	135
15183	Stability of epitaxial BiXO <sub>3</sub> phases by density-functional theory. APL Materials, 2020, 8, .	2.2	4
15184	Cation and Anion Co-doped Perovskite Nanofibers for Highly Efficient Electrocatalytic Oxygen Evolution. ACS Applied Materials & Interfaces, 2020, 12, 41259-41268.	4.0	39
15185	Interface engineering of Ag-Ni <sub>3</sub> S <sub>2</sub> heterostructures toward efficient alkaline hydrogen evolution. Nanoscale, 2020, 12, 19333-19339.	2.8	19
15186	Insight and performance of LC-DFT vs DFT in the NMR shielding and chemical shift calculations: Case of CHCl <sub>3</sub> -CH <sub>2</sub> CF <sub>3</sub> . International Journal of Quantum Chemistry, 2020, 120, e26408.	1.0	1
15187	Deriving approximate functionals with asymptotics. Faraday Discussions, 2020, 224, 98-125.	1.6	3
15188	Efficient yet accurate dispersion-corrected semilocal exchange-correlation functionals for non-covalent interactions. Journal of Chemical Physics, 2020, 153, 084117.	1.2	10
15189	Electronic and photocatalytic properties of two-dimensional boron phosphide/SiC van der Waals heterostructure with direct type-II band alignment: a first principles study. RSC Advances, 2020, 10, 32027-32033.	1.7	18
15190	Optical, half-metallic and thermoelectric properties of the Co <sub>2</sub> TaAl [001] film. Indian Journal of Physics, 2021, 95, 1709-1721.	0.9	3
15191	<sc>DFT</sc>, <sc>DLPNO-CCSD</sc>(T), and <sc>NEVPT2</sc> benchmark study of the reaction between ferrocenium and trimethylphosphine. Journal of Computational Chemistry, 2020, 41, 2388-2397.	1.5	12
15192	Experimental and Density Functional Theory Study of the Adsorption Characteristics of CaO for SeO <sub>2</sub> in Simulated Flue Gas and the Effect of CO <sub>2</sub> . Energy & Fuels, 2020, 34, 10872-10881.	2.5	23
15193	Facilitating Phase Evolution for a High-Energy-Efficiency, Low-Cost O <sub>3</sub> -Type Na <sub>x</sub> Cu <sub>0.18</sub> Fe <sub>0.3</sub> Mn <sub>0.52</sub> O <sub>2</sub> Sodium Ion Battery Cathode. Inorganic Chemistry, 2020, 59, 13792-13800.	1.9	15
15194	Vacancy-induced anion and cation redox chemistry in cation-deficient F-doped anatase TiO <sub>2</sub> . Journal of Materials Chemistry A, 2020, 8, 20393-20401.	5.2	8
15195	Thermal effects on the electronic properties of sodium electride under high pressures. Physical Review B, 2020, 102, .	1.1	10
15196	Density Functional Theory Calculations of the Stability and Statistical Disorder in Crystals of the Kappa Phase of Me <sub>3</sub> W <sub>10</sub> C <sub>3</sub> (Me = Fe, Co, Ni). Russian Journal of Physical Chemistry A, 2020, 94, 0.1369-1374.		0
15197	Wide range zero-thermal-quenching ultralong phosphorescence from zero-dimensional metal halide hybrids. Nature Communications, 2020, 11, 4649.	5.8	164





#	ARTICLE	IF	CITATIONS
15216	Development of a fragment kinetic Monte Carlo method for efficient prediction of ionic diffusion in perovskite crystals. <i>Computational Materials Science</i> , 2020, 184, 109844.	1.4	2
15217	Detachment of human mesenchymal stem cells from a gold substrate using electric current. <i>Materialia</i> , 2020, 13, 100866.	1.3	0
15218	Nonlinear propagating modes beyond the phonons in fluorite-structured crystals. <i>Communications Physics</i> , 2020, 3, .	2.0	17
15219	The First-Principles Prediction of Two Dimensional Monolayer Puckered WCAZ2 as the Anode Material of Li-ion Batteries. <i>Materials Today Communications</i> , 2020, 25, 101587.	0.9	1
15220	Hyper oxygen incorporation in CeF <sub>3</sub> : a new intermediate-band photocatalyst for antibiotic degradation under visible/NIR light. <i>RSC Advances</i> , 2020, 10, 38798-38804.	1.7	8
15221	Calculation of elastic constants at high pressure from first-principles. <i>AIP Conference Proceedings</i> , 2020, , .	0.3	1
15222	Gas flow through atomic-scale apertures. <i>Science Advances</i> , 2020, 6, .	4.7	22
15223	Understanding Catalyst Structureâ€“Selectivity Relationships in Pd-Catalyzed Enantioselective Methoxycarbonylation of Styrene. <i>Organometallics</i> , 2020, 39, 4544-4556.	1.1	17
15224	Preferential location of zirconium dopants in cerium dioxide nanoparticles and the effects of doping on their reducibility: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26568-26582.	1.3	6
15225	Intermediate Band Studies of Substitutional V <sup>2+</sup> , Cr <sup>2+</sup> , and Mn <sup>2+</sup> Defects in ZnTe Alloys. <i>Applied Sciences (Switzerland)</i> , 2020, 10, 8937.	1.3	2
15226	Anatomy of Magnetic Anisotropy and Voltage-Controlled Magnetic Anisotropy in Metal Oxide Heterostructure from First Principles. <i>Crystals</i> , 2020, 10, 1118.	1.0	1
15227	Shock compression of vanadium at extremes: Theory and experiment. <i>Physical Review B</i> , 2020, 102, .	1.1	13
15228	Tuning the structure of the skyrmion lattice system Cu <sub>2</sub> OSeO <sub>3</sub> under pressure. <i>Physical Review B</i> , 2020, 102, .	1.1	1
15229	Deep machine learning interatomic potential for liquid silica. <i>Physical Review E</i> , 2020, 102, 052125.	0.8	25
15230	Structural, electronic and mechanical properties of SnTe and selenium doped SnTe-Ab initio study. <i>Materials Today: Proceedings</i> , 2022, 50, 2741-2744.	0.9	6
15231	Diradical Character of Neutral Heteroleptic Bis(1,2-dithiolene) Metal Complexes: Case Study of [Pd(Me <sub>2</sub> timdt)(mnt)] (Me <sub>2</sub> timdt = 1,3-Dimethyl-2,4,5-trithioximidazolidine; Tj ETQq1 1.0.7843145rgBT /Ov	1.0	1
15232	Density Functional Theory for Moleculeâ€“Metal Surface Reactions: When Does the Generalized Gradient Approximation Get It Right, and What to Do If It Does Not. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 10552-10560.	2.1	37
15233	Computational and Experimental Mechanistic Insights into the Ethanol-to-Butanol Upgrading Reaction over MgO. <i>ACS Catalysis</i> , 2020, 10, 15162-15177.	5.5	16

#	ARTICLE	IF	CITATIONS
15234	Elemental Core Level Shift in High Entropy Alloy Nanoparticles <i>via</i> X-ray Photoelectron Spectroscopy Analysis and First-Principles Calculation. ACS Nano, 2020, 14, 17704-17712.	7.3	48
15235	Interrelated Mechanism by Which the Methide Quinone Celastrol, Obtained from the Roots of <i>Tripterygium wilfordii</i> , Inhibits Main Protease 3CL <sup>pro</sup> of COVID-19 and Acts as Superoxide Radical Scavenger. International Journal of Molecular Sciences, 2020, 21, 9266.	1.8	16
15236	The Effect of Interaction Weight on Dipole Field Calculations to Reconstruct the $\text{La}_{2/3}\text{Sr}_{1/3}\text{CuO}_4$ $\mu\text{SR}$ Spectrum. Key Engineering Materials, 0, 860, 165-170.	0.4	0
15237	Function of Interface Deposition of Calcium Sulfate in Pressure Acid Leaching of Black Shale-Hosted Vanadium. Minerals (Basel, Switzerland), 2020, 10, 952.	0.8	4
15238	Unraveling the Hidden Role of the Counteranion in $\alpha$ -Cation in a Cage-Systems. Journal of Physical Chemistry A, 2020, 124, 8040-8049.	1.1	3
15239	Highly Enhanced Gas Sensing Performance Using a 1T/2H Heterophase $\text{MoS}_2$ Field-Effect Transistor at Room Temperature. ACS Applied Materials & Interfaces, 2020, 12, 50610-50618.	4.0	64
15240	Electro-oxidation of furfural on gold is limited by furoate self-assembly. Journal of Catalysis, 2020, 391, 327-335.	3.1	30
15241	Theoretical Studies of $\text{Au}_3^{+}$ Clusters Using Density Functional Theory. Key Engineering Materials, 2020, 862, 94-98.	0.4	0
15242	The Effect of Carbon Defects in the Coal-Pyrite Vacancy on the Electronic Structure and Optical Properties: A DFT + U Study. Minerals (Basel, Switzerland), 2020, 10, 815.	0.8	2
15243	Investigation of alkali-ion (Li, Na and K) intercalation in manganese hexacyanoferrate $\text{K}_x\text{MnFe}(\text{CN})_6$ as cathode material. Chemical Engineering Journal, 2020, 396, 125269.	6.6	44
15244	Structural evolution and magnetic properties of $\text{ScLi}_n$ ( $n = 2-13$ ) clusters: A PSO and DFT investigation*. Chinese Physics B, 2020, 29, 077101.	0.7	5
15245	A new mixed-anion phosphate $\text{Cs}_2\text{Bi}_2\text{Sr}(\text{P}_2\text{O}_7)(\text{PO}_4)_2$ : Synthesis, characterization, structure and its $\text{Eu}^{3+}$ -activated luminescence. Journal of Solid State Chemistry, 2020, 288, 121411.	1.4	9
15246	Density Functional Theory Study of Decarboxylation and Decarbonylation of Acetic Acid on Pd(111). Journal of Physical Chemistry C, 2020, 124, 13082-13093.	1.5	13
15247	Electrocatalytic reduction of $\text{CO}_2$ to ethylene and ethanol through hydrogen-assisted $\text{C}-\text{C}$ coupling over fluorine-modified copper. Nature Catalysis, 2020, 3, 478-487.	16.1	788
15248	The one-electron self-interaction error in 74 density functional approximations: a case study on hydrogenic mono- and dinuclear systems. Physical Chemistry Chemical Physics, 2020, 22, 15805-15830.	1.3	27
15249	Electrochemical Li Intercalation in Black Phosphorus: In Situ and Ex Situ Studies. Journal of Physical Chemistry C, 2020, 124, 10710-10718.	1.5	18
15250	Understanding Zn Functions on Hydrothermal Stability in a One-Pot-Synthesized $\text{Cu}\&\text{Zn-SSZ-13}$ Catalyst for $\text{NH}_3$ Selective Catalytic Reduction. ACS Catalysis, 2020, 10, 6197-6212.	5.5	65
15251	Gd impurity effect on the magnetic and electronic properties of hexagonal Sr ferrites: A case study by DFT. Chinese Physics B, 2020, 29, 077505.	0.7	2

#	ARTICLE	IF	CITATIONS
15252	Enhancing adhesion of Al <sub>2</sub> O <sub>3</sub> scale on Ti-Al intermetallics by alloying: A first principles study. Computational Materials Science, 2020, 181, 109756.	1.4	9
15253	Characteristics of dopant distribution and surface oxygen vacancy formation for modified Fe <sub>2</sub> O <sub>3</sub> in chemical looping combustion. Fuel, 2020, 276, 117942.	3.4	38
15254	Accurate simulations of atomic diffractive scattering from KCl(0 0 1) under fast grazing incidence conditions. Nuclear Instruments & Methods in Physics Research B, 2020, 476, 1-9.	0.6	5
15255	Two-dimensional $CP\bar{3}$ monolayer and its fluorinated derivative with promising electronic and optical properties: A theoretical study. Physical Review B, 2020, 101, .	1.1	27
15256	Two-Dimensional van der Waals Supramolecular Frameworks from Co-Hosted Molecular Assembly and C <sub>60</sub> Dimerization. Journal of Physical Chemistry C, 2020, 124, 12589-12595.	1.5	7
15257	Ligand Effect on Geometry and Electronic Structures of Face-Centered Cubic Ag <sub>14</sub> and Ag <sub>23</sub> Nanoclusters. Journal of Physical Chemistry C, 2020, 124, 13421-13426.	1.5	4
15258	Effects of B on the Segregation Behavior of Mo at the Fe-Cr(111)/Cr <sub>2</sub> O <sub>3</sub> (0001) Interface: A First-Principles Study. Metals, 2020, 10, 577.	1.0	6
15259	Cu Anchored Ti <sub>2</sub> NO <sub>2</sub> as High Performance Electrocatalyst for Oxygen Evolution Reaction: A Density Functional Theory Study. ChemCatChem, 2020, 12, 4059-4066.	1.8	27
15260	Investigation on Martensitic Transformation and Magnetic Properties of all-d-Metal Pd <sub>2</sub> MnTi and Pt <sub>2</sub> MnTi by First-Principle Calculations. Journal of Superconductivity and Novel Magnetism, 2020, 33, 2245-2250.	0.8	4
15261	Single Vanadium Atoms Anchored on Graphitic Carbon Nitride as a High-Performance Catalyst for Non-oxidative Propane Dehydrogenation. ACS Nano, 2020, 14, 5772-5779.	7.3	73
15262	AgFeS <sub>2</sub> nanoparticles as a novel photothermal platform for effective artery stenosis therapy. Nanoscale, 2020, 12, 11288-11296.	2.8	15
15263	High-temperature ion-thermal behavior from average-atom calculations. Physical Review E, 2020, 101, 053201.	0.8	6
15264	Theoretical anchoring effect of new phosphorus allotropes for lithium-sulfur batteries. Nanoscale, 2020, 12, 11095-11111.	2.8	10
15265	Synergy between a Silver-Copper Surface Alloy Composition and Carbon Dioxide Adsorption and Activation. ACS Applied Materials & Interfaces, 2020, 12, 25374-25382.	4.0	19
15266	Grafting of Lanthanum Complexes on a Functionalized Graphene Surface: Theoretical Investigation on Ethylene and 1,3-Butadiene Homo- and Copolymerization. Chemistry - A European Journal, 2020, 26, 13213-13225.	1.7	3
15267	Trends in the Adsorption of Oxygen and Li <sub>2</sub> O <sub>2</sub> on Transition-Metal Carbide Surfaces: A Theoretical Study. Journal of Physical Chemistry C, 2020, 124, 7716-7724.	1.5	9
15268	A physics-based machine learning study of the behavior of interstitial helium in single crystal W-Mo binary alloys. Journal of Applied Physics, 2020, 127, .	1.1	10
15269	Superconducting boron allotropes. Physical Review B, 2020, 101, .	1.1	18

#	ARTICLE	IF	CITATIONS
15270	Dependence on co-adsorbed water in the reforming reaction of ethanol on a Rh(111) surface. RSC Advances, 2020, 10, 17787-17794.	1.7	0
15271	Antioxidant Properties of Embelin in Cell Culture. Electrochemistry and Theoretical Mechanism of Scavenging. Potential Scavenging of Superoxide Radical through the Cell Membrane. Antioxidants, 2020, 9, 382.	2.2	32
15272	Charge doping induced reversible multistep structural phase transitions and electromechanical actuation in two-dimensional $1T\text{-MoS}_2$ . Nanoscale, 2020, 12, 12541-12550.	2.8	19
15273	Stable edge structures and electronic states in zigzag $1T\text{-dichalcogenide}$ nanoribbons. Journal of Physics Condensed Matter, 2020, 32, 365303.	0.7	1
15274	Structure and reactivity of flotation reagents. , 2020, , 181-236.		1
15275	Electronic, optical, and thermoelectric properties of sodium pnictogen chalcogenides: A first principles study. Computational Materials Science, 2020, 183, 109818.	1.4	21
15276	Vacancy Occupation-Driven Polymorphic Transformation in Cobalt Ditetelluride for Boosted Oxygen Evolution Reaction. ACS Nano, 2020, 14, 6968-6979.	7.3	100
15277	Computational prediction of $\text{Au}^{+4}$ oxidation state in Au via compressed $\text{AuO}_2$ compound. Journal of Physics Condensed Matter, 2020, 32, 015402.	0.7	2
15278	First-principles study of superior hydrogen storage performance of Li-decorated $\text{Be}_2\text{N}_6$ monolayer. International Journal of Hydrogen Energy, 2020, 45, 19465-19478.	3.8	24
15279	Unified and transferable description of dynamics of $\text{H}_2$ dissociative adsorption on multiple copper surfaces via machine learning. Physical Chemistry Chemical Physics, 2020, 22, 13958-13964.	1.3	37
15280	Origin of magnetic inhomogeneity in Cr- and V-doped topological insulators. Physical Review B, 2020, 101, .	1.1	6
15281	Effect of Zn/S non-stoichiometric ratio on the structural, optical and electronic properties of nano-ZnS. Applied Physics A: Materials Science and Processing, 2020, 126, 1.	1.1	17
15282	Orbital Overlapping through Induction Bonding Overcomes the Intrinsic Delamination of 3D-Printed Cementitious Binders. ACS Nano, 2020, 14, 9466-9477.	7.3	22
15283	Enhancing Energy Product and Thermal Stability of $\text{SmFe}_{12}$ by Interstitial Doping. Physical Review Applied, 2020, 13, .	1.5	16
15284	First-principle calculations on the structures and electronic properties of the CO-adsorbed $(\text{SnO}_2)_2$ clusters. Structural Chemistry, 2020, 31, 1861-1867.	1.0	4
15285	Application of SPS in the fabrication of UN and (U,Th)N pellets from microspheres. Journal of Nuclear Materials, 2020, 536, 152181.	1.3	10
15286	Validation of Pseudopotential Calculations for the Electronic Band Gap of Solids. Journal of Chemical Theory and Computation, 2020, 16, 3620-3627.	2.3	25
15287	Catalytic Conversion Furfuryl Alcohol to Tetrahydrofurfuryl Alcohol and 2-Methylfuran at Terrace, Step, and Corner Sites on Ni. ACS Catalysis, 2020, 10, 7240-7249.	5.5	31

#	ARTICLE	IF	CITATIONS
15288	Structural and electronic properties of the adsorption of nitric oxide molecule on copper clusters CuN(N $\hat{A}$ = $\hat{A}$ 1 $\hat{A}$ “7): A DFT study. <i>Chemical Physics Letters</i> , 2020, 753, 137543.	1.2	6
15289	Green synthesis of antibacterial and antifungal silver nanoparticles using Citrus limetta peel extract: Experimental and theoretical studies. <i>Journal of Environmental Chemical Engineering</i> , 2020, 8, 104019.	3.3	88
15290	Super-hygroscopic film for wearables with dual functions of expediting sweat evaporation and energy harvesting. <i>Nano Energy</i> , 2020, 75, 104873.	8.2	52
15291	First-Principles Calculation of Optimizing the Performance of Germanene-Based Supercapacitors by Vacancies and Metal Atoms. <i>Journal of Physical Chemistry C</i> , 2020, 124, 12346-12358.	1.5	16
15292	Neural network interpolation of exchange-correlation functional. <i>Scientific Reports</i> , 2020, 10, 8000.	1.6	14
15293	CNT $\hat{A}$ Assembled Octahedron Carbon $\hat{A}$ Encapsulated Cu <sub>3</sub> /Cu Heterostructure by In Situ MOF $\hat{A}$ Derived Engineering for Superior Lithium Storage: Investigations by Experimental Implementation and First $\hat{A}$ Principles Calculation. <i>Advanced Science</i> , 2020, 7, 2000736.	5.6	66
15294	Interfacial properties and fracture behavior of the L12-Al3Sc   Al interface: Insights from a first-principles study. <i>Applied Surface Science</i> , 2020, 515, 146017.	3.1	20
15295	BC3 graphene-like monolayer as a drug delivery system for nitrosourea anticancer drug: A first-principles perception. <i>Applied Surface Science</i> , 2020, 525, 146577.	3.1	44
15296	The importance of atomic charge distributions of solid boron material in N2 electrochemical reduction. <i>Applied Surface Science</i> , 2020, 526, 146606.	3.1	13
15297	Vacancy effect of antimony on shear deformation mechanisms of CoSb3 thermoelectric material. <i>Computational Materials Science</i> , 2020, 182, 109761.	1.4	6
15298	Exploring the microscopic reaction mechanism of H2S and COS with CuO oxygen carrier in chemical looping combustion. <i>Fuel Processing Technology</i> , 2020, 205, 106431.	3.7	20
15299	The roles of native defects and transition metal additives in the dehydrogenation mechanism of Mg(AlH4)2. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 17625-17636.	3.8	1
15300	B12Y12 (Y: N, P) fullerene-like cages for exemestane-delivery; molecular modeling investigation. <i>Journal of Molecular Structure</i> , 2020, 1217, 128455.	1.8	16
15301	Crystal structure and properties of iodine monofluoride compounds at high pressure. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 385404.	0.7	3
15302	Electronic properties and superior CO2 capture selectivity of metal nitride (XN) and phosphide (XP) (X $\hat{A}$ =Al, Ga and In) sheets. <i>Applied Surface Science</i> , 2020, 527, 146445.	3.1	7
15303	Extraction Behavior of Acidic Phosphorus-Containing Compounds to Some Metal Ions: A Combination Research of Experimental and Theoretical Investigations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5033-5041.	1.1	2
15304	Structural transformation of energetic cyclo-pentazolate salt under the pressure. <i>Structural Chemistry</i> , 2020, 31, 1887-1896.	1.0	1
15305	Introduction of density functional theory. , 2020, , 1-12.		6



#	ARTICLE	IF	CITATIONS
15306	Interaction of water and oxygen with sulfide mineral surface. , 2020, , 113-179.		0
15307	Electronic structures and surface adsorption of impurity-bearing sulfide minerals. , 2020, , 307-359.		0
15308	Investigation on mechanical and optical properties of the Ti-doped NbAl <sub>3</sub> compound by first-principle calculation. Physica B: Condensed Matter, 2020, 593, 412276.	1.3	6
15309	Relationships between Orbital Energies, Optical and Fundamental Gaps, and Exciton Shifts in Approximate Density Functional Theory and Quasiparticle Theory. Journal of Chemical Theory and Computation, 2020, 16, 4337-4350.	2.3	21
15310	Comparative Insertion Reactivity of CO, CO <sub>2</sub> , tBuCN, and tBuNC into Thorium and Uranium-Phosphorus Bonds. Organometallics, 2020, 39, 2152-2161.	1.1	19
15311	Anion-modulated nickel-based nanoheterostructures as high performance electrocatalysts for hydrogen evolution reaction. Journal of Materials Chemistry A, 2020, 8, 12013-12027.	5.2	10
15312	First-principles study of the adsorption of 3d transition metals on BaO- and TiO <sub>2</sub> -terminated cubic-phase BaTiO <sub>3</sub> (001) surfaces. Journal of Chemical Physics, 2020, 152, 204701.	1.2	10
15313	Effects of self-interstitial atom on behaviors of hydrogen and helium in tungsten. Physica Scripta, 2020, 95, 075708.	1.2	7
15314	First-principles Hubbard $U$ and Hund's $J$ corrected approximate density functional theory predicts an accurate fundamental gap in rutile and anatase $\text{TiO}_2$ clusters. Theoretical Chemistry Accounts, 2020, 139, 1.	1.1	31
15315	Relativistic effects on the energetic stability of $\text{Pb}_5$ clusters. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	0
15316	Phase transformations in novel hot-deformed Al-Zn-Mg-Cu-Si-Mn-Fe-Sc-Zr alloys. Materials and Design, 2020, 193, 108821.	3.3	21
15317	Stability and energetics of $\text{HnVm}$ complexes in Fe-Cr alloys: Ab initio study. Materials Chemistry and Physics, 2020, 253, 123314.	2.0	4
15318	Calorimetric study of Nd <sub>2</sub> Fe <sub>14</sub> B: Heat capacity, standard Gibbs energy of formation and magnetic entropy. Thermochimica Acta, 2020, 690, 178672.	1.2	7
15319	Solution enthalpy calculation for impurity in liquid metal by first-principles calculations: A benchmark test for oxygen impurity in liquid sodium. Journal of Chemical Physics, 2020, 152, 154503.	1.2	4
15320	Comparing the performance of density functionals in describing the adsorption of atoms and small molecules on Ni(111). Surface Science, 2020, 700, 121675.	0.8	8
15321	Assessment of the DLPNO Binding Energies of Strongly Noncovalent Bonded Atmospheric Molecular Clusters. ACS Omega, 2020, 5, 7601-7612.	1.6	38
15322	Relationship between hydrogen binding energy and activity for hydrogen evolution reaction by palladium supported on sulfur-doped ordered mesoporous carbon. Journal of Industrial and Engineering Chemistry, 2020, 89, 361-367.	2.9	11
15323	Effects of pressure on structural, mechanical, and electronic properties of trigonal and monoclinic MgSiO <sub>3</sub> . Solid State Sciences, 2020, 105, 106261.	1.5	7



#	ARTICLE	IF	CITATIONS
15324	Enhancement of the tensile strength by introducing alloy element Fe for Ti based alloy. Solid State Communications, 2020, 318, 113982.	0.9	16
15325	Search for stable cocrystals of energetic materials using the evolutionary algorithm USPEX. Physical Chemistry Chemical Physics, 2020, 22, 16822-16830.	1.3	21
15326	The strategy for improving the stability of nitroform derivativesâ€™ high-energetic oxidant based on hexanitroethane. Journal of Molecular Modeling, 2020, 26, 181.	0.8	3
15327	Thermoelasticity of tremolite amphibole: Geophysical implications. American Mineralogist, 2020, 105, 904-916.	0.9	11
15328	Understanding the role of boron and stoichiometric ratio in the catalytic performance of amorphous Co-B catalyst. Applied Surface Science, 2020, 518, 146199.	3.1	7
15329	Uncovering the Zr segregation behavior and its effect on the fracture strength of Al $\hat{\text{5}}$ (210) [100] symmetrical tilt grain boundary: Insight from first principles calculation. Materials Today Communications, 2020, 25, 101268.	0.9	2
15330	Delocalization in Substituted Benzene Dications: A Magnetic Point of View. ChemistryOpen, 2020, 9, 657-661.	0.9	4
15331	Biogenic silver nanoparticle synthesis and stabilization for apoptotic activity; insights from experimental and theoretical studies. Chemical Papers, 2020, 74, 4089-4101.	1.0	18
15332	On the excitation mechanism of visible responsible Er-TiO <sub>2</sub> system proved by experimental and theoretical investigations for boosting photocatalytic activity. Applied Surface Science, 2020, 527, 146815.	3.1	14
15333	Insight into the intrinsic mechanism of improving electrochemical performance via constructing the preferred crystal orientation in lithium cobalt dioxide. Chemical Engineering Journal, 2020, 399, 125708.	6.6	13
15334	The influence of transition metal solutes on the dissolution and diffusion of oxygen in tungsten. Journal of Nuclear Materials, 2020, 537, 152250.	1.3	5
15335	Adsorption and diffusion behaviors of H <sub>2</sub> , H <sub>2</sub> S, NH <sub>3</sub> , CO and H <sub>2</sub> O gases molecules on MoO <sub>3</sub> monolayer: A DFT study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126533.	0.9	34
15336	Dielectrophoretic borophene tweezer: Sub-10â€™mV nano-particle trapping. Applied Surface Science, 2020, 527, 146859.	3.1	4
15337	Molecular Interpretation of Pharmaceuticalsâ€™™ Adsorption on Carbon Nanomaterials: Theory Meets Experiments. Processes, 2020, 8, 642.	1.3	29
15338	Influence of (Mn or Co)-doping on structural, magnetic and electronic properties of nano Zn <sub>0.75</sub> Cd <sub>0.25</sub> S. Chinese Journal of Physics, 2020, 67, 414-427.	2.0	13
15339	Probing the Hydrogen Bonding in Microsolvated Clusters of Au <sub>1,2</sub> â€™ (Solv) <sub>n</sub> (Solv =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 147 Td (C <sub>sub&gt;2&gt;</sub>	1.1	6
15340	Multifunctional Lateral Transitionâ€™Metal Disulfides Heterojunctions. Advanced Functional Materials, 2020, 30, 2002939.	7.8	86
15341	Reversing abnormal hole localization in high-Al-content AlGa <sub>N</sub> quantum well to enhance deep ultraviolet emission by regulating the orbital state coupling. Light: Science and Applications, 2020, 9, 104.	7.7	25

#	ARTICLE	IF	CITATIONS
15342	Investigation on Adsorption and Decomposition Properties of CL-20/FOX-7 Molecules on MgH <sub>2</sub> (110) Surface by First-Principles. <i>Molecules</i> , 2020, 25, 2726.	1.7	5
15343	Lithiation of Sulfur-Graphene Compounds Using Reactive Force-Field Molecular Dynamics Simulations. <i>Journal of the Electrochemical Society</i> , 2020, 167, 100555.	1.3	10
15344	Dipole Relaxation in Semiconducting Zn <sub>2-x</sub> Mg <sub>x</sub> InV <sub>3</sub> O <sub>11</sub> Materials (Where x = 0.0, 0.4, 1.0, 1.6, and 2.0). <i>Materials</i> , 2020, 13, 2425.	1.3	1
15345	Type-II band alignment AlN/InSe van der Waals heterostructure: Vertical strain and external electric field. <i>Applied Surface Science</i> , 2020, 528, 146782.	3.1	26
15346	Uncertainty in the separation properties of functionalized porous graphenes. <i>Applied Surface Science</i> , 2020, 525, 146524.	3.1	6
15347	LaCrO <sub>3</sub> -Coated La <sub>0.6</sub> Sr <sub>0.4</sub> Co <sub>0.2</sub> Fe <sub>0.8</sub> O <sub>3-<math>\delta</math></sub> Core-Shell Structured Cathode with Enhanced Cr Tolerance for Intermediate-Temperature Solid Oxide Fuel Cells. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 29133-29142.	4.0	4
15348	Co nanoparticle-embedded N,O-codoped porous carbon nanospheres as an efficient peroxydisulfate activator: singlet oxygen dominated catalytic degradation of organic pollutants. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15340-15353.	1.3	35
15349	Raman spectra of MXenes Zr <sub>2</sub> X(X=C and N). <i>Nanotechnology</i> , 2020, 31, 405708.	1.3	7
15350	Density Functional Theory Calculations on Copper-Mediated Peroxide Decomposition Reactions: Implications for Jet Fuel Autoxidation. <i>Energy &amp; Fuels</i> , 2020, 34, 7439-7447.	2.5	9
15351	Molecular and dissociative adsorption of CO and SO on the surface of Ir(111). <i>AIP Advances</i> , 2020, 10, 035021.	0.6	2
15352	Characterization of the Equiatomic Quaternary Heusler Alloy ZnCdRhMn: Structural, Electronic, and Magnetic Properties. <i>Journal of Superconductivity and Novel Magnetism</i> , 2020, 33, 3087-3095.	0.8	48
15353	Molecular simulation study of strontium doping on the adsorption of methanol on CaO(100) surface. <i>Journal of Fuel Chemistry and Technology</i> , 2020, 48, 172-178.	0.9	4
15354	The correlation between chemical effect and segregation behavior in metallic Al liquid. <i>Computational Materials Science</i> , 2020, 175, 109611.	1.4	1
15355	Theoretical study of CH <sub>4</sub> adsorption and dissociation on W-Cu(110) surface. <i>Computational and Theoretical Chemistry</i> , 2020, 1186, 112890.	1.1	5
15356	Revealing the effect of phosphorus doping on Co@carbon in boosting oxygen evolution catalytic activity. <i>Journal of Alloys and Compounds</i> , 2020, 843, 156001.	2.8	8
15357	Theoretical and Experimental Study on Exciton Properties of Ti <sub>2</sub> O <sub>5</sub> . <i>Journal of Physical Chemistry C</i> , 2020, 124, 15066-15075.	1.5	19
15358	Existence and Properties of Isolated Catalytic Sites on the Surface of $\beta$ -Cristobalite-Supported, Doped Tungsten Oxide Catalysts (WO <sub>x</sub> / $\beta$ -SiO <sub>2</sub> ). <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 107 Td (Na-WO<sub>x</sub>)</i>	5.5	33
15359	Oxidative Coupling of Methane (OCM): A Combined Periodic DFT and Experimental Study. <i>ACS Catalysis</i> , 2020, 10, 4580-4592.		
15359	Effect of Electrolyte on the Proton Transport through Graphane in the Electrochemical Cell: A First-Principles Study. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3025-3031.	2.1	6

#	ARTICLE	IF	CITATIONS
15360	High throughput screening of $M_3C_2$ MXenes for efficient $CO_2$ reduction conversion into hydrocarbon fuels. <i>Nanoscale</i> , 2020, 12, 7660-7673.	2.8	64
15361	Mechanism and activity of the oxygen reduction reaction on $WTe_2$ transition metal dichalcogenide with Te vacancy. <i>RSC Advances</i> , 2020, 10, 8460-8469.	1.7	11
15362	Assessing model-dielectric-dependent hybrid functionals on the antiferromagnetic transition-metal monoxides MnO, FeO, CoO, and NiO. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 015502.	0.7	30
15363	First-principles study of stability, electronic structure and quantum capacitance of B-, N- and O-doped graphynes as supercapacitor electrodes. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 215501.	0.7	9
15364	Effect of copper concentration on the structure and properties of Al-Cu-Fe and Al-Cu-Ni melts. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 224003.	0.7	10
15365	Copper, gold, and platinum under femtosecond irradiation: Results of first-principles calculations. <i>Physical Review B</i> , 2020, 101, .	1.1	30
15366	Hydrolytic dehydrogenation of $NH_3BH_3$ catalyzed by ruthenium nanoparticles supported on magnesium-aluminum layered double-hydroxides. <i>RSC Advances</i> , 2020, 10, 9996-10005.	1.7	16
15367	Enhancing hydrogen storage by metal substitution in MIL-88A metal-organic framework. <i>Adsorption</i> , 2020, 26, 509-519.	1.4	15
15368	Effects of carboxylic acid auxiliary ligands on the magnetic properties of azido-Cu(II) complexes: A density functional theory study. <i>Polyhedron</i> , 2020, 182, 114506.	1.0	14
15369	Highly Effective Work Function Reduction of $\pm$ Borophene via Caesium Decoration: A First-Principles Investigation. <i>Advanced Theory and Simulations</i> , 2020, 3, 1900249.	1.3	8
15370	Intermetallic Reactivity: $Ca_3Cu_7.8Al_{26.2}$ and the Role of Electronegativity in the Stabilization of Modular Structures. <i>Inorganic Chemistry</i> , 2020, 59, 5018-5029.	1.9	10
15371	General synthesis of two-dimensional van der Waals heterostructure arrays. <i>Nature</i> , 2020, 579, 368-374.	13.7	393
15372	Stability and electronic properties of Au atom doped hexagonal boron nitride sheet on Ni(111) support: Role of vacancy defects and supports towards single atom catalysis. <i>Applied Surface Science</i> , 2020, 515, 145978.	3.1	10
15373	The Aromatic 2-Iminomethylphenyltellurenyl Cation. A Lewis Superacid Despite the Intramolecularly Coordinating N-Donor Ligand. <i>Organometallics</i> , 2020, 39, 1202-1212.	1.1	10
15374	Investigation on $Cu_2O$ Surface Reconstruction and Catalytic Performance of $NH_3$ -SCO by Experimental and DFT Studies. <i>ACS Applied Energy Materials</i> , 2020, 3, 3465-3476.	2.5	25
15375	<i>In situ</i> construction of a MOF-derived carbon-encapsulated $LiCoO_2$ heterostructure as a superior cathode for elevated-voltage lithium storage: from experimental to theoretical study. <i>Journal of Materials Chemistry A</i> , 2020, 8, 6607-6618.	5.2	46
15376	Crystal facet dependence of carbon chain growth mechanism over the Hcp and Fcc Co catalysts in the Fischer-Tropsch synthesis. <i>Applied Catalysis B: Environmental</i> , 2020, 269, 118847.	10.8	29
15377	Effect of indole alkaloids from roots of <i>Rauvolfia ligustrina</i> in the noradrenergic neurotransmission. <i>FÄ-toterapÄ-Äç</i> , 2020, 143, 104545.	1.1	4

#	ARTICLE	IF	CITATIONS
15378	Pd <sub>3</sub> Ag(111) as a Model System for Hydrogen Separation Membranes: Combined Effects of CO Adsorption and Surface Termination on the Activation of Molecular Hydrogen. <i>Topics in Catalysis</i> , 2020, 63, 750-761.	1.3	13
15379	Comparative study on the activities of different MgO surfaces in CO <sub>2</sub> activation and hydrogenation. <i>Catalysis Today</i> , 2020, 356, 535-543.	2.2	18
15380	Oxygen adsorption on ideal ZrB <sub>2</sub> and ZrC surfaces. <i>Journal of Alloys and Compounds</i> , 2020, 830, 154655.	2.8	11
15381	Synergistic trifunctional electrocatalysis of pyridinic nitrogen and single transition-metal atoms anchored on pyrazine-modified graphdiyne. <i>Science Bulletin</i> , 2020, 65, 995-1002.	4.3	34
15382	Electronic structures and strain responses of group VA/VA two-dimensional van der waals heterostructures. <i>Vacuum</i> , 2020, 176, 109296.	1.6	12
15383	Direct Synthesis of Semimetal Phthalocyanines on a Surface with Insights into Interfacial Properties. <i>Journal of Physical Chemistry C</i> , 2020, 124, 8247-8256.	1.5	3
15384	Extension and evaluation of the D4 London-dispersion model for periodic systems. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8499-8512.	1.3	138
15385	Complex-time shredded propagator method for large-scale $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle G \langle \text{mml:mi} \rangle \langle \text{mml:mi} \rangle W \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle$ calculations. <i>Physical Review B</i> , 2020, 101, .		
15386	X-Ray structures, Mössbauer hyperfine parameters, and molecular orbital descriptions of the phthalocyaninato iron(II) azole complexes. <i>Journal of Porphyrins and Phthalocyanines</i> , 2020, 24, 894-903.	0.4	10
15387	Comment on "Local, solvation pressures and conformational changes in ethylenediamine aqueous solutions probed using Raman spectroscopy" by M. Cárceles, A. Lobato, N. J. Mendoza, L. J. Bonales and V. G. Baonza, <i>Phys. Chem. Chem. Phys.</i> , 2016, 18, 26192. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 7119-7125.	1.3	1
15388	First principle study of the structural and electronic properties of Nihonium. <i>MRS Advances</i> , 2020, 5, 1175-1183.	0.5	1
15389	A DFT screening of single transition atoms supported on MoS <sub>2</sub> as highly efficient electrocatalysts for the nitrogen reduction reaction. <i>Nanoscale</i> , 2020, 12, 10035-10043.	2.8	94
15390	Inorganic photovoltaic cells based on BiFeO <sub>3</sub> : spontaneous polarization, lattice matching, light polarization and their relationship with photovoltaic performance. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8658-8666.	1.3	6
15391	DFT study of electronic and optical properties of (Mn) co-doped SrTiO <sub>3</sub> for enhanced photocatalytic hydrogen production. <i>Solid State Communications</i> , 2020, 312, 113893.	0.9	22
15392	Optimization of Pt-Oxygen-Containing Species Anodes for Ethanol Oxidation Reaction: High Performance of Pt-AuSnO <sub>x</sub> Electrocatalyst. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 2846-2853.	2.1	11
15393	Pressure-Stabilized Zinc Trifluoride. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 2854-2858.	2.1	7
15394	Designing catalysts for water splitting based on electronic structure considerations. <i>Electronic Structure</i> , 2020, 2, 023001.	1.0	43
15395	Intersecting nodal rings in orthorhombic-type BaLi <sub>2</sub> Sn compound. <i>Journal of Materials Chemistry C</i> , 2020, 8, 5461-5466.	2.7	16

#	ARTICLE	IF	CITATIONS
15396	Electronic structures and optoelectronic properties of $\text{ATiOPO}_4$ ( $A = \text{H, Li, Na, K, Rb, Cs, Fr}$ ) and photo-degradation. <i>Materials Research Express</i> , 2020, 7, 045901.	0.8	6
15397	Multi-coefficients correlation methods. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1474.	6.2	4
15398	Photoisomerization of IC <sub>3</sub> N. An experimental and theoretical study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 395, 112470.	2.0	1
15399	Effects of nanoporous Au on ATP synthase. <i>MRS Communications</i> , 2020, 10, 173-178.	0.8	1
15400	First-principles studies of chalcopyrite-type (Cu, Li)GaS <sub>2</sub> and (Cu, Li)InS <sub>2</sub> systems. <i>Japanese Journal of Applied Physics</i> , 2020, 59, SCCB18.	0.8	0
15401	Molecular Distribution of Indomethacin: Impact on the Precipitation of Glassy Curcumin pH-Responsive Nanoparticles with Enhanced Solubility. <i>Crystal Growth and Design</i> , 2020, 20, 2377-2389.	1.4	6
15402	Atomic-scale simulations for lithium dendrite growth driven by strain gradient. <i>Applied Mathematics and Mechanics (English Edition)</i> , 2020, 41, 533-542.	1.9	5
15403	Post-redox engineering electron configurations of atomic thick C <sub>3</sub> N <sub>4</sub> nanosheets for enhanced photocatalytic hydrogen evolution. <i>Applied Catalysis B: Environmental</i> , 2020, 270, 118855.	10.8	40
15404	A systematic investigation of the catalytic performances of monolayer carbon nitride nanosheets C <sub>3</sub> N <sub>x</sub> . <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 6772-6782.	1.3	9
15405	Impact of electron transfer of atomic metals on adjacent graphene layers on electrochemical water splitting. <i>Nanoscale</i> , 2020, 12, 7814-7821.	2.8	16
15406	The devil in the details: A tutorial review on some undervalued aspects of density functional theory calculations. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26332.	1.0	63
15407	Interpretation of vibrational optical activity spectra of proteins. , 2020, , 219-248.		0
15408	Insights into the tribochemistry of sliding iron oxide surfaces lubricated by sodium silicate glasses: An ab initio molecular dynamics study. <i>Applied Surface Science</i> , 2020, 528, 147008.	3.1	12
15409	DFT studies of 2-mercaptobenzothiazole and 2-mercaptobenzimidazole as corrosion inhibitors for copper. <i>Corrosion Science</i> , 2020, 174, 108840.	3.0	58
15410	The comparative study of XO <sub>2</sub> (X = C, N, S) gases adsorption and dissociation on pristine and defective graphene supported Pt <sub>13</sub> . <i>Materials Chemistry and Physics</i> , 2020, 247, 122712.	2.0	8
15411	Closing the Gap Between Experiment and Theory: Reactive Scattering of HCl from Au(111). <i>Journal of Physical Chemistry C</i> , 2020, 124, 15944-15960.	1.5	18
15412	Predicting the Effect of Dopants on CO <sub>2</sub> Adsorption in Transition Metal Carbides: Case Study on TiC (001). <i>Journal of Physical Chemistry C</i> , 2020, 124, 15969-15976.	1.5	10
15413	Using principal component analysis for neural network high-dimensional potential energy surface. <i>Journal of Chemical Physics</i> , 2020, 152, 234103.	1.2	11

#	ARTICLE	IF	CITATIONS
15414	Strong influence of strain gradient on lithium diffusion: flexo-diffusion effect. <i>Nanoscale</i> , 2020, 12, 15175-15184.	2.8	9
15415	High-loaded single Cu atoms decorated on N-doped graphene for boosting Fenton-like catalysis under neutral pH. <i>Journal of Materials Chemistry A</i> , 2020, 8, 13685-13693.	5.2	104
15416	Studies on magnetic and electronic properties of $\text{Pu}^{\text{X}}_3$		

#	ARTICLE	IF	CITATIONS
15432	Effects of rare earth elements on the microstructure and wear properties of TiB <sub>2</sub> reinforced aluminum matrix composite coatings: Experiments and first principles calculations. <i>Applied Surface Science</i> , 2020, 530, 147051.	3.1	29
15433	Robust tuning metal/carbon heterointerfaces via ketonic oxygen enables hydrogen evolution reaction outperforming Pt/C. <i>Applied Surface Science</i> , 2020, 529, 147080.	3.1	3
15434	Exploring the hydrogen evolution capabilities of earth-abundant ternary metal borides for neutral and alkaline water-splitting. <i>Electrochimica Acta</i> , 2020, 354, 136738.	2.6	30
15435	Effects of oxygen impurity concentration on the interfacial properties of Ta <sub>3</sub> N <sub>5</sub> /Ta <sub>5</sub> N <sub>6</sub> composite photoelectrode: A DFT calculation. <i>Applied Catalysis B: Environmental</i> , 2020, 278, 119296.	10.8	6
15436	Adsorption and decomposition properties of HMX on MgH <sub>2</sub> (111) surface: A first Principles study. <i>Chemical Physics</i> , 2020, 538, 110875.	0.9	5
15437	Chemical looping steam reforming of bio-oil for hydrogen-rich syngas production: Effect of doping on LaNi <sub>0.8</sub> Fe <sub>0.2</sub> O <sub>3</sub> perovskite. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 21123-21137.	3.8	38
15438	Highly efficient light-driven methane coupling under ambient conditions based on an integrated design of a photocatalytic system. <i>Green Chemistry</i> , 2020, 22, 4669-4675.	4.6	54
15439	Study on the adsorption of OH <sup>-</sup> and CaOH <sup>+</sup> on Fe (100) surface and their effect on passivation of steel bar: Experiments and DFT modelling. <i>Corrosion Science</i> , 2020, 174, 108804.	3.0	20
15440	First principles study of sarin nerve gas adsorption on graphene nanoribbon with single molecule resolution. <i>Materials Today: Proceedings</i> , 2020, 28, 1985-1989.	0.9	3
15441	Photocatalytic hydrogen production over Rh-loaded TiO <sub>2</sub> : What is the origin of hydrogen and how to achieve hydrogen production from water?. <i>Applied Catalysis B: Environmental</i> , 2020, 278, 119316.	10.8	73
15442	Lithium vacancy migration in Li <sub>2</sub> O <sub>2</sub> : From first principles studies. <i>Computational Materials Science</i> , 2020, 184, 109873.	1.4	6
15443	The effect of structural changes on the half metallic properties by using Tran Blaha modified Becke Johnson (TB_mBJ) method. <i>Journal of Magnetism and Magnetic Materials</i> , 2020, 514, 167198.	1.0	12
15444	Interfacial chemical binding and improved kinetics assisting stable aqueous Zn-MnO <sub>2</sub> batteries. <i>Materials Today Energy</i> , 2020, 17, 100475.	2.5	53
15445	First-principles investigations of intrinsic point defects and helium impurities in vanadium monocarbide. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2020, 479, 163-170.	0.6	3
15446	Optical spectra of 2D monolayers from time-dependent density functional theory. <i>Faraday Discussions</i> , 2020, 224, 467-482.	1.6	8
15447	Unleashing ultra-fast sodium ion storage mechanisms in interface-engineered monolayer MoS <sub>2</sub> /C interoverlapped superstructure with robust charge transfer networks. <i>Journal of Materials Chemistry A</i> , 2020, 8, 15002-15011.	5.2	26
15448	Origins of Unconventional <sup>13</sup> C Site Selectivity in Palladium-Catalyzed C(sp <sup>3</sup> )-H Activation and Arylation of Aliphatic Alcohols. <i>Organic Letters</i> , 2020, 22, 1464-1468.	2.4	18
15449	Investigation on <sup>13</sup> C to <sup>12</sup> C transition in an IN718G superalloy during heat treatment, using first principle. <i>Materials Characterization</i> , 2020, 162, 110168.	1.9	8



#	ARTICLE	IF	CITATIONS
15450	Pursuing the high-temperature quantum anomalous Hall effect in $\text{MnBi}$ heterostructures. <i>Physical Review B</i> , 2020, 101, .	1.2	2
15451	First-Principles Calculations of the Electronic Structure and Optical Properties of Yttrium-Doped ZnO Monolayer with Vacancy. <i>Materials</i> , 2020, 13, 724.	1.3	13
15452	Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials. <i>Chemical Reviews</i> , 2020, 120, 2215-2287.	23.0	231
15453	A new model for evaluating the diffraction elastic constants of WC-Co. <i>Materials Science and Technology</i> , 2020, 36, 334-341.	0.8	1
15454	On the existence of a local dipolar plasmon mode in doped small gold atomic arrays. <i>Physical Review B</i> , 2020, 101, .	1.1	2
15455	Effects of alloy compositions on hydrogen behaviors at a nickel grain boundary and a coherent twin boundary. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 10951-10961.	3.8	14
15456	Double-network hydrogel templated FeS/graphene with enhanced PMS activation performance: considering the effect of the template and iron species. <i>Environmental Science: Nano</i> , 2020, 7, 817-828.	2.2	19
15457	Mechanical, structural, and thermodynamic properties of TaC-ZrC ultra-high temperature ceramics using first principle methods. <i>Materials Research Express</i> , 2020, 7, 036502.	0.8	9
15458	Evaluating the exfoliation of two-dimensional materials with a Green's function surface model. <i>Physical Review B</i> , 2020, 101, .	1.1	32
15459	Surface oxygen vacancies promoted photodegradation of benzene on TiO <sub>2</sub> film. <i>Applied Surface Science</i> , 2020, 511, 145597.	3.1	60
15460	Photodecomposition properties of brominated flame retardants (BFRs). <i>Ecotoxicology and Environmental Safety</i> , 2020, 192, 110272.	2.9	15
15461	Effect of 3d heterometallic ions on the magnetic properties of azido-Cu(II) with isonicotinic acid coligands: A theoretical perspective. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 97, 107562.	1.3	11
15462	Evidence of Hydronium Formation in Water@Chabazite Zeolite Using Inelastic Neutron Scattering Experiments and ab Initio Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2020, 124, 5436-5443.	1.5	7
15463	Yolk@shell or yolk-in-shell nanocatalysts? A proof-of-concept study. <i>Journal of Materials Chemistry A</i> , 2020, 8, 10217-10225.	5.2	14
15464	An ab initio study on the effects of Na passivation on friction reduction of an iron oxide surface. <i>Journal of Applied Physics</i> , 2020, 127, 065305.	1.1	6
15465	Chemisorption characteristics of pyridine on Rh, Pd, Pt and Ni(111). <i>Electronic Structure</i> , 2020, 2, 015001.	1.0	2
15466	The Mode of Incorporation of As(-I) and Se(-I) in Natural Pyrite Revisited. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 379-390.	1.2	18
15467	High-efficiency direct methane conversion to oxygenates on a cerium dioxide nanowires supported rhodium single-atom catalyst. <i>Nature Communications</i> , 2020, 11, 954.	5.8	152

#	ARTICLE	IF	CITATIONS
15468	WIEN2k: An APW+lo program for calculating the properties of solids. Journal of Chemical Physics, 2020, 152, 074101.	1.2	1,185
15469	Symmetry transformation in Pd quasicrystals upon heating and hydrogenation. Computational Materials Science, 2020, 177, 109582.	1.4	0
15470	Gas adsorption and light interaction mechanism in phosphorene-based field-effect transistors. Physical Chemistry Chemical Physics, 2020, 22, 5949-5958.	1.3	14
15471	Quantum chemical and kinetic study of the $\text{CCl}_2 + \text{HCl} \rightarrow \text{CHCl}_3$ insertion reaction. Computational and Theoretical Chemistry, 2020, 1176, 112742.	1.1	4
15472	The Enantiomers of Trinorbornane and Derivatives Thereof. Helvetica Chimica Acta, 2020, 103, e2000019.	1.0	3
15473	MoS <sub>2</sub> -Supported Fe <sub>2</sub> Clusters Catalyzing Nitrogen Reduction Reaction to Produce Ammonia. Journal of Physical Chemistry C, 2020, 124, 6260-6266.	1.5	69
15474	Shedding light on the bonding situation of triangular and square heterometallic clusters: computational insight. New Journal of Chemistry, 2020, 44, 5079-5087.	1.4	2
15475	Modification of 1D TiO <sub>2</sub> nanowires with GaO <sub>x</sub> N <sub>y</sub> by atomic layer deposition for TiO <sub>2</sub> @GaO <sub>x</sub> N <sub>y</sub> core-shell nanowires with enhanced photoelectrochemical performance. Nanoscale, 2020, 12, 7159-7173.	2.8	22
15476	Emodin Scavenging of Superoxide Radical Includes $\pi\text{-}\pi$ Interaction. X-Ray Crystal Structure, Hydrodynamic Voltammetry and Theoretical Studies. Antioxidants, 2020, 9, 194.	2.2	17
15477	Interaction of nitric oxide with the (110) surface of cobalt spinel nanocubes – A comprehensive DFT, atomistic thermodynamic, IR and TPD account. Applied Surface Science, 2020, 513, 145835.	3.1	10
15478	Improving desorption temperature and kinetic properties in MgH <sub>2</sub> by vacancy defects: DFT study. International Journal of Hydrogen Energy, 2020, 45, 10806-10813.	3.8	23
15479	Co-doped graphene edge for enhanced N <sub>2</sub> -to-NH <sub>3</sub> conversion. Journal of Energy Chemistry, 2020, 48, 322-327.	7.1	40
15480	The effect of ionic liquid compounds on the exfoliation of the two-dimensional layer of molybdenum disulfide. Microporous and Mesoporous Materials, 2020, 299, 110127.	2.2	1
15481	Simple Automated Tool for Exchange-Correlation Functional Fitting. Journal of Physical Chemistry A, 2020, 124, 2700-2707.	1.1	5
15482	Large Enantiospecificity of Step-kink Metal Surfaces: Contributions from the Backbone and Side Chain of L-Amino Acids. Journal of Physical Chemistry C, 2020, 124, 742-748.	1.5	5
15483	Accelerating Atomic Catalyst Discovery by Theoretical Calculations – Machine Learning Strategy. Advanced Energy Materials, 2020, 10, 1903949.	10.2	99
15484	Unveiling dislocation characteristics in $N_3$ from stacking fault energy and ideal strength: A first-principles study via pure shear deformation. Physical Review B, 2020, 101, .	1.1	18
15485	Large optical polarizability causing positive effects on the birefringence of planar-triangular BO <sub>3</sub> groups in ternary borates. Dalton Transactions, 2020, 49, 3284-3292.	1.6	15

#	ARTICLE	IF	CITATIONS
15486	A density functional theory study on reduction-induced structural transformation of copper-oxide-based oxygen carrier. <i>Journal of Chemical Physics</i> , 2020, 152, 054709.	1.2	8
15487	An effective interface-regulating mechanism enabled by non-sacrificial additives for high-voltage nickel-rich cathode. <i>Journal of Power Sources</i> , 2020, 453, 227852.	4.0	26
15488	DFT study of Se and SeO <sub>2</sub> adsorbed on CaO (001) surface: Role of oxygen. <i>Applied Surface Science</i> , 2020, 510, 145488.	3.1	22
15489	CoSe <sub>2</sub> modified Se-decorated CdS nanowire Schottky heterojunctions for highly efficient photocatalytic hydrogen evolution. <i>Chemical Engineering Journal</i> , 2020, 389, 124431.	6.6	57
15490	Out-of-plane ionicity versus in-plane covalency interplay and electron-phonon coupling in MgB <sub>2</sub> superconductor. <i>Chinese Journal of Physics</i> , 2020, 64, 287-294.	2.0	1
15491	Self-supported MoS <sub>2</sub> /V <sub>2</sub> O <sub>3</sub> heterostructures as efficient hybrid catalysts for hydrogen evolution reaction. <i>Journal of Alloys and Compounds</i> , 2020, 827, 154262.	2.8	7
15492	Stable zigzag edges of transition-metal dichalcogenides with high catalytic activity for oxygen reduction. <i>Electrochimica Acta</i> , 2020, 338, 135865.	2.6	14
15493	A density functional theory study on the selective catalytic reduction of NO by NH <sub>3</sub> reactivity of $\lambda$ -Fe <sub>2</sub> O <sub>3</sub> (001) catalyst doped by Mn, Ti, Cr and Ni. <i>Fuel</i> , 2020, 267, 117147.	3.4	37
15494	Enthalpies and elastic properties of Ni-Co binary system by ab initio calculations and an energy comparison with the CALPHAD approach. <i>Materials Today Communications</i> , 2020, 23, 100905.	0.9	5
15495	Theoretical study of the structural, electronic and magnetic properties of equiatomic quaternary CoTcCrZ (Z=Si, Ge, P) Heusler alloys. <i>Chinese Journal of Physics</i> , 2020, 64, 123-137.	2.0	23
15496	Effect of external pressure on the structural stability, electronic structure, band gap engineering and optical properties of LiNbO <sub>3</sub> : An ab-initio calculation. <i>Materials Today Communications</i> , 2020, 23, 100919.	0.9	25
15497	Spherical Metal Oxides with High Tap Density as Sulfur Host to Enhance Cathode Volumetric Capacity for Lithium-Sulfur Battery. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 5909-5919.	4.0	76
15498	Cooperative Effect of Multiple Active Sites and Hierarchical Chemical Bonds in Metal-Organic Compounds for Improving Cathode Performance. <i>ACS Energy Letters</i> , 2020, 5, 477-485.	8.8	10
15499	Modeling amino-acid side chain infrared spectra: the case of carboxylic residues. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 3008-3016.	1.3	10
15500	Oxygen Reduction Reaction on a Cu <sup>II</sup> Complex of 3,5-Diamino-1,2,4-triazole: A DFT Approach. <i>ACS Omega</i> , 2020, 5, 1581-1585.	1.6	4
15501	Self-assembled CoTiO <sub>3</sub> nanorods with controllable oxygen vacancies for the efficient photochemical reduction of CO <sub>2</sub> to CO. <i>Catalysis Science and Technology</i> , 2020, 10, 2040-2046.	2.1	22
15502	Electronic and elastic properties of brownmillerite. <i>Materials Research Express</i> , 2020, 7, 015516.	0.8	5
15503	Influences of MgO(001) and TiO <sub>2</sub> (101) Supports on the Structures and Properties of Au Nanoclusters. <i>Catalysts</i> , 2020, 10, 16.	1.6	0

#	ARTICLE	IF	CITATIONS
15504	Functional group-directed self-installing doors in porous graphene: a theoretical study. <i>Journal of Materials Science</i> , 2020, 55, 5111-5122.	1.7	3
15505	A density functional theory study of CO <sub>2</sub> hydrogenation to methanol over Pd/TiO <sub>2</sub> catalyst: The role of interfacial site. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 6328-6340.	3.8	35
15506	A Periodic DFT Study of the Synergistic Mechanisms between Extraframework Aluminum Species and Brønsted Acid Sites in HY Zeolites. <i>Industrial &amp; Engineering Chemistry Research</i> , 2020, 59, 2736-2744.	1.8	7
15507	Nitrogen and sulfur dual-doped high-surface-area hollow carbon nanospheres for efficient CO <sub>2</sub> reduction. <i>Chinese Journal of Catalysis</i> , 2020, 41, 830-838.	6.9	49
15508	Efficient hydrogen production from ethanol steam reforming over layer-controlled graphene-encapsulated Ni catalysts. <i>Journal of Cleaner Production</i> , 2020, 252, 119907.	4.6	25
15509	New benzothiazole based copper(II) hydrazone Schiff base complexes for selective and environmentally friendly oxidation of benzylic alcohols: The importance of the bimetallic species tuned by the choice of the counterion. <i>Journal of Molecular Liquids</i> , 2020, 302, 112590.	2.3	19
15510	Isolated Molybdenum(VI) and Tungsten(VI) Oxide Species on Partly Dehydroxylated Silica: A Computational Perspective. <i>Journal of Physical Chemistry C</i> , 2020, 124, 3002-3013.	1.5	15
15511	Electronic and optical properties of monolayer MoS <sub>2</sub> under the influence of polyethyleneimine adsorption and pressure. <i>RSC Advances</i> , 2020, 10, 4201-4210.	1.7	17
15512	Dimerization of pentacyclopentacorannulene C <sub>30</sub> H <sub>10</sub> as a strategy to produce C <sub>60</sub> H <sub>20</sub> as a precursor for C <sub>60</sub> . <i>RSC Advances</i> , 2020, 10, 3689-3693.	1.7	3
15513	Structural, elastic, electronic and optical properties of lithium halides (LiF, LiCl, LiBr, and LiI): First-principle calculations. <i>Materials Chemistry and Physics</i> , 2020, 244, 122733.	2.0	22
15514	Integrated experimental and theoretical approach to probe the synergistic effect of ammonia in methanesulfonic acid reactions with small alkylamines. <i>Environmental Sciences: Processes and Impacts</i> , 2020, 22, 305-328.	1.7	18
15515	Exsolution of Cu nanoparticles in (LaSr) <sub>0.9</sub> Fe <sub>0.9</sub> Cu <sub>0.1</sub> O <sub>4</sub> Ruddlesden-Popper oxide as symmetrical electrode for solid oxide cells. <i>Applied Surface Science</i> , 2020, 511, 145525.	3.1	40
15516	Proximity enforced oxidative addition of a strong unpolar $\sigma$ -Si-Si bond at rhodium( $\sigma$ ). <i>Dalton Transactions</i> , 2020, 49, 1731-1735.	1.6	3
15517	Electrochemical Polarization Dependence of the Elastic and Electrostatic Driving Forces to Aliovalent Dopant Segregation on LaMnO <sub>3</sub> . <i>Journal of the American Chemical Society</i> , 2020, 142, 3548-3563.	6.6	50
15518	Effect of bromine deficiency on large elastic moduli of alpha-phase diisopropyl ammonium bromide ( $\pm$ -DIPAB) molecular crystals. <i>European Physical Journal B</i> , 2020, 93, 1.	0.6	4
15519	Room temperature ferromagnetism in carbon doped MoO <sub>3</sub> for spintronic applications: A DFT study. <i>Journal of Magnetism and Magnetic Materials</i> , 2020, 502, 166503.	1.0	19
15520	Achieving superior high-capacity batteries with the lightest Ti <sub>2</sub> C MXene anode by first-principles calculations: Overarching role of S-functionate (Ti <sub>2</sub> CS <sub>2</sub> ) and multivalent cations carrier. <i>Journal of Power Sources</i> , 2020, 451, 227791.	4.0	84
15521	Synthesis, DFT and kinetic studies of chromic S-methylidithione. <i>Polyhedron</i> , 2020, 179, 114386.	1.0	0

#	ARTICLE	IF	CITATIONS
15522	HCOOH dissociation over the Pd-decorated Cu bimetallic catalyst: The role of the Pd ensemble in determining the selectivity and activity. Applied Surface Science, 2020, 511, 145554.	3.1	18
15523	Abnormally Low Activation Energy in Cubic Na <sub>3</sub> SbS <sub>4</sub> Superionic Conductors. Chemistry of Materials, 2020, 32, 2264-2271.	3.2	35
15524	Exploring the origin of electrochemical performance of Cr-doped LiNi <sub>0.5</sub> Mn <sub>1.5</sub> O <sub>4</sub> . Physical Chemistry Chemical Physics, 2020, 22, 3831-3838.	1.3	13
15525	Atomically Dispersed Single Ni Site Catalysts for Nitrogen Reduction toward Electrochemical Ammonia Synthesis Using N <sub>2</sub> and H <sub>2</sub> O. Small Methods, 2020, 4, 1900821.	4.6	148
15526	Prediction of new thermodynamically stable ZnN <sub>2</sub> O <sub>3</sub> at high pressure. Physical Chemistry Chemical Physics, 2020, 22, 10941-10948.	1.3	1
15527	Conductivity and mixed conductivity of a novel dense diffusion barrier and the sensing properties of limiting current oxygen sensors. Dalton Transactions, 2020, 49, 6682-6692.	1.6	59
15528	Vacancy induced robust magnetism in graphene hexagonal-boron nitride in-plane hybrids with hexagonal shaped islands. Journal of Magnetism and Magnetic Materials, 2020, 502, 166530.	1.0	4
15529	Revealing the Interplay Between Covalent and Non-Covalent Interactions Driving the Adsorption of Monosubstituted Thiourea Derivatives on the Au(111) Surface. Journal of Physical Chemistry C, 2020, 124, 9924-9939.	1.5	2
15530	Interaction of C <sub>3</sub> ≡C <sub>5</sub> Alkenes with Zeolitic Brønsted Sites: $\pi$ -Complexes, Alkoxides, and Carbenium Ions in H-FER. Journal of Physical Chemistry C, 2020, 124, 10067-10078.	1.5	41
15531	The formation and effect of O-vacancies in doped TiO <sub>2</sub> . New Journal of Chemistry, 2020, 44, 8559-8571.	1.4	7
15532	Sensitivity of positrons at hydrogen storage sites in FeCr alloy containing vacancy and helium atom. International Journal of Hydrogen Energy, 2020, 45, 15571-15577.	3.8	15
15533	Manipulatable Interface Electric Field and Charge Transfer in a 2D/2D Heterojunction Photocatalyst via Oxygen Intercalation. Catalysts, 2020, 10, 469.	1.6	5
15534	Trends in transition metal solute diffusion in metals: The case of tungsten. Computational Materials Science, 2020, 179, 109638.	1.4	5
15535	An efficient mechanism for enhancing the thermoelectricity of twin graphene nanoribbons by introducing defects. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 122, 114160.	1.3	10
15536	Adsorption and Gas Sensing Properties of the Pt <sub>3</sub> -MoSe <sub>2</sub> Monolayer to SOF <sub>2</sub> and SO <sub>2</sub> F <sub>2</sub> . ACS Omega, 2020, 5, 7722-7728.	1.6	24
15537	In-situ resonant band engineering of solution-processed semiconductors generates high performance n-type thermoelectric nano-inks. Nature Communications, 2020, 11, 2069.	5.8	23
15538	Formation of Hexagonal PdSe <sub>2</sub> for Electronics and Catalysis. Journal of Physical Chemistry C, 2020, 124, 10935-10940.	1.5	16
15539	Hydrangea-Like CuS with Irreversible Amorphization Transition for High-Performance Sodium-Ion Storage. Advanced Science, 2020, 7, 1903279.	5.6	57

#	ARTICLE	IF	CITATIONS
15540	A new database and benchmark of the bond energies of noble gas-containing molecules. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26238.	1.0	6
15541	Theoretical study of the reduction in sensitivity of copper azide following encapsulation in carbon nanotubes. <i>Journal of Molecular Modeling</i> , 2020, 26, 90.	0.8	5
15542	Nanoscale All-Oxide-Heterostructured Bio-inspired Optoresponsive Nociceptor. <i>Nano-Micro Letters</i> , 2020, 12, 83.	14.4	33
15543	A single-phase ScTiZrHf high-entropy alloy with thermally stable hexagonal close-packed structure. <i>Intermetallics</i> , 2020, 122, 106802.	1.8	27
15544	Atomic-scale investigation on the structural evolution and deformation behaviors of Cu-Cr nanocrystalline alloys processed by high-pressure torsion. <i>Journal of Alloys and Compounds</i> , 2020, 832, 154994.	2.8	4
15545	Modulation of the electronic structure and magnetism performance of V-doped monolayer MoS <sub>2</sub> by strain engineering. <i>Journal of Physics and Chemistry of Solids</i> , 2020, 142, 109459.	1.9	9
15546	First-principles investigation of high pressure effect on structure, mechanical and electronic properties of Mo <sub>2</sub> ScAlC <sub>2</sub> . <i>Physica B: Condensed Matter</i> , 2020, 588, 412171.	1.3	1
15547	Structural, electronic, magnetic properties and critical behavior of the equiatomic quaternary Heusler alloy CoFeTiSn. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126453.	0.9	52
15548	First-principles computation of magnesium doped CaZrO <sub>3</sub> perovskite: A study of phase transformation, bandgap engineering and optical response for optoelectronic applications. <i>Solid State Communications</i> , 2020, 313, 113907.	0.9	29
15549	Construction of a Molecular Switch Based on Two Metastable States of Fullerene on Cu(111). <i>Journal of Physical Chemistry C</i> , 2020, 124, 11158-11164.	1.5	6
15550	Mechanism of Proton Conduction in Doped Barium Cerates: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 8024-8033.	1.5	22
15551	Separation Properties of Porous MoS <sub>2</sub> Membranes Decorated with Small Molecules. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 20096-20102.	4.0	18
15552	Insight into the Effects of Water on the Ethene to Aromatics Reaction with HZSM-5. <i>ACS Catalysis</i> , 2020, 10, 5288-5298.	5.5	39
15553	Morphology and reactivity of size-selected titanium oxide nanoclusters on Au(111). <i>Journal of Chemical Physics</i> , 2020, 152, 054714.	1.2	12
15554	Pressure-induced superconductivity in SnSb <sub>2</sub> Te <sub>4</sub> . <i>Journal of Physics Condensed Matter</i> , 2020, 32, 235901.	0.7	5
15555	Electronic Structure and Polarization of NaMgF <sub>3</sub> /NaCaF <sub>3</sub> Superlattices: Insight from First-Principles. <i>IOP Conference Series: Materials Science and Engineering</i> , 2020, 774, 012016.	0.3	0
15556	Experimental evidence of monolayer AlB <sub>2</sub> with symmetry-protected Dirac cones. <i>Physical Review B</i> , 2020, 101, .	1.1	20
15557	Dynamics Studies of O <sub>2</sub> Collision on Pt(111) Using a Global Potential Energy Surface. <i>Journal of Physical Chemistry C</i> , 2020, 124, 10573-10583.	1.5	7



#	ARTICLE	IF	CITATIONS
15558	Unraveling the single-atom electrocatalytic activity of transition metal-doped phosphorene. <i>Nanoscale Advances</i> , 2020, 2, 2410-2421.	2.2	23
15559	Using strain to alter the energy bands of the monolayer MoSe <sub>2</sub> : A systematic study covering both tensile and compressive states. <i>Applied Surface Science</i> , 2020, 521, 146398.	3.1	20
15560	Helium behaviors at Mn <sub>6</sub> Ni <sub>16</sub> Si <sub>7</sub> precipitate in $\hat{\Gamma}$ -Fe: Insights from ab initio modeling. <i>Computational Materials Science</i> , 2020, 181, 109735.	1.4	2
15561	First-principles calculation of interface binding strength and fracture performance of $\hat{\Gamma}$ -Al interface in Al-Mg-Si-Cu alloy. <i>Journal of Alloys and Compounds</i> , 2020, 830, 154515.	2.8	12
15562	First-principles study of bcc Fe-Cr-Si binary and ternary random alloys from special quasi-random structure. <i>Physica B: Condensed Matter</i> , 2020, 586, 412085.	1.3	8
15563	Can We Predict the Pressure Induced Phase Transition of Urea? Application of Quantum Molecular Dynamics. <i>Molecules</i> , 2020, 25, 1584.	1.7	13
15564	Effect of anomalous behavior of Be-doping on structural stability, bandgap and optical properties in comparison with Mg-doped BaZrO <sub>3</sub> perovskite: insights from DFT calculations. <i>Optical and Quantum Electronics</i> , 2020, 52, 1.	1.5	15
15565	Ab initio study of He, Ne, Ar, Kr incorporation in zirconium carbide. <i>Journal of Nuclear Materials</i> , 2020, 534, 152154.	1.3	2
15566	Metallic Ni <sub>3</sub> Mo <sub>3</sub> N Porous Microrods with Abundant Catalytic Sites as Efficient Electrocatalyst for Large Current Density and Superstability of Hydrogen Evolution Reaction and Water Splitting. <i>Applied Catalysis B: Environmental</i> , 2020, 272, 118956.	10.8	138
15567	Mechanism of formaldehyde advanced interaction and degradation on Fe <sub>3</sub> O <sub>4</sub> ( $1\hat{1}\bar{1}$ ) catalyst: Density functional theory study. <i>Applied Surface Science</i> , 2020, 520, 146324.	3.1	4
15568	Theoretical prediction of eliminating the buffer layer and achieving charge neutrality for epitaxial graphene on 6H-SiC(0001) via boron compound intercalations. <i>Carbon</i> , 2020, 161, 323-330.	5.4	3
15569	Ab initio phase diagram of WSe based on crystal structure prediction. <i>Computational Materials Science</i> , 2020, 181, 109732.	1.4	3
15570	Theoretical investigation of structural and mechanical stability of Mo <sub>2</sub> N. <i>Solid State Communications</i> , 2020, 314-315, 113919.	0.9	4
15571	Adsorption of Organic Acids and Phosphate to an Iron (Oxyhydr)oxide Mineral: A Combined Experimental and Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3249-3260.	1.1	9
15572	Optimization of Anticorrosive Zinc Coatings: Tuning the Adhesion of Zinc/Silica Contact by Interfacial Ternary Oxide Formation. <i>Journal of Physical Chemistry C</i> , 2020, 124, 9337-9344.	1.5	2
15573	Dynamic electrocatalyst with current-driven oxyhydroxide shell for rechargeable zinc-air battery. <i>Nature Communications</i> , 2020, 11, 1952.	5.8	185
15574	CO activation and methanation mechanism on hexagonal close-packed Co catalysts: effect of functionals, carbon deposition and surface structure. <i>Catalysis Science and Technology</i> , 2020, 10, 3387-3398.	2.1	5
15575	Nature inspired solid-liquid phase amphibious adhesive. <i>Soft Matter</i> , 2020, 16, 5854-5860.	1.2	3



#	ARTICLE	IF	CITATIONS
15576	Incoherent tilt grain boundaries stabilized by stacking faults and solute-cluster segregation: a case-study of an Mg-Gd alloy. <i>Materials Research Letters</i> , 2020, 8, 268-274.	4.1	11
15577	Hydrogen storage capacity on Li-decorated covalent organic framework-1: A first-principles study. <i>Materials Research Express</i> , 2020, 7, 035506.	0.8	19
15578	BaHgSn: A Dirac semimetal with surface hourglass fermions. <i>Physical Review B</i> , 2020, 101, .	1.1	6
15579	Plastic and Superionic Helium Ammonia Compounds under High Pressure and High Temperature. <i>Physical Review X</i> , 2020, 10, .	2.8	28
15580	Monolayer Honeycomb Borophene: A Promising Anode Material with a Record Capacity for Lithium-Ion and Sodium-Ion Batteries. <i>Journal of the Electrochemical Society</i> , 2020, 167, 090527.	1.3	28
15581	Elucidating the Molecular Basis of Avibactam-Mediated Inhibition of Class A $\beta$ -Lactamases. <i>Chemistry - A European Journal</i> , 2020, 26, 9639-9651.	1.7	9
15582	Rational design of an efficient descriptor for single-atom catalysts in the hydrogen evolution reaction. <i>Journal of Materials Chemistry A</i> , 2020, 8, 9202-9208.	5.2	41
15583	Probing the Geometric and Electronic Effects of Aluminum-Magnesium Clusters on Reactivity Toward Oxygen. <i>Journal of Cluster Science</i> , 2021, 32, 445-460.	1.7	2
15584	$\text{CO}_2$ reduction to acetic acid on the greigite $\text{Fe}_3\text{S}_4\{111\}$ surface. <i>Faraday Discussions</i> , 2021, 229, 35-49.	1.6	12
15585	First-principles study of electronic structure and optical properties of Er:Lu $2\text{O}_3$ . <i>Journal of Rare Earths</i> , 2021, 39, 453-459.	2.5	13
15586	Infrared spectra of surface nitrates: Revision of the current opinions based on the case study of ceria. <i>Journal of Catalysis</i> , 2021, 394, 245-258.	3.1	53
15587	Adsorption and diffusion of oxygen on metal surfaces studied by first-principle study: A review. <i>Journal of Materials Science and Technology</i> , 2021, 62, 180-194.	5.6	78
15588	Hf doping for enhancing the thermoelectric performance in layered $\text{Na}_{0.75}\text{CoO}_2$ . <i>Materials Today: Proceedings</i> , 2021, 42, 1542-1546.	0.9	1
15589	Stable high-entropy TiZrHfNbVCrMoMnFeCoNiAl Laves phase. <i>Scripta Materialia</i> , 2021, 193, 108-111.	2.6	21
15590	The active site of ethanol formation from syngas over $\text{Cu}_4$ cluster modified $\text{MoS}_2$ catalyst: A theoretical investigation. <i>Applied Surface Science</i> , 2021, 540, 148301.	3.1	4
15591	Li-decorated $\text{Al}_2\text{C}$ monolayer as a potential template for hydrogen storage: A first-principles perspective. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26528.	1.0	22
15592	Mechanism of the autothermal reforming reaction of methane on Pt(111) surfaces: A density functional theory study. <i>Applied Surface Science</i> , 2021, 539, 148288.	3.1	5
15593	Cementitious grain-boundary passivation for flexible perovskite solar cells with superior environmental stability and mechanical robustness. <i>Science Bulletin</i> , 2021, 66, 527-535.	4.3	54

#	ARTICLE	IF	CITATIONS
15594	Toxic volatile organic compounds sensing by Al <sub>2</sub> C monolayer: A first-principles outlook. <i>Journal of Hazardous Materials</i> , 2021, 403, 123600.	6.5	22
15595	Free-standing nanoporous NiMnFeMo alloy: An efficient non-precious metal electrocatalyst for water splitting. <i>Chemical Engineering Journal</i> , 2021, 404, 126530.	6.6	88
15596	Fitting elephants in the density functionals zoo: Statistical criteria for the evaluation of density functional theory methods as a suitable replacement for counting parameters. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26379.	1.0	7
15597	A highly efficient Fenton-like catalyst based on isolated diatomic Fe-Co anchored on N-doped porous carbon. <i>Chemical Engineering Journal</i> , 2021, 404, 126376.	6.6	143
15598	Structure and electronic properties of $\hat{\Gamma}$ -Bi <sub>2</sub> O <sub>3</sub> tuned by vacancy and doping: A first-principles study. <i>Ceramics International</i> , 2021, 47, 205-213.	2.3	8
15599	First-principles study of de-twinning in a FCC alloy. <i>Journal of Solid State Chemistry</i> , 2021, 293, 121765.	1.4	4
15600	Hydrogen storage on pristine and Li-decorated BC <sub>6</sub> N monolayer from first-principles insights. <i>Molecular Physics</i> , 2021, 119, e1827177.	0.8	24
15601	Theoretical investigation of CoTa <sub>2</sub> O <sub>6</sub> /graphene heterojunctions for oxygen evolution reaction. <i>Frontiers of Physics</i> , 2021, 16, 1.	2.4	6
15602	Efficient sulfur resistance of Fe, La and Ce doped hierarchically structured catalysts for low-temperature methanation integrated with electric internal heating. <i>Fuel</i> , 2021, 283, 118984.	3.4	31
15603	Two-dimensional transition metal borides as highly efficient N <sub>2</sub> fixation catalysts. <i>Applied Surface Science</i> , 2021, 536, 147742.	3.1	58
15604	Tuning structural-transformation temperature toward giant magnetocaloric effect in MnCoGe alloy: A theoretical study. <i>Journal of Alloys and Compounds</i> , 2021, 854, 157063.	2.8	8
15605	Bio-synthesised black $\hat{\Gamma}$ -Cr <sub>2</sub> O <sub>3</sub> nanoparticles; experimental analysis and density function theory calculations. <i>Journal of Alloys and Compounds</i> , 2021, 850, 156671.	2.8	24
15606	Density functional characterization of Bi-based photocatalysts: BiTaO <sub>4</sub> , Bi <sub>4</sub> Ta <sub>2</sub> O <sub>11</sub> and Bi <sub>7</sub> Ta <sub>3</sub> O <sub>18</sub> . <i>Materials Science in Semiconductor Processing</i> , 2021, 121, 105447.	1.9	33
15607	Two-dimensional WSe <sub>2</sub> /SnSe p-n junctions secure ultrahigh thermoelectric performance in n-type Pb/I Co-doped polycrystalline SnSe. <i>Materials Today Physics</i> , 2021, 16, 100306.	2.9	51
15608	Feasibility of Ca <sub>12</sub> O <sub>12</sub> Nanocluster in Lithium and Sodium Atom/Ion Batteries: DFT Study. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2021, 31, 1006-1014.	1.9	5
15609	Density functional theory study on the electronic and photocatalytic properties of different phases for Ba <sub>2</sub> BiTaO <sub>6</sub> . <i>Journal of Solid State Chemistry</i> , 2021, 293, 121790.	1.4	7
15610	Catalytic oxidation mechanism of NO to HNO <sub>3</sub> on TiO <sub>2</sub> (101) and (001) surfaces and the influence factors on NO removal: A DFT study. <i>Journal of Environmental Chemical Engineering</i> , 2021, 9, 104643.	3.3	6
15611	Highly active multivalent multielement catalysts derived from hierarchical porous TiNb <sub>2</sub> O <sub>7</sub> nanospheres for the reversible hydrogen storage of MgH <sub>2</sub> . <i>Nano Research</i> , 2021, 14, 148-156.	5.8	68

#	ARTICLE	IF	CITATIONS
15612	Catalytic activity of Ni <sub>3</sub> Mo surfaces for hydrogen evolution reaction: A density functional theory approach. <i>Applied Surface Science</i> , 2021, 537, 147894.	3.1	25
15613	The exploration of metal-free catalyst g-C <sub>3</sub> N <sub>4</sub> for NO degradation. <i>Journal of Hazardous Materials</i> , 2021, 404, 124153.	6.5	24
15614	Antioxidant studies by hydrodynamic voltammetry and DFT, quantitative analyses by HPLC-DAD of clovamide, a natural phenolic compound found in <i>Theobroma Cacao</i> L. beans. <i>Food Chemistry</i> , 2021, 341, 128260.	4.2	11
15615	New Icosahedra-based B <sub>4</sub> N phases by particle swarm optimization. <i>Journal of Alloys and Compounds</i> , 2021, 854, 157255.	2.8	5
15616	Two-dimensional transition metal phthalocyanine sheet as a promising electrocatalyst for nitric oxide reduction: a first principle study. <i>Environmental Science and Pollution Research</i> , 2021, 28, 7191-7199.	2.7	22
15617	Investigation on elastic properties and electronic structure of dilute Ir-based alloys by first-principles calculations. <i>Journal of Alloys and Compounds</i> , 2021, 850, 156548.	2.8	18
15618	ADP potential for the Au-Rh system and its application in element segregation of nanoparticles. <i>Computational Materials Science</i> , 2021, 186, 110002.	1.4	8
15619	Mechanistic investigations <i>via</i> DFT support the cooperative heterobimetallic C-H and O-H bond activation across Ta $\epsilon$ multiple bonds. <i>Dalton Transactions</i> , 2021, 50, 504-510.	1.6	13
15620	Artificial Intelligence and QM/MM with a Polarizable Reactive Force Field for Next-Generation Electrocatalysts. <i>Matter</i> , 2021, 4, 195-216.	5.0	29
15621	Control of the single atom/nanoparticle ratio in Pd/C catalysts to optimize the cooperative hydrogenation of alkenes. <i>Catalysis Science and Technology</i> , 2021, 11, 984-999.	2.1	30
15622	Rational design of Lithium-Sulfur battery cathodes based on differential Atom Electronegativity. <i>Energy Storage Materials</i> , 2021, 35, 577-585.	9.5	25
15623	Stuffed Tridymite Structures: Synthesis, Structure, Second Harmonic Generation, Optical, and Multiferroic Properties. <i>Chemistry - A European Journal</i> , 2021, 27, 1995-2008.	1.7	5
15624	Systematic investigations of the electron, phonon, elastic and thermal properties of monolayer so-MoS <sub>2</sub> by first-principles calculations. <i>Applied Surface Science</i> , 2021, 539, 148248.	3.1	11
15625	Insights into the catalytic activity of trimetallic Al/Zn/Cu surfaces for the water gas shift reaction. <i>Applied Surface Science</i> , 2021, 542, 148589.	3.1	12
15626	Theoretical insight into the oxidation mechanism of NO <sub>2</sub> and SO <sub>2</sub> on TiO <sub>2</sub> surface: The role of H <sub>2</sub> O, NH <sub>3</sub> and SO <sub>4</sub> <sup>2-</sup> . <i>Atmospheric Environment</i> , 2021, 246, 118068.	1.9	3
15627	First-principles survey on the pristine BC <sub>2</sub> N monolayer as a promising vehicle for delivery of $\beta$ -lapachone anticancer drug. <i>Journal of Molecular Liquids</i> , 2021, 321, 114917.	2.3	22
15628	Lithiophilic diffusion barrier layer on stainless steel mesh for dendrite suppression and stable lithium metal anode. <i>Applied Materials Today</i> , 2021, 22, 100896.	2.3	8
15629	Size effect in two-dimensional oxide-on-metal catalysts of CO oxidation and its connection to oxygen bonding: An experimental and theoretical approach. <i>Journal of Catalysis</i> , 2021, 393, 100-106.	3.1	7

#	ARTICLE	IF	CITATIONS
15630	From antiferromagnetic to ferromagnetic exchange in a family of phenoxido-bridged heterodinuclear Cu(II)-Mn(II) complexes: A magneto-structural theoretical study. <i>Polyhedron</i> , 2021, 194, 114955.	1.0	7
15631	Electronic, optical, vibrational and thermodynamic properties of phaBN structure: A first principles study. <i>Computational Materials Science</i> , 2021, 188, 110210.	1.4	11
15632	Elastic, mechanical, optical and magnetic properties of Ru <sub>2</sub> MnX (X=ÅNb, Ta, V) Heusler alloys. <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 523, 167614.	1.0	24
15633	Mechanism on catalytic cracking tar with CaO-based catalysts for hydrogen-rich gas by DFT and experiments. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 6522-6531.	3.8	8
15634	Facet-dependent gold nanocrystals for effective photothermal killing of bacteria. <i>Journal of Hazardous Materials</i> , 2021, 407, 124617.	6.5	94
15635	Atomically targeting NiFe LDH to create multivacancies for OER catalysis with a small organic anchor. <i>Nano Energy</i> , 2021, 81, 105606.	8.2	204
15636	Coercivity dependence of cation distribution in Co-based spinel: correlating theory and experiments. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 433-443.	3.0	5
15637	SAMPL7: Host-guest binding prediction by molecular dynamics and quantum mechanics. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 63-77.	1.3	9
15638	"Materials Studio" Simulation Study of the Adsorption and Polymerization Mechanism of Sodium Silicate on Active Silica Surface at Different Temperatures. <i>International Journal of Metalcasting</i> , 2021, 15, 1091-1098.	1.5	17
15639	Monolayer h-BN/C3B lateral heterostructures with promising electronic and optical properties: A first-principles study. <i>Chemical Physics</i> , 2021, 541, 111042.	0.9	2
15640	First principles investigation of the structural, elastic, electronic and vibrational properties of vanadium-based V <sub>3</sub> X (X = Fe, Co, and Ni) compounds. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 150, 109854.	1.9	4
15641	Ammonia electro-oxidation mechanism on the platinum (100) surface. <i>Catalysis Today</i> , 2021, 371, 50-57.	2.2	28
15642	Influence of deposition angle on structural, optical, and electronic properties of zinc sulfide nano-layers and optical relation between Kramers-Kronig and DFT calculations. <i>Journal of the Australian Ceramic Society</i> , 2021, 57, 237-248.	1.1	0
15643	Enabling selective, room-temperature gas detection using atomically dispersed Zn. <i>Sensors and Actuators B: Chemical</i> , 2021, 329, 129221.	4.0	10
15644	Low-Index Stoichiometric Surfaces of CuBiW <sub>2</sub> O <sub>8</sub> . <i>Surface Science</i> , 2021, 705, 121762.	0.8	1
15645	Insights into the Bond Behavior and Mechanical Properties of Hafnium Carbide under High Pressure and High Temperature. <i>Inorganic Chemistry</i> , 2021, 60, 515-524.	1.9	20
15646	Structural, electronic and magnetic properties of Mn doped CeO <sub>2</sub> : An ab-initio study. <i>Physica B: Condensed Matter</i> , 2021, 601, 412443.	1.3	20
15647	Molecular structure and mild steel/HCl corrosion inhibition of 4,5-Dicyanoimidazole: Vibrational, electrochemical and quantum mechanical calculations. <i>Journal of Molecular Structure</i> , 2021, 1230, 129647.	1.8	43

#	ARTICLE	IF	CITATIONS
15648	Novel structural phase and superconductivity of W-Te compounds under high pressures. Computational Materials Science, 2021, 188, 110222.	1.4	4
15649	Electronic modulation of oxygen evolution on metal doped NiFe layered double hydroxides. Journal of Colloid and Interface Science, 2021, 587, 385-392.	5.0	35
15650	Behavior of enrichment and migration path of Cu <sup>2+</sup> Ag <sup>+</sup> Pd <sup>2+</sup> Bi <sup>3+</sup> Pb in the recovery of waste multilayer ceramic capacitors by eutectic capture of copper. Journal of Cleaner Production, 2021, 287, 125469.	4.6	5
15651	Insight into enhanced thermoluminescence property of (Mg, Cu, Ag)-Doped LiF:A DFT study. Journal of Luminescence, 2021, 231, 117779.	1.5	8
15652	Band structure and absorption spectra of NH <sub>4</sub> XI <sub>3</sub> (X = Pb, Mg) based hybrid Perovskite for UV ray protector and electrochromic materials applications. Journal of Physics and Chemistry of Solids, 2021, 151, 109860.	1.9	4
15653	Designing new SRP density functionals including non-local vdW-DF2 correlation for H <sub>2</sub> + Cu(111) and their transferability to H <sub>2</sub> + Ag(111), Au(111) and Pt(111). Physical Chemistry Chemical Physics, 2021, 23, 7875-7901.	1.3	9
15654	Theoretical insights into the poisoning effect of Na and K on $\hat{\Gamma}$ -Fe <sub>2</sub> O <sub>3</sub> catalyst for selective catalytic reduction of NO with NH <sub>3</sub> . Applied Catalysis A: General, 2021, 610, 117968.	2.2	9
15655	Few-layered CuInP <sub>2</sub> S <sub>6</sub> nanosheet with sulfur vacancy boosting photocatalytic hydrogen evolution. CrystEngComm, 2021, 23, 591-598.	1.3	25
15656	Half metallicity and ferromagnetism of vanadium nitride nanoribbons: a first-principles study. Physical Chemistry Chemical Physics, 2021, 23, 1127-1138.	1.3	14
15657	Semiconducting properties of pyridyl appended linear dicarboxylate based coordination polymers: theoretical prediction via DFT study. Dalton Transactions, 2021, 50, 270-278.	1.6	8
15658	Tuning the Conduction Band Potential of Bi <sub>2</sub> Se <sub>3</sub> based Semiconductors Using a Combination of Organic Ligands. ChemSusChem, 2021, 14, 892-897.	3.6	7
15659	Investigation of Aviation Lubricant Aging under Engine Representative Conditions. Tribology Transactions, 2021, 64, 501-512.	1.1	7
15660	Sn <sub>2</sub> B <sub>5</sub> O <sub>9</sub> Br as an Outstanding Bifunctional Material with Strong Second Harmonic Generation Effect and Large Birefringence. Advanced Optical Materials, 2021, 9, 2001734.	3.6	49
15661	Mechanistic insights into efficient reversible hydrogen storage in ferrotitanium. International Journal of Hydrogen Energy, 2021, 46, 906-921.	3.8	11
15662	Enhanced N <sub>2</sub> affinity of 1T-MoS <sub>2</sub> with a unique pseudo-six-membered ring consisting of Na <sup>+</sup> Li <sup>+</sup> Sa <sup>+</sup> Mo <sup>+</sup> Sa <sup>+</sup> Mo for high ambient ammonia electrosynthesis performance. Journal of Materials Chemistry A, 2021, 9, 1230-1239.	5.2	44
15663	Theoretical investigation of the water splitting photocatalytic properties of pristine, Nb and V doped, and Nb-V co-doped (1 1 1) TaON nanosheets. Applied Surface Science, 2021, 541, 148572.	3.1	11
15664	Highly efficient H <sub>2</sub> generation over Cu <sub>2</sub> Se decorated Cd <sub>0.95</sub> Se <sub>0.05</sub> nanowires by photocatalytic water reduction. Chemical Engineering Journal, 2021, 409, 128157.	6.6	22
15665	Redox Performance of Cu-Doped Fe <sub>2</sub> O <sub>3</sub> /Al <sub>2</sub> O <sub>3</sub> as Oxygen Carriers for Chemical Looping Hydrogen Production. Energy & Fuels, 2021, 35, 626-635.	2.5	20

#	ARTICLE	IF	CITATIONS
15666	Identification of hydrogen species on Pt/Al <sub>2</sub> O <sub>3</sub> by <i>in situ</i> inelastic neutron scattering and their reactivity with ethylene. Catalysis Science and Technology, 2021, 11, 116-123.	2.1	6
15667	The mechanical properties of ice X with particular emphasis on its auxetic potential. Journal of Physics and Chemistry of Solids, 2021, 150, 109717.	1.9	8
15668	Analysis of an all-solid state nanobattery using molecular dynamics simulations under an external electric field. Physical Chemistry Chemical Physics, 2021, 23, 597-606.	1.3	16
15669	Modeling microsolvation clusters with electronic-structure calculations guided by analytical potentials and predictive machine learning techniques. Physical Chemistry Chemical Physics, 2021, 23, 1738-1749.	1.3	10
15670	Chemisorption, diffusion and permeation of hydrogen isotopes in bcc bulk cr and cr(100) surface: First-principles dft simulations. Journal of Nuclear Materials, 2021, 543, 152538.	1.3	11
15671	Assessment of multiscale hydrogen desorption models from (0001) Be surfaces. Journal of Nuclear Materials, 2021, 543, 152595.	1.3	7
15672	Growth mechanism and electronic and magnetic properties of AgnTi alloy clusters. Journal of Physics and Chemistry of Solids, 2021, 148, 109757.	1.9	20
15673	The first-principles study of the adsorption of Cu <sub>n</sub> ( <i>n</i> = 2-4) clusters on graphene doped with B. Molecular Physics, 2021, 119, .	0.8	6
15674	Structural, Electronic, and Magnetic Properties of 3d Transition Metal-Doped BP Nanotubes by First Principle Calculations. Journal of Superconductivity and Novel Magnetism, 2021, 34, 749-761.	0.8	1
15675	Stress-induced phase stabilization and transformation in equiatomic CuZr B19'™ martensite: A DFT study. Journal of Alloys and Compounds, 2021, 860, 157906.	2.8	2
15676	Chemiresistive I <sup>2</sup> -Tellurene nanosheets for detecting 2-Butanone and 2-Pentanone - a first-principles study. Materials Today Communications, 2021, 26, 101758.	0.9	9
15677	Interaction mechanism among CO, H <sub>2</sub> S and CuO oxygen carrier in chemical looping combustion: A density functional theory calculation study. Proceedings of the Combustion Institute, 2021, 38, 5281-5288.	2.4	11
15678	Glass-forming ability, structure and magnetocaloric effect in Gd-Sc-Co-Ni-Al bulk metallic glasses. Journal of Alloys and Compounds, 2021, 854, 157170.	2.8	13
15679	Structural, magnetic and electronic properties of Fe-Ga-Tb (0 ≤ x ≤ 1.85) alloys: Density-functional theory study. Journal of Alloys and Compounds, 2021, 857, 157540.	2.8	6
15680	Band gaps of the solar perovskites photovoltaic CsXCl <sub>3</sub> (X=Sn, Pb or Ge). Materials Science in Semiconductor Processing, 2021, 122, 105484.	1.9	67
15681	Effective carrier separation in zinc oxide and boron phosphide van der Waals heterostructure. Applied Surface Science, 2021, 535, 147825.	3.1	22
15682	Adsorption mechanism of decomposition gas of SF <sub>6</sub> circuit breaker on MOF-505 analogue. Vacuum, 2021, 183, 109816.	1.6	15
15683	Promotion of CO <sub>2</sub> methanation at low temperature over hydrotalcite-derived catalysts-effect of the tunable metal species and basicity. International Journal of Hydrogen Energy, 2021, 46, 518-530.	3.8	37



#	ARTICLE	IF	CITATIONS
15684	Role of Ta and Nb alloying elements on the viscosity of Fe-B-Si melts. <i>Journal of Molecular Liquids</i> , 2021, 323, 114636.	2.3	4
15685	Electronic structure, elastic, optical and thermal properties of chalcopyrite CuBY2 (B = In, Ga, In0.5) Tj ETQq1 1 0.784314 rgBT /Overlo	0.9	2
15686	Can density functional theory $\hat{\sim}$ Cope $\hat{\sim}$ ™ with highly fluxional shapeshifting molecules?. <i>Chemical Physics</i> , 2021, 540, 111013.	0.9	15
15687	Magnesium vacancies and hydrogen doping in MgH2 for improving gravimetric capacity and desorption temperature. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 2322-2329.	3.8	11
15688	The 1H and 13C chemical shifts of 5 $\hat{\sim}$ 5 lignin model dimers: An evaluation of DFT functionals. <i>Journal of Molecular Structure</i> , 2021, 1226, 129300.	1.8	5
15689	Revisiting surface chemistry in TiO2: A critical role of ionic passivation for pH-independent and anti-corrosive photoelectrochemical water oxidation. <i>Chemical Engineering Journal</i> , 2021, 407, 126929.	6.6	11
15690	Effect of calcium to silica ratio on the synthesis of calcium silicate hydrate in high alkaline desilication solution. <i>Journal of the American Ceramic Society</i> , 2021, 104, 535-547.	1.9	12
15691	Structural, Electronic, Magnetic, Elastic, Thermodynamic, and Thermoelectric Properties of the Half-Heusler RhFeX (with X = Ge, Sn) Compounds. <i>Journal of Superconductivity and Novel Magnetism</i> , 2021, 34, 211-225.	0.8	18
15692	DFT investigation of 2-mercaptobenzothiazole adsorption on model oxidized copper surfaces and relationship with corrosion inhibition. <i>Applied Surface Science</i> , 2021, 537, 147802.	3.1	47
15693	The philosophy of carbon: meso-entropy materials. <i>Faraday Discussions</i> , 2021, 227, 80-90.	1.6	10
15694	Time-Dependent Density Functional Theory Study of Copper(II) Oxo Active Sites for Methane-to-Methanol Conversion in Zeolites. <i>Inorganic Chemistry</i> , 2021, 60, 1149-1159.	1.9	10
15695	Silicon Nanowire Parameter Extraction Using DFT and Comparative Performance Analysis of SiNWFET and CNTFET Devices. <i>Semiconductors</i> , 2021, 55, 100-107.	0.2	3
15696	Electronic structure of solids and molecules. <i>Interface Science and Technology</i> , 2021, , 325-373.	1.6	2
15697	Surface oxidation for enhancing the hydrogen evolution reaction of metal nitrides: a theoretical study on vanadium nitride. <i>Materials Advances</i> , 0, , .	2.6	4
15698	Temperature and pressure-induced strains in anhydrous iron trifluoride polymorphs. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2825-2835.	1.3	1
15699	Tuning the electronic and magnetic properties of hydrogen saturated zigzag silicene nanoribbon doped with B atoms chain. <i>Ferroelectrics</i> , 2021, 570, 77-87.	0.3	0
15700	Improvement of alkali metal ion batteries <i>&lt;i&gt;via&lt;/i&gt;</i> interlayer engineering of anodes: from graphite to graphene. <i>Nanoscale</i> , 2021, 13, 12521-12533.	2.8	14
15701	Controlling the off-center positions of anions through thermodynamics and kinetics in flexible perovskite-like materials. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4491-4499.	1.3	2



#	ARTICLE	IF	CITATIONS
15721	Pressure-induced Na <sup>+</sup> Au compounds with novel structural units and unique charge transfer. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6455-6461.	1.3	8
15722	B <sub>3</sub> O <sub>3</sub> monolayer: an emerging 2D material for CO <sub>2</sub> capture. <i>New Journal of Chemistry</i> , 2021, 45, 15328-15335.	1.4	20
15723	An artificial hybrid interphase for an ultrahigh-rate and practical lithium metal anode. <i>Energy and Environmental Science</i> , 2021, 14, 4115-4124.	15.6	376
15724	Study of the structural and optoelectronic properties of dye solar cells based on phosphonic acid anchoring by DFT functionals. <i>New Journal of Chemistry</i> , 2021, 45, 2723-2733.	1.4	12
15725	A Simple Range-Separated Double-Hybrid Density Functional Theory for Excited States. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 927-942.	2.3	38
15726	Electronic Transport and Corrosion Mechanisms of Graphite-Like Nanocrystalline Carbon Films Used on Metallic Bipolar Plates in Proton-Exchange Membrane Fuel Cells. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 3825-3835.	4.0	21
15727	Critical benchmarking of popular composite thermochemistry models and density functional approximations on a probabilistically pruned benchmark dataset of formation enthalpies. <i>Journal of Chemical Physics</i> , 2021, 154, 044113.	1.2	10
15728	Disorder effects of vacancies on the electronic transport properties of realistic topological insulator nanoribbons: The case of bismuthene. <i>Physical Review Materials</i> , 2021, 5, .	0.9	14
15729	New graphane: inspiration from the structure correlation with phosphorene. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15302-15312.	1.3	2
15730	H4,4,4-graphyne with double Dirac points as high-efficiency bifunctional electrocatalysts for water splitting. <i>Journal of Materials Chemistry A</i> , 2021, 9, 4082-4090.	5.2	28
15731	Novel graphitic carbon nitride g-C <sub>9</sub> N <sub>10</sub> as a promising platform to design efficient photocatalysts for dinitrogen reduction to ammonia: the first-principles investigation. <i>Journal of Materials Chemistry A</i> , 2021, 9, 20615-20625.	5.2	21
15732	Boosting electrochemical nitrogen reduction reaction performance of two-dimensional Mo porphyrin monolayers <i>via</i> turning the coordination environment. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4178-4186.	1.3	6
15733	Sliver Doped Sodium Antimonate with Greatly Reduced the Band Gap for Efficiently Enhanced Photocatalytic Activities Under Visible Light (Experiment and DFT Calculation). <i>Materials Research</i> , 2021, 24, .	0.6	9
15734	A two-dimensional arsenene/g-C <sub>3</sub> N <sub>4</sub> van der Waals heterostructure: a highly efficient photocatalyst for water splitting. <i>Sustainable Energy and Fuels</i> , 2021, 5, 2249-2256.	2.5	20
15735	Computational exploration of heterometal substitution into the decaniobate framework, [Nb <sub>10</sub> O <sub>28</sub> ] <sup>6+</sup> . <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10402-10408.	1.3	0
15736	Novel ReSe semiconductor designed by structure prediction and phase diagram calculation. <i>Journal of Materials Science</i> , 2021, 56, 6878-6890.	1.7	2
15737	Curvature-induced bandgap reduction in TiO <sub>2</sub> double-walled nanotubes. <i>Journal of Applied Physics</i> , 2021, 129, 024303.	1.1	0
15738	Ab initio molecular dynamics of hydrogen on tungsten surfaces. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7919-7925.	1.3	1

#	ARTICLE	IF	CITATIONS
15739	Electron localization function implementation in the exact muffin-tin orbitals method. <i>Physical Review B</i> , 2021, 103, .	1.1	7
15740	First-Principles Investigation of Structural, Electronic, and Optical Response of SnZrO <sub>3</sub> with Al Inclusion for Optoelectronic Applications. <i>Physics of the Solid State</i> , 2021, 63, 134-140.	0.2	15
15741	An Ab-initio Study of Structural, Elastic, Electronic, Vibrational and Optical Properties of Semiconductor NaAlSi Compound for Optoelectronic Applications. <i>Advances in Material Research and Technology</i> , 2021, , 125-144.	0.3	0
15742	Single metal atom anchored on a CN monolayer as an excellent electrocatalyst for the nitrogen reduction reaction. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2658-2662.	1.3	10
15743	Adsorption of chloroquine and hydroxychloroquine as potential drugs for SARS-CoV-2 infection on BC <sub>3</sub> nanosheets: a DFT study. <i>New Journal of Chemistry</i> , 2021, 45, 17976-17983.	1.4	16
15744	Revised local atomic potential method for predicting properties of energetic materials. <i>Journal of Energetic Materials</i> , 0, , 1-17.	1.0	0
15745	Prediction of low-Z collinear and noncollinear antiferromagnetic compounds having momentum-dependent spin splitting even without spin-orbit coupling. <i>Physical Review Materials</i> , 2021, 5, .	0.9	64
15746	Screening of effective NRR electrocatalysts among the Si-based MSi <sub>2</sub> N <sub>4</sub> (M = Tj ETQq1 1.0.784314 rgBT /Qv 5.2 34	1.0	34
15747	Two-dimensional materials as a stabilized interphase for the solid-state electrolyte Li <sub>10</sub> GeP <sub>2</sub> S <sub>12</sub> in lithium metal batteries. <i>Journal of Materials Chemistry A</i> , 2021, 9, 4810-4821.	5.2	12
15748	A systematic computational investigation of the water splitting and N <sub>2</sub> reduction reaction performances of monolayer MBenes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6613-6622.	1.3	9
15749	Computational study of the staircase molecular conductivity of polyoxovanadates adsorbed on Au(111). <i>Dalton Transactions</i> , 2021, 50, 5540-5551.	1.6	7
15750	Iron-Nanoparticle-Loaded Nitrogen-Doped Carbon Nanotube/Carbon Sheet Composites Derived from MOF as Electrocatalysts for an Oxygen Reduction Reaction. <i>ACS Applied Nano Materials</i> , 2021, 4, 459-477.	2.4	35
15751	Self-cascade MoS <sub>2</sub> nanozymes for efficient intracellular antioxidation and hepatic fibrosis therapy. <i>Nanoscale</i> , 2021, 13, 12613-12622.	2.8	31
15752	A hierarchical Co <sub>3</sub> O <sub>4</sub> /CoS microbox heterostructure as a highly efficient bifunctional electrocatalyst for rechargeable Zn-air batteries. <i>Journal of Materials Chemistry A</i> , 2021, 9, 17344-17352.	5.2	40
15753	Monolayer 2D semiconducting tellurides for high-mobility electronics. <i>Physical Review Materials</i> , 2021, 5, .	0.9	13
15754	Factors controlling oxophilicity and carbophilicity of transition metals and main group metals. <i>Journal of Materials Chemistry A</i> , 2021, 9, 22325-22333.	5.2	16
15755	Triethanolamine interface modification of crystallized ZnO nanospheres enabling fast photocatalytic hazard-free treatment of Cr(vi) ions. <i>Nanotechnology Reviews</i> , 2021, 10, 847-856.	2.6	6
15756	Probing the formation and optical properties of Ti <sub>3</sub> +TiO <sub>2</sub> with (001) exposed crystal facet by ethanol-assisted fluorination. <i>New Journal of Chemistry</i> , 2021, 45, 12453-12463.	1.4	5

#	ARTICLE	IF	CITATIONS
15757	Theoretical insight into the deoxygenation molecular mechanism of butyric acid catalyzed by a Ni <sub>12</sub> P <sub>6</sub> cluster. <i>Catalysis Science and Technology</i> , 2021, 11, 6425-6437.	2.1	2
15759	BaTi(BO <sub>3</sub> ) <sub>2</sub> : an excellent birefringent material with highly coplanar isolated [BO <sub>3</sub> ] groups. <i>New Journal of Chemistry</i> , 2021, 45, 7065-7068.	1.4	7
15760	Complexes of divalent europium with dotp and dotpph. <i>New Journal of Chemistry</i> , 2021, 45, 5879-5889.	1.4	9
15761	How many shades of grey? On the proximity of density functional approximation to ab initio method via calculations of electric multipole moments. <i>Journal of Physics: Conference Series</i> , 2021, 1730, 012126.	0.3	0
15762	Ferromagnetic coupling in a dicopper(II) oxamate complex bridged by carboxylate groups. <i>CrystEngComm</i> , 2021, 23, 1885-1897.	1.3	7
15763	Reactions of ruthenium cyclopentadienyl precursor in the metal precursor pulse of Ru atomic layer deposition. <i>Journal of Materials Chemistry C</i> , 2021, 9, 2919-2932.	2.7	5
15764	Na <sub>1.7</sub> Li <sub>0.3</sub> BaZn <sub>7</sub> (TeO <sub>6</sub> ) <sub>3</sub> : The first mixed alkali metal and alkaline earth metal zinc tellurate. <i>Inorganic Chemistry Communication</i> , 2021, 123, 108363.	1.8	0
15765	Mechanism of Pd-catalysed C(sp <sup>3</sup> )–H arylation of thioethers with Ag(I) additives. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 6766-6770.	1.5	3
15766	Charge pumping enabling Co–NC to outperform benchmark Pt catalyst for pH-universal hydrogen evolution reaction. <i>Energy and Environmental Science</i> , 2021, 14, 3160-3173.	15.6	81
15767	Robust half-metallicity in CoZrMnZ (Z = P, As and Sb) quaternary Heusler alloys. <i>Philosophical Magazine</i> , 2021, 101, 892-904.	0.7	4
15768	Catalytic mechanism for the isomerization of glucose into fructose over an aluminium-MCM-41 framework. <i>Catalysis Science and Technology</i> , 2021, 11, 1537-1543.	2.1	8
15769	First-principles Study on Nanoscale Tungsten Oxide: a Review. <i>Wuji Cailiao Xuebao/Journal of Inorganic Materials</i> , 2021, 36, 1125.	0.6	4
15770	First-principles-based kinetic Monte Carlo simulations of CO oxidation on catalytic Au(110) and Ag(110) surfaces. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 14037-14050.	1.3	7
15771	Heterovalent cations substitution to design asymmetric chalcogenides with promising nonlinear optical performances. <i>Journal of Materials Chemistry C</i> , 2021, 9, 8659-8665.	2.7	25
15772	Insights into the Mechanism of Low-Valent Cobalt-Catalyzed C–H Activation. <i>ACS Catalysis</i> , 2021, 11, 1505-1515.	5.5	32
15773	Hydrogen induced interface engineering in Fe <sub>2</sub> O <sub>3</sub> –TiO <sub>2</sub> heterostructures for efficient charge separation for solar-driven water oxidation in photoelectrochemical cells. <i>RSC Advances</i> , 2021, 11, 4297-4307.	1.7	16
15774	Computational approaches to dissociative chemisorption on metals: towards chemical accuracy. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8962-9048.	1.3	47
15775	Ultrasonic Plasma Engineering Toward Facile Synthesis of Single-Atom M-N <sub>4</sub> /N-Doped Carbon (M = Fe, Tj ETQq1 1 0.784314 13, 60.	14.4	63

#	ARTICLE	IF	CITATIONS
15776	Crystal structures and superconductivity of lithium and fluorine implanted gold hydrides under high pressures. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21544-21553.	1.3	3
15777	Balancing Stability and Li-ion Conductivity of Li <sub>10</sub> SiP <sub>2</sub> O <sub>12</sub> for Solid-State Electrolytes with Assistance of body-centered cubic oxygen framework. <i>Journal of Materials Chemistry A</i> , 0, , .	5.2	2
15778	Structural Origins of Elastic and 2D Plastic Flexibility of Molecular Crystals Investigated with Two Polymorphs of Conformationally Rigid Coumarin. <i>Chemistry of Materials</i> , 2021, 33, 1053-1060.	3.2	50
15779	Copper confined in vesicle-like BCN cavities promotes electrochemical reduction of nitrate to ammonia in water. <i>Journal of Materials Chemistry A</i> , 2021, 9, 23675-23686.	5.2	42
15780	Replacing hybrid density functional theory: motivation and recent advances. <i>Chemical Society Reviews</i> , 2021, 50, 8470-8495.	18.7	80
15781	Halogenated Ti <sub>3</sub> C <sub>2</sub> MXenes with Electrochemically Active Terminals for High-Performance Zinc Ion Batteries. <i>ACS Nano</i> , 2021, 15, 1077-1085.	7.3	183
15782	Origins of ligand-controlled diastereoselectivity in dirhodium-catalysed direct amination of aliphatic C(sp <sup>3</sup> )-H bonds. <i>Catalysis Science and Technology</i> , 2021, 11, 6960-6964.	2.1	2
15783	Ag (111) surface for ambient electrolysis of nitrogen to ammonia. <i>Journal of Molecular Modeling</i> , 2021, 27, 38.	0.8	15
15784	Predicting the structure and NMR coupling constant <sup>1</sup> J( <i>i</i> ) of XeF <sub>6</sub> using quantum mechanics methods. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7240-7246.	1.3	2
15785	A new acentric borate-nitrate Cs <sub>3</sub> B <sub>8</sub> O <sub>13</sub> (NO <sub>3</sub> ) with interpenetrating porous 3D covalent and ionic lattices. <i>Dalton Transactions</i> , 2021, 50, 8676-8679.	1.6	4
15786	Defect structures of sodium and chloride co-substituted hydroxyapatite and its osseointegration capacity. <i>Journal of Materials Science</i> , 2021, 56, 5493-5508.	1.7	4
15787	First-principles calculations of hybrid inorganic-organic interfaces: from state-of-the-art to best practice. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8132-8180.	1.3	36
15788	Assessment of the performance of DFT functionals in the fulfillment of off-diagonal hypervirial relationships. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15268-15274.	1.3	13
15789	Nonadiabatic couplings from a variational excited state method based on constrained DFT. <i>Journal of Chemical Physics</i> , 2021, 154, 014110.	1.2	6
15790	Terahertz Spectroscopy and Molecular Modeling of Barbituric Acid. <i>Journal of Applied Spectroscopy</i> , 2021, 87, 1000-1005.	0.3	1
15791	Theoretical Combined Experimental Study of Unique He Behaviors in High-Entropy Alloys. <i>Inorganic Chemistry</i> , 2021, 60, 1388-1397.	1.9	12
15792	Gas-sensing performance of BC <sub>3</sub> nanotubes for detecting poisonous cyanogen gas: a periodic DFT approach. <i>New Journal of Chemistry</i> , 2021, 45, 11574-11584.	1.4	14
15793	Novel structural phases and the properties of LaX (X = P, As) under high pressure: first-principles study. <i>RSC Advances</i> , 2021, 11, 3058-3070.	1.7	4



#	ARTICLE	IF	CITATIONS
15794	Insight into the charging&#x2014;discharging of magnetite electrodes: <i>in situ</i> XAS and DFT study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6051-6061.	1.3	5
15795	Theoretical study on the Y-Ba-H hydrides at high pressure. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2021, 390, 127109.	0.9	7
15796	Quantum chemistry study of SCR-NH <sub>3</sub> nitric oxide reduction on Ce-doped $\gamma$ -Fe <sub>2</sub> O <sub>3</sub> catalyst surface. <i>Molecular Catalysis</i> , 2021, 502, 111373.	1.0	11
15797	Alteration impact of electronic properties of c-SrTiO <sub>3</sub> on optical response due to Ca inclusion: A DFT study. <i>Physica B: Condensed Matter</i> , 2021, 602, 412553.	1.3	9
15798	High-Throughput Screening of Synergistic Transition Metal Dual-Atom Catalysts for Efficient Nitrogen Fixation. <i>Nano Letters</i> , 2021, 21, 1871-1878.	4.5	223
15799	Improving the stability of perovskite by covering graphene on <i>ABX<sub>3</sub></i> surface. <i>International Journal of Energy Research</i> , 2021, 45, 10808-10820.	2.2	7
15800	First-Principles Investigation on Electrochemical Performance of Na-Doped LiNi <sub>1/3</sub> Co <sub>1/3</sub> Mn <sub>1/3</sub> O <sub>2</sub> . <i>Frontiers in Physics</i> , 2021, 8, .	1.0	13
15801	Tuning of the Optical Properties of Monolayer Blue Phosphorene. <i>Plasmonics</i> , 2021, 16, 1213-1221.	1.8	4
15802	Structural and electronic properties of realistic two-dimensional amorphous topological insulators. <i>2D Materials</i> , 2021, 8, 025032.	2.0	16
15803	Examining Experimental Raman Mode Behavior in Mono- and Bilayer 2H-TaSe <sub>2</sub> via Density Functional Theory: Implications for Quantum Information Science. <i>ACS Applied Nano Materials</i> , 2021, 4, 1810-1816.	2.4	2
15804	A Nanometer-Sized Graphite/Boron-Doped Diamond Electrochemical Sensor for Sensitive Detection of Acetaminophen. <i>ACS Omega</i> , 2021, 6, 6326-6334.	1.6	30
15805	Design of Lewis Pairs via Interface Engineering of Oxide&#x2014;Metal Composite Catalyst for Water Activation. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 1443-1452.	2.1	18
15806	Half-Metallicity and Magnetism in the Full Heusler Alloy Fe <sub>2</sub> MnSn with L2 <sub>1</sub> and XA Stability Ordering Phases. <i>Journal of Low Temperature Physics</i> , 2021, 202, 343-359.	0.6	52
15807	The nuts and bolts of core-hole constrained <i>ab initio</i> simulation for K-shell x-ray photoemission and absorption spectra. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 154005.	0.7	20
15808	Catalytic mechanism of oxygen reduction on two types of <i>AB<sub>4</sub></i> @graphene : A density functional study. <i>International Journal of Energy Research</i> , 2021, 45, 10858-10868.	2.2	6
15809	Characterization of Li&#x2014;S Batteries Using Laboratory Sulfur X-ray Emission Spectroscopy. <i>ACS Applied Energy Materials</i> , 2021, 4, 2357-2364.	2.5	8
15810	First principles study of electronic, elastic, optical and magnetic properties of Rh <sub>2</sub> MnX (X = Ti, Hf, Sc). <i>Journal of Applied Physics</i> , 2021, 124, 104301.	1.0	14
15811	Quantitative characterisation of the ring normal modes. Pyridine as a study case. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 119026.	2.0	11

#	ARTICLE	IF	CITATIONS
15812	A computational insight into the relationship between side chain IR line shapes and local environment in fibril-like structures. <i>Journal of Chemical Physics</i> , 2021, 154, 084105.	1.2	1
15813	Precipitation of dopants on acceptor-doped $\text{LaMnO}_3$ revealed by defect chemistry from first principles. <i>Journal of Chemical Physics</i> , 2021, 154, 064702.	1.2	4
15814	Morphology evolution of $\text{SmCo}_x$ permanent magnetic nanoparticles. <i>Science China: Physics, Mechanics and Astronomy</i> , 2021, 64, 1.	2.0	2
15815	Investigation of fluorinated ether-containing electrolytes for high energy-density nickel-rich $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}$ . <i>International Journal of Energy Research</i> , 2021, 45, 9936-9947.	2.2	4
15816	Atomistic Imaging of Competition between Surface Diffusion and Phase Transition during the Intermetallic Formation of Faceted Particles. <i>ACS Nano</i> , 2021, 15, 5284-5293.	7.3	17
15817	Finding Short-Wavelength Birefringent Crystals with Large Optical Anisotropy Activated by $\pi$ -Conjugated $[\text{C}(\text{NH}_2)_3]$ Units. <i>Crystal Growth and Design</i> , 2021, 21, 1869-1877.	1.4	15
15818	Li interaction-induced phase transition from black to blue phosphorene. <i>Physical Review Materials</i> , 2021, 5, .	0.9	11
15819	Elucidating the origin of selective dehydrogenation of propane on $\gamma$ -alumina under $\text{H}_2\text{S}$ treatment and co-feed. <i>Journal of Catalysis</i> , 2021, 394, 142-156.	3.1	21
15821	The Activation and Reduction of $\text{N}_2$ by Single/Double-Atom Electrocatalysts: A First-Principle Study. <i>ChemistrySelect</i> , 2021, 6, 1787-1794.	0.7	6
15822	First-principles study of hydrogen trapping and diffusion at grain boundaries in $\gamma$ -Fe. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 7589-7600.	3.8	29
15823	Data-Driven Discovery and Understanding of Ultrahigh-Modulus Crystals. <i>Chemistry of Materials</i> , 2021, 33, 1276-1284.	3.2	16
15824	Metal-Organic Framework-Derived Hierarchical $\text{MnO}/\text{Co}$ with Oxygen Vacancies toward Elevated-Temperature Li-Ion Battery. <i>ACS Nano</i> , 2021, 15, 4594-4607.	7.3	121
15825	Do Secondary Electrostatic Interactions Influence Multiple Dihydrogen Bonds? A 2D Array on an Amine-Borane Azacoronand: Theoretical Studies and Synthesis. <i>ChemPhysChem</i> , 2021, 22, 593-605.	1.0	9
15826	Effect of trichloroacetic acid on iron oxidation: Implications on the control of DBPs and deposits in drinking water. <i>Water Research</i> , 2021, 189, 116632.	5.3	13
15827	Constructing Surface Plasmon Resonance on $\text{Bi}_2\text{WO}_6$ to Boost High-Selective $\text{CO}_2$ Reduction for Methane. <i>ACS Nano</i> , 2021, 15, 3529-3539.	7.3	113
15828	-block elemental-atom-embedded $\text{C}_3$	0.9	0
15829	The sequential activation of $\text{H}_2$ and $\text{N}_2$ mediated by the gas-phase $\text{Sc}_3\text{N}^+$ clusters: Formation of amido unit. <i>Journal of Chemical Physics</i> , 2021, 154, 054307.	1.2	11
15830	Relative stability of Cu, Ag, and Pt at high pressures and temperatures from <i>ab initio</i> calculations. <i>Physical Review B</i> , 2021, 103, .	1.1	14

#	ARTICLE	IF	CITATIONS
15831	Ammonia deep chemical looping combustion on perfect and reduced $\text{Fe}_2\text{O}_3$ : A theoretical account. International Journal of Energy Research, 2021, 45, 10562-10571.	2.2	3
15832	IrN <sub>4</sub> and IrN <sub>7</sub> as potential high-energy-density materials. Journal of Chemical Physics, 2021, 154, 054706.	1.2	11
15833	Thermodynamic and Kinetic Competition between C-H and O-H Bond Formation Pathways during Electrochemical Reduction of CO on Copper Electrodes. ACS Catalysis, 2021, 11, 2422-2434.	5.5	20
15834	First-principles study of co-adsorption behavior of $\text{O}_2$ and $\text{CO}_2$ molecules on $\text{f-Pu}(100)$ surface. Chinese Physics B, 2021, 30, 026601.	0.7	5
15835	Platinum supported on early transition metal carbides: Efficient electrocatalysts for methanol electro-oxidation reaction in alkaline electrolyte. Chemical Engineering Journal, 2021, 406, 126670.	6.6	28
15836	Modeling the structure of the $\text{TiO}_2(\text{rutile})/\text{SrTiO}_3$ heterointerface. IOP Conference Series: Materials Science and Engineering, 2021, 1093, 012031.	0.3	2
15837	Two-dimensional Dirac dispersion in the layered compound $\text{BaCdSb}$ . Physical Review B, 2021, 103, .	1.1	2
15838	First-principles study on band gaps and transport properties of van der Waals $\text{WSe}_2/\text{WTe}_2$ heterostructure. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2021, 76, 361-370.	0.7	5
15839	Connecting experimental synthetic variables with the microstructure and electronic properties of doped ferroelectric perovskites for solar cell applications using high-throughput frameworks. Acta Materialia, 2021, 204, 116466.	3.8	4
15840	Chemosensing nature of black phosphorene nanotube towards $\text{C}_{14}\text{H}_9\text{Cl}_5$ and $\text{C}_{10}\text{H}_5\text{Cl}_7$ molecules – A first-principles insight. Computational and Theoretical Chemistry, 2021, 1196, 113109.	1.1	11
15841	Elucidating the Structure of Bimetallic $\text{NiW}/\text{SiO}_2$ Catalysts and Its Consequences on Selective Deoxygenation of <i>m</i> -Cresol to Toluene. ACS Catalysis, 2021, 11, 2935-2948.	5.5	32
15842	Gd-Ru Nanoparticles Supported on $\text{Zr}_{0.5}\text{Ce}_{0.5}\text{O}_2$ Nanorods for Dry Methane Reforming. ACS Applied Nano Materials, 2021, 4, 2547-2557.	2.4	13
15843	Electronic and Transport Properties of Bilayer Phosphorene Nanojunction: Effect of Paired Substitution Doping. ACS Applied Electronic Materials, 2021, 3, 733-742.	2.0	13
15844	Experimental and computational studies of an antiplasmodial derivative of allantoin; antimycobacterial essential oil from Cordia batesii WERNHAM (Boraginaceae). BMC Chemistry, 2021, 15, 15.	1.6	3
15845	&lt;i>Ab Initio&lt;/i> Study of Helium in Tantalum: Interaction, Migration, and Clustering with Helium and Vacancies. Materials Science Forum, 0, 1024, 121-126.	0.3	0
15846	Hydrogen effect on $\text{CoRhMnSi}$ and thermoelectric properties of $\text{CoRhMnSi}$ [001] film. International Journal of Energy Research, 2021, 45, 13055-13070.	2.2	8
15847	Vibrational State-to-State Scattering of Water from $\text{Cu}(111)$ : Comparison of Quantum and Quasiclassical Methods with Normal Mode and Adiabatic Switching Sampling. Journal of Physical Chemistry C, 2021, 125, 4995-5005.	1.5	5
15848	Density of $\text{Fe-Ni-C}$ Liquids at High Pressures and Implications for Liquid Cores of Earth and the Moon. Journal of Geophysical Research: Solid Earth, 2021, 126, e2020JB021089.	1.4	5

#	ARTICLE	IF	CITATIONS
15849	Pragmatic Improvement of Magnetic Exchange Couplings from Subsystem Density-Functional Theory through Orthogonalization of Subsystem Orbitals. <i>Journal of Physical Chemistry C</i> , 2021, 125, 6176-6188.	1.5	3
15850	High-throughput screening of transition metal single-atom catalyst anchored on Janus MoSSe basal plane for hydrogen evolution reaction. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 10337-10345.	3.8	30
15851	DFT study of the interaction between carbon monoxide and Rh-Cu bimetallic nanoclusters. <i>Materials Today Communications</i> , 2021, 26, 102013.	0.9	5
15852	Activating two-dimensional Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> -MXene with single-atom cobalt for efficient CO <sub>2</sub> photoreduction. <i>Cell Reports Physical Science</i> , 2021, 2, 100371.	2.8	80
15853	DFT and TDDFT studies of the new inorganic perovskite CsPbI <sub>3</sub> for solar cell applications. <i>Chemical Physics Letters</i> , 2021, 766, 138347.	1.2	68
15854	Density Functional Theory Studies on Sulfurâ€“Polyacrylonitrile as a Cathode Host Material for Lithiumâ€“Sulfur Batteries. <i>ACS Omega</i> , 2021, 6, 9700-9708.	1.6	11
15855	Variation in electronic and optical responses due to phase transformation of SrZrO <sub>3</sub> from cubic to orthorhombic under high pressure: a computational insight. <i>Indian Journal of Physics</i> , 2022, 96, 1-9.	0.9	10
15856	Atomistic insights into lithium adsorption and migration on phosphorusâ€“doped graphene. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26659.	1.0	6
15857	Accurate Prediction of MÃ“ssbauer Hyperfine Parameters in Bis-Axially Coordinated Iron(II) Phthalocyanines Using Density Functional Theory Calculations: A Story of a Single Orbital Revealed by Natural Bond Orbital Analysis. <i>Inorganic Chemistry</i> , 2021, 60, 3690-3706.	1.9	13
15858	Polarization-resolved Raman spectra of $\hat{I}\pm$ -PtO <sub>2</sub> *. <i>Chinese Physics B</i> , 2021, 30, 047102.	0.7	2
15859	First-principles study on growth mechanism of TiN on MgO (1 0 0) and (1 1 0) surfaces. <i>Computational Materials Science</i> , 2021, 189, 110257.	1.4	5
15860	Effects of surface spatial structures and electronic properties of chalcopyrite and pyrite on Z-200 selectivity. <i>Minerals Engineering</i> , 2021, 163, 106803.	1.8	28
15861	Shock-induced polymorphic transitions of $F_2$ up to 1 TPa and their implications for the universal behavior of shocked compounds. <i>Physical Review B</i> , 2021, 103, .	1.1	2
15862	Structural, optical, and electronic characteristics of non-stoichiometric nanocadmium sulfide. <i>Journal of Materials Science: Materials in Electronics</i> , 2021, 32, 9517-9530.	1.1	7
15863	Monolayer Fe <sub>3</sub> GeX <sub>2</sub> (X = S, Se, and Te) as Highly Efficient Electrocatalysts for Lithiumâ€“Sulfur Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 11845-11851.	4.0	45
15864	Pressure effect of the mechanical, electronics and thermodynamic properties of Mgâ€“B compounds A first-principles investigations. <i>Scientific Reports</i> , 2021, 11, 6096.	1.6	5
15865	Understanding contact electrification at liquidâ€“solid interfaces from surface electronic structure. <i>Nature Communications</i> , 2021, 12, 1752.	5.8	56
15866	Perovskite Light-Emitting Diodes with Near Unit Internal Quantum Efficiency at Low Temperatures. <i>Advanced Materials</i> , 2021, 33, e2006302.	11.1	16

#	ARTICLE	IF	CITATIONS
15867	Self-Healable Recoverable Mechanically Induced Instant Luminescence from Cr <sup>3+</sup> -Doped LiGa <sub>5</sub> O <sub>8</sub> . <i>Advanced Functional Materials</i> , 2021, 31, 2010685.	7.8	84
15868	Interaction studies of nitrotoluene and toluidine molecules on novel square-octagon arsenene nanotubes based on DFT method. <i>Journal of Molecular Liquids</i> , 2021, 325, 115260.	2.3	18
15869	Understanding heterogeneous metal-mediated interfacial enhancement mechanisms in graphene-embedded copper matrix composites. <i>Applied Surface Science</i> , 2021, 541, 148524.	3.1	11
15870	Nanodevices engineering and spin transport properties of MnBi <sub>2</sub> Te <sub>4</sub> monolayer. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	53
15871	Unraveling the Control Mechanism of Carbon Nanotubes on the Oxygen Reduction Reaction and Product Growth Behavior in Lithium-Air Batteries. <i>ACS Applied Energy Materials</i> , 2021, 4, 2148-2157.	2.5	6
15872	Anionic Activation of CO <sub>2</sub> via (M <sub>n</sub> ) <sup>+</sup> -CO <sub>2</sub> <sup>-</sup> Complex on Magic-Numbered Anionic Coinage Metal Clusters M <sub>n</sub> <sup>+</sup> (M =) Tj ETQq1 1 0.784314 rg	1.0	1
15873	Effects of thermal expansion and degeneracy on ambipolar carrier mobility of non-peripherally hexyl-substituted phthalocyanine. <i>Applied Physics Express</i> , 2021, 14, 041001.	1.1	0
15874	Single-metal-atom site with high-spin state embedded in defective BN nanosheet promotes electrocatalytic nitrogen reduction. <i>Nano Research</i> , 2021, 14, 4211-4219.	5.8	55
15875	Adsorption and cracking of propane by zeolites of different pore size. <i>Journal of Catalysis</i> , 2021, 395, 117-128.	3.1	29
15876	Enabling a Stable Room-Temperature Sodium-Sulfur Battery Cathode by Building Heterostructures in Multichannel Carbon Fibers. <i>ACS Nano</i> , 2021, 15, 5639-5648.	7.3	70
15877	Correlation between mixing enthalpy and structural order in liquid Mg-Si system. <i>Transactions of Nonferrous Metals Society of China</i> , 2021, 31, 853-864.	1.7	1
15878	Overcoming Pd-TiO <sub>2</sub> Deactivation during H <sub>2</sub> Production from Photoreforming Using Cu@Pd Nanoparticles Supported on TiO <sub>2</sub> . <i>ACS Applied Nano Materials</i> , 2021, 4, 3204-3219.	2.4	17
15879	Interfacial Polarization and Ionic Structure at the Ionic Liquid-Metal Interface Studied by Vibrational Spectroscopy and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2741-2753.	1.2	9
15880	Frustrated Packing in Simple Structures: Chemical Pressure Hindrance to Isolobal Bonds in the TiAl <sub>3</sub> type and ZrAl <sub>2.6</sub> Sn <sub>0.4</sub> . <i>Inorganic Chemistry</i> , 2021, 60, 4779-4791.	1.9	7
15881	Re-evaluation of the electronic structure and thermoelectric properties of narrow-gap semiconducting $\sqrt{2}\times\sqrt{2}$ -SrSi <sub>2</sub> : A complementary experimental and first-principles hybrid-functional approach. <i>Journal of Applied Physics</i> , 2021, 129, .	1.1	6
15882	Synthesis, Characterization, and Comparative Theoretical Investigation of Dinitrogen-Bridged Group 6-Gold Heterobimetallic Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 5545-5562.	1.9	11
15883	Large magnetic anisotropy in an OsIr dimer anchored in defective graphene. <i>Nanotechnology</i> , 2021, 32, 230001.	1.3	10
15884	High-throughput screening to modulate electronic and optical properties of alloyed Cs <sub>2</sub> AgBiCl <sub>6</sub> for enhanced solar cell efficiency. <i>JPhys Materials</i> , 2021, 4, 025005.	1.8	14

#	ARTICLE	IF	CITATIONS
15885	Thermodynamic assessment of Au-Pt-Ni system. <i>Materials Today Communications</i> , 2021, 26, 102061.	0.9	0
15886	Adsorption Property of Starch-Based Microporous Carbon Materials with High Selectivity and Uptake for C1/C2/C3 Separation. <i>Industrial &amp; Engineering Chemistry Research</i> , 2021, 60, 4668-4676.	1.8	13
15887	Regulation of vertical and biaxial strain on electronic and optical properties of G-GaN-G sandwich heterostructure. <i>Journal of Materials Science</i> , 2021, 56, 11402-11413.	1.7	3
15888	Adsorption of Ag on M-doped graphene: First principle calculations. <i>International Journal of Minerals, Metallurgy and Materials</i> , 2021, 28, 487-494.	2.4	14
15889	Static dipole polarizabilities of polyacenes using self-interaction-corrected density functional approximations. <i>Journal of Chemical Physics</i> , 2021, 154, 114305.	1.2	12
15890	Pristine B3CN4 monolayer for hydrogen storage: A first-principles approach. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2021, 391, 127116.	0.9	20
15891	Spinterface Formation at $\pm$ -Sexithiophene/Ferromagnetic Conducting Oxide. <i>Journal of Physical Chemistry C</i> , 2021, 125, 6073-6081.	1.5	6
15892	Shock-compressed silicon: Hugoniot and sound speed up to 2100 GPa. <i>Physical Review B</i> , 2021, 103, .	1.1	13
15893	Electronic and optical properties of fluorinated graphene within many-body Green's function framework. <i>Journal of Chemical Physics</i> , 2021, 154, 104705.	1.2	4
15894	Investigation on half-metallic ferromagnetism in Phosphorous doped SmN-Band structure study. <i>Journal of Physics: Conference Series</i> , 2021, 1770, 012093.	0.3	0
15895	Theoretical Assessment of Hinge-Type Models for Electron Donors in Reaction Centers of Photosystems I and II as well as of Purple Bacteria. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3066-3079.	1.2	6
15896	Morphology-dependent NO <sub>2</sub> gas sensing for needle-like In <sub>2</sub> O <sub>3</sub> chemiresistor nanosensors. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2021, 265, 115011.	1.7	9
15897	Construction of poly-naphthalocyanine linked by [4]-radialene-like structures on silver surfaces. <i>Nano Research</i> , 2021, 14, 4563.	5.8	2
15898	Theoretical analysis of the adsorption of phosphoric acid and model phosphate monoesters on CeO <sub>2</sub> (111). <i>Surface Science</i> , 2021, 705, 121776.	0.8	6
15899	N-Doped Graphene-Supported Diatomic Ni-Fe Catalyst for Synergistic Oxidation of CO. <i>Journal of Physical Chemistry C</i> , 2021, 125, 5616-5622.	1.5	23
15900	Comparative study of single-atom gold and iridium on CeO <sub>2</sub> {111}. <i>Journal of Chemical Physics</i> , 2021, 154, 164703.	1.2	2
15901	Facile synthesis of nitrogen-doped and boron-doped reduced graphene oxide using radio-frequency plasma for supercapacitors. <i>Journal Physics D: Applied Physics</i> , 2021, 54, 265501.	1.3	10
15902	Investigation of optoelectronic properties of AgIn <sub>1-x</sub> Ga <sub>x</sub> Y <sub>2</sub> (Y = Se, Te) semiconductors. <i>Indian Journal of Physics</i> , 0, , 1.	0.9	0



#	ARTICLE	IF	CITATIONS
15903	High-contrast, reversible change of thermal conductivity in hexagonal nickel-iron sulfides. <i>Acta Materialia</i> , 2021, 208, 116709.	3.8	13
15904	Electronic and Magnetic Properties of (Ti, V, Cr, Mn, and Co)-Doped CdS. <i>Journal of Superconductivity and Novel Magnetism</i> , 2021, 34, 1923-1931.	0.8	8
15905	Modulating Curie Temperature and Magnetic Anisotropy in Nanoscale-Layered Cr <sub>2</sub> Te <sub>3</sub> Films: Implications for Room-Temperature Spintronics. <i>ACS Applied Nano Materials</i> , 2021, 4, 4810-4819.	2.4	25
15906	An Ab Initio Perspective on the Key Vacancy Defects of KMgF <sub>3</sub> . <i>Journal of Physical Chemistry C</i> , 2021, 125, 8253-8267.	1.5	5
15907	Prediction of theoretical strength of diamond under complex loadings. <i>Extreme Mechanics Letters</i> , 2021, 44, 101233.	2.0	11
15908	A highly efficient Fe-doped Ni <sub>3</sub> S <sub>2</sub> electrocatalyst for overall water splitting. <i>Nano Research</i> , 2021, 14, 4740-4747.	5.8	52
15909	Revealing the Effect of Sodium on Iron-Based Catalysts for CO <sub>2</sub> Hydrogenation: Insights from Calculation and Experiment. <i>Journal of Physical Chemistry C</i> , 2021, 125, 7637-7646.	1.5	20
15910	Afterglow-Catalysis and Self-Reporting of Pollutant Degradation by Ethylenediaminetetraacetic Acid Disodium-Etched Cr:ZnGa <sub>2</sub> O <sub>4</sub> . <i>Journal of Physical Chemistry C</i> , 2021, 125, 9096-9106.	1.5	7
15911	Accommodation and diffusion of Nd in uranium silicide - U <sub>3</sub> Si <sub>2</sub> . <i>Journal of Nuclear Materials</i> , 2021, 547, 152794.	1.3	0
15912	Materials Studio simulation for the adsorption properties of CO <sub>2</sub> molecules at the surface of sodium silicate and potassium silicate solution under different pressure conditions. <i>International Journal of Metalcasting</i> , 2022, 16, 242-251.	1.5	8
15913	Tunable Negative Poisson's Ratio in Van der Waals Superlattice. <i>Research</i> , 2021, 2021, 1904839.	2.8	5
15914	Enhancing the Hydrogen Evolution Properties of Kesterite Absorber by Si Doping in the Surface of CZTS Thin Film. <i>Advanced Materials Interfaces</i> , 2021, 8, 2002124.	1.9	8
15915	Structural, Electronic, Magnetic, and Elastic Properties of Co <sub>x</sub> Cr <sub>2</sub> Z (X = Sc, Ti; Z = Al, Ga) Quaternary Heusler Alloys: First-Principles Study. <i>Physica Status Solidi (B): Basic Research</i> , 2021, 258, 2100004.	0.7	4
15916	Reaction mechanism of methane conversion over Ca <sub>2</sub> Fe <sub>2</sub> O <sub>5</sub> oxygen carrier in chemical looping hydrogen production. <i>Fuel</i> , 2021, 290, 120094.	3.4	16
15917	Microstructure Maps of Complex Perovskite Materials from Extensive Monte Carlo Sampling Using Machine Learning Enabled Energy Model. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3591-3599.	2.1	16
15918	Theoretical insights into strong intrinsic piezoelectricity of blue-phosphorus-like group-IV monochalcogenides. <i>Nano Research</i> , 2022, 15, 209-216.	5.8	17
15919	The cage-like structure enhanced magnetic moment in Sc <sub>n</sub> (n = 2-12) clusters: A first-principles jointed particle swarm optimization investigation. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26654.	1.0	2
15920	First-Principles Study of Graphene-6H SiC Surface Interactions. <i>Balkan Journal of Electrical and Computer Engineering</i> , 2021, 9, 171-177.	0.4	0

#	ARTICLE	IF	CITATIONS
15921	Cd(II) coordination polymer of fumaric acid and pyridyl-hydrazide Schiff base: Structure, photoconductivity and theoretical interpretation. <i>Inorganica Chimica Acta</i> , 2021, 518, 120253.	1.2	17
15922	Influence of anisotropic strain and temperature on hydrogen dissolution in tungsten. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2021, 29, 055011.	0.8	0
15923	Oxidation behavior of different La <sub>2</sub> O <sub>3</sub> -content modified SiC ceramic at 1700 °C. <i>Ceramics International</i> , 2021, 47, 11560-11567.	2.3	8
15924	Effect of doping and pressure on the electronic and magnetic properties of the quaternary Heusler alloys. <i>Materials Research Express</i> , 2021, 8, 046527.	0.8	2
15925	First principles study of behavior of helium at Fe(110) "graphene interface". <i>Chinese Physics B</i> , 2021, 30, 046802.	0.7	2
15926	Mechanical Vibrational Relaxation of NO Scattering from Metal and Insulator Surfaces: When and Why They Are Different. <i>Physical Review Letters</i> , 2021, 126, 156101.	2.9	16
15927	Synthesis, crystal structure and physical properties of a new chalcogenides Rb <sub>3</sub> Ga <sub>3</sub> Ge <sub>7</sub> S <sub>20</sub> . <i>Journal of Solid State Chemistry</i> , 2021, 296, 121945.	1.4	5
15928	A New Monolayer B <sub>4</sub> C <sub>4</sub> with Robust Stability and Excellent Performance for Spontaneous Water Splitting Under Visible Light. <i>Advanced Theory and Simulations</i> , 2021, 4, 2100015.	1.3	1
15929	Maximized crystal water content and charge-shielding effect in layered vanadate render superior aqueous zinc-ion battery. <i>Materials Today Energy</i> , 2021, 21, 100757.	2.5	18
15930	Energy disposal into the vibrational degrees of freedom of bimolecular reaction products: Key factors and simple model. <i>Chemical Physics</i> , 2021, 544, 111098.	0.9	4
15931	First-principles calculations of diffusion activation energies for designing anti-self-aging biodegradable zinc alloys. <i>Journal of Materials Research</i> , 2021, 36, 1475-1486.	1.2	6
15932	Multiconfiguration Density-Coherence Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2775-2782.	2.3	12
15933	Insights into thermodynamic properties of CsCl-type HfTM (TM = Fe, Ru, Os) compounds from first-principles calculations. <i>Applied Physics A: Materials Science and Processing</i> , 2021, 127, 1.	1.1	0
15934	Metastable 1T <sup>-2</sup> -phase group VIB transition metal dichalcogenide crystals. <i>Nature Materials</i> , 2021, 20, 1113-1120.	13.3	119
15935	Study of Anharmonicity in Zirconium Hydrides Using Inelastic Neutron Scattering and Ab-Initio Computer Modeling. <i>Inorganics</i> , 2021, 9, 29.	1.2	3
15936	Theoretical investigation of physical properties of the spinel ZnFe <sub>2</sub> O <sub>4</sub> compound: Ab-initio calculation. <i>Phase Transitions</i> , 2021, 94, 134-146.	0.6	2
15937	(6-Diphenylphosphinoacenaphth-5-yl)indium and -nickel Compounds: Synthesis, Structure, Transmetalation, and Cross-Coupling Reactions. <i>Organometallics</i> , 2021, 40, 1284-1295.	1.1	5
15938	CS <sub>2</sub> Removal from C <sub>5</sub> Distillates by Reactive Molecular Dynamics Simulations. <i>Industrial &amp; Engineering Chemistry Research</i> , 2021, 60, 5816-5825.	1.8	4

#	ARTICLE	IF	CITATIONS
15939	Atomistic insight into hydrogen trapping at MC/BCC-Fe phase boundaries: The role of local atomic environment. <i>Acta Materialia</i> , 2021, 208, 116744.	3.8	36
15940	Photocatalytic and Photoelectrochemical Hydrogen Evolution from Water over Cu <sub>2</sub> Sn <sub>x</sub> Ge <sub>1-x</sub> S <sub>3</sub> Particles. <i>Journal of the American Chemical Society</i> , 2021, 143, 5698-5708.	6.6	33
15941	A full configuration interaction quantum Monte Carlo study of ScO, TiO, and VO molecules. <i>Journal of Chemical Physics</i> , 2021, 154, 164302.	1.2	11
15942	The liquid exfoliation of graphene in polar solvents. <i>Applied Surface Science</i> , 2021, 546, 149046.	3.1	36
15943	Ferromagnetism in Mn-Doped ZnO: A Joint Theoretical and Experimental Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 7734-7745.	1.5	24
15944	Doping of MoS <sub>2</sub> by Cu and V: An Efficient Strategy for the Enhancement of Hydrogen Evolution Activity. <i>Langmuir</i> , 2021, 37, 4847-4858.	1.6	22
15945	Unlocking the Optimal Aqueous Bi-Bi <sub>2</sub> O <sub>3</sub> Anode via Unifying Octahedrally Liberated Bi-Atoms and Spilled Nano-Bi Exsolution. <i>Energy Storage Materials</i> , 2021, 36, 376-386.	9.5	37
15946	High capacity reversible hydrogen storage in zirconium doped 2D-covalent triazine frameworks: Density Functional Theory investigations. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 14520-14531.	3.8	41
15947	Computational Investigation of MgH <sub>2</sub> /NbO <sub>x</sub> for Hydrogen Storage. <i>Journal of Physical Chemistry C</i> , 2021, 125, 8862-8868.	1.5	9
15948	Identifying the convergent reaction path from pre-designed assembled structures: Dissymmetrical dehalogenation of Br <sub>2</sub> Py on Ag(111). <i>Nano Research</i> , 0, , 1.	5.8	20
15949	The best density functional theory functional for the prediction of <sup>1</sup> H and <sup>13</sup> C chemical shifts of protonated alkylpyrroles. <i>Journal of Computational Chemistry</i> , 2021, 42, 1248-1262.	1.5	5
15950	Effects of Zn and Mg Segregations on the Grain Boundary Sliding and Cohesion in Al: Ab Initio Modeling. <i>Metals</i> , 2021, 11, 631.	1.0	8
15951	A DFT study in bulk magnetic moment of Fe <sub>x</sub> Co <sub>1-x</sub> (0 ≤ x ≤ 1). <i>Bulletin of Materials Science</i> , 2021, 44, 1.	0.8	2
15952	BiSbWO <sub>6</sub> : Properties of a mixed 5s/6s lone-pair-electron system. <i>Chemical Physics</i> , 2021, 544, 111117.	0.9	4
15953	Modelling the primary damage in Fe and W: Influence of the short range interactions on the cascade properties: Part 1 – Energy transfer. <i>Journal of Nuclear Materials</i> , 2021, 547, 152816.	1.3	10
15954	Effects of IIIA element doping on structure stability, electronic structure and optical properties of T-carbon. <i>Chemical Physics</i> , 2021, 544, 111095.	0.9	2
15955	First-principles calculations of effects of pressure on paramagnetic, ferromagnetic, and antiferromagnetic spin-web Cu <sub>3</sub> TeO <sub>6</sub> . <i>Journal of Molecular Modeling</i> , 2021, 27, 129.	0.8	1
15956	High-Performance Hydrogen Storage Properties of Li-Decorated B <sub>2</sub> N <sub>2</sub> Nanosheets: A Periodic Density Functional Theory Study. <i>Energy &amp; Fuels</i> , 2021, 35, 6858-6867.	2.5	33

#	ARTICLE	IF	CITATIONS
15957	Ba with Unusual Oxidation States in Ba Chalcogenides under Pressure. Journal of Physical Chemistry Letters, 2021, 12, 4203-4210.	2.1	11
15958	Diverse electronic and magnetic properties of CrS <sub>2</sub> enabling strain-controlled 2D lateral heterostructure spintronic devices. Npj Computational Materials, 2021, 7, .	3.5	35
15959	Bandgap engineering of Gallium oxides by crystalline disorder. Materials Today Physics, 2021, 18, 100369.	2.9	44
15960	A joint experimental and theoretical study on structural, electronic, and magnetic properties of MnGen <sup>n+</sup> (n = 3-14) clusters. Journal of Chemical Physics, 2021, 154, 204302.	1.2	24
15961	Synergistic Effects of Tungsten Doping and Sulfur Vacancies in MoS <sub>2</sub> on Enhancement of Hydrogen Evolution. Journal of Physical Chemistry C, 2021, 125, 11369-11379.	1.5	17
15962	A Water-Soluble Schiff Base Turn-on Fluorescent Chemosensor for the Detection of Al <sup>3+</sup> and Zn <sup>2+</sup> Ions at the Nanomolar Level: Application in Live-Cell Imaging. Journal of Fluorescence, 2021, 31, 1277-1290.	1.3	14
15963	Steric hindrance effect on adsorption of xanthate on sphalerite surface: A DFT study. Minerals Engineering, 2021, 165, 106834.	1.8	20
15964	Formulation of 3D<math>\text{H}_4\text{SiO}_4</math> xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg" ><math>\text{H}_4</math><math>\text{SiO}_4</math></math> xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg" ><math>\text{H}_4</math><math>\text{SiO}_4</math></math>		

#	ARTICLE	IF	CITATIONS
15975	First-principles calculations of metal surfaces. I. Slab-consistent bulk reference for convergent surface properties. <i>Physical Review B</i> , 2021, 103, .	1.1	3
15976	Low-Dimensional Organic Metal Halide Hybrids with Excitation-Dependent Optical Waveguides from Visible to Near-Infrared Emission. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 26451-26460.	4.0	23
15977	Vacancies-Engineered $M_{2}CO_{2}$ MXene as an Efficient Hydrogen Evolution Reaction Electrocatalyst. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4805-4813.	2.1	31
15978	Assessment of Performance of Density Functionals for Predicting Potential Energy Curves in Hydrogen Storage Applications. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4245-4257.	1.1	2
15979	Computational Mechanistic Study of Brønsted Acid-Catalyzed Unsymmetrical 1,2,4,5-Tetrazines Synthesis. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4715-4726.	1.1	2
15980	Atomically precise noble metal clusters (Ag <sub>10</sub> , Au <sub>10</sub> , Pd <sub>10</sub> and Pt <sub>10</sub> ) on alumina support: A comprehensive DFT study for oxidative catalysis. <i>Applied Surface Science</i> , 2021, 547, 149160.	3.1	7
15981	Effect of Ru Doping on the Properties of LiFePO <sub>4</sub> /C Cathode Materials for Lithium-Ion Batteries. <i>ACS Omega</i> , 2021, 6, 14122-14129.	1.6	34
15982	A DFT study of the equiatomic quaternary Heusler alloys ZnCdXMn (X=Pd, Ni or Pt). <i>Solid State Communications</i> , 2021, 331, 114292.	0.9	39
15983	Density functional theory study of formaldehyde adsorption and decomposition on Co-doped defective CeO <sub>2</sub> (110) surface*. <i>Chinese Physics B</i> , 2021, 30, 103101.	0.7	1
15984	Structural, Elastic, Electronic, and Magnetic Properties of XPtBi (X=Er and Ho) Using FP-LAPW Method. <i>Journal of Superconductivity and Novel Magnetism</i> , 2021, 34, 1865-1873.	0.8	3
15985	Structure sensitivity of ammonia electro-oxidation on transition metal surfaces: A first-principles study. <i>Journal of Catalysis</i> , 2021, 397, 137-147.	3.1	31
15986	Distance synergy of single Ag atoms doped MoS <sub>2</sub> for hydrogen evolution electrocatalysis. <i>Applied Surface Science</i> , 2021, 547, 149113.	3.1	24
15987	Visible-light-driven CO <sub>2</sub> reduction to ethylene on CdS: Enabled by structural relaxation-induced intermediate dimerization and enhanced by ZIF-8 coating. <i>Applied Catalysis B: Environmental</i> , 2021, 285, 119834.	10.8	71
15988	Hydroxylapatite and Related Minerals in Bone and Dental Tissues: Structural, Spectroscopic and Mechanical Properties from a Computational Perspective. <i>Biomolecules</i> , 2021, 11, 728.	1.8	15
15989	Magnetic, Electronic, and Mechanical Properties of Bulk $\mu\text{-Fe}_{2}\text{N}$ Synthesized at High Pressures. <i>ACS Omega</i> , 2021, 6, 12591-12597.	1.6	4
15990	Induced magnetization in Cu atoms at the Fe-Co/Cu <sub>3</sub> Au(001) interface: X-ray magnetic circular dichroism experiments and theoretical results. <i>Applied Surface Science</i> , 2021, 548, 149215.	3.1	1
15991	Cold-plasma technique enabled supported Pt single atoms with tunable coordination for hydrogen evolution reaction. <i>Applied Catalysis B: Environmental</i> , 2021, 285, 119861.	10.8	38
15992	Learning to Model G-Quadruplexes: Current Methods and Perspectives. <i>Annual Review of Biophysics</i> , 2021, 50, 209-243.	4.5	21

#	ARTICLE	IF	CITATIONS
15993	Comparison of charge transport and opto-electronic properties of pyrene and anthracene derivatives for OLED applications. <i>Journal of Molecular Modeling</i> , 2021, 27, 174.	0.8	6
15994	Pseudo-copper Ni-Zn alloy catalysts for carbon dioxide reduction to C2 products. <i>Frontiers of Physics</i> , 2021, 16, 1.	2.4	19
15995	Thermally Strain-Induced Band Gap Opening on Platinum Diselenide-Layered Films: A Promising Two-Dimensional Material with Excellent Thermoelectric Performance. <i>Chemistry of Materials</i> , 2021, 33, 3490-3498.	3.2	18
15996	Assessing the Activity of Ni Clusters Supported on TiC(001) toward CO <sub>2</sub> and H <sub>2</sub> Dissociation. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12019-12027.	1.5	15
15997	Energy Decomposition to Access the Stability Changes Induced by CO Adsorption on Transition-Metal 13-Atom Clusters. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2294-2301.	2.5	6
15998	Zinc Complex-Based Multifunctional Reactive Lithium Polysulfide Trapper Approaching Its Theoretical Efficiency. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 23936-23944.	4.0	12
15999	Ce-introduced effects on modification of acidity and Pt electronic states on Pt-Sn/Al <sub>2</sub> O <sub>3</sub> catalysts for catalytic reforming. <i>Applied Catalysis A: General</i> , 2021, 617, 118116.	2.2	17
16000	Elucidating the Mechanism of Ambient-Temperature Aldol Condensation of Acetaldehyde on Ceria. <i>ACS Catalysis</i> , 2021, 11, 8621-8634.	5.5	14
16001	Nitrogen doping in non-magnetic yttrium oxide: Induction of room temperature ferromagnetism from first principles simulations. <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 528, 167840.	1.0	5
16002	Helium incorporation induced direct-gap silicides. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	6
16003	Structural Diversity and Argentophilic Interactions in Small Phosphine Silver(I) Thiolate Clusters. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 2702-2711.	1.0	9
16004	Improving the applicability of the Pauli kinetic energy density based semilocal functional for solids. <i>New Journal of Physics</i> , 2021, 23, 063007.	1.2	13
16005	BaYOBO <sub>3</sub> : A deep-ultraviolet rare-earth oxy-borate with a large second harmonic generation response. <i>Science China Chemistry</i> , 2021, 64, 1184-1191.	4.2	22
16006	Photocatalytic conversion of CO to fuels with water by B-doped graphene/g-C <sub>3</sub> N <sub>4</sub> heterostructure. <i>Science Bulletin</i> , 2021, 66, 1186-1193.	4.3	19
16007	Stability, and electronic and optical properties of ternary nitride phases of MgSnN <sub>2</sub> : A first-principles study. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 153, 110011.	1.9	21
16008	Requirements for an accurate dispersion-corrected density functional. <i>Journal of Chemical Physics</i> , 2021, 154, 230902.	1.2	39
16009	Ethylene oxidation on unpromoted silver catalysts: Reaction pathway and selectivity analysis using DFT calculations. <i>Surface Science</i> , 2021, 708, 121834.	0.8	6
16010	An effective scheme to determine surface energy and its relation with adsorption energy. <i>Acta Materialia</i> , 2021, 212, 116895.	3.8	16



#	ARTICLE	IF	CITATIONS
16011	First-principles study of N <sub>2</sub> O decomposition on (001) facet of perovskite LaBO <sub>3</sub> (B = Mn, Co, Ni). <i>Molecular Catalysis</i> , 2021, 510, 111713.	1.0	3
16012	Different Reactivities of (5-Ph <sub>2</sub> -P-Ace-6)-MeSiH toward the Rhodium(I) Chlorides [(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> RhCl] <sub>2</sub> and [(CO) <sub>2</sub> RhCl] <sub>2</sub> . Hirshfeld Atom Refinement of a Rh-HA·A·Si Interaction. <i>Organometallics</i> , 2021, 40, 2027-2038.	1.1	6
16013	Revealing the boosting role of NO for soot combustion over CeO <sub>2</sub> (111): A first-principles microkinetic modeling. <i>Molecular Catalysis</i> , 2021, 509, 111582.	1.0	3
16014	Cobalt Metal ALD: Understanding the Mechanism and Role of Zinc Alkyl Precursors as Reductants for Low-Resistivity Co Thin Films. <i>Chemistry of Materials</i> , 2021, 33, 5045-5057.	3.2	16
16015	Co and Mo Co-doped Fe <sub>2</sub> O <sub>3</sub> for Selective Ethylene Production via Chemical Looping Oxidative Dehydrogenation. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 8002-8011.	3.2	21
16016	Local Temperature as a Chemical Reactivity Descriptor. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5623-5630.	2.1	17
16017	High-entropy ferroelastic rare-earth tantalite ceramic: (Y <sub>0.2</sub> Ce <sub>0.2</sub> Sm <sub>0.2</sub> Gd <sub>0.2</sub> Dy <sub>0.2</sub> )TaO <sub>4</sub> . <i>Journal of the American Ceramic Society</i> , 2021, 104, 5873-5882.		49
16018	Thermodynamic properties of forming methanol-water and ethanol-water clusters at various temperatures and pressures and implications for atmospheric chemistry: A DFT study. <i>Chemosphere</i> , 2021, 272, 129846.	4.2	9
16019	Enhanced Electrochemical Property of Li <sub>1.2</sub> xNa <sub>x</sub> Mn <sub>0.54</sub> Ni <sub>0.13</sub> Co <sub>0.13</sub> O <sub>2</sub> Cathode Material for the New Optoelectronic Devices. <i>Frontiers in Physics</i> , 2021, 9, .	1.0	1
16020	Bias-dependent diffusion of a H <sub>2</sub> O molecule on metal surfaces by the first-principles method under the grand canonical ensemble. <i>Physical Review Materials</i> , 2021, 5, .	0.9	9
16021	Strong influence of nonmagnetic ligands on the momentum-dependent spin splitting in antiferromagnets. <i>Physical Review B</i> , 2021, 103, .	1.1	16
16022	Evaluation of density functional theory for a large and diverse set of organic and inorganic equilibrium structures. <i>Journal of Computational Chemistry</i> , 2021, 42, 1590-1601.	1.5	44
16023	Identifying the key steps determining the selectivity of toluene methylation with methanol over HZSM-5. <i>Nature Communications</i> , 2021, 12, 3725.	5.8	26
16024	Stepping Out of Transition Metals: Activating the Dual Atomic Catalyst through Main Group Elements. <i>Advanced Energy Materials</i> , 2021, 11, 2101404.	10.2	33
16025	Bi <sub>2</sub> Se <sub>3</sub> /Bi <sub>2</sub> Se <sub>3</sub> and TlSe/TlSe junctions: enhanced coupling of topological interface states by intercalation. <i>Journal Physics D: Applied Physics</i> , 2021, 54, 345301.	1.3	3
16026	Bromine heavy-atom induced persistent room temperature phosphorescence of [ZnBr <sub>2</sub> ] based coordination polymer. <i>Journal of Solid State Chemistry</i> , 2021, 298, 122135.	1.4	1
16027	Dual Dirac points and odd-even oscillated energy gap in zigzag chlorinated stanene nanoribbon. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 325303.	0.7	2
16028	Interplay of quantum capacitance with Van der Waals forces, intercalation, co-intercalation, and the number of MoS <sub>2</sub> layers. <i>Materials Today Energy</i> , 2021, 20, 100677.	2.5	17

#	ARTICLE	IF	CITATIONS
16029	CO oxidation activity of Pt/CeO <sub>2</sub> catalysts below 0 °C: platinum loading effects. <i>Applied Catalysis B: Environmental</i> , 2021, 286, 119931.	10.8	83
16030	Novel insights into the reoxidation of direct reduced iron (DRI) during ball-mill treatment: A combined experimental and computational study. <i>Applied Surface Science</i> , 2021, 552, 149485.	3.1	8
16031	A density functional theory study on thermal properties of perfect and defective graphene. <i>Journal of Physics: Conference Series</i> , 2021, 1948, 012219.	0.3	0
16032	Predictions of Chemical Shifts for Reactive Intermediates in CO <sub>2</sub> Reduction under Operando Conditions. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 31554-31560.	4.0	12
16033	Superconductive Sodium Carbides with Pentagon Carbon at High Pressures. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5850-5856.	2.1	16
16034	Current Density Calculations of an Octahedral Fe Nanocluster for Selective Electrocatalytic for Nitrogen Reduction. <i>ACS Applied Nano Materials</i> , 2021, 4, 7758-7770.	2.4	14
16035	Factors controlling segregation tendency of solute Ti, Ag and Ta into different symmetrical tilt grain boundaries of tungsten: First-principles and experimental study. <i>Acta Materialia</i> , 2021, 211, 116868.	3.8	22
16036	Electrochemical Detection of Tryptophan Metabolites via Kynurenine Pathway by Using Nanocarbon Films. <i>Electroanalysis</i> , 2022, 34, 709-716.	1.5	6
16037	Theoretical Predictions of the Structural and Mechanical Properties of Tungsten-Rare Earth Element Alloys. <i>Materials</i> , 2021, 14, 3046.	1.3	5
16038	The Strain-Tuned Spin Seebeck Effect, Spin Polarization, and Giant Magnetoresistance of a Graphene Nanobubble in Zigzag Graphene Nanoribbons. <i>ACS Omega</i> , 2021, 6, 15308-15315.	1.6	2
16039	Spin-Scaled Range-Separated Double-Hybrid Density Functional Theory for Excited States. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4211-4224.	2.3	25
16040	Ab initio modelling of helium behavior in $\delta$ -Fe-TaC interface. <i>Nuclear Materials and Energy</i> , 2021, 27, 100956.	0.6	2
16041	Structural, Electronic, and Magnetic Properties of the Rare Earth-Based Solar Perovskites: GdAlO <sub>3</sub> , DyAlO <sub>3</sub> , and HoAlO <sub>3</sub> . <i>Journal of Superconductivity and Novel Magnetism</i> , 2021, 34, 2371-2380.	0.8	25
16042	Mechanism of improving the SCR NO removal activity of Fe <sub>2</sub> O <sub>3</sub> catalyst by doping Mn. <i>Journal of Alloys and Compounds</i> , 2021, 867, 158787.	2.8	29
16043	Development of Bimetallic PdNi Electrocatalysts toward Mitigation of Catalyst Poisoning in Direct Borohydride Fuel Cells. <i>ACS Catalysis</i> , 2021, 11, 8417-8430.	5.5	28
16044	The Relationship between Natural Pyrite and Impurity Element Semiconductor Properties: A Case Study of Vein Pyrite from the Zaozigou Gold Deposit in China. <i>Minerals (Basel, Switzerland)</i> , 2021, 11, 596.	0.8	4
16045	Theoretical scanning of bimetallic alloy for designing efficient N <sub>2</sub> electroreduction catalyst. <i>Materials Today Energy</i> , 2021, 20, 100684.	2.5	21
16046	Multifunctional Ca <sub>10</sub> (PO <sub>4</sub> ) <sub>6</sub> F <sub>2</sub> as a host for radioactive waste immobilization: Am <sup>3+</sup> /Eu <sup>3+</sup> ions distribution, phosphor characteristics and radiation induced changes. <i>Journal of Hazardous Materials</i> , 2021, 411, 125025.	6.5	19

#	ARTICLE	IF	CITATIONS
16047	DFT insights into the hydrodenitrogenation mechanism of quinoline catalyzed by different Ni-promoted MoS <sub>2</sub> edge sites: Effect of the active phase morphology. Journal of Hazardous Materials, 2021, 411, 125127.	6.5	11
16048	Uniform and robust TiN/HfO <sub>2</sub> /Pt memristor through interfacial Al-doping engineering. Applied Surface Science, 2021, 550, 149274.	3.1	34
16049	Computational screening study of double transition metal carbonitrides M <sub>2</sub> CNO <sub>2</sub> -MXene as catalysts for hydrogen evolution reaction. Npj Computational Materials, 2021, 7, .	3.5	63
16050	Linear and nonlinear optical response of g-C <sub>3</sub> N <sub>4</sub> -based quantum dots*. Chinese Physics B, 2021, 30, 077802.	0.7	0
16051	Assessing the role of mineral particles in the atmospheric photooxidation of typical carbonyl compound. Journal of Environmental Sciences, 2021, 105, 56-63.	3.2	3
16052	Migration and coordination of vanadium separating from black shale involved by fluoride. Separation and Purification Technology, 2021, 266, 118552.	3.9	15
16053	Ab Initio Modeling of fcc Fe-Co-Cr-Ni High Entropy Alloys with Full Composition Range. Journal of Phase Equilibria and Diffusion, 2021, 42, 656-672.	0.5	7
16054	Light Harvesting from Oxygen Vacancies and A- and B-Site Dopants in CaSnO <sub>3</sub> Perovskite through Efficient Photon Utilization and Local Site Engineering. ACS Applied Electronic Materials, 2021, 3, 3256-3270.	2.0	11
16055	Unraveling the anomalous mechanoluminescence intensity change and pressure-induced red-shift for manganese-doped zinc sulfide. Nano Energy, 2021, 85, 106005.	8.2	19
16056	How the Copper Dopant Alters the Geometric and Photoelectronic Properties of the Lead-free Cs <sub>2</sub> AgSbCl <sub>6</sub> Double Perovskite. Advanced Theory and Simulations, 2021, 4, 2100142.	1.3	6
16057	Promoting Reversible Cathode Reactions in Magnesium Rechargeable Batteries Using Metastable Cubic MgMn <sub>2</sub> O <sub>4</sub> Spinel Nanoparticles. ACS Applied Nano Materials, 2021, 4, 8328-8333.	2.4	17
16058	Hydricity of 3d Transition Metal Complexes from Density Functional Theory: A Benchmarking Study. Molecules, 2021, 26, 4072.	1.7	19
16059	Theoretical Approach toward Optimum Anion-Doping on MXene Catalysts for Hydrogen Evolution Reaction: an Ab Initio Thermodynamics Study. ACS Applied Materials & Interfaces, 2021, 13, 37035-37043.	4.0	17
16060	Spectroscopic Analysis of Rare-Earth Silicide Structures on the Si(111) Surface. Materials, 2021, 14, 4104.	1.3	3
16061	Assessing the structural, electronic, elastic and thermoelectric properties of PtTiSn and PdLaBi transition metal alloys from the first-principles prospective. Materials Science in Semiconductor Processing, 2021, 129, 105796.	1.9	3
16062	Investigations of adsorption behavior and anti-cancer activity of curcumin on pure and platinum-functionalized B <sub>12</sub> N <sub>12</sub> nanocages. Journal of Molecular Liquids, 2021, 334, 116516.	2.3	39
16063	The early growth process of helium blistering in tungsten and molybdenum: First-principles and statistical model calculations. Journal of Nuclear Materials, 2021, 550, 152938.	1.3	2
16064	Strontium Stannate as an Alternative Anode Material for Li-Ion Batteries. Journal of Physical Chemistry C, 2021, 125, 14947-14956.	1.5	9

#	ARTICLE	IF	CITATIONS
16065	In-situ growth of heterophase Ni nanocrystals on graphene for enhanced catalytic reduction of 4-nitrophenol. <i>Nano Research</i> , 2022, 15, 1230-1237.	5.8	21
16066	Three-dimensional acetylenic modified graphene for high-performance optoelectronics and topological materials. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	4
16067	First-principles studies on sensing properties of delta arsenene nanoribbons towards hexane and heptane molecules. <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113256.	1.1	14
16068	Unraveling the Intermediate Reaction Complexes and Critical Role of Support-Derived Oxygen Atoms in CO Oxidation on Single-Atom Pt/CeO <sub>2</sub> . <i>ACS Catalysis</i> , 2021, 11, 8701-8715.	5.5	51
16069	Effects of yttrium on mechanical and cohesion properties of zirconium diboride. <i>Vacuum</i> , 2021, 189, 110246.	1.6	4
16070	Constructing Active Sites from Atomic-Scale Geometrical Engineering in Spinel Oxide Solid Solutions for Efficient and Robust Oxygen Evolution Reaction Electrocatalysts. <i>Advanced Science</i> , 2021, 8, e2101653.	5.6	31
16071	Structural and mechanical properties of Ti-B-C coatings prepared by dual magnetron sputtering. <i>Thin Solid Films</i> , 2021, 730, 138723.	0.8	4
16072	Cobalt Telluride: A Highly Efficient Trifunctional Electrocatalyst for Water Splitting and Oxygen Reduction. <i>ACS Applied Energy Materials</i> , 2021, 4, 8158-8174.	2.5	36
16073	Density Functional Geometries and Zero-Point Energies in Ab Initio Thermochemical Treatments of Compounds with First-Row Atoms (H, C, N, O, F). <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4872-4890.	2.3	22
16074	On the structure sensitivity of and CO coverage effects on formic acid decomposition on Pd surfaces. <i>Surface Science</i> , 2021, 709, 121846.	0.8	11
16075	Resistivity scaling in epitaxial MAX-phase Ti <sub>4</sub> SiC <sub>3</sub> (0001) layers. <i>Journal of Applied Physics</i> , 2021, 130, .	1.1	8
16076	Enhancing Catalytic Properties of Iron- and Nitrogen-Doped Carbon for Nitrogen Reduction through Structural Distortion: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 16004-16012.	1.5	14
16077	Surface Magnetism in Pristine $\sqrt{3} \times \sqrt{3}$ Rhombohedral Boron and Intersurface Exchange Coupling Mechanism of Boron Icosahedra. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6812-6817.	2.1	5
16078	Few-Layer PdSe <sub>2</sub> Nanofilm/Si Heterojunction for Sensing NO <sub>2</sub> at Room Temperature. <i>ACS Applied Nano Materials</i> , 2021, 4, 7358-7370.	2.4	18
16079	Optical and electronic properties of TiO <sub>2</sub> /GOQDs composites: A combined experimental and first-principles calculations study. <i>Computational Materials Science</i> , 2021, 195, 110503.	1.4	11
16080	An integrated experimental and computational investigation of defect and microstructural effects on thermal transport in thorium dioxide. <i>Acta Materialia</i> , 2021, 213, 116934.	3.8	26
16081	Structure-sensitivity of direct oxidation methane to methanol over Rhn/ZrO <sub>2-x</sub> (1 0 1) (n=1, 4, 10) surfaces: A DFT study. <i>Applied Surface Science</i> , 2021, 555, 149690.	3.1	11
16082	Is Mg <sub>17</sub> Al <sub>12</sub> ductile or brittle? A theoretical insight. <i>Journal of Magnesium and Alloys</i> , 2023, 11, 936-944.	5.5	12

#	ARTICLE	IF	CITATIONS
16083	Extension of the Linear Response Function of Electron Density to a Plane-wave Basis and the First Application to Periodic Surface Systems. <i>Chemistry Letters</i> , 2021, 50, 1801-1805.	0.7	2
16084	Designing an Electron-Deficient Pd/NiCo <sub>2</sub> O <sub>4</sub> Bifunctional Electrocatalyst with an Enhanced Hydrodechlorination Activity to Reduce the Consumption of Pd. <i>Environmental Science &amp; Technology</i> , 2021, 55, 10087-10096.	4.6	64
16085	Theoretical Inspection of M <sub>1</sub> /PMA Single-Atom Electrocatalyst: Ultra-High Performance for Water Splitting (HER/OER) and Oxygen Reduction Reactions (OER). <i>ACS Catalysis</i> , 2021, 11, 8929-8941.	5.5	121
16086	Computer simulation of crystals formed from 4-6-12 and 5-7 fluorographene layers. <i>Journal of Physics: Conference Series</i> , 2021, 1967, 012058.	0.3	0
16087	Single boron atom anchored on graphitic carbon nitride nanosheet (B/g-C <sub>2</sub> N) as a photocatalyst for nitrogen fixation: A first-principles study*. <i>Chinese Physics B</i> , 2021, 30, 083101.	0.7	3
16088	Structural phase transformation, insulator to semiconductor transition by Be/Sr doping and impact on optical properties of KMgF <sub>3</sub> fluoro-perovskite. <i>Molecular Physics</i> , 2021, 119, .	0.8	0
16089	Mechanism for anisotropic diffusion of liquid-like Cu atoms in hexagonal $\hat{I}^2$ Cu <sub>2</sub> S. <i>Physical Review Materials</i> , 2021, 5, .	0.9	4
16090	Impact of Se in Structural, Mechanical, Thermal, Thermoelectric and Optical Properties of n-type SnTe. <i>ECS Journal of Solid State Science and Technology</i> , 2021, 10, 071016.	0.9	8
16091	First-Principles Calculations of Structural, Electronic, Optical, and Thermoelectric Properties of LuNiBi and LuNiSb Half-Heusler. <i>Journal of Superconductivity and Novel Magnetism</i> , 2021, 34, 2689-2698.	0.8	11
16092	Linear and Nonlinear Optical Properties of Centrosymmetric Sb <sub>4</sub> O <sub>5</sub> SO <sub>4</sub> and Noncentrosymmetric Sb <sub>4</sub> O <sub>4</sub> (SO <sub>4</sub> )(OH) <sub>2</sub> Induced by Lone Pair Stereoactivity. <i>Inorganic Chemistry</i> , 2021, 60, 11648-11654.	1.9	33
16093	Supramolecular Anchoring Strategy for Facile Production of Ruthenium Nanoparticles Embedded in N-Doped Mesoporous Carbon Nanospheres for Efficient Hydrogen Generation. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 32997-33005.	4.0	11
16094	Theory-Guided Discovery of Novel Materials. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6499-6513.	2.1	11
16095	Thermoelectric properties of phosphorus-doped van der Waals crystal Ta <sub>4</sub> SiTe <sub>4</sub> . <i>Materials Today Physics</i> , 2021, 19, 100417.	2.9	13
16096	Pseudo-Periodically Coupling Ni <sub>2</sub> O Lattice with Ce <sub>2</sub> O Lattice in Ultrathin Heteronanowire Arrays for Efficient Water Oxidation. <i>Small</i> , 2021, 17, e2101727.	5.2	39
16097	Bandgap engineering in MnPS <sub>3</sub> and ZnPS <sub>3</sub> for photocatalytic water splitting: A first-principles study. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 26950-26960.	3.8	11
16098	Comment on "Thermoelectricity: The physico-chemical mechanics view". <i>J. Chem. Phys.</i> 154, 024112 (2021). <i>Journal of Chemical Physics</i> , 2021, 155, 087101.	1.2	8
16099	Potential energy surface and band gap landscape of molybdenum and titanium disulfides. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26803.	1.0	1
16100	Vacancy-defect modulated pathway of photoreduction of CO <sub>2</sub> on single atomically thin AgInP <sub>2</sub> S <sub>6</sub> sheets into olefiant gas. <i>Nature Communications</i> , 2021, 12, 4747.	5.8	128

#	ARTICLE	IF	CITATIONS
16101	Prominently enhanced corrosive gas NO <sub>2</sub> resistibility for silicone rubber composite coatings by incorporation of functional g-C <sub>3</sub> N <sub>4</sub> nanosheets. <i>Progress in Organic Coatings</i> , 2021, 157, 106292.	1.9	3
16102	Improvement of the High-Performance Al-Doped LiNi <sub>1/3</sub> Co <sub>1/3</sub> Mn <sub>1/3</sub> O <sub>2</sub> Cathode Material for New Electro-Optical Conversion Devices. <i>Frontiers in Physics</i> , 2021, 9, .	1.0	2
16103	Effects of alloying elements on the stability and mechanical properties of $\hat{I}^2$ -Ti <sub>0.5</sub> X <sub>0.5</sub> (X = V, Cr, Mn, Fe;) Tj ETQq0 0 0 rgBT /Overlock 10 Communications, 2021, 334-335, 114395.	0.9	1
16104	Facile one-pot synthesis of superfine palladium nanoparticles on polydopamine-functionalized carbon nanotubes as a nanocatalyst for the Heck reaction. <i>Journal of Materials Science and Technology</i> , 2021, 82, 197-206.	5.6	16
16105	Structural, electronic, optical and thermoelectric analysis of perovskites XRuO <sub>3</sub> (X=Ca, Sr). <i>Physica B: Condensed Matter</i> , 2021, 614, 412962.	1.3	8
16106	Theoretical screening of 2D materials supported transition-metal single atoms as efficient electrocatalysts for hydrogen evolution reaction. <i>Materialia</i> , 2021, 18, 101168.	1.3	4
16107	Comprehension of defect states induced by fluorine ions substituting for oxygen ions in Sr <sub>3</sub> MgSi <sub>2</sub> O <sub>8</sub> by first principles calculation. <i>Functional Materials Letters</i> , 2021, 14, 2151039.	0.7	3
16108	Adsorption of Si(OH) <sub>4</sub> and Al(OH) <sub>4</sub> onto arsenopyrite surface: Exploring the sealing feasibility of geopolymer to arsenopyrite. <i>Minerals Engineering</i> , 2021, 170, 107017.	1.8	12
16109	Single-atom doping in carbon black nanomaterials for photothermal antibacterial applications. <i>Cell Reports Physical Science</i> , 2021, 2, 100535.	2.8	8
16110	C(sp <sup>3</sup> )-F Bond Activation and Hydrodefluorination of the CF <sub>3</sub> Group Catalyzed by a Nickel(II) Hydride Complex: Theoretical Insight into the Mechanism with a Spin-State Change and Two Ion-Pair Intermediates. <i>ACS Catalysis</i> , 2021, 11, 10681-10693.	5.5	5
16111	A New Type of Large-Gap Quantum Spin Hall Insulator Material ZrSe <sub>5</sub> . <i>Physica Status Solidi (B): Basic Research</i> , 2021, 258, 2100256.	0.7	2
16112	Enhanced electrochemical performance and storage mechanism of LiFePO <sub>4</sub> doped by Co, Mn and S elements for lithium-ion batteries. <i>Electrochimica Acta</i> , 2021, 388, 138592.	2.6	31
16113	Hot Carrier Dynamics at Ligated Silicon(111) Surfaces: A Computational Study. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 7504-7511.	2.1	3
16114	Orbital-scale understanding on high-selective hydrogenation of acetylene over Pt <sub>1</sub> -Cu(1 1 1) catalyst. <i>Chemical Engineering Science</i> , 2021, 240, 116664.	1.9	12
16115	Structure and Absolute Configuration of Phenanthro-erylene Quinone Pigments from the Deep-Sea Crinoid <i>Hyalocrinus naresianus</i> . <i>Marine Drugs</i> , 2021, 19, 445.	2.2	6
16116	CoAsS Kristalinin Bazı Fiziksel Özelliklerinin Basınçta İncelenmesi. <i>Yıldırım Dergisi Fen Bilimleri Enstitüsü Dergisi</i> , 0, , .	0,0	0
16117	Impact of NO <sub>x</sub> and NH <sub>3</sub> addition on toluene oxidation over MnO <sub>x</sub> -CeO <sub>2</sub> catalyst. <i>Journal of Hazardous Materials</i> , 2021, 416, 125939.	6.5	37
16118	Density functional theory calculation of the Renner-Teller effect in NCO : Preliminary assessment of exact exchange energy on the accuracy of the Renner coefficient. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26804.	1.0	1



#	ARTICLE	IF	CITATIONS
16119	Designing highly incompressible transition metal nitrides: A new class of $W_{0.5}Al_{0.5}N$ phases. Journal of Applied Physics, 2021, 130, 065105.	1.1	1
16120	Dependence of the substituent energy on the level of theory. Journal of Computational Chemistry, 2021, 42, 2079-2088.	1.5	6
16121	Strain induced structural phase transition in $TM_6X_6$ (TM = Mo, W; X = S, Se, Te) nanowires. Journal of Solid State Chemistry, 2021, 300, 122194.	1.4	3
16122	Optical and Thermodynamic Properties of Half-Heusler Compound $TaIrSn$ : Using Modified Becke-Johnson (mBJ). Journal of Superconductivity and Novel Magnetism, 2021, 34, 2865-2877.	0.8	6
16123	Arene and functionalized arene based two dimensional organic-inorganic hybrid perovskites for photovoltaic applications. Journal of Computational Chemistry, 2021, 42, 1982-1990.	1.5	16
16124	In situ study on the compression deformation of $MoNbTaVW$ high-entropy alloy. Journal of Alloys and Compounds, 2021, 871, 159557.	2.8	7
16125	Adsorption and activation of $CO_2$ on $Pt/CeO_x/TiO_2(110)$ : Role of the Pt-CeOx interface. Surface Science, 2021, 710, 121852.	0.8	5
16126	Theoretical study on structural, excitonic and electronic properties of $Nb_2O_5$ with five crystal structures. Materials Science in Semiconductor Processing, 2021, 130, 105831.	1.9	3
16127	Solvent-free synthesis of N-doped carbon-based catalyst for high-efficient reduction of 4-nitrophenol. Journal of Environmental Chemical Engineering, 2021, 9, 105649.	3.3	8
16128	Catalytic Role of Adsorption of Electrolyte/Molecules as Functional Ligands on Two-Dimensional $TM-N_4$ Monolayer Catalysts for the Electrocatalytic Nitrogen Reduction Reaction. ACS Applied Materials & Interfaces, 2021, 13, 40590-40601.	4.0	11
16129	Preparation and characterization of $Ag_2ZnSn(S,Se)_4$ and its application in improvement of power conversion efficiency of $Cu_2ZnSn(S,Se)_4$ -based solar cells. Ceramics International, 2021, 47, 34473-34480.	2.3	4
16130	Electronic Mechanism of Martensitic Transformation in Nb-doped NiTi Alloys: A First-Principles Investigation. ACS Omega, 2021, 6, 22033-22038.	1.6	2
16131	Surface structure of mass-selected niobium oxide nanoclusters on Au(111). Nanotechnology, 2021, 32, 475601.	1.3	7
16132	Toward the Proper Selection of Carbon Electrode Materials for Energy Storage Applications: Experimental and Theoretical Insights. Energy & Fuels, 2021, 35, 13426-13437.	2.5	12
16133	A DFT Investigation of the Adsorption of Phosphate Ions on Co- and Ni-Doped Graphene. Nano, 2021, 16, .	0.5	2
16134	Anomalies in the dynamics of a metallic glass-forming liquid under super-high pressure. Journal of Molecular Liquids, 2021, 335, 116138.	2.3	1
16135	Evolution of Ferromagnetic and Antiferromagnetic States in Iron Nitride Clusters $Fe_nN$ and $Fe_nN_2$ ( $n = 1-10$ ). Journal of Physical Chemistry A, 2021, 125, 7891-7899.	1.1	4
16136	Electronic, optical, and vibrational properties of $B_3N_3H_6$ from first-principles calculations. Journal of Molecular Modeling, 2021, 27, 241.	0.8	0

#	ARTICLE	IF	CITATIONS
16137	Modulation of the Second Order Nonlinear Optical Properties of Helical Graphene Nanoribbons Through Introducing Azulene Defects or/and BN Units. Chemical Research in Chinese Universities, 2022, 38, 974-984.	1.3	3
16138	Study of the solar perovskite CsMBr <sub>3</sub> (M=Pb or Ge) photovoltaic materials: Band-gap engineering. Solid State Sciences, 2021, 118, 106679.	1.5	20
16139	Stability, electronic structure, and magnetic moment of vanadium phthalocyanine grafted to the Au(111) surface. Journal of Chemical Physics, 2021, 155, 074701.	1.1	0
16140	Chirality recognition and separation of 4-ethynyltriphenylamine induced by chiral Kagomé network on Cu(111). Chemical Physics, 2021, 548, 111216.	0.9	0
16141	Catalytic performance of Pt <sub>3</sub> Ni cluster toward ethane activation. Chemical Physics, 2021, 548, 111204.	0.9	2
16142	Dissociation of water on atomic oxygen-covered Rh nanoclusters supported on graphene/Ru(0001). Journal of Chemical Physics, 2021, 155, 074701.	1.2	1
16143	Surface fluorinated nickel-graphene nanocomposites for high-efficiency methanol electrooxidation. International Journal of Hydrogen Energy, 2021, 46, 27138-27148.	3.8	5
16144	Hydrogen storage on Li-decorated B <sub>4</sub> N: a first-principle calculation insight. Journal Physics D: Applied Physics, 2021, 54, 445501.	1.3	15
16145	Distortion of the Coordination Structure and High Symmetry of the Crystal Structure in In <sub>4</sub> SnS <sub>8</sub> Microflowers for Enhancing Visible-Light Photocatalytic CO <sub>2</sub> Reduction. ACS Catalysis, 2021, 11, 11029-11039.	5.5	37
16146	Synthesis and Characterization of a complex mixture based on cobalt and tin and study of its application towards production of hydrogen gas from ethanol. IOP Conference Series: Materials Science and Engineering, 2021, 1170, 012002.	0.3	0
16147	Formation and influence of surface hydroxyls on product selectivity during CO <sub>2</sub> hydrogenation by Ni/SiO <sub>2</sub> catalysts. Journal of Catalysis, 2021, 400, 228-233.	3.1	27
16148	Reliable TDDFT Protocol Based on a Local Hybrid-Functional for the Prediction of Vibronic Phosphorescence Spectra Applied to Tris(2,2'-bipyridine)-Metal Complexes. Journal of Physical Chemistry A, 2021, 125, 7099-7110.	1.1	13
16149	Ab initio four-band Wannier tight-binding model for generic twisted graphene systems. Physical Review B, 2021, 104, .	1.1	12
16150	Investigation of photocatalytic properties based on Fe and Ce Co-doped ZnO via hydrothermal method and first principles. Materials Science in Semiconductor Processing, 2021, 131, 105835.	1.9	21
16151	Unraveling the decisive role of surface CeO <sub>2</sub> nanoparticles in the Pt-CeO <sub>2</sub> /MnO <sub>2</sub> hetero-catalysts for boosting toluene oxidation: Synergistic effect of surface decorated and intrinsic O-vacancies. Chemical Engineering Journal, 2021, 418, 129399.	6.6	132
16152	Investigation of the photocatalytic properties of U-Mo alloys with respect to composition and temperature in the U-Mo system. Journal of Nuclear Materials, 2021, 552, 152970.	1.3	10
16153	Stepwise Evolution of Photocatalytic Spinel-Structured (Co,Cr,Fe,Mn,Ni) <sub>3</sub> O <sub>4</sub> High Entropy Oxides from First-Principles Calculations to Machine Learning. Crystals, 2021, 11, 1035.	1.0	11
16154	Sulfur doping effect on the electronic properties of zirconium dioxide ZrO <sub>2</sub> . Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2021, 270, 115200.	1.7	28

#	ARTICLE	IF	CITATIONS
16155	Structural, elastic, vibrational, electronic and optical properties of SmFeO <sub>3</sub> using density functional theory. <i>Physica B: Condensed Matter</i> , 2021, 615, 413061.	1.3	14
16156	Various Exchange-Correlation Effects on Structural, Electronic, and Optical Properties of Brookite TiO <sub>2</sub> . <i>ECS Journal of Solid State Science and Technology</i> , 2021, 10, 083010.	0.9	8
16157	Effects of the Goethite Surface Hydration Microstructure on the Adsorption of the Collectors Dodecylamine and Sodium Oleate. <i>Langmuir</i> , 2021, 37, 10052-10060.	1.6	18
16158	C2-selective alkylation of pyridines by rhodium–aluminum complexes. <i>Tetrahedron</i> , 2021, 95, 132339.	1.0	19
16159	GFCCLib: Scalable and efficient coupled-cluster Green's function library for accurately tackling many-body electronic structure problems. <i>Computer Physics Communications</i> , 2021, 265, 108000.	3.0	8
16160	First-Principles Study of Hydrogen Storage of Sc-Modified Semiconductor Covalent Organic Framework-1. <i>ACS Omega</i> , 2021, 6, 21985-21993.	1.6	10
16161	Design single nonmetal atom doped 2D Ti <sub>2</sub> CO <sub>2</sub> electrocatalyst for hydrogen evolution reaction by coupling electronic descriptor. <i>Applied Surface Science</i> , 2021, 556, 149778.	3.1	15
16162	Effect of sulfur deficiency on the structural, optical and electronic properties of MnS nanostructures. <i>Chemical Physics Letters</i> , 2021, 779, 138877.	1.2	20
16163	Ab-initio study on physical properties of intermetallic LiPb compound. <i>Journal of Computational Science</i> , 2021, 54, 101428.	1.5	3
16164	Trimetallic Metal–Organic Framework Nanoframe Superstructures: A Stress–Buffering Architecture Engineering of Anode Material toward Boosted Lithium Storage Performance. <i>Energy and Environmental Materials</i> , 2023, 6, .	7.3	7
16165	TiN inducing ferrite nucleation based on the bcc-Fe/TiN interfaces formation at atomic scale by first-principles calculation. <i>Computational Materials Science</i> , 2021, 197, 110570.	1.4	16
16166	Regulation mechanism of the solvent coligands on the magnetic properties of azido-Cu(II) complexes by mixed carboxylate/alkanols ligands: A theoretical exploration. <i>Polyhedron</i> , 2021, 205, 115312.	1.0	5
16167	Free energies of iron phases at high pressure and temperature: Molecular dynamics study. <i>Physical Review B</i> , 2021, 104, .	1.1	18
16168	Tailoring the Structural and Electronic Properties of Graphene through Ion Implantation. <i>Materials</i> , 2021, 14, 5080.	1.3	3
16169	Computer simulation of the three-dimensional structure of fluorinated graphene crystals. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2022, 30, 160-166.	1.0	1
16170	Li-decorated B <sub>2</sub> O as potential candidates for hydrogen storage: A DFT simulations study. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 33486-33495.	3.8	35
16171	Benzothiazole–based chemosensor: a quick dip into its anion sensing mechanism. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, e4283.	0.9	2
16172	Relevance of Dispersion and the Electronic Spin in the DFT + <i>U</i> Approach for the Description of Pristine and Defective TiO <sub>2</sub> Anatase. <i>ACS Omega</i> , 2021, 6, 23170-23180.	1.6	4

#	ARTICLE	IF	CITATIONS
16173	Robust large-gap topological insulator phase in transition-metal chalcogenide $ZrTe_4$ Se. <i>New Journal of Physics</i> , 2021, 23, 093046.	1.2	0
16174	Coronene-Based 2D Metal-Organic Frameworks: A New Family of Promising Single-Atom Catalysts for Nitrogen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2021, 125, 20870-20876.	1.5	13
16175	Ab-Initio Predictions of the Energy Harvesting Performance of L-Arginine and L-Valine Single Crystals. <i>Frontiers in Mechanical Engineering</i> , 2021, 7, .	0.8	5
16176	Characterizing the defects and ferromagnetism in metal oxides: The case of magnesium oxide. <i>Materials Characterization</i> , 2021, 179, 111366.	1.9	9
16177	Fluorine incorporation into calcite, aragonite and vaterite $CaCO_3$ : Computational chemistry insights and geochemistry implications. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 308, 384-392.	1.6	6
16178	Influence of hydrogen isotopes on vacancy formation and antisite defect diffusion in palladium and vanadium metals. <i>Computational Materials Science</i> , 2021, 197, 110641.	1.4	3
16179	Zn-air battery operated with a 3DOM trimetallic spinel ( $Mn_{0.5}Ni_{0.5}Co_2O_4$ ) as the oxygen electrode. <i>Electrochimica Acta</i> , 2021, 391, 138900.	2.6	26
16180	The interaction of flotation reagents with metal ions in mineral surfaces: A perspective from coordination chemistry. <i>Minerals Engineering</i> , 2021, 171, 107067.	1.8	101
16181	Machine learning for materials discovery: Two-dimensional topological insulators. <i>Applied Physics Reviews</i> , 2021, 8, .	5.5	34
16182	Anomalous heavy doping in chemical-vapor-deposited titanium trisulfide nanostructures. <i>Physical Review Materials</i> , 2021, 5, .	0.9	3
16183	Comparison of sulfur poisoning resistance of Ce/Mn doped $\hat{1}^3$ -Fe $2O_3$ (0 0 1) surface in $NH_3$ -SCR reaction with DFT method. <i>Applied Surface Science</i> , 2021, 561, 149847.	3.1	20
16184	The 3d transition-metals doping tunes the electronic and magnetic properties of 2D monolayer $InP_3$ . <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 533, 168026.	1.0	11
16185	Fe@B $6H_6$ aggregates: from simple building blocks to graphene analogue. <i>Journal of Molecular Modeling</i> , 2021, 27, 273.	0.8	0
16186	Superior room-temperature power factor in GeTe systems via multiple valence band convergence to a narrow energy range. <i>Materials Today Physics</i> , 2021, 20, 100484.	2.9	5
16187	Molecular orbital study of Fe(II) and Fe(III) complexation with salicylate and citrate ligands: Implications for soil biogeochemistry. <i>Soil Science Society of America Journal</i> , 2022, 86, 181-194.	1.2	3
16188	Effects of Temperature on Enantiomerization Energy and Distribution of Isomers in the Chiral $Cu_{13}$ Cluster. <i>Molecules</i> , 2021, 26, 5710.	1.7	8
16189	Associative vs. dissociative mechanism: Electrocatalysis of nitric oxide to ammonia. <i>Chinese Chemical Letters</i> , 2022, 33, 1051-1057.	4.8	61
16190	Promotional Role of a Cation Intermediate Complex in $C_2$ Formation from Electrochemical Reduction of $CO_2$ over Cu. <i>ACS Catalysis</i> , 2021, 11, 12336-12343.	5.5	60

#	ARTICLE	IF	CITATIONS
16191	A member of p-type TCO family: Sn <sub>2</sub> TaxNb <sub>2-x</sub> O <sub>7</sub> with a tunable band gap and controllable hole mobility. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2021, 271, 115255.	1.7	0
16192	Theoretical Insights into Optoelectronic Properties of Non-Fullerene Acceptors for the Design of Organic Photovoltaics. <i>ACS Applied Energy Materials</i> , 2021, 4, 11090-11100.	2.5	6
16193	Study the effect of silver ion implantation on the structural, optical, and electrical properties of copper oxide thin films: an experimental and theoretical approach. <i>European Physical Journal Plus</i> , 2021, 136, 1.	1.2	4
16194	Synthesis and structural, crystallographic, electronic, chemical and optical characterizations of alpha-diisopropylammonium bromide (I±-DIPAB) thin films. <i>Optik</i> , 2021, 241, 167014.	1.4	5
16195	Interaction studies of dichlobenil and isoproturon on square-octagon phosphorene nanotube based on DFT frame work. <i>Chemical Physics Letters</i> , 2021, 778, 138773.	1.2	26
16196	Architecture of NaFe(MoO <sub>4</sub> ) <sub>2</sub> as a novel anode material for rechargeable lithium and sodium ion batteries. <i>Applied Surface Science</i> , 2021, 559, 149903.	3.1	7
16197	Modeling twin boundary structures in body centered cubic transition metals. <i>Computational Materials Science</i> , 2021, 197, 110649.	1.4	10
16198	Metal-free boron and sulphur co-doped carbon nanofibers with optimized p-band centers for highly efficient nitrogen electroreduction to ammonia. <i>Applied Catalysis B: Environmental</i> , 2021, 292, 120144.	10.8	55
16199	DFT study of Se and Te doped SrTiO <sub>3</sub> for enhanced visible-light driven photocatalytic hydrogen production. <i>Optical and Quantum Electronics</i> , 2021, 53, 1.	1.5	11
16200	Double Transition Metal Carbides MXenes (D-MXenes) as Promising Electrocatalysts for Hydrogen Reduction Reaction: <i>Ab Initio</i> Calculations. <i>ACS Omega</i> , 2021, 6, 23676-23682.	1.6	14
16201	Nanomolecular Metallurgy: Transformation from Au <sub>144</sub> (SCH <sub>2</sub> CH <sub>2</sub> Ph) <sub>60</sub> to Au <sub>279</sub> (SPh-t-Bu) <sub>84</sub> . <i>Journal of Physical Chemistry C</i> , 2021, 125, 20488-20502.	1.5	4
16202	Graphite to AlB <sub>2</sub> and MgB <sub>2</sub> : a comparative study of their tight-binding model and Dirac nodal line. <i>Philosophical Magazine</i> , 0, , 1-15.	0.7	1
16203	Surface-Plasmon Properties of Noble Metals with Exotic Phases. <i>Journal of Physical Chemistry C</i> , 2021, 125, 21521-21532.	1.5	5
16204	Density-functional theory calculation of magnetic properties of BiFeO <sub>3</sub> and BiCrO <sub>3</sub> under epitaxial strain. <i>Journal of Applied Physics</i> , 2021, 130, .	1.1	2
16205	Understanding chemical short-range ordering/demixing coupled with lattice distortion in solid solution high entropy alloys. <i>Acta Materialia</i> , 2021, 216, 117140.	3.8	52
16206	Corrosion inhibition of locally de-passivated surfaces by DFT study of 2-mercaptobenzothiazole on copper. <i>Npj Materials Degradation</i> , 2021, 5, .	2.6	15
16207	Insights into the borohydride electrooxidation reaction on metallic nickel from operando FTIRS, on-line DEMS and DFT. <i>Electrochimica Acta</i> , 2021, 389, 138721.	2.6	14
16208	Reproduction of Melting and Crystallization of Sodium by Machine-Learning Interatomic Potential Based on Artificial Neural Networks. <i>Journal of the Physical Society of Japan</i> , 2021, 90, 094603.	0.7	2

#	ARTICLE	IF	CITATIONS
16209	Basic physical behavior of impurity carbon in molybdenum for nuclear material: A systematical first-principles simulation. <i>Nuclear Materials and Energy</i> , 2021, 28, 101053.	0.6	1
16210	Spin-polarized gap in the magnetic Weyl semimetal $\text{CoS}_2$ . <i>Physical Review B</i> , 2021, 104, .	1.1	9
16211	Recent developments in two-dimensional layered tungsten dichalcogenides based materials for gas sensing applications. <i>Materials Today Communications</i> , 2021, 28, 102717.	0.9	6
16212	Interfacial Proton Transfer for Hydrogen Evolution at the Sub-Nanometric Platinum/Electrolyte Interface. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 47252-47261.	4.0	4
16213	A systematic computational study to understand the effect of metals (Mg, Ca, Sr) doping and external isotropic static pressure on phase stability, electronic band structure and optical properties of $\text{KNbO}_3$ . <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2021, 271, 115261.	1.7	7
16214	Effects of Interfacial Termination, Oxidation, and Film Thickness on the Magnetic Anisotropy in $\text{Mn}_{2.25}\text{Co}_{0.75}\text{Ga}_{0.5}\text{Sn}_{0.5}/\text{MgO}$ Heterostructures. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 47293-47301.	4.0	3
16215	First principles calculations on the novel high pressure phase of HfC. <i>International Journal of Modern Physics B</i> , 2021, 35, .	1.0	0
16216	Benchmark test of a dispersion corrected revised Tao-Mo semilocal functional for thermochemistry, kinetics, and noncovalent interactions of molecules and solids. <i>Journal of Chemical Physics</i> , 2021, 155, 114102.	1.2	4
16217	In Situ Defect Induction in Close-Packed Lattice Plane for the Efficient Zinc Ion Storage. <i>Small</i> , 2021, 17, e2101944.	5.2	24
16218	Interface-strain-confined synthesis of amorphous $\text{TiO}_2$ mesoporous nanosheets with stable pseudocapacitive lithium storage. <i>Chemical Engineering Journal</i> , 2021, 420, 129894.	6.6	28
16219	Strategy to utilize amorphous phase of semiconductor toward excellent and reliable photochemical water splitting performance: Roles of interface dipole moment and reaction parallelization. <i>International Journal of Energy Research</i> , 2022, 46, 3674-3685.	2.2	5
16220	Electric field polarized sulfonated carbon dots/NiFe layered double hydroxide as highly efficient electrocatalyst for oxygen evolution reaction. <i>Chemical Engineering Journal</i> , 2021, 420, 129690.	6.6	16
16221	System Theoretical Study on the Effect of Variable Nonmetallic Doping on Improving Catalytic Activity of $2\text{D-Ti}_3\text{C}_2\text{O}_2$ for Hydrogen Evolution Reaction. <i>Nanomaterials</i> , 2021, 11, 2497.	1.9	6
16222	Engineering microstructure of $\text{LiFe}(\text{MoO}_4)_2$ as an advanced anode material for rechargeable lithium-ion battery. <i>Journal of Materials Science: Materials in Electronics</i> , 2021, 32, 24273-24284.	1.1	7
16223	Theoretical Insights into $\text{Na}_5\text{M}(\text{PO}_4)_2\text{F}_2$ (M = Cr, V): A Fluorophosphate-Based High-Performance Cathode System for Sodium-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2021, 125, 19593-19599.	1.5	3
16224	Metal-free tellurene cocatalyst with tunable bandgap for enhanced photocatalytic hydrogen production. <i>Materials Today Energy</i> , 2021, 21, 100720.	2.5	18
16225	Molecular Modeling and Reactivity of Thermally Altered Coals by Molecular Simulation Techniques. <i>Energy &amp; Fuels</i> , 0, , .	2.5	10
16226	Bandgap of two-dimensional materials: Thorough assessment of modern exchange-correlation functionals. <i>Journal of Chemical Physics</i> , 2021, 155, 104103.	1.2	26



#	ARTICLE	IF	CITATIONS
16227	Performance improvement of $\text{B}_3$ borophene in nitrogen fixation using single-atom anchoring: A first-principles study. Applied Surface Science, 2021, 560, 149667.	3.1	11
16228	Coordination Chemistry and Sensing Properties Towards Anions and Metal Ions of a Simple Fluorescent Urea. European Journal of Inorganic Chemistry, 2021, 2021, 3878.	1.0	3
16229	Kinetic analysis of the effect of $\text{O}_2$ on $\text{SF}_6$ over-thermal decomposition. Journal Physics D: Applied Physics, 2021, 54, 495502.	1.3	12
16230	Ethylene production by direct conversion of methane over isolated single active centers. Chemical Engineering Journal, 2021, 420, 130493.	6.6	20
16231	Absence of spillover of hydrogen adsorbed on small palladium clusters anchored to graphene vacancies. Applied Surface Science, 2021, 559, 149835.	3.1	17
16232	$\text{CaCl}_2$ and $\text{CaCl}_2 \cdot 2\text{H}_2\text{O}$ on $\text{Pt}(\text{111})$ and $\text{Pt}(\text{110})$ surfaces: A DFT study. Applied Surface Science, 2021, 559, 149835.	3.1	17
16233	Flux growth synthesis, single crystal and electronic structure of the new intermetallic compound $\text{Pt}_2\text{Ca}_{17}\text{Ta}_3$ . Computational Materials Science, 2021, 197, 110591.	1.4	0
16234	Van der Waals heterostructure $\text{Pt}/\text{Pt}(\text{111})/\text{Pt}(\text{110})$ for topological valleytronics. Physical Review B, 2021, 104, .	1.4	0
16235	Synthesis and characterization of Layered Double Hydroxides aimed at encapsulation of sodium diclofenac: Theoretical and experimental study. Journal of Molecular Liquids, 2021, 338, 116677.	2.3	6
16236	Fe-doped effects on phase transition and electronic structure of $\text{CeO}_2$ under compressed conditions from ab initio calculations. Applied Physics A: Materials Science and Processing, 2021, 127, 1.	1.1	3
16237	Synthesis, crystal and electronic structure of $\text{CaNi}_2\text{Al}_8$ . Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2021, 76, 659-668.	0.3	2
16238	Dimensional-Dependent Effects in Platinum Core-Shell-Based Catalysts for Fuel Cell Applications. ACS Applied Nano Materials, 2021, 4, 9697-9708.	2.4	13
16239	Ni-based catalysts derived from Ni-Zr-Al ternary hydrotalcites show outstanding catalytic properties for low-temperature $\text{CO}_2$ methanation. Applied Catalysis B: Environmental, 2021, 293, 120218.	10.8	62
16240	High uptake and fixation ability of BC monolayer for CO and NO toxic gases: a computational analysis. Journal of Materials Science, 2021, 56, 18566-18580.	1.7	0
16241	Effect of Potassium on Methanol Steam Reforming on the Cu(111) and Cu(110) Surfaces: A DFT Study. Journal of Physical Chemistry C, 2021, 125, 20905-20918.	1.5	12
16242	$\text{Na}_2\text{SO}_4/\text{NaCl}$ binary eutectic salt roasting to enhance extraction of lithium from pyrometallurgical slag of spent lithium-ion batteries. Chinese Journal of Chemical Engineering, 2022, 41, 294-300.	1.7	10
16243	An energetic phase of $\text{ZnN}_6$ at ambient conditions. Physica B: Condensed Matter, 2021, 617, 413139.	1.3	3
16244	Substrate orientation dependent structural, electronic and magnetic properties of V and Cr linear chains. Physica B: Condensed Matter, 2021, 617, 413132.	1.3	0

#	ARTICLE	IF	CITATIONS
16245	Combinations of density functionals for accurate molecular properties of Be/W/H compounds. Nuclear Materials and Energy, 2021, 28, 101026.	0.6	0
16246	Can We Predict the Isosymmetric Phase Transition? Application of DFT Calculations to Study the Pressure Induced Transformation of Chlorothiazide. International Journal of Molecular Sciences, 2021, 22, 10100.	1.8	4
16247	Stabilization of ferromagnetism in carbon doped Mg <sub>2</sub> Mn <sub>2</sub> O <sub>7</sub> clusters. International Journal of Computational Materials Science and Engineering, 0, , 2150022.	0.5	0
16248	Anomalous thermophysical properties and electrone transition in fcc potassium. Physical Review B, 2021, 104, .	1.1	0
16249	Metal heteroatom (Mg, Cu and Co) and porous carbon co-doped MIL-101 composites with superior acetone capture capacity. Chemical Engineering Journal, 2022, 430, 132656.	6.6	11
16250	Atomic-scale mechanism of rhombohedral twinning in sapphire. Acta Materialia, 2021, 216, 117137.	3.8	8
16251	Uncovering the Promotion of CeO <sub>2</sub> /CoS <sub>1.97</sub> Heterostructure with Specific Spatial Architectures on Oxygen Evolution Reaction. Advanced Materials, 2021, 33, e2102593.	11.1	118
16252	Ligand-to-Metal Charge-Transfer Photophysics and Photochemistry of Emissive d <sup>0</sup> Titanocenes: A Spectroscopic and Computational Investigation. Inorganic Chemistry, 2021, 60, 14399-14409.	1.9	17
16253	Sensitive H <sub>2</sub> gas sensors based on SnO <sub>2</sub> nanowires. Sensors and Actuators B: Chemical, 2021, 345, 130334.	4.0	82
16254	Factors affecting the vacancy formation energy in Fe <sub>70</sub> Ni <sub>10</sub> Cr <sub>20</sub> random concentrated alloy. Computational Materials Science, 2021, 198, 110669.	1.4	10
16255	A novel Hf <sub>2</sub> CO <sub>2</sub> /WS <sub>2</sub> van der Waals heterostructure as a potential candidate for overall water splitting photocatalyst. Materials Science in Semiconductor Processing, 2021, 133, 105947.	1.9	17
16256	The helium behavior and thermal stability of W/Ta bilayer nanocomposite investigated by neutron reflectometry. Nuclear Instruments & Methods in Physics Research B, 2021, 504, 43-49.	0.6	1
16257	Superhard carbon-rich C <sub>6</sub> N compounds hidden in compression of the mixture of carbon black and tetracyanoethylene. Carbon, 2021, 184, 846-854.	5.4	5
16258	La-doped TiO <sub>2</sub> nanorods toward boosted electrocatalytic N <sub>2</sub> -to-NH <sub>3</sub> conversion at ambient conditions. Chinese Journal of Catalysis, 2021, 42, 1755-1762.	6.9	35
16259	Robust type-II BP/AlN van der Waals heterostructure: A first-principles study. Chemical Physics Letters, 2021, 781, 138989.	1.2	3
16260	A rechargeable 6-electron Al <sub>2</sub> Se battery with high energy density. Energy Storage Materials, 2021, 41, 667-676.	9.5	44
16261	First-principles calculations to investigate electronic structure and transport properties of CrC monolayers: A new horizon for spintronic application. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2021, 272, 115379.	1.7	17
16262	Microscopic and atomistic mechanisms of sliding friction of MoS <sub>2</sub> : Effects of undissociated and dissociated H <sub>2</sub> O. Applied Surface Science, 2021, 563, 150270.	3.1	18

#	ARTICLE	IF	CITATIONS
16263	Investigation of material properties of halide mixed lead - Free double perovskite for optoelectronic applications using first-principles study. <i>Materials Science in Semiconductor Processing</i> , 2021, 133, 105963.	1.9	11
16264	Structural, electronics and optical properties of sodium based fluoroperovskites NaXF <sub>3</sub> (X = Ca, Mg, Sr). <i>Journal of Applied Physics</i> , 2021, 412, 127574.	0.9	31
16265	Meso-scale simulation on mechanism of Na <sup>+</sup> -gated water-conducting nanochannels in zeolite NaA. <i>Journal of Membrane Science</i> , 2021, 635, 119462.	4.1	5
16266	Advanced lithium-sulfur batteries enabled by a SnS <sub>2</sub> -Hollow carbon nanofibers Flexible Electro-catalytic Membrane. <i>Carbon</i> , 2021, 184, 1-11.	5.4	27
16267	Oxygen migration triggering molybdenum exposure in oxygen vacancy-rich ultra-thin Bi <sub>2</sub> MoO <sub>6</sub> nanoflakes: Dual binding sites governing selective CO <sub>2</sub> reduction into liquid hydrocarbons. <i>Journal of Energy Chemistry</i> , 2021, 61, 281-289.	7.1	40
16268	Optimized electrocatalytic performance of PtZn intermetallic nanoparticles for methanol oxidation by designing catalyst support and fine-tuning surface composition. <i>Electrochimica Acta</i> , 2021, 394, 139106.	2.6	6
16269	Tensile strain induced surface reactions for co-adsorption of H <sub>2</sub> O and OH <sup>-</sup> on vacancy Al (111) surface. <i>Vacuum</i> , 2021, 192, 110459.	1.6	2
16270	Influence of the Fe-doping on hydrogen behavior on the ZrCo surface. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 33877-33888.	3.8	10
16271	Enhancing the hydrogen evolution reaction by non-precious transition metal (Non-metal) atom doping in defective MoSi <sub>2</sub> N <sub>4</sub> monolayer. <i>Applied Surface Science</i> , 2021, 563, 150388.	3.1	49
16272	Molecular-level insights into the immobilization of vapor-phase mercury on Fe/Co/Ni-doped hierarchical molybdenum selenide. <i>Journal of Hazardous Materials</i> , 2021, 420, 126583.	6.5	7
16273	Performance enhancement of ZnGa <sub>2</sub> O <sub>4</sub> Schottky type deep-ultraviolet photodetectors by oxygen supercritical fluid treatment. <i>Results in Physics</i> , 2021, 29, 104764.	2.0	12
16274	Origin of ferromagnetism and the origin of covalent bonding in double perovskite compound Sr <sub>2</sub> CoRuO <sub>6</sub> . <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 535, 168175.	1.0	7
16275	Synergistic utilization of 3D materials merits and unidirectional electrons transfer of Schottky junction for optimizing optical absorption and charge kinetics. <i>Applied Catalysis B: Environmental</i> , 2021, 295, 120278.	10.8	23
16276	Assessment of density functional theory in studying on the transition states of a Diiron-mediated N-N bond cleavage reaction. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113418.	1.1	1
16277	Interaction studies of tuberculosis biomarker vapours on novel beta arsenene sheets - A DFT insight. <i>Computational and Theoretical Chemistry</i> , 2021, 1205, 113426.	1.1	15
16278	Density functional study of trans,trans,trans-[Pt(N <sub>3</sub> ) <sub>2</sub> (OH) <sub>2</sub> (Py) <sub>2</sub> ] on molecular structure and vibrational spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 261, 120022.	2.0	3
16279	Sorption studies of sulfadimethoxine and tetracycline molecules on $\hat{\Gamma}$ -antimonene nanotube - A first-principles insight. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 108, 107988.	1.3	14
16280	Formation of ordered B structure on W(100). <i>Surface Science</i> , 2021, 713, 121906.	0.8	7

#	ARTICLE	IF	CITATIONS
16281	Sensing ability of 2D Al <sub>2</sub> C monolayer toward toxic pnictogen hydrides: A first-principles perspective. <i>Sensors and Actuators A: Physical</i> , 2021, 331, 113000.	2.0	10
16282	Magnetic properties of Pr bulk and clusters determined using density functional theory calculations. <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 538, 168286.	1.0	0
16283	Electronic, optical, magneto-optical, and thermoelectric properties of the SrS graphene-like under Cr impurity. <i>Chemical Physics</i> , 2021, 551, 111355.	0.9	9
16284	Modulating CoFe <sub>2</sub> O <sub>4</sub> nanocube with oxygen vacancy and carbon wrapper towards enhanced electrocatalytic nitrogen reduction to ammonia. <i>Applied Catalysis B: Environmental</i> , 2021, 297, 120452.	10.8	42
16285	Highly disordering nanoporous frameworks of lanthanide-dicarboxylates for catalysis of CO <sub>2</sub> cycloaddition with epoxides. <i>Journal of Solid State Chemistry</i> , 2021, 303, 122464.	1.4	5
16286	Natural Honeycomb-like structure cork carbon with hierarchical Micro-Mesopores and N-containing functional groups for VOCs adsorption. <i>Applied Surface Science</i> , 2021, 565, 150550.	3.1	38
16287	A first-principles study of thiadiazole and dimercapto-thiadiazole adsorption on copper and silver surfaces. <i>Materials Chemistry and Physics</i> , 2021, 273, 125057.	2.0	6
16288	Effect of TiC surface oxide overlayer on the control of Li O behavior in lithium-oxygen batteries: Implications for cathode catalyst design. <i>Applied Surface Science</i> , 2021, 567, 150785.	3.1	1
16289	Functional group tuning of two-dimensional carbon nanosheets for boosting oxygen reduction electrocatalysis. <i>Carbon</i> , 2021, 185, 395-403.	5.4	10
16290	Coupling Ru-MoS <sub>2</sub> heterostructure with silicon for efficient photoelectrocatalytic water splitting. <i>Chemical Engineering Journal</i> , 2021, 423, 130231.	6.6	15
16291	Deformation strengthening mechanism of in situ TiC/TC4 alloy nanocomposites produced by selective laser melting. <i>Composites Part B: Engineering</i> , 2021, 225, 109305.	5.9	29
16292	The ground state structures and spectra of Ag <sub>20</sub> clusters and the adsorption to carbon monoxide. <i>Materials Chemistry and Physics</i> , 2021, 273, 125134.	2.0	8
16293	C-doped ZnS-ZnO/Rh nanosheets as multijunctioned photocatalysts for effective H <sub>2</sub> generation from pure water under solar simulating light. <i>Applied Catalysis B: Environmental</i> , 2021, 297, 120473.	10.8	45
16294	Effects of pressure on structural, electronic, optical, and mechanical properties of ZrTe <sub>5</sub> : A density functional theory study. <i>Physica B: Condensed Matter</i> , 2021, 620, 413286.	1.3	3
16295	Short-range ordering governs brittleness and ductility in W-Ta solid solution: Insights from Pugh's shear-to-bulk modulus ratio. <i>Scripta Materialia</i> , 2021, 204, 114136.	2.6	21
16296	Triggering in-plane defect cluster on MoS <sub>2</sub> for accelerated dinitrogen electroreduction to ammonia. <i>Journal of Energy Chemistry</i> , 2021, 62, 359-366.	7.1	40
16297	Press dependent electronic structure and optical property of Ba <sub>2</sub> Mg(PO <sub>4</sub> ) <sub>2</sub> :Eu <sup>2+</sup> . <i>Journal of Alloys and Compounds</i> , 2021, 883, 160870.	2.8	1
16298	Molecular structure, tautomer's, reactivity and inhibition studies on 6-Methyl-2-thiouracil for mild steel corrosion in aqueous HCl (1.00 M): Experimental and Theoretical Studies. <i>Journal of Molecular Structure</i> , 2021, 1244, 130927.	1.8	31

#	ARTICLE	IF	CITATIONS
16299	Magnetic properties and half metallic behavior of the Full-Heusler Co <sub>2</sub> FeGe alloy: DFT and Monte Carlo studies. <i>Journal of Solid State Chemistry</i> , 2021, 304, 122534.	1.4	32
16300	Hydrogen embrittlement of bulk W-0.5 wt% ZrC alloy induced by annealing in hydrogen atmosphere. <i>Journal of Nuclear Materials</i> , 2021, 556, 153177.	1.3	4
16301	Efficient photocatalytic H <sub>2</sub> O <sub>2</sub> production from oxygen and pure water over graphitic carbon nitride decorated by oxidative red phosphorus. <i>Applied Catalysis B: Environmental</i> , 2021, 298, 120522.	10.8	68
16302	Implications for the Nb aggregation inherited from melt to $\hat{\text{I}}^3$ phase of U-Nb alloy. <i>Journal of Alloys and Compounds</i> , 2021, 885, 160537.	2.8	0
16303	DFT simulation-based screening of single transition metals supported on g-C <sub>3</sub> N <sub>4</sub> for the catalytic oxidation of Hg <sup>0</sup> . <i>Fuel</i> , 2021, 305, 121456.	3.4	8
16304	A potential application of a crystal triazine organic framework in energy: Photocatalytic decomposition of water. <i>Physica B: Condensed Matter</i> , 2021, 623, 413342.	1.3	6
16305	Single Ni supported on Ti <sub>3</sub> C <sub>2</sub> O <sub>2</sub> for uninterrupted CO <sub>2</sub> catalytic hydrogenation to formic acid: A DFT study. <i>Separation and Purification Technology</i> , 2021, 279, 119722.	3.9	14
16306	Electrically-tuned transition of band alignment in arsenene/MoTe <sub>2</sub> van der Waals heterostructures. <i>Vacuum</i> , 2021, 194, 110612.	1.6	3
16307	Supercapattery electrode materials by Design: Plasma-induced defect engineering of bimetallic oxyphosphides for energy storage. <i>Journal of Colloid and Interface Science</i> , 2021, 603, 478-490.	5.0	30
16308	Sc <sub>2</sub> CO-MXene/h-BN heterostructure with synergetic effect as an anchoring and catalytic material for lithium-sulfur battery. <i>Journal of Alloys and Compounds</i> , 2021, 887, 161273.	2.8	15
16309	Electronic tuning of SrIrO <sub>3</sub> perovskite nanosheets by sulfur incorporation to induce highly efficient and long-lasting oxygen evolution in acidic media. <i>Applied Catalysis B: Environmental</i> , 2021, 298, 120562.	10.8	55
16310	The roles of Cl <sup>•</sup> and OH <sup>•</sup> in the dissociation of H <sub>2</sub> O molecules on an Al surface: A first-principles calculation. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 159, 110281.	1.9	2
16311	Cubic to tetragonal structural phase transformation in NaNbO <sub>3</sub> with peculiar Mg and Ca doping and its repercussions on optoelectronic properties. <i>Optik</i> , 2021, 247, 168017.	1.4	3
16312	First-principles study of helium in austenitic Fe 6.3 at% Cr alloys: Structural, stability, energetics, and clustering with vacancies. <i>Materials Today Communications</i> , 2021, 29, 102837.	0.9	4
16313	Probing the role of surface hydroxyls for Bi, Sn and In catalysts during CO <sub>2</sub> Reduction. <i>Applied Catalysis B: Environmental</i> , 2021, 298, 120581.	10.8	54
16314	A supramolecular H <sub>12</sub> SubPcB-OPhCOPh/TiO <sub>2</sub> Z-scheme hybrid assembled via dimeric concave-ligand $\pi$ - $\pi$ interaction for visible photocatalytic oxidation of tetracycline. <i>Applied Catalysis B: Environmental</i> , 2021, 298, 120550.	10.8	43
16315	First-principles study of vacancy interaction with grain boundaries of tungsten under tensile strains. <i>Computational Materials Science</i> , 2021, 200, 110760.	1.4	3
16316	Green synthesis of antimicrobial silver nanoparticles using fruit extract of <i>Glycosmis pentaphylla</i> and its theoretical explanations. <i>Journal of Molecular Structure</i> , 2022, 1247, 131361.	1.8	35

#	ARTICLE	IF	CITATIONS
16317	Sulfurized-polyacrylonitrile in lithium-sulfur batteries: Interactions between undercoordinated carbons and polymer structure under low lithiation. <i>Journal of Energy Chemistry</i> , 2022, 66, 587-596.	7.1	13
16318	Fluorine-doped graphene oxide prepared by direct plasma treatment for supercapacitor application. <i>Chemical Engineering Journal</i> , 2022, 428, 132086.	6.6	41
16319	Unraveling U6+, Am3+&Eu3+ ionâ€™s distribution in Ca10(PO4)6F2for radioactive waste immobilization and the associated U6+â†’ Eu3+energy transfer dynamics for tunable emission characteristics. <i>Journal of Hazardous Materials</i> , 2022, 423, 126980.	6.5	6
16320	Revealing the Al/L12-Al3Zr inter-facial properties: Insights from first-principles calculations. <i>Vacuum</i> , 2022, 195, 110620.	1.6	15
16321	A theoretical study of the twinned ZnO nanostructures. <i>Applied Surface Science</i> , 2022, 571, 151295.	3.1	0
16322	Metallic phase WO.9Mo0.1S2 for high-performance anode of sodium ion batteries through suppressing the dissolution of polysulfides. <i>Journal of Energy Chemistry</i> , 2022, 66, 356-365.	7.1	13
16323	Study the electronic and magnetic properties of MnxZn1-xO supercell using first principle calculation. <i>Materials Science in Semiconductor Processing</i> , 2022, 137, 106179.	1.9	0
16324	Short-range order clusters in the long-period stacking/order phases with an intrinsic-I type stacking fault in Mg-Co-Y alloys. <i>Scripta Materialia</i> , 2022, 207, 114282.	2.6	30
16325	Application of hybrid MOF composite in extraction of f-block elements: Experimental and computational investigation. <i>Chemosphere</i> , 2022, 287, 132232.	4.2	12
16326	The formation of atomic and sub-nano scale pores under tensile strain in oxide films on Zr alloys: A first-principles study. <i>Applied Surface Science</i> , 2022, 571, 151316.	3.1	2
16327	Taming the challenges of activity and selectivity in catalysts for electrochemical N2 fixation via single metal atom supported on WS2. <i>Applied Surface Science</i> , 2022, 571, 151357.	3.1	16
16328	First principles study on the oxygen reduction reaction of Ir@Pt core-shell structure. <i>Chemical Physics</i> , 2022, 552, 111356.	0.9	3
16329	Enhanced sorption of the UV filter 4-methylbenzylidene camphor on aged PET microplastics from both experimental and theoretical perspectives. <i>RSC Advances</i> , 2021, 11, 32494-32504.	1.7	10
16330	Stacking fault energy and electronic structure of molybdenum under solid solution softening/hardening. <i>Journal of Central South University</i> , 2021, 28, 39-47.	1.2	5
16331	Induction of Room Temperature Ferromagnetism in N-Doped Yttrium Oxide: Ab Initio Calculation. <i>JETP Letters</i> , 2021, 113, 120-126.	0.4	0
16332	Can ultra-thin Si FinFETs work well in the sub-10 nm gate-length region?. <i>Nanoscale</i> , 2021, 13, 5536-5544.	2.8	15
16333	Nb-Doped nickel nitride-derived catalysts for electrochemical water splitting. <i>Catalysis Science and Technology</i> , 2021, 11, 6455-6461.	2.1	6
16334	Assembling organicâ€™inorganic building blocks for high-capacity electrode design. <i>Materials Horizons</i> , 2021, 8, 1825-1834.	6.4	1



#	ARTICLE	IF	CITATIONS
16335	Structure, intermolecular interactions, and dynamic properties of NTO crystals with impurity defects: a computational study. <i>CrystEngComm</i> , 2021, 23, 2455-2468.	1.3	14
16336	The mechanism behind the photochromism and photomagnetism of type II biindenylidenediones: multiconfigurational, perturbative and density functional theory studies. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17453-17465.	1.3	0
16337	Predictive Modeling of Ceramic Materials. , 2021, , 475-480.		0
16338	Assessing Nickel Titanium Binary Systems Using Structural Search Methods and Ab Initio Calculations. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1578-1591.	1.5	3
16339	High-throughput screening of single metal atom anchored on N-doped boron phosphide for N <sub>2</sub> reduction. <i>Nanoscale</i> , 2021, 13, 13437-13450.	2.8	18
16340	A sandwich-like Ga <sub>2</sub> FeS <sub>4</sub> -supported single metal atom as a promising bifunctional electrocatalyst for overall water splitting. <i>Journal of Materials Chemistry A</i> , 2021, 9, 18594-18603.	5.2	4
16341	Sulfur-doped g-C <sub>3</sub> N <sub>4</sub> for efficient photocatalytic CO <sub>2</sub> reduction: insights by experiment and first-principles calculations. <i>Catalysis Science and Technology</i> , 2021, 11, 1725-1736.	2.1	51
16342	Unraveling the site-specific energy transfer driven tunable emission characteristics of Eu <sup>3+</sup> & Tb <sup>3+</sup> co-doped Ca <sub>10</sub> (PO <sub>4</sub> ) <sub>6</sub> F <sub>2</sub> phosphors. <i>RSC Advances</i> , 2021, 11, 31421-31432.	1.7	8
16343	Tailoring the catalytic performance of single platinum anchored on graphene by vacancy engineering for propane dehydrogenation: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22004-22013.	1.3	4
16344	DFT insight into the effect of Cu atoms on adsorption and dissociation of CO <sub>2</sub> over a Pd <sub>8</sub> /TiO <sub>2</sub> (101) surface. <i>RSC Advances</i> , 2021, 11, 17391-17398.	1.7	4
16345	Computational modelling of Pd-catalysed alkoxy carbonylation of alkenes and alkynes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15869-15880.	1.3	7
16346	First-principles study of properties of rare-earth-doped LiFePO <sub>4</sub> . <i>Wuli Xuebao/Acta Physica Sinica</i> , 2021, 70, 158203.	0.2	4
16347	N-type and p-type molecular doping on monolayer MoS <sub>2</sub> . <i>RSC Advances</i> , 2021, 11, 8033-8041.	1.7	15
16348	Defects in H/He neutral beam irradiated potassium doped tungsten alloy by positron annihilation technique. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2021, 70, 167803.	0.2	3
16350	Synthesis, characterization and ab initio study of WO <sub>3</sub> nanocubes with peculiar electrochemical properties. <i>Journal of Nanoparticle Research</i> , 2021, 23, 1.	0.8	6
16351	Host dependent electrocatalytic hydrogen evolution of Ni/TiO <sub>2</sub> composites. <i>Journal of Materials Chemistry A</i> , 2021, 9, 6325-6334.	5.2	10
16352	Modelling high performance potassium-ion battery anode materials with two-dimensional vanadium carbide MXene: the role of surface O- and S-terminations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 3898-3904.	1.3	12
16353	The spin-dependent transport properties of defected zigzag graphene nanoribbons with graphene nanobubbles. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2753-2761.	1.3	5

#	ARTICLE	IF	CITATIONS
16354	Rational design of Ti-based oxygen redox layered oxides for advanced sodium-ion batteries. <i>Journal of Materials Chemistry A</i> , 2021, 9, 11762-11770.	5.2	11
16355	Structural Determination of a Graphite/Hexagonal Boron Nitride Superlattice Observed in the Experiment. <i>Inorganic Chemistry</i> , 2021, 60, 2598-2603.	1.9	6
16356	Machine learning to tame divergent density functional approximations: a new path to consensus materials design principles. <i>Chemical Science</i> , 2021, 12, 13021-13036.	3.7	23
16357	Low in-plane atomic density phosphorene anodes for lithium-/sodium-ion batteries. <i>Journal of Materials Chemistry C</i> , 2021, 9, 6802-6814.	2.7	8
16358	Impact of fluorination and chlorination on the electronic structure, topology and in-plane ring normal modes of pyridines. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18958-18974.	1.3	5
16359	How well do self-interaction corrections repair the overestimation of static polarizabilities in density functional calculations?. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18678-18685.	1.3	14
16360	Investigation of vanadia- $\alpha$ -alumina catalysts with solid-state NMR spectroscopy and DFT. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19352-19363.	1.3	1
16361	First-principles molecular dynamics study on the surface chemistry and nanotribological properties of MgAl layered double hydroxides. <i>Nanoscale</i> , 2021, 13, 5014-5025.	2.8	12
16362	Computational Investigation of MgH <sub>2</sub> /Graphene Heterojunctions for Hydrogen Storage. <i>Journal of Physical Chemistry C</i> , 2021, 125, 2357-2363.	1.5	33
16363	On the structure of Au <sub>11</sub> (SR) <sub>9</sub> and Au <sub>13</sub> (SR) <sub>11</sub> clusters. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19636-19646.	1.3	3
16364	Strain-controlled single Cr-embedded nitrogen-doped graphene achieves efficient nitrogen reduction. <i>Materials Advances</i> , 2021, 2, 5704-5711.	2.6	9
16365	Engineering Bimetallic NiFe-Based Hydroxides/Selenides Heterostructure Nanosheet Arrays for Highly Efficient Oxygen Evolution Reaction. <i>Small</i> , 2021, 17, e2007334.	5.2	103
16366	Electrochemically synthesized SnO <sub>2</sub> with tunable oxygen vacancies for efficient electrocatalytic nitrogen fixation. <i>Nanoscale</i> , 2021, 13, 16307-16315.	2.8	13
16367	Sulfur vacancies in Co <sub>9</sub> S <sub>8</sub> /N-doped graphene enhancing the electrochemical kinetics for high-performance lithium-sulfur batteries. <i>Journal of Materials Chemistry A</i> , 2021, 9, 10704-10713.	5.2	53
16368	A comparative DFT study of the oxidation of Al crystals and nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24004-24015.	1.3	9
16369	Adsorption energy as a promising single-parameter descriptor for single atom catalysis in the oxygen evolution reaction. <i>Journal of Materials Chemistry A</i> , 2021, 9, 6442-6450.	5.2	18
16374	Combining Electronic Structure Calculations and Spectroscopy to Unravel the Structure of Grafted Organometallic Complexes. , 0, , 359-374.		1
16375	Synthesis and Molecular Structure of Pseudo-Hexacoordinated Pnictines Bearing $\alpha$ -Phenylpyridine Ligands. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 4373-4379.	1.0	4

#	ARTICLE	IF	CITATIONS
16376	XYO <sub>3</sub> (X=K, Na; Y=Nb, Ta) based superlattices for photocatalysis. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2017, 14, 1700026.	0.8	6
16377	New structural motif of 18 valence electron molecules with a planar tetracoordinate heavier group 14 center: Unique stabilization effect of a $\pi$ -type skeleton. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25436.	1.0	3
16378	Electronic Modulation of Hierarchical Spongy Nanosheets toward Efficient and Stable Water Electrolysis. <i>Small</i> , 2021, 17, e2006881.	5.2	35
16379	Quantum-mechanical and Classical Simulations of Mg-Ca Carbonates. <i>Topics in Molecular Organization and Engineering</i> , 1997, , 113-156.	0.1	5
16380	Modelling of Oxide-Supported Metals. <i>Progress in Theoretical Chemistry and Physics</i> , 2001, , 109-147.	0.2	2
16381	An Ab-Initio Study of Mechanical Behavior for (A <sub>n</sub> -O) <sub>n</sub> Nanorods. , 2006, , 23-32.		1
16383	Hohenberg-Kohn-Sham Density Functional Theory. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2007, , 153-201.	0.6	1
16384	Orbital-Dependent Functionals for the Exchange-Correlation Energy: A Third Generation of Density Functionals. <i>Lecture Notes in Physics</i> , 2003, , 56-122.	0.3	45
16386	Analysis and modelling of atomic and molecular kohn-sham potentials. <i>Topics in Current Chemistry</i> , 1996, , 107-167.	4.0	31
16387	A Critical Assessment of Density Functional Theory with Regard to Applications in Organometallic Chemistry. <i>Topics in Organometallic Chemistry</i> , 1999, , 109-163.	0.7	59
16388	Applications of Computer Simulations and Statistical Mechanics in Surface Electrochemistry. <i>Modern Aspects of Electrochemistry</i> , 2009, , 131-149.	0.2	2
16389	Density-Functional Theory in External Electric and Magnetic Fields. <i>Modern Aspects of Electrochemistry</i> , 2009, , 341-408.	0.2	1
16390	Ab Initio Study of Ideal Shear Strength. <i>Solid Mechanics and Its Applications</i> , 2004, , 401-410.	0.1	4
16391	Tight-Binding Total Energy Methods for Magnetic Materials and Multi-Element Systems. , 2005, , 275-305.		1
16392	Secondary Magnetic Properties. , 2003, , 131-184.		1
16393	Density Functional Theory for The Study of Single-Molecule Electronic Systems. , 1999, , 439-450.		3
16395	Metallic Surfaces and Density Functional Theory. <i>NATO ASI Series Series B: Physics</i> , 1995, , 393-430.	0.2	3
16396	Energetics of Solid Surfaces: Clusters and Anticlusters, Generalized Liquid-Drop Model, Energy Density, Stress Field, and Rigorous Theorems. <i>NATO ASI Series Series B: Physics</i> , 1995, , 559-577.	0.2	4

#	ARTICLE	IF	CITATIONS
16397	Density Gradient Expansion of the Electronic Exchange-Correlation Energy, and its Generalization. NATO ASI Series Series B: Physics, 1995, , 51-64.	0.2	3
16398	A Local View of Bonding and Diffusion at Metal Surfaces. NATO ASI Series Series B: Physics, 1997, , 11-22.	0.2	1
16399	Density-Functional Theory of Surface Diffusion and Epitaxial Growth of Metals. NATO ASI Series Series B: Physics, 1997, , 83-101.	0.2	7
16400	Mixing Exact Exchange with GGA: When to Say When. , 1998, , 57-68.		32
16401	Density Functional Theory, Its Gaussian Implementation and Applications to Complex Systems. NATO ASI Series Series B: Physics, 1994, , 411-445.	0.2	10
16402	Photovoltaic Materials Design by Computational Studies: Metal Sulfides. , 2020, , 123-138.		2
16403	Making Computer Materials Real: The Predictive Power of First-Principles Molecular Dynamics. Springer Series in Materials Science, 2020, , 3-21.	0.4	1
16404	DFT-Parameterized Object Kinetic Monte Carlo Simulations of Radiation Damage. , 2020, , 2457-2488.		1
16405	Linear Scaling DFT for defects in metals. , 2014, , 265-272.		1
16406	Theoretical Investigation of the Self-Diffusion on Au(100). , 2007, , 171-185.		1
16407	Mechanism of Chiral Growth of 6, 13-Pentacenequinone Films on Si (111). Advances in Materials Research, 2008, , 281-293.	0.2	1
16408	Hydride Vapor Phase Epitaxy of GaN. Springer Series in Materials Science, 2010, , 31-60.	0.4	12
16409	Dispersion corrected density functionals applied to the water naphthalene cluster. Lecture Notes in Computational Science and Engineering, 2004, , 205-214.	0.1	1
16410	Reactivity of Metal Carbene Clusters Pt n CH 2 + and PtMCH 2 + (M = Cu, Ag, Au, Pt, Rh) Toward O2 and NH3: A Computational Study. , 2012, , 169-218.		1
16411	O2 Adsorption Dynamics at Metal Surfaces: Non-adiabatic Effects, Dissociation and Dissipation. Springer Series in Surface Sciences, 2013, , 389-419.	0.3	15
16412	Role of step sites on water dissociation on stoichiometric ceria surfaces. Highlights in Theoretical Chemistry, 2014, , 19-25.	0.0	1
16413	Density Functional Theory. Lecture Notes in Quantum Chemistry II, 1994, , 91-124.	0.3	15
16414	Density Functional Theory Study of Self-Diffusion on the (111) Surfaces of Ni, Pd, Pt, Cu, Ag and Au. Springer Series in Solid-state Sciences, 1996, , 173-182.	0.3	5

#	ARTICLE	IF	CITATIONS
16415	The Generalized-Gradient Approximation to Density Functional Theory and Bonding. , 1998, , 37-50.		5
16416	Steering and Isotope Effects in the Dissociative Adsorption of H <sub>2</sub> /Pd(100). , 1998, , 285-292.		1
16417	Molecular-Dynamic Simulations of Structure Formation in Complex Materials. , 1996, , 294-328.		2
16418	Potential Energy Surfaces for Reaction Catalyzed by Metalloenzymes from Quantum Chemical Computations. NATO Science for Peace and Security Series A: Chemistry and Biology, 2009, , 275-313.	0.5	1
16419	First Steps Towards Quantum Refinement of Protein X-Ray Structures. , 2012, , 87-120.		7
16420	Heusler Compounds: Applications in Spintronics. , 2016, , 335-364.		11
16421	Electronic Properties, Spectroscopic Properties and Monomolecular Isomerization Processes of Prototype OLED Compound Aluminum Tris(Quinolin-8-Olate) Facial and Meridional Isomers. , 2003, , 321-341.		1
16422	Substrate-Mediated Interaction on Ag(111) Surfaces from First Principles. NATO Science Series Series II, Mathematics, Physics and Chemistry, 2001, , 225-236.	0.1	2
16424	The Status of Density Functional Theory for Chemical Physics. , 1994, , 87-100.		3
16425	Electronic Structure of Vanadia Systems: Systematic Theoretical Studies. , 2000, , 417-438.		1
16426	Bonding and Electronic Structure of Minerals. , 1999, , 201-264.		3
16427	Optimized Effective Potential for Atoms and Molecules. Topics in Molecular Organization and Engineering, 1997, , 27-50.	0.1	6
16428	Quantum Chemical Studies of Transition Metal Catalyzed Enzyme Reactions. , 1997, , 233-253.		4
16429	Crystal ab initio Investigations of Ice II, VIII and IX. , 1994, , 411-418.		1
16430	Density Functional Theory, Calculations of Potential Energy Surfaces and Reaction Paths. , 1995, , 161-189.		4
16431	Theory of Adsorption and Surface Reactions. , 1997, , 285-351.		69
16432	Relativistic Density Functional Theory. Progress in Theoretical Chemistry and Physics, 2003, , 439-486.	0.2	3
16433	Sulphur Bonding in Transition Metal Sulphides and MoS <sub>2</sub> Based Structures. , 1998, , 155-168.		3

#	ARTICLE	IF	CITATIONS
16434	A Quantum Chemistry Approach for the Design and Analysis of Nanosensors for Fissile Materials. Challenges and Advances in Computational Chemistry and Physics, 2014, , 1-29.	0.6	1
16435	Functionalized Graphene and Cobalt Phthalocyanine Based Materials with Potential Use for Electrical Conduction. Challenges and Advances in Computational Chemistry and Physics, 2014, , 185-215.	0.6	1
16436	Interaction with Substrates. SpringerBriefs in Applied Sciences and Technology, 2020, , 45-64.	0.2	1
16437	Structure and stability of sodium-doped helium snowballs through DFT calculations. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	5
16438	SAMPL6 logP challenge: machine learning and quantum mechanical approaches. Journal of Computer-Aided Molecular Design, 2020, 34, 495-510.	1.3	11
16439	DFT study of small aluminum and boron hydrides: isomeric composition and physical properties. , 2018, 29, 49.		1
16440	First principles investigation on the applicability of ruthenium as a potential ORR catalyst. Journal of Chemical Sciences, 2020, 132, 1.	0.7	4
16441	Spectroscopic and kinetic responses of Cu-SSZ-13 to SO <sub>2</sub> exposure and implications for NO <sub>x</sub> selective catalytic reduction. Applied Catalysis A: General, 2019, 574, 122-131.	2.2	48
16442	Highly dispersed CuFe-nitrogen active sites electrode for synergistic electrochemical CO <sub>2</sub> reduction at low overpotential. Applied Energy, 2020, 269, 115029.	5.1	36
16443	Molecular design of porphyrin dyes using different electron-withdrawing moieties for high performance dye-sensitized solar cells. Computational and Theoretical Chemistry, 2020, 1182, 112846.	1.1	5
16444	Magnetic and electronic properties of double perovskite Lu <sub>2</sub> MnCoO <sub>6</sub> : Ab-initio calculations and Monte Carlo simulation. Chemical Physics Letters, 2017, 685, 191-197.	1.2	34
16445	Ab initio calculation of helium behavior in the spallation tungsten. Fusion Engineering and Design, 2017, 125, 479-483.	1.0	3
16446	Subtle atomistic processes of S-phase formation in Al-Cu-Mg alloys. Journal of Alloys and Compounds, 2020, 838, 155677.	2.8	14
16447	Insight into interface cohesion and impurity-induced embrittlement in carbide dispersion strengthen tungsten from first principles. Journal of Nuclear Materials, 2020, 538, 152223.	1.3	14
16448	Strain dependent tuning electronic properties of noble metal di chalcogenides PdX <sub>2</sub> (X=As, Se) mono-layer. Materials Chemistry and Physics, 2017, 198, 162-166.	2.0	32
16449	Thermodynamic origin of solute-enriched stacking-fault in dilute Mg-Zn-Y alloys. Materials and Design, 2020, 188, 108452.	3.3	27
16450	Crl <sub>3</sub> magnetic nanotubes: A comparative DFT and DFT+U study, and strain effect. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 123, 114205.	1.3	12
16451	Optimizing hybrid density functionals by means of quantum molecular similarity techniques. Advances in Molecular Similarity, 1999, , 187-203.	0.5	2



#	ARTICLE	IF	CITATIONS
16452	Insight into the Oxidation Mechanism of a Cu-Based Oxygen Carrier (Cu <sup>+</sup> Cu <sub>2</sub> O <sup>+</sup> CuO) in Chemical Looping Combustion. <i>Energy &amp; Fuels</i> , 2020, 34, 8718-8725.	2.5	34
16453	Sodium Rivals Silver as Single-Atom Active Centers for Catalyzing Abatement of Formaldehyde. <i>Environmental Science &amp; Technology</i> , 2017, 51, 7084-7090.	4.6	70
16454	Selective Synthesis of $\hat{I}^{\pm}$ , $\hat{I}^2$ , and $\hat{I}^3$ -Ag <sub>2</sub> WO <sub>4</sub> Polymorphs: Promising Platforms for Photocatalytic and Antibacterial Materials. <i>Inorganic Chemistry</i> , 2021, 60, 1062-1079.	1.9	18
16455	Computational Investigation of the Spin-Density Asymmetry in Photosynthetic Reaction Center Models from First Principles. <i>Journal of Physical Chemistry B</i> , 2020, 124, 4873-4888.	1.2	13
16456	Reaction Mechanism of the Metal Precursor Pulse in Plasma-Enhanced Atomic Layer Deposition of Cobalt and the Role of Surface Facets. <i>Journal of Physical Chemistry C</i> , 2020, 124, 11990-12000.	1.5	4
16457	Lead Free Two-Dimensional Mixed Tin and Germanium Halide Perovskites for Photovoltaic Applications. <i>Journal of Physical Chemistry C</i> , 2021, 125, 74-81.	1.5	29
16458	Conductance Switching in Molecular Self-Assembled Monolayers for Application of Data Storage. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1069-1074.	1.5	6
16459	Generation of $\hat{\alpha}$ -Graphene Arch-Bridge $\hat{\alpha}$ on a Diamond Surface by Si Doping: A First-Principles Computational Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 26379-26386.	1.5	2
16460	Facilitated Dissociation of Water in the Presence of Lithium Metal at Ambient Temperature as a Requisite for Lithium $\hat{\alpha}$ Gas Reactions. <i>Journal of Physical Chemistry C</i> , 2018, 122, 16016-16022.	1.5	10
16461	Unusual Electronic Structure of the Donor $\hat{\alpha}$ Acceptor Cocrystal Formed by Dithieno[3,2- <i>a</i> :2 $\hat{\alpha}$ 2,3 $\hat{\alpha}$ 2- <i>c</i> ]phenazine and 7,7,8,8-Tetracyanoquinodimethane. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4510-4515.	2.1	15
16462	Why In <sub>2</sub> O <sub>3</sub> Can Make 0.7 nm Atomic Layer Thin Transistors. <i>Nano Letters</i> , 2021, 21, 500-506.	4.5	99
16463	Interface Engineering of Silver-Based Heterostructures for CO <sub>2</sub> Reduction Reaction. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 56642-56649.	4.0	27
16464	Morphology and Surface Reactivity Relationship in the Li <sub>1+x</sub> Mn <sub>2<math>\hat{\alpha}</math></sub> O <sub>4</sub> Spinel with $x = 0.05$ and $0.10$ : A Combined First-Principle and Experimental Study. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 44922-44930.	4.0	21
16465	Diphenylalanine-Derivative Peptide Assemblies with Increased Aromaticity Exhibit Metal-like Rigidity and High Piezoelectricity. <i>ACS Nano</i> , 2020, 14, 7025-7037.	7.3	59
16466	Synergized Cu/Pb Core/Shell Electrocatalyst for High-Efficiency CO <sub>2</sub> Reduction to C <sub>2+</sub> Liquids. <i>ACS Nano</i> , 2021, 15, 1039-1047.	7.3	64
16467	Determining the Effect of Hot Electron Dissipation on Molecular Scattering Experiments at Metal Surfaces. <i>Jacs Au</i> , 2021, 1, 164-173.	3.6	33
16468	Platinum single-atom and cluster catalysis of the hydrogen evolution reaction. , 0, .		1
16469	Dissociative adsorption of O <sub>2</sub> on strained Pt(111). <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17927-17933.	1.3	12

#	ARTICLE	IF	CITATIONS
16470	Interfacial structure-governed SO <sub>2</sub> resistance of Cu/TiO <sub>2</sub> catalysts in the catalytic oxidation of CO. <i>Catalysis Science and Technology</i> , 2020, 10, 1661-1674.	2.1	20
16471	A DFT study for silicene quantum dots embedded in silicane: controllable magnetism and tuneable band gap by hydrogen. <i>RSC Advances</i> , 2019, 9, 32782-32790.	1.7	2
16472	Quantum Monte Carlo calculations on dissociative chemisorption of H <sub>2</sub> + Al(110): Minimum barrier heights and their comparison to DFT values. <i>Journal of Chemical Physics</i> , 2020, 153, 224701.	1.2	16
16473	State-to-state quantum dynamics of H <sub>2</sub> O/HOD scattering from Cu(111): Mode- and bond-selective vibrational energy transfer. <i>Journal of Chemical Physics</i> , 2020, 153, 214702.	1.2	8
16474	A Sesquiterpene Isonitrile with a New Tricyclic Skeleton from the Indo-Pacific Nudibranch <i>Phyllidiella pustulosa</i> : Spectroscopic and Computational Studies. <i>Australian Journal of Chemistry</i> , 2020, 73, 129.	0.5	9
16475	Semiconducting phase in borophene: role of defect and strain. <i>Journal Physics D: Applied Physics</i> , 2017, 50, 405103.	1.3	17
16476	Insight the process of hydrazine gas adsorption on layered WS <sub>2</sub> : a first principle study. <i>Nanotechnology</i> , 2020, 31, 495703.	1.3	6
16477	Retention of hydrogen in W-Ti-C, W-Ta-C and W-Zr-C alloys: <i>ab initio</i> study. <i>Physica Scripta</i> , 2020, 95, 105707.	1.2	4
16478	First-principles spin-polarized calculations on the adsorption of ethanethiol molecule upon the nonpolar (100) ZnO surface. <i>Physica Scripta</i> , 2021, 96, 015803.	1.2	1
16479	Theoretical study on martensitic-type transformation path from rutile phase to $\hat{\Gamma}$ -PbO <sub>2</sub> phase of Ti <sub>2</sub> O. <i>Chinese Physics B</i> , 2020, 29, 076101.	0.7	2
16480	Parameters setup for first-principles on well-formedness and thermodynamic properties of bulk and habit surfaces of Mg <sub>2</sub> Si. <i>Materials Research Express</i> , 2020, 7, 076513.	0.8	2
16481	Evaluation of photocatalytic activity of commercial red phosphorus towards the disinfection of <i>E. coli</i> and reduction of Cr (VI) under direct sunlight. <i>Materials Research Express</i> , 2020, 7, 104002.	0.8	13
16482	The magnetic, optical and electronic properties of Mn <sup>2+</sup> (X <sup>2+</sup> =As, Se, Te, Po) co-doped MoS <sub>2</sub> monolayers via first principle calculation. <i>Materials Research Express</i> , 2020, 7, 116301.	0.8	11
16483	Structural, elastic, electronic, and magnetic properties of MnNbZ (Z = As, Sb) and FeNbZ (Z = Sn, Pb) semi-Heusler alloys. <i>Materials Research Express</i> , 2020, 7, 116527.	0.8	3
16484	Effect of As and Ga doping on the electronic structure and photoelectric properties of cubic Ca <sub>2</sub> Ge. <i>Materials Research Express</i> , 2020, 7, 126304.	0.8	6
16485	An accurate machine learning calculator for the lithium-graphite system. <i>JPhys Energy</i> , 2021, 3, 014005.	2.3	11
16486	Zero-point energies prevent a trigonal to simple cubic transition in high-pressure sulfur. <i>Electronic Structure</i> , 2020, 2, 045003.	1.0	1
16487	First-principles study of the nontrivial topological phase in chains of 3d transition metals. <i>Physical Review B</i> , 2020, 101, .	1.1	7

#	ARTICLE	IF	CITATIONS
16488	Compensation of band-edge positions in titanium-doped $N_5$ photoanode for enhanced water splitting performance: A first-principles insight. Physical Review Materials, 2017, 1, .	0.9	11
16489	Thermodynamic properties of paramagnetic $\hat{I}_\pm$ - and $\hat{I}^2$ Mn from first principles: The effect of transverse spin fluctuations. Physical Review Materials, 2017, 1, .	0.9	4
16490	Assessment of the GLLB-SC potential for solid-state properties and attempts for improvement. Physical Review Materials, 2018, 2, .	0.9	44
16491	Resolving phase stability in the Ti-O binary with first-principles statistical mechanics methods. Physical Review Materials, 2018, 2, .	0.9	17
16492	High-temperature thermophysical properties of $\hat{I}^3$ - and $\hat{I}$ -Mn from first principles. Physical Review Materials, 2018, 2, .	0.9	2
16493	Nexus networks in carbon honeycombs. Physical Review Materials, 2018, 2, .	0.9	16
16494	Experimental and theoretical electronic structure and symmetry effects in ultrathin NbSe2 films. Physical Review Materials, 2018, 2, .	0.9	11
16495	Atomistic study of the electronic contact resistivity between the half-Heusler alloys (HfCoSb), Tj ETQq1 1 0.784314, rgBT /Overlock 10 T	0.9	4
16496	Plasmon spectroscopy: Robust metallicity of Au wires on Si(557) upon oxidation. Physical Review Materials, 2018, 2, .	0.9	10
16497	First-principles study of vibrational entropy effects on the PbTe-SrTe phase diagram. Physical Review Materials, 2018, 2, .	0.9	8
16498	Domain morphology and mechanics of the $T$ transition metal dichalcogenide monolayers. Physical Review Materials, 2018, 2, .	0.9	18
16499	Intermolecular coupling and superconductivity in $S_8$ and other Chevrel phase compounds. Physical Review Materials, 2018, 2, .	0.9	9
16500	High-throughput screening for spin-gapless semiconductors in quaternary Heusler compounds. Physical Review Materials, 2019, 3, .	0.9	79
16501	High-throughput design of $211$ M2AX compounds. Physical Review Materials, 2019, 3, .	0.9	21
16502	Dielectric-dependent hybrid functionals for heterogeneous materials. Physical Review Materials, 2019, 3, .	0.9	36
16503	Strain-controlled magnetic and optical properties of monolayer $H\hat{a}$ TaS <sub>2</sub> . Physical Review Materials, 2019, 3, .	0.9	9
16504	Impact of organic molecule rotation on the optoelectronic properties of hybrid halide perovskites. Physical Review Materials, 2019, 3, .	0.9	20
16505	Polar or not polar? The interplay between reconstruction, Sr enrichment, and reduction at the $La_{0.75}Sr_{0.25}$ (001) surface. Physical Review Materials, 2020, 4, .	0.9	21



#	ARTICLE	IF	CITATIONS
16524	Magnetic-Adsorbate-Induced Spin Polarization in Carbon Materials â€œTwo Fe Atoms on Planar C10and C10H8â€œ. Journal of the Physical Society of Japan, 2003, 72, 2413-2416.	0.7	5
16525	Relation between Surface Composition and Electronic Properties of Native Oxide Films on an Aluminium-Copper Alloy Studied by DFT. Journal of the Electrochemical Society, 2020, 167, 161501.	1.3	13
16526	Fundamental Concepts in Molecular Simulation of NOx Catalysis. , 2005, , 233-268.		5
16527	Vibrational Excitations of Polyatomic Molecules. , 2011, , 263-282.		1
16528	The Magnetism of (Pb <sub>1-x</sub> /sub>Sr <sub>x</sub> /sub>)TiO <sub>3</sub> and the Effect of Oxygen Vacancy on Its Magnetism by First-Principles Study. Advances in Condensed Matter Physics, 2016, 05, 45-51.	0.1	2
16529	Effect of Al Substitution on the Electronic and Magnetic Properties of GdCo5. Acta Physica Polonica A, 2002, 101, 525-536.	0.2	2
16530	Electronic Structure and X-Ray Photoelectron Spectra of YNi <sub>4</sub> B Compound. Acta Physica Polonica A, 2003, 104, 487-494.	0.2	5
16531	Behaviour of Di-Transition-Metal Nitride Ti <sub>1-x</sub> Zr <sub>x</sub> N Alloy at High Pressure. Acta Physica Polonica A, 2009, 116, 1085-1089.	0.2	5
16532	Magnetism in Doped Two-Dimensional Honeycomb Structures of III-V Binary Compounds. Acta Physica Polonica A, 2012, 121, 1240-1241.	0.2	1
16533	Structural and Magnetic Properties of Co Thin Films on Au(111) Substrates. Acta Physica Polonica A, 2012, 121, 653-659.	0.2	7
16534	A DFT Study of the Strain Effect on the Optical Properties of Linear and Dimerized Titanium Nanochains. Acta Physica Polonica A, 2016, 129, 344-347.	0.2	1
16535	First Principles Study of Gas Adsorption Dynamics on Pristine and Defected Graphene. Acta Physica Polonica A, 2016, 129, A-142-A-144.	0.2	4
16536	The effect of strain on the electronic properties of MoS <sub>2</sub> monolayers. Multiscale and Multiphysics Mechanics, 2016, 1, 77-86.	0.3	2
16537	â€œConjugate Channelingâ€•Effect in Dislocation Core Diffusion: Carbon Transport in Dislocated BCC Iron. PLoS ONE, 2013, 8, e60586.	1.1	26
16538	H2 Dissociative Adsorption at the Zigzag Edges of Graphite. E-Journal of Surface Science and Nanotechnology, 2004, 2, 77-80.	0.1	27
16539	First-Principles Study of Field-Effect Doping in Nano-Scale Systems by the Enforced Fermi-Energy Difference Method. E-Journal of Surface Science and Nanotechnology, 2005, 3, 453-456.	0.1	3
16540	Epitaxial growth of ZnO crystal on the Si-terminated 6H-SiC(0001) surface using the first-principles calculation. E-Journal of Surface Science and Nanotechnology, 2006, 4, 254-257.	0.1	3
16541	Hydrogen atom quantum migration on platinum. E-Journal of Surface Science and Nanotechnology, 2006, 4, 619-623.	0.1	15

#	ARTICLE	IF	CITATIONS
16542	First Principles Investigations on Fuel Cell Reactions: H <sub>2</sub> -Pt(111) Interactions. E-Journal of Surface Science and Nanotechnology, 2008, 6, 134-137.	0.1	3
16543	First-principle calculations of effective mass of silicon crystal with vacancy defects. Materials Science-Poland, 2016, 34, 916-923.	0.4	9
16544	Microstructure and Phase Control in Zr-Fe-Cr-Ni Alloys: Thermodynamic and Kinetic Aspects. Journal of ASTM International, 2005, 2, 12771.	0.2	8
16546	Electronic structure of PbSnS <sub>3</sub> and PbGeS <sub>3</sub> semiconductor compounds with the mixed cation coordination. Semiconductor Physics, Quantum Electronics and Optoelectronics, 2015, 18, 12-19.	0.3	3
16547	Quantum Confinement and Piezoresistivity Simulation in 3C-SiC Nanosheet. IEEJ Transactions on Sensors and Micromachines, 2016, 136, 465-472.	0.0	1
16548	An approach to determine enthalpies of formation for ternary compounds. Journal of Mining and Metallurgy, Section B: Metallurgy, 2010, 46, 1-9.	0.3	18
16549	Formation and Stability of Solute Enriched Stacking Fault in the Mg-Co-Y, Mg-Co-Zn-Y and Mg-Zn-Ca Ternary Systems. Materials Transactions, 2020, 61, 839-848.	0.4	12
16550	The LPSO Structure with an Extra Order beyond Stacking Periodicity. Materials Transactions, 2020, 61, 833-838.	0.4	16
16551	Amino Acid Adsorption Effects on Nanotube Electronics. Shinku/Journal of the Vacuum Society of Japan, 2006, 49, 440-442.	0.2	1
16552	Shinku/Journal of the Vacuum Society of Japan, 2006, 49, 514-519.		
16553	A Behavior of a Hydrogen Atom of Pd <sub>0.75</sub> Ag <sub>0.25</sub> (111). Shinku/Journal of the Vacuum Society of Japan, 2007, 50, 440-443.	0.2	2
16554	The Na-H system: from first-principles calculations to thermodynamic modeling. International Journal of Materials Research, 2006, 97, 845-853.	0.1	13
16557	Direct Observations of Precursor Short-Range Order Clusters of Solute Atoms in a LPSO-Forming Mg-Zn-Gd Ternary Alloy. Frontiers in Materials, 2019, 6, .	1.2	16
16558	First-Principles Forecast of Gapless Half-Metallic and Spin-Gapless Semiconducting Materials: Case Study of Inverse Ti <sub>2</sub> CoSi-Based Compounds. Applied Sciences (Switzerland), 2020, 10, 782.	1.3	3
16559	Computational Surface Modelling of Ices and Minerals of Interstellar Interest—Insights and Perspectives. Minerals (Basel, Switzerland), 2021, 11, 26.	0.8	13
16560	Removal Mechanism Investigation of Ultraviolet Induced Nanoparticle Colloid Jet Machining. Molecules, 2021, 26, 68.	1.7	7
16561	Customizable Ligand Exchange for Tailored Surface Property of Noble Metal Nanocrystals. Research, 2020, 2020, 2131806.	2.8	13
16562	The Structures and Properties of Y-Substituted Mg <sub>2</sub> Ni Alloys and Their Hydrides: A First-Principles Study. American Journal of Analytical Chemistry, 2016, 07, 67-74.	0.3	5



#	ARTICLE	IF	CITATIONS
16563	Ab Initio Study of Electronic Properties of a Armchair (7,7) Carbon Nanotube. <i>Advances in Materials Physics and Chemistry</i> , 2012, 02, 159-162.	0.3	9
16564	A DFT/ECP-Small Basis Set Modelling of Cisplatin: Molecular Structure and Vibrational Spectrum. <i>Computational Molecular Bioscience</i> , 2012, 02, 35-44.	0.6	16
16565	A Comparative Study of Electronic Properties of Bulk MoS <sub>2</sub> and Its Monolayer Using DFT Technique: Application of Mechanical Strain on MoS <sub>2</sub> Monolayer. <i>Graphene</i> , 2014, 03, 52-59.	0.3	130
16566	First Principles Studies on the Electronic Structure and Band Structure of Paraelectric SrTiO <sub>3</sub> by Different Approximations. <i>Journal of Modern Physics</i> , 2011, 02, 934-943.	0.3	14
16567	A Density Functional Theory Study of Methoxy and Atomic Hydrogen Chemisorption on Au(100) Surface. <i>Journal of Modern Physics</i> , 2013, 04, 409-417.	0.3	6
16568	Non Local Corrections to the Electronic Structure of Non Ideal Electron Gases: The Case of Graphene and Tyrosine. <i>Journal of Modern Physics</i> , 2013, 04, 522-527.	0.3	2
16569	Investigation of the Optical Properties of CdBr <sub>2</sub> . <i>Optics and Photonics Journal</i> , 2011, 01, 1-4.	0.3	7
16570	Structural, Magnetic, and Electronic Properties of Fe: A Screened Hybrid Functional Study. <i>Journal of Magnetism</i> , 2011, 16, 201-205.	0.2	13
16571	Effect of Basis Set Superposition Error on the MP2 Relative Energies of Gold Cluster Au <sub>6</sub> . <i>Bulletin of the Korean Chemical Society</i> , 2009, 30, 794-796.	1.0	6
16572	First-Principles Study of the Three Polymorphs of Crystalline 1,1-Diamino-2,2-dinitroethylene. <i>Bulletin of the Korean Chemical Society</i> , 2013, 34, 2281-2285.	1.0	4
16573	Molecular structure, vibrational spectroscopic and HOMO/LUMO studies of some organotellurium compounds by quantum chemical investigations. <i>European Journal of Chemistry</i> , 2015, 6, 248-253.	0.3	6
16574	Analysis of the electronic structure of the primary electron donor of photosystem I of <i>Spirodela oligorrhiza</i> by photochemically induced dynamic nuclear polarization (photo-CIDNP) solid-state nuclear magnetic resonance (NMR). <i>Magnetic Resonance</i> , 2020, 1, 261-274.	0.8	6
16575	First-principles study of electronic transport properties of C <sub>20</sub> F <sub>20</sub> molecule. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2010, 59, 2010.	0.2	4
16576	Adsorption and diffusion of oxygen on Pt (111) surface and subsurface. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2012, 61, 076802.	0.2	2
16577	First-principles calculation for mechanical properties of metal dihydrides. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2012, 61, 108801.	0.2	10
16578	First-principles study on the elastic, electronic and thermodynamic properties of ErNi <sub>2</sub> B <sub>2</sub> C under high pressure. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2013, 62, 107402.	0.2	5
16579	First-principles study on elastic properties of hexagonal phase ErA <sub>x</sub> (A=H, He). <i>Wuli Xuebao/Acta Physica Sinica</i> , 2013, 62, 116201.	0.2	7
16580	First principles study of Au-Sn intermetallic compounds. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2013, 62, 247102.	0.2	10

#	ARTICLE	IF	CITATIONS
16581	Effect of strain on Li adsorption on silicene. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 217101.	0.2	1
16582	Structural and electronic properties of hydrogenated bilayer silicene. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 076801.	0.2	2
16583	First principles study on the H <sub>2</sub> diffusion and desorption at the Li-doped MgH <sub>2</sub> (001) surface. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 056801.	0.2	2
16584	The first-principle calculation on the Li cluster adsorbed on graphene. Wuli Xuebao/Acta Physica Sinica, 2017, 66, 057301.	0.2	3
16585	Electronic structures and ferroelectric properties of Ba-doped ZnO. Wuli Xuebao/Acta Physica Sinica, 2018, 67, 107701.	0.2	2
16586	Electronic structure calculation of Cr content effect on corrosion resistance of Ti-Nb-Cr alloy. Wuli Xuebao/Acta Physica Sinica, 2018, 67, 197101.	0.2	2
16587	First-principles calculations of magnetic and optical properties of Ga <sub>1-x</sub> Cr <sub>x</sub> Sb (x = 0.25, 0.50, 0.75). Wuli Xuebao/Acta Physica Sinica, 2019, 68, 176301.	0.2	2
16588	Density Functional Theory Investigation on the Dissociation and Adsorption Processes of N <sub>2</sub> on Pd(111) and Pd <sub>3</sub> Ag(111) Surfaces. Japanese Journal of Applied Physics, 2011, 50, 045701.	0.8	3
16589	First Principles Calculations of Defect Formation in In-Free Photovoltaic Semiconductors Cu <sub>2</sub> ZnSnS <sub>4</sub> and Cu <sub>2</sub> ZnSnSe <sub>4</sub> . Japanese Journal of Applied Physics, 2011, 50, 04DP07.	0.8	50
16590	Adsorption and Diffusion of Li and Ni on Graphene with Boron Substitution for Hydrogen Storage: <i>Ab-initio</i> Method. Japanese Journal of Applied Physics, 2011, 50, 06GJ02.	0.8	6
16591	Controllability of Electrical Conductivity by Oxygen Vacancies and Charge Carrier Trapping at Interface between CoO and Electrodes. Japanese Journal of Applied Physics, 2011, 50, 071101.	0.8	5
16592	Crystalline InGaZnO Density of States and Energy Band Structure Calculation Using Density Function Theory. Japanese Journal of Applied Physics, 2011, 50, 091102.	0.8	24
16593	Theoretical Simulation of Deformed Carbon Nanotubes with Adsorbed Metal Atoms: Enhanced Reactivity by Deformation. Japanese Journal of Applied Physics, 2011, 50, 105101.	0.8	2
16594	First-Principles Study on Cd Doping in Cu <sub>2</sub> ZnSnS <sub>4</sub> and Cu <sub>2</sub> ZnSnSe <sub>4</sub> . Japanese Journal of Applied Physics, 2012, 51, 10NC11.	0.8	31
16595	Surface Stabilities of Various Crystal Faces of CuInSe <sub>2</sub> and Related Compounds by First-Principles Calculation. Japanese Journal of Applied Physics, 2012, 51, 10NC22.	0.8	4
16596	First-Principles Studies of Er <sub>2</sub> O <sub>3</sub> (110) Heteroepitaxy on Si(001). International Journal of Applied Physics and Mathematics, 2014, 4, 108-112.	0.3	2
16597	Modular synthesis of antimalarial quinoline-based PGM metallarectangles. Dalton Transactions, 2021, 50, 15274-15286.	1.6	5
16598	Designed borophene/TMDs hybrid catalysts for enhanced hydrogen evolution reactions. Journal of Materials Chemistry C, 2021, 9, 15877-15885.	2.7	15

#	ARTICLE	IF	CITATIONS
16599	Ab-initio Description of Solids. , 2021, , 9-101.		0
16600	Steric effects in the hydrogen evolution reaction based on the TMX <sub>4</sub> active center: Fe <sup>2+</sup> BHT as a case study. Physical Chemistry Chemical Physics, 2021, 23, 25239-25245.	1.3	4
16601	Controllable fabrication and photocatalytic performance of nanoscale single-layer MoSe <sub>2</sub> islands with substantial edges on an Ag(111) substrate. Nanoscale, 2021, 13, 19165-19171.	2.8	5
16602	K <sub>2</sub> ZnMoP <sub>2</sub> O <sub>10</sub> : a novel nonlinear optical molybdophosphate with a strong second harmonic generation response and moderate birefringence. Journal of Materials Chemistry C, 2021, 9, 15321-15328.	2.7	14
16603	Understanding the role of axial O in CO <sub>2</sub> electroreduction on NiN <sub>4</sub> single-atom catalysts <i>via</i> simulations in realistic electrochemical environment. Journal of Materials Chemistry A, 2021, 9, 23515-23521.	5.2	45
16604	Single-atom Ru catalyst for selective synthesis of 3-pentanone <i>via</i> ethylene hydroformylation. Green Chemistry, 2021, 23, 9038-9047.	4.6	14
16605	Large magnetoresistance of a compensated metal Cu <sub>2</sub> Sb correlated with its Fermi surface topology. Physical Review Materials, 2021, 5, .	0.9	0
16606	Sintering Rate and Mechanism of Supported Pt Nanoparticles by Multiscale Simulation. Langmuir, 2021, 37, 12529-12538.	1.6	5
16607	Adsorption performance of modified graphene toward Ti: a first-principles investigation. Journal of Molecular Modeling, 2021, 27, 321.	0.8	1
16608	Gram-scale Synthesis of Nanosized Li <sub>3</sub> HoBr <sub>6</sub> Solid Electrolyte for All-solid-state Li-ion Battery. Small Methods, 2021, 5, e2101002.	4.6	22
16609	Engineering catalyst supports to stabilize PdOx two-dimensional rafts for water-tolerant methane oxidation. Nature Catalysis, 2021, 4, 830-839.	16.1	86
16610	Crystal structure and photo-physical properties in a perovskite-type semiconducting hybrid phase: {(m-C <sub>6</sub> H <sub>7</sub> N <sub>2</sub> O <sub>2</sub> ) <sub>2</sub> CdCl <sub>4</sub> } <sub>n</sub> . Journal of Molecular Structure, 2022, 1250, 131789.	1.8	1
16611	Experimental studies and DFT calculations to predict atomic arrangements at twin boundaries and distribution behaviors of different solutes in complex intermetallics. Journal of Physics and Chemistry of Solids, 2022, 161, 110453.	1.9	4
16612	Engineering Tetrahedral Co <sup>2+</sup> -Exposed Co <sub>3</sub> O <sub>4</sub> Nanosheets toward Highly Efficient Styrene Epoxidation. Industrial & Engineering Chemistry Research, 2021, 60, 15106-15114.	1.8	4
16613	Ab initio investigation for the adsorption of acrolein onto the surface of C <sub>60</sub> , C <sub>59</sub> Si, and C <sub>59</sub> Ge: NBO, QTAIM, and NCI analyses. Structural Chemistry, 2022, 33, 363-378.	1.0	26
16614	Understanding the Catalytic Activity of the Preferred Nitrogen Configuration on the Carbon Nanotube Surface and Its Implications for Li-O <sub>2</sub> Batteries. Journal of Physical Chemistry C, 2021, 125, 22570-22580.	1.5	5
16615	Computational Insights into the Role of External and Local Electric Fields in Macrocyclic Chemical and Biological Systems. ChemPhysChem, 2021, 22, 2484-2492.	1.0	1
16616	Phase stability, band gap engineering and optical response of Li-, Be- and Mg-doped SrZrO <sub>3</sub> perovskite: Theoretical perspective with GGA-PBE. European Physical Journal Plus, 2021, 136, 1.	1.2	5



#	ARTICLE	IF	CITATIONS
16635	Capturing polysulfides by sulfurized polyacrylonitrile in lithium-sulfur batteries and the sulfur chain effects through Density Functional Theory. <i>Electrochemical Science Advances</i> , 2022, 2, .	1.2	2
16636	Multi-state formulation of the frozen-density embedding quasi-diabatization approach. <i>Journal of Chemical Physics</i> , 2021, 155, 174104.	1.2	4
16637	A search for a DFT functional for actinide compounds. <i>Journal of Chemical Physics</i> , 2021, 155, 161103.	1.2	6
16638	Tuning Site Energy by $XO_6$ Units in $Li_2(PO_4)_3$ Enables High Li Ion Conductivity and Improved Stability. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 50948-50956.	4.0	7
16639	TM3 (TM = V, Fe, Mo, W) single-cluster catalyst confined on porous BN for electrocatalytic nitrogen reduction. <i>Journal of Materials Science and Technology</i> , 2022, 108, 46-53.	5.6	19
16640	Low thermal conductivity of complex thermoelectric barium silicide film epitaxially grown on Si. <i>Applied Physics Letters</i> , 2021, 119, .	1.5	7
16641	Compensating Electronic Effect Enables Fast Site-to-Site Electron Transfer over Ultrathin RuMn Nanosheet Branches toward Highly Electroactive and Stable Water Splitting. <i>Advanced Materials</i> , 2021, 33, e2105308.	11.1	73
16642	Atomically Dispersed Tin-Modified $\gamma$ -alumina for Selective Propane Dehydrogenation under $H_2/S$ Co-feed. <i>ACS Catalysis</i> , 2021, 11, 13472-13482.	5.5	8
16643	FeCo alloy encased in nitrogen-doped carbon for efficient formaldehyde removal: Preparation, electronic structure, and d-band center tailoring. <i>Journal of Hazardous Materials</i> , 2022, 424, 127593.	6.5	11
16644	Effective Repeatable Mechanoluminescence in Heterostructured $LiNi_xNa_{1-x}NbO_3$ : $Pr^{3+}$ . <i>Small</i> , 2021, 17, e2103441.	5.2	26
16645	Static isotropic pressure induced ultra-wide band gap response of $NaCaF_3$ fluoro-perovskite and its repercussions on optical properties: ab initio calculation. <i>Molecular Simulation</i> , 2021, 47, 1549-1557.	0.9	6
16646	Structural, electronic and magnetic properties of the equiatomic quaternary Heusler $CoRuMnGe$ alloy: a DFT study. <i>Ferroelectrics</i> , 2021, 582, 155-163.	0.3	2
16647	Pressure-induced superconductivity in Li-Te electrides. <i>Physical Review B</i> , 2021, 104, .	1.1	14
16648	Emerging Yttrium Phosphides with Tetrahedron Phosphorus and Superconductivity under High Pressures. <i>Chemistry - A European Journal</i> , 2021, 27, 17420-17427.	1.7	5
16649	Effects of the Gas Molecules ( $H_2$ , $CO$ , $NO$ ) and Transition Metal Atoms ( $Cr$ , $Au$ ) Adsorbed on Hexagonal Boron Nitride Layers. <i>Journal of the Physical Society of Japan</i> , 2021, 90, 114601.	0.7	1
16650	Porous graphene membranes under small tensile strains exhibit higher percolation barriers to the passing molecules. <i>Surfaces and Interfaces</i> , 2021, 27, 101526.	1.5	0
16651	Hybridization of carbon nanotube tissue and $MnO_2$ as a generic advanced air cathode in metal-air batteries. <i>Journal of Power Sources</i> , 2021, 514, 230597.	4.0	5
16652	Bead-milling and recrystallization from natural marmatite to Fe-doping $ZnS-C$ materials for lithium-ion battery anodes. <i>Electrochimica Acta</i> , 2021, 399, 139430.	2.6	12

#	ARTICLE	IF	CITATIONS
16653	Photoelectric properties of monolayer WS <sub>2</sub> -MoS <sub>2</sub> lateral heterojunction from first principles. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2021, 420, 127771.	0.9	8
16654	Ab initio simulations on the pure Cr lattice stability at OK: Verification with the Fe-Cr and Ni-Cr binary systems. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2021, 75, 102359.	0.7	14
16655	A theoretical screening of the O Hâ€¦â€¦â€¦ interaction between water and benzene using density-functional approaches: Effects of nonlocal exchange and long-range dispersion corrections in the true minimum. <i>Computational and Theoretical Chemistry</i> , 2021, 1206, 113464.	1.1	5
16656	Preparation of superhydrophobic nanoplate iron oxide surface on a carbon steel for anti-wetting applications. <i>Materials and Design</i> , 2021, 211, 110169.	3.3	10
16657	Dataset of the crystal structures, electrical transport properties, and first-principles electronic structures of GeTe-rich GeTe-Sb <sub>2</sub> Te <sub>3</sub> thermoelectric materials. <i>Data in Brief</i> , 2021, 39, 107462.	0.5	2
16658	Theoretical investigation of the effect of auxiliary ligands on dipyrazole-bridged binuclear Cu(II) complexes. <i>Chemical Physics Letters</i> , 2021, 784, 139102.	1.2	6
16659	Direct thermal annealing synthesis of FeO nanodots anchored on N-doped carbon nanosheet for long-term electrocatalytic oxygen reduction. <i>Electrochimica Acta</i> , 2021, 398, 139361.	2.6	15
16660	Structures and Properties of Atoms and Molecules Confined in Nanospaces. Proton Relay Dissociation of Water Molecules on a Si(001) Surface.. <i>Hyomen Kagaku</i> , 2000, 21, 39-48.	0.0	1
16661	AB-INITIO MOLECULAR DYNAMICS SIMULATION OF AMORPHOUS SILICA SURFACE. , 2000, , 371-390.		0
16662	What Can We Learn About Perfect and Defective MgO (001) Surface Using Density Functional Theory?. , 2000, , 49-60.		0
16663	Ab-Initio Study of The Influence of Epitaxial Strain on Magnetoelastic Properties. , 2002, , 439-447.		0
16664	First-Principles Parameter Estimation for Dynamic Monte Carlo of a Lattice-Gas Model. <i>Springer Proceedings in Physics</i> , 2002, , 40-44.	0.1	0
16665	Ab Initio Modeling of Free Energy Profiles in Thermally Activated Processes. , 2002, , 19-29.		0
16669	Demonstrating the Effectiveness of a Nonlocal Density Functional Description of Exchange and Correlation. <i>Progress in Theoretical Chemistry and Physics</i> , 2003, , 169-183.	0.2	0
16670	Electronic Structure and Chemisorption Properties of Supported Metal Clusters. , 2003, , .		0
16672	Optimum designs of additional elements from first-principles simulations. <i>Keikin-zoku/Journal of Japan Institute of Light Metals</i> , 2004, 54, 82-89.	0.1	24
16675	Current and Force Spectroscopy. <i>Nanoscience and Technology</i> , 2006, , 221-257.	1.5	0
16676	Trends in the First-principles Theoretical Study on Catalysis. <i>Hyomen Kagaku</i> , 2006, 27, 354-359.	0.0	2



#	ARTICLE	IF	CITATIONS
16677	Density Functional Study on the Interaction of Hydrogen with Pt <sub>3</sub> Ti(111). Shinku/Journal of the Vacuum Society of Japan, 2006, 49, 298-301.	0.2	1
16678	Electronic Properties and Fragmentation Dynamics of Organic Species Deposited on Silicon Surfaces. Challenges and Advances in Computational Chemistry and Physics, 2007, , 505-532.	0.6	0
16679	Density Functional Molecular Orbital Calculations on Longer DNA“DNA and PNA“DNA Double Strands. , 2007, , 299-303.		0
16680	First-Principles Atomic-Scale Study of Superlow Friction. Nanoscience and Technology, 2007, , 201-217.	1.5	0
16683	Tailoring the Surface Reactivity: Comparison of Pd/Nb(110) and Rh/Nb(110). Collection of Czechoslovak Chemical Communications, 2008, 73, 745-754.	1.0	1
16684	Selected High-Impact Journal Articles on Defects in Microelectronic Materials and Devices. , 2008, , .		2
16685	Computational Approach in Zeolite Science. , 2009, , 223-250.		0
16686	Effects of molecular adsorption on optical losses of silver surfaces. , 2009, , .		0
16688	Design of Heterogeneous Catalysts and the Application to the Oxygen Reduction Reaction. , 2010, , 303-328.		0
16689	Electronic Properties and Reactivities of Perfect, Defected, and Doped Single-Walled Carbon Nanotubes. Challenges and Advances in Computational Chemistry and Physics, 2010, , 421-471.	0.6	1
16690	Electronic Structure Methods Based on Density Functional Theory. , 2009, , 478-488.		0
16691	Effect of hydrogen on ferroelectric properties of Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub> during forming gas annealing. Wuli Xuebao/Acta Physica Sinica, 2010, 59, 8042.	0.2	1
16692	First-principles study of the thermal transport property of Y <sub>3</sub> Al <sub>5</sub> O <sub>12</sub> . Wuli Xuebao/Acta Physica Sinica, 2010, 59, 2697.	0.2	2
16693	Influence of surface effect to the performance of LiMn <sub>2</sub> O <sub>4</sub> cathode material for lithium ion batteries. Wuli Xuebao/Acta Physica Sinica, 2010, 59, 5863.	0.2	3
16694	Understanding Long-range Indirect Interactions Between Surface Adsorbed Molecules. , 2010, , 75-84.		0
16695	First-principles calculation of structural stability and electronic properties of ZnO atomic chains. Wuli Xuebao/Acta Physica Sinica, 2010, 59, 2051.	0.2	3
16696	A low coverage investigation on Al adsorption on the (111) surface of Pt, Ir and Au. Wuli Xuebao/Acta Physica Sinica, 2010, 59, 4143.	0.2	4
16697	Antisite defect of LiFePO <sub>4</sub> : A first-principles study. Wuli Xuebao/Acta Physica Sinica, 2010, 59, 5135.	0.2	3

#	ARTICLE	IF	CITATIONS
16698	First-principles study on chemisorption of Cl on $\hat{1}^3$ -TiAl(111) surface. Wuli Xuebao/Acta Physica Sinica, 2010, 59, 7278.	0.2	9
16699	Methanol Electro-Oxidation by Methanol Dehydrogenase Enzymatic Catalysts: A Computational Study. Modern Aspects of Electrochemistry, 2010, , 243-274.	0.2	1
16700	A Density Functional Theory Study of 2-Chlorothiophene Adsorption on Rh(111) Surface. Chinese Journal of Catalysis, 2010, 31, 49-55.	6.9	0
16702	First-principles calculations of magnetism of Fe atomic sheet. Wuli Xuebao/Acta Physica Sinica, 2011, 60, 047502.	0.2	3
16703	First principles investigation of electronic structures and stabilities of Mg <sub>2</sub> Ni and its complex hydrides. Wuli Xuebao/Acta Physica Sinica, 2011, 60, 077103.	0.2	3
16704	Mechanism of the influence of the interaction between interstitial H atom and doped atom on the dehydrogenation performance of LiNH <sub>2</sub> . Wuli Xuebao/Acta Physica Sinica, 2011, 60, 117101.	0.2	1
16705	Helicity effects on Rh adsorption behavior inside and outside the single-wall carbon nanotubes. Wuli Xuebao/Acta Physica Sinica, 2011, 60, 087102.	0.2	2
16706	Evaluation of the Oxygen Diffusion Coefficient in Nickel-Base Alloys. , 2011, , 1463-1475.		0
16707	Atomic-Scale Investigation on the Ti/Fe(001) Interface Structure: Molecular Dynamics Simulations and Ab initio Calculations. Japanese Journal of Applied Physics, 2011, 50, 01BE07.	0.8	0
16708	First principles study on substitution behavior and alloying effects of Nb in Ni <sub>3</sub> Al. Wuli Xuebao/Acta Physica Sinica, 2011, 60, 047103.	0.2	5
16709	Theoretical research of TiO <sub>2</sub> adsorption on GaN(0001) surface. Wuli Xuebao/Acta Physica Sinica, 2011, 60, 106801.	0.2	2
16710	Electronic Structures and Magnetism of Al/Fe(001) Thin-Film Systems: First-Principles Calculations. Japanese Journal of Applied Physics, 2011, 50, 01BF03.	0.8	0
16711	The Mechanical Properties of CaX <sub>6</sub> (X = B and C). , 2011, , 127-133.		0
16712	A first principles study of the lattice dynamics property of LiFePO <sub>4</sub> . Wuli Xuebao/Acta Physica Sinica, 2011, 60, 028201.	0.2	5
16713	The structural stability and electronic properties of monolayer BC <sub>2</sub> N. Wuli Xuebao/Acta Physica Sinica, 2011, 60, 127305.	0.2	0
16714	First-principles calculation for elastic constants of $\hat{1}^{\pm}$ -ScD <sub>x</sub> (D=H, He). Wuli Xuebao/Acta Physica Sinica, 2011, 60, 076201.	0.2	7
16715	Na effect on the electronic transport properties of C <sub>20</sub> H <sub>20</sub> molecule. Wuli Xuebao/Acta Physica Sinica, 2011, 60, 017302.	0.2	4
16716	First principles study of H <sub>2</sub> molecule adsorption on Li <sub>3</sub> N(110) surfaces. Wuli Xuebao/Acta Physica Sinica, 2011, 60, 086801.	0.2	2

#	ARTICLE	IF	CITATIONS
16718	Mechanism for Lower Resistivity of Niobium-Doped Anatase Titanium Dioxide Obtained in Oxygen-Reduced Atmosphere: Investigation by Generalized Gradient Approximation +UMethod. Japanese Journal of Applied Physics, 2011, 50, 041102.	0.8	0
16719	Structural Analysis of Nitride Phosphors. Series in Optics and Optoelectronics, 2011, , 203-261.	0.0	0
16720	Structures of Butylthiolate Self-Assembled Monolayers on Au(111) with Gold Adatoms. Bulletin of the Korean Chemical Society, 2011, 32, 3614-3617.	1.0	0
16721	First-Principles Study of Electronic Structure and Optical Properties of Tetragonal PbMoO <sub>4</sub> . ISRN Condensed Matter Physics, 2011, 2011, 1-7.	0.0	0
16722	First-principles study of FeAl(B2) microalloyed with La, Ac, Sc and Y. Wuli Xuebao/Acta Physica Sinica, 2012, 61, 137102.	0.2	7
16723	Study on the electronic structures and energy band properties of Cd-doped wurtzite BeO. Wuli Xuebao/Acta Physica Sinica, 2012, 61, 177102.	0.2	2
16724	Energy band properties and phase stability of Be <sub>1-x</sub> Mg <sub>x</sub> O alloy. Wuli Xuebao/Acta Physica Sinica, 2012, 61, 237101.	0.2	2
16725	The Standard ASW Method. Lecture Notes in Physics, 2012, , 5-44.	0.3	0
16726	Density Functional Study of the Origin of the Strongly Delocalized Electronic Structure of the CuA Site in Cytochrome c Oxidase. Progress in Theoretical Chemistry and Physics, 2012, , 513-524.	0.2	0
16727	The vibration and dissociation of NO onPt (111) surface. Wuli Xuebao/Acta Physica Sinica, 2012, 61, 226801.	0.2	2
16728	Study on the lattice constants and energy band properties of Be and Ca doped wurtzite ZnO. Wuli Xuebao/Acta Physica Sinica, 2012, 61, 227101.	0.2	4
16729	First principles investigations of the structural stability and thermal dynamical properties of metal Ba under high pressure. Wuli Xuebao/Acta Physica Sinica, 2012, 61, 146301.	0.2	4
16730	Structural and electronic properties of Al-doped spinel LiMn <sub>2</sub> O <sub>4</sub> . Wuli Xuebao/Acta Physica Sinica, 2012, 61, 187306.	0.2	1
16732	First principles investigation of dynamic performance in the process of lithium intercalation into black phosphorus. Wuli Xuebao/Acta Physica Sinica, 2012, 61, 247101.	0.2	6
16733	Adsorption of successive layers of H <sub>2</sub> molecules on a model copper surface: performances of second- to fifth-rung exchange-correlation functionals. Highlights in Theoretical Chemistry, 2013, , 281-289.	0.0	0
16734	The effect of Si co-doping on defect-induced intrinsic magnetism in GaN. Hongwai Yu Haomibo Xuebao/Journal of Infrared and Millimeter Waves, 2012, 30, 229-231.	0.2	0
16736	Magnetic Properties of Iron on Strained Graphene: Density Functional Theory Study. Japanese Journal of Applied Physics, 2012, 51, 06FD13.	0.8	0
16738	The effect of Ga/N co-doping on electronic structure of InSb. Hongwai Yu Haomibo Xuebao/Journal of Infrared and Millimeter Waves, 2012, 31, 231-234.	0.2	0

#	ARTICLE	IF	CITATIONS
16741	Analysis of the origin of lateral interactions in the adsorption of small organic molecules on oxide surfaces. Highlights in Theoretical Chemistry, 2014, , 177-183.	0.0	0
16742	Lithium Niobate Dielectric Function and Second-Order Polarizability Tensor From Massively Parallel Ab Initio Calculations. , 2013, , 93-104.		0
16743	First-principles calculation and experimental study of metal magnetic memory effects. Wuli Xuebao/Acta Physica Sinica, 2013, 62, 086201.	0.2	3
16744	Theoretical Studies on Ethene Formation from Ethyl-Palladium(II) Complexes by Using DFT Method Including Solvent Effects. Journal of Computer Chemistry Japan, 2013, 12, 71-85.	0.0	0
16745	Occupancy sites of uranium atom in goethite by first-principles calculation. Wuli Xuebao/Acta Physica Sinica, 2013, 62, 087101.	0.2	0
16746	First-Principles Study for Phase Diagrams of Cd <sup>2+</sup> -Ca and Cd <sup>2+</sup> -Y Tsai-Type Approximants Under Pressure. , 2013, , 195-201.		1
16747	An Evaluation of Density Functional Theory for CO Adsorption on Pt(111). Progress in Theoretical Chemistry and Physics, 2013, , 195-210.	0.2	0
16748	First-principles study of pressure induced phase transition, electronic structure and elastic properties of CdS. Wuli Xuebao/Acta Physica Sinica, 2013, 62, 087104.	0.2	4
16749	A Safari Through Density Functional Theory. , 2013, , 465-478.		1
16750	First-principles study on the energy bandgap bowing parameter of wurtzite Be <sub>x</sub> Zn <sub>1-x</sub> O. Wuli Xuebao/Acta Physica Sinica, 2013, 62, 037102.	0.2	0
16751	Effect of substitution Fe <sup>2+</sup> on physical properties of MgSiO <sub>3</sub> perovskite at high temperature and high pressure. Wuli Xuebao/Acta Physica Sinica, 2013, 62, 049101.	0.2	2
16752	First-Principles Investigation of the Surface Properties of LiNiO <sub>2</sub> as Cathode Material for Lithium-ion Batteries. Journal of the Korean Electrochemical Society, 2013, 16, 169-176.	0.1	1
16753	Benchmarking the Performance of DHDFs for the Main Group Chemistry. Springer Briefs in Molecular Science, 2014, , 47-77.	0.1	0
16754	An Overview of Modern Density Functional Theory. Springer Briefs in Molecular Science, 2014, , 1-24.	0.1	0
16755	Electronic structures, band-gap origins and magnetisms of Ti <sub>2</sub> Cr-based alloys with CuHg <sub>2</sub> Ti-type structure. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 107103.	0.2	0
16756	Surface Stabilities and Helium Trapping of Nano-Sized Oxide Phases in Nano-Structured Ferritic Alloys: A First Principles Study. , 2014, , 163-170.		0
16757	Magnetic and electronic properties of fluorographene sheet with foreign atom substitutions. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 046102.	0.2	5
16758	First-principle study on the effects of Tl doping on the band gap and the band-edge of optical absorption of InI. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 147102.	0.2	3

#	ARTICLE	IF	CITATIONS
16760	Structural and electronic properties of hydrogenated bilayer boron nitride. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 016801.	0.2	1
16761	First-principles study on the effect of Ge-doping on the conductivity of InI. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 237101.	0.2	1
16763	Hydrocarbon Clusters: Building Blocks for New Materials. , 1993, , 157-165.		0
16764	Simple Views of Metallic Clusters. NATO ASI Series Series B: Physics, 1995, , 323-338.	0.2	0
16765	Density Functional Theory: Improving the Functionals, Extending the Applications. , 1996, , 359-394.		1
16766	Total Energy and Related Properties. Lecture Notes in Quantum Chemistry II, 1996, , 179-207.	0.3	4
16768	Density Functional Calculations on Special Clusters. , 1996, , 97-121.		0
16769	Calculation of Mineral Properties with the Electron Gas Model. Topics in Molecular Organization and Engineering, 1997, , 63-79.	0.1	0
16770	Fullerene Footprints: Cycloadducts of Carbon Rings. , 1997, , 261-274.		0
16771	Lattice Relaxation and the Stability of Plutonium-Based Alloys and Intermetallics. , 1998, , 109-112.		0
16772	Brief Introduction to Density Functional Theory. , 1998, , 3-18.		1
16773	Density Functionals for Energies and Eigenvalues: Local Mass Approximation. , 1998, , 299-309.		0
16774	Ab Initio Investigations of the Dynamical Properties of Ice. , 1999, , 175-184.		0
16775	A Brief Report on Density Functional Theory. , 1999, , 47-58.		0
16776	Molecular Properties from First Principles. , 1999, , 249-258.		0
16777	Molecular Electronics: Switchable and Programmable Device Models. , 0, , 2674-2691.		0
16778	DFT Study for Adsorption and Decomposition Mechanism of Trimethylene Oxide on Al(111) Surface. Bulletin of the Korean Chemical Society, 2014, 35, 2013-2018.	1.0	0
16779	Magnetic Properties of Strained L1<sub>0</sub>-ordered FePt and CoPt: An ab initio Study. Applied Science and Convergence Technology, 2014, 23, 273-278.	0.3	0

#	ARTICLE	IF	CITATIONS
16780	Molecular Dynamics Simulation: From "Ab Initio" to "Coarse Grained", 2015, , 1-61.		0
16782	Relativistic Density Functional Theory. , 2015, , 1-29.		2
16783	Creation of the ab initio theoretical high-pressure mineral physics. Ganseki Kobutsu Kagaku, 2015, 44, 10-24.	0.1	0
16784	Treating Relativistic Effects in Transition Metal Complexes. Springer Theses, 2015, , 23-36.	0.0	0
16787	Discovering Electronic Signatures for Phase Stability of Intermetallics via Machine Learning. Springer Series in Materials Science, 2016, , 223-238.	0.4	1
16788	Submonolayer Rare Earth Silicide Thin Films on the Si(111) Surface. , 2016, , 163-175.		0
16789	Single spin channels in Ni-doped CoTiSb semiconductor. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 087102.	0.2	0
16790	Electronic transport properties of oligo phenylene ethynylene molecule modified by the (CH <sub>3</sub> ) <sub>2</sub> and (NH <sub>2</sub> ) <sub>2</sub> groups. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 073102.	0.2	0
16791	First-principle study of the oxygen adsorption on Zr surface with Nb or Ge. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 096802.	0.2	0
16792	Research on THz wave reflection based on volume phase grating. , 2016, , .		0
16793	Quantum Mechanics for Quantum Chemistry. , 2016, , 357-549.		0
16794	Na-Ion Anode Based on Na(Li,Ti)O <sub>2</sub> System: Effects of Mg Addition. Journal of the Korean Ceramic Society, 2016, 53, 282-287.	1.1	0
16795	Experimental and Theoretical Approaches for the Surface Interaction between Copper and Activated Sludge Microorganisms at Molecular Scale. , 2016, , 3-22.		0
16796	Synthesis of Micron-sized Gold Nanoplates at Low Precursor Concentration Using Ionic Liquid as Novel Subphase Solvent. International Journal of Chemical Engineering and Applications (IJCEA), 2016, 7, 173-177.	0.3	3
16797	Density Functional Investigation of the Inclusion of Gold Clusters on a CH <sub>3</sub> Self-Assembled Lattice on Au(111). Advances in Chemistry, 2016, 2016, 1-8.	1.1	1
16798	Chapter 4 Theoretical Aspects of Gold Nanocatalyst for Ethanol and Glucose Oxidation. , 2016, , 145-176.		0
16800	First-principles study on adsorption mechanism of hydrogen on tungsten trioxide surface. Wuli Xuebao/Acta Physica Sinica, 2017, 66, 086801.	0.2	1
16801	The Composition of the Protosolar Disk and the Formation Conditions for Comets. , 2017, , 151-190.		0



#	ARTICLE	IF	CITATIONS
16802	Theoretical Modelling Methods. Springer Theses, 2017, , 37-66.	0.0	0
16803	First principle study of electronic structures and optical absorption properties of O and S doped graphite phase carbon nitride (g-C <sub>3</sub> N <sub>4</sub> ) <sub>6</sub> quantum dots. Wuli Xuebao/Acta Physica Sinica, 2017, 66, 187102.	0.2	2
16804	First-principles study of absorption mechanism of hydrogen on W <sub>2</sub> O <sub>5</sub> (010) surface. Wuli Xuebao/Acta Physica Sinica, 2017, 66, 246801.	0.2	2
16805	Experimental and Theoretical Methods. Springer Theses, 2017, , 31-43.	0.0	0
16806	Efectos de intercambio y correlaci3n en las propiedades estructurales y electr3nicas del TiO <sub>2</sub> en la fase rutilo. Ciencia En Desarrollo, 2017, 8, .	0.1	2
16807	Ru <sub>2</sub> FeGa Heusler alaÄ±mÄ±n yapÄ±sal, elektronik, elastik ve fonon Ä±zelliklerinin ilk prensip Ä±salÄ±masÄ±. Sakarya University Journal of Science, 0, , 1-1.	0.3	1
16808	Determination of the total energy of a many-particle system. , 2018, , 28-37.		0
16809	An overview of hydrogen storage system in Ni-MH batteries. , 2018, , 389-455.		0
16810	First-principles study on Jahn-Teller effect in Cr monolayer film. Wuli Xuebao/Acta Physica Sinica, 2018, 67, 237301.	0.2	2
16811	Lityum Bor KarbÄ±r (LiBC) BileÄ±inin YapÄ±sal, Elektronik ve Mekanik Ä±zelliklerinin BasÄ±nÄ± AltÄ±nda DeÄ±Ä±mi. Journal of the Faculty of Engineering and Architecture of Gazi University, 2018, 33, .	0.3	0
16812	Effects of Point Defects on Properties of B <sub>2</sub> NiAl: A First-principles Study. Rare Metal Materials and Engineering, 2018, 47, 2687-2692.	0.8	0
16813	First-principles study of structure, electronic structure and thermoelectric properties for Co<sub>2</sub>-based Heusler alloys Co<sub>2</sub>/FeAl<sub>1-x</sub>/Si<sub>x</sub> (x = 0.25, x = 0.5, x =) Tj ETCq1 1 0.784314	0.2	2
16814	First-principles study of rare-earth-doped cathode materials Li<sub>2</sub>/MnO<sub>3</sub> in Li-ion batteries. Wuli Xuebao/Acta Physica Sinica, 2019, 68, 138201.	0.2	4
16815	Optimized Li storage performance of B, N doped graphyne as Li-ion battery anode materials. Wuli Xuebao/Acta Physica Sinica, 2019, 68, 213601.	0.2	4
16816	First-principles study of electronic structure, magnetic and optical properties of laminated molybdenum oxides. Wuli Xuebao/Acta Physica Sinica, 2019, 68, 057101.	0.2	1
16817	Atomistic Simulations of Metal-Al <sub>2</sub> O <sub>3</sub> Interfaces. , 2019, , 199-239.		0
16818	Density Functional Methods. Springer Theses, 2019, , 29-70.	0.0	0
16819	Multiscale Simulation of Precipitation in Copper-Alloyed Pipeline Steels and in Cu-Ni-Si Alloys. , 2019, , 241-281.		1

#	ARTICLE	IF	CITATIONS
16820	Electronic structures and Li diffusion in cathode material $\text{Li}_2\text{FeO}_2$ of Li-ion batteries. Wuli Xuebao/Acta Physica Sinica, 2019, 68, 157201.	0.2	2
16821	Effect of mechanical deformations on absorption spectrum of metallic films of nanometer thickness. , 2019, , .		0
16822	Production of zinc oxide thin films and crystals in different deposition times and investigation of their structural, optical and electronic properties. Materials Science-Poland, 2019, 37, 90-99.	0.4	0
16823	Controlling factors for alignment of solute clusters in magnesium alloys: A first-principles analysis. Keikinokoku/Journal of Japan Institute of Light Metals, 2019, 69, 471-478.	0.1	0
16824	First-principles study of the single- and double-walled nanotubes of $\text{TiO}_2$ . , 2019, , .		0
16825	Investigation of Structural, Electronic, Optic and Elastic Properties of Perovskite $\text{RbGeCl}_3$ Crystal: A First Principles Study. Gazi University Journal of Science, 2019, 32, 1008-1019.	0.6	4
16826	Dimensionally driven crossover from semimetal to direct semiconductor in layered SbAs. Physical Review Materials, 2019, 3, .	0.9	1
16827	Simulation Studies for Black Phosphorus: From Theory to Experiment. Engineering Materials, 2020, , 101-115.	0.3	0
16828	Observing quantum trapping on $\text{MoS}_2$ through the lifetimes of resonant electrons: revealing the Pauli exclusion principle. Nanoscale Advances, 2020, 2, 5848-5856.	2.2	4
16829	Exact nonadiabatic part of the Kohn-Sham potential and its fluidic approximation. Physical Review Materials, 2020, 4, .	0.9	2
16830	Study on the reaction mechanism of acetylene selective hydrogenation catalysts $\text{Pd-Ag/Al}_2\text{O}_3$ . Inorganic and Nano-Metal Chemistry, 2021, 51, 70-77.	0.9	6
16831	Electronic structure and electrical transport properties of $\text{MoS}_2$ single-walled nanotubes based on first principles. International Journal of Modern Physics B, 2021, 35, .	1.0	1
16832	Non-covalent interactions in hexanuclear polyoxidometalates $[\text{VIV}_6\text{B}_2\text{O}_{50}\text{H}_8]^{8-}$ . An experimental and theoretical approach. Polyhedron, 2021, 211, 115553.	1.0	2
16833	Structure, Stability, Properties, and Application of Atomically Thin Coinage Metal Flatland in Graphene Pore: A Density Functional Theory Calculation. Physica Status Solidi (B): Basic Research, 2022, 259, 2100489.	0.7	10
16834	Electronic structure, optical and thermoelectric properties of $\text{Ge}_2\text{SeS}$ monolayer via first-principles study. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 136, 115022.	1.3	15
16835	Subnanometer high-entropy alloy nanowires enable remarkable hydrogen oxidation catalysis. Nature Communications, 2021, 12, 6261.	5.8	169
16836	X-ray Structure Determination, Antioxidant Voltammetry Studies of Butein and $2\text{-diOH}$ -Dihydroxy-3,4-dimethoxychalcone. Computational Studies of 4 Structurally Related $2\text{-diOH}$ Chalcones to Examine Their Antimalarial Activity by Binding to Falcipain-2. Molecules, 2021, 26, 6511.	1.7	6
16837	Comprehensive Mechanism of $\text{CO}_2$ Electroreduction on Non-Noble Metal Single-Atom Catalysts of $\text{Mo}_2\text{CS}_2$ -MXene. Chemistry - A European Journal, 2021, 27, 17900-17909.	1.7	16

#	ARTICLE	IF	CITATIONS
16838	Research on the Effects of Sn Dopants of V2O5 Based on the First Principles. Journal of Electronic Materials, 0, , 1.	1.0	4
16839	Prediction of lattice constants for the full-Heusler alloys by vector regression model and Artificial Neural Networks. Computational Condensed Matter, 2021, 29, e00605.	0.9	0
16840	Balancing Anchoring and Diffusion for Screening of Metal Oxide Cathode Materials in Lithium-Sulfur Batteries. Journal of Physical Chemistry C, 2021, 125, 24318-24327.	1.5	3
16841	Constructing Pd/ferroelectric Bi4Ti3O12 nanoflake interfaces for O2 activation and boosting NO photo-oxidation. Applied Catalysis B: Environmental, 2022, 302, 120876.	10.8	19
16842	Effects of hydrogen/halogen edge termination on structural, electronic, and optical properties of planar silicene nanoribbons SiNRs. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 136, 115046.	1.3	5
16843	The special chemical short-range order and solidification behavior of Cu-Fe-P immiscible alloys. Journal of Molecular Liquids, 2021, 344, 117936.	2.3	7
16844	Electronic theoretical study on sensing behaviors of defects and doping coexistence of black phosphorene to formaldehyde. Wuli Xuebao/Acta Physica Sinica, 2020, 69, 237101.	0.2	3
16845	Atomistic Modeling of Oxide Defects. , 2020, , 609-648.		4
16846	First-Principles Modeling of Interface Effects in Oxides. , 2020, , 1119-1149.		0
16847	DFT Study of MAX Phase Surfaces for Electrocatalyst Support Materials in Hydrogen Fuel Cells. Materials, 2021, 14, 77.	1.3	7
16848	CO Diffusion and Bond Weakening on Cu(410) Probing Surface Structure. E-Journal of Surface Science and Nanotechnology, 2020, 18, 307-311.	0.1	0
16849	Study on the optical properties for the F-type color center in BeO crystal with first-principles. Modern Physics Letters B, 2021, 35, 2150148.	1.0	2
16850	Strain and support effects on phase transition and surface reactivity of ultrathin ZnO films: DFT insights. AIP Advances, 2020, 10, .	0.6	4
16851	First-principles study on structural mechanical and thermodynamic properties of HfMoTaTiZr. Journal of Physics: Conference Series, 2020, 1706, 012148.	0.3	1
16852	Vibrational properties and Raman spectra of octagonal structure nitrogen. Journal of Raman Spectroscopy, 2021, 52, 626-634.	1.2	0
16853	Optimizing Configurations for Determining the Electromagnetic Properties of CsFeF3, NaFeF3, and RbFeF3 Fluorides: GGA vs GGA+U and TB-mBj Approaches. Annals of West University of Timisoara: Physics, 2020, 62, 71-94.	0.2	0
16854	Structural Stability and Magnetic Ordering in BiFeO3 Perovskite Oxide: A Comparative Study GGA+U vs L(S)DA+U. Annals of West University of Timisoara: Physics, 2020, 62, 52-70.	0.2	1
16855	Complexes of In(III) with 8-hydroxyquinoline-5-sulfonate in solution: Structural studies and the effect of cationic surfactants on the photophysical behaviour. Dalton Transactions, 2021, 50, 16970-16983.	1.6	2

#	ARTICLE	IF	CITATIONS
16856	Catalytic superlubricity via in-situ formation of graphene during sliding friction on Au@a-C:H films. <i>Carbon</i> , 2022, 186, 180-192.	5.4	26
16857	Oxidation mechanism of the arsenopyrite surface by oxygen with and without water: Experimental and theoretical analysis. <i>Applied Surface Science</i> , 2022, 573, 151574.	3.1	14
16858	Pressure effects on electronic structure and electrical conductivity of TiZrHfNb high-entropy alloy. <i>Intermetallics</i> , 2022, 140, 107394.	1.8	12
16859	Van der Waals heterostructure of graphene Defected&Doped X(X = Au, N) composite ZnO monolayer: A First Principle study. <i>Materials Science in Semiconductor Processing</i> , 2022, 138, 106247.	1.9	5
16860	In situ construction of S-scheme AgBr/BiOBr heterojunction with surface oxygen vacancy for boosting photocatalytic CO <sub>2</sub> reduction with H <sub>2</sub> O. <i>Applied Catalysis B: Environmental</i> , 2022, 301, 120802.	10.8	289
16861	Density functional theory studies on ortho-position adsorption of SO <sub>3</sub> at step sites of a CaO surface with SO <sub>2</sub> and CO <sub>2</sub> . <i>Fuel</i> , 2022, 310, 122174.	3.4	5
16862	Few-layer fluorine-functionalized graphene hole-selective contacts for efficient inverted perovskite solar cells. <i>Chemical Engineering Journal</i> , 2022, 430, 132831.	6.6	13
16863	Synergistic coupling between Fe <sub>7</sub> S <sub>8</sub> -MoS <sub>2</sub> heterostructure and few layers MoS <sub>2</sub> -embedded N/P-doping carbon nanocapsule enables superior Li-S battery performances. <i>Applied Surface Science</i> , 2022, 574, 151586.	3.1	25
16864	Light emission of Lu <sub>2</sub> Sn <sub>2</sub> O <sub>7</sub> pyrochlore driven by oxygen vacancy and local site engineering. <i>Journal of Alloys and Compounds</i> , 2022, 893, 162249.	2.8	5
16865	CO <sub>2</sub> reduction mechanism on the Nb <sub>2</sub> CO <sub>2</sub> MXene surface: Effect of nonmetal and metal modification. <i>Computational Materials Science</i> , 2022, 202, 110971.	1.4	16
16866	Electronic structure investigation of intrinsic and extrinsic defects in LiF. <i>Computational Materials Science</i> , 2022, 202, 110977.	1.4	11
16867	First-principles investigation on electronic structure and solar radiation shielding performance of Ti <sub>0.33</sub> WO <sub>3</sub> . <i>Wuli Xuebao/Acta Physica Sinica</i> , 2020, 69, 047102.	0.2	0
16868	Energetic Ground State Calculations, Electronic Band Structure at Surfaces. <i>Springer Handbooks</i> , 2020, , 471-498.	0.3	0
16869	Achieving flexible large-scale reactivity tuning by controlling the phase, thickness and support of two-dimensional ZnO. <i>Chemical Science</i> , 2021, 12, 15284-15290.	3.7	3
16870	Recent Developments in Density Functional Approximations. , 2020, , 213-226.		3
16871	Interaction of flotation reagents with mineral surface. , 2020, , 237-305.		0
16872	A Theoretical Perspective to the Magnetism of Nanoalloys. , 2020, , 225-265.		0
16873	First-principles study of magnetism in some novel MXene materials. <i>RSC Advances</i> , 2020, 10, 44430-44436.	1.7	11

#	ARTICLE	IF	CITATIONS
16874	Shock compression of niobium oxides from first-principles. AIP Conference Proceedings, 2020, , .	0.3	0
16875	Experimental and Computational Methods. Springer Theses, 2020, , 33-64.	0.0	0
16876	Progress of refactoring first principle package of Beijing Simulation Tool for Atom TEchnology. Wuli Xuebao/Acta Physica Sinica, 2020, 69, 043101.	0.2	0
16877	Interaction of Hydrogen with Graphitic Surfaces, Clean and Doped with Metal Clusters. , 2020, , 545-566.		0
16878	Optical properties of mono and bilayer plumbene: A DFT study. AIP Conference Proceedings, 2020, , .	0.3	1
16879	Visible Light-Promoted Carbon Dioxide Reforming of Methane Over Pt/TaN Catalysts. Springer Theses, 2020, , 75-91.	0.0	0
16880	Current Problems in Computer Simulation of Variability of Three-Dimensional Structure of DNA. Progress in Theoretical Chemistry and Physics, 2020, , 233-253.	0.2	1
16881	Site Preference of the Alloying Additions on Mechanical Properties of L12 Ni3Co Alloys. Minerals, Metals and Materials Series, 2020, , 1763-1774.	0.3	0
16882	Iron- and Silicon-Intercalated Graphene on Silicon Carbide: from Hybridization to Quasi-Freestanding Bilayer Graphene. Reviews on Advanced Materials and Technologies, 2020, 2, 42-46.	0.1	0
16883	High-pressure crystal structure and properties of BrCl. Journal of Physics Condensed Matter, 2020, 33, 095401.	0.7	2
16884	Nickel-based metal-organic framework-derived Ni/NC/KB as a separator coating for high capacity lithium-sulfur batteries. Sustainable Energy and Fuels, 2021, 5, 6372-6380.	2.5	6
16885	Unraveling Site Selective Magnetic Properties of Cobalt Sites in Critical Elements Lean RE(TM)5 Magnet Materials. Jom, 2021, 73, 3894-3900.	0.9	0
16886	Theoretical considerations of superconducting HfBH2 and HfB2H under high pressure. Journal of Applied Physics, 2021, 130, 153904.	1.1	3
16887	Prediction of stable Cu structure and phase transition mechanism at ultra-high pressure: A comprehensive properties characterization by DFT calculation. Physica B: Condensed Matter, 2022, 625, 413538.	1.3	1
16888	Spherical vs non-spherical and symmetry-preserving vs symmetry-breaking densities of open-shell atoms in density functional theory. Journal of Chemical Physics, 2021, 155, 234110.	1.2	5
16889	Defluorination and adsorption of tetrafluoroethylene (TFE) on TiO2(110) and Cr2O3(0001). Scientific Reports, 2021, 11, 21551.	1.6	0
16890	Ce-modified SrFeO3- for ethane oxidative dehydrogenation coupled with CO2 splitting via a chemical looping scheme. Applied Catalysis B: Environmental, 2022, 303, 120894.	10.8	47
16891	Accelerated Discovery of Single-Atom Catalysts for Nitrogen Fixation via Machine Learning. Energy and Environmental Materials, 2023, 6, .	7.3	26

#	ARTICLE	IF	CITATIONS
16892	Crystallographic, electronic and magnetic properties of Sr <sub>2</sub> FeW <sub>1-x</sub> MoxO <sub>6</sub> double perovskite oxides. Inorganic Chemistry Communication, 2021, 134, 109047.	1.8	4
16893	Quantum anomalous Hall effect in $\text{MnBi}_2\text{Te}_4$ van der Waals heterostructures. Physical Review Materials, 2021, 5, .	0.9	0
16894	Tris(6-diphenylphosphinoacenaphth-5-yl)gallium: Z-Type Ligand and Transmetalation Reagent. Organometallics, 2021, 40, 3785-3796.	1.1	3
16895	Theoretical Study of Weakly Bound Adsorbates on Au(111): Tests on van der Waals Density Functionals. Journal of Physical Chemistry C, 2021, 125, 24958-24966.	1.5	2
16896	Eco-friendly Utilization of silicon-rich lye: Synthesis of amorphous calcium silicate hydrate and its application for recovering heavy metals. Separation and Purification Technology, 2022, 282, 120092.	3.9	9
16897	Theoretical study on low temperature reverse water gas shift (RWGS) mechanism on monatomic transition metal M doped C <sub>2</sub> N catalyst (M=Cu, Co, Fe). Molecular Catalysis, 2021, 516, 111992.	1.0	6
16898	First-principles studies on two-dimensional B <sub>2</sub> O <sub>3</sub> adsorbent as a potential drug delivery platform for TEPA anticancer drug. Journal of Molecular Modeling, 2021, 27, 347.	0.8	16
16899	Superior Infrared Nonlinear Optical Performance Achieved by Synergetic Functional Motif and Vacancy Site Modulations. Chemistry of Materials, 2021, 33, 8831-8837.	3.2	23
16900	Dual-Silicon-Doped Graphitic Carbon Nitride Sheet: An Efficient Metal-Free Electrocatalyst for Urea Synthesis. Journal of Physical Chemistry Letters, 2021, 12, 10837-10844.	2.1	40
16901	Thermodynamic analysis of the gas phase reaction of Mg-doped GaN growth by HVPE using MgO. Japanese Journal of Applied Physics, 2020, 59, 088001.	0.8	5
16902	Gold nanostructures on iron oxide surfaces and their interaction with CO. Journal of Physics Condensed Matter, 2020, 32, 433001.	0.7	1
16903	Covalent Carbon Compounds: From Diamond Crystallites to Fullerene-Assembled Polymers. , 2002, , 111-130.		0
16904	Theoretical Methods for Modeling Chemical Processes on Semiconductor Surfaces. , 2004, , 246-265.		0
16906	Investigation of the Magnetic Hyperfine Field at <sup>140</sup> Ce on Gd Sites in GdCo <sub>2</sub> Compound. , 2005, , 189-193.		0
16907	Frontiers in surface analysis: Experiments and modeling. , 2007, , 391-414.		0
16910	Reaction Processes on Catalytically Active Surfaces. , 2007, , 311-340.		0
16912	Large-Scale Ab initio Simulations for Embedded Nanodots. , 2007, , 153-160.		0
16913	Redox Catalysis and Reactivity of Metalloporphyrines. , 2009, , 201-212.		0



#	ARTICLE	IF	CITATIONS
16914	Long-Range Chiral Recognition Due to Substrate Locking and Substrate-Adsorbate Charge Transfer. , 2009, , 641-648.		0
16915	The Standard ASW Method. , 2007, , 5-45.		0
16916	The Basic Structure of Ti-Si-N Superhard Nanocomposite Coatings: Ab Initio Studies. , 2008, , 117-136.		0
16917	Understanding Molecular Recognition and Self-Assembly from Large-Scale Numerical Simulations. , 2009, , 129-137.		0
16918	Statistical study of vacancy diffusion in TiC and TaC. Physical Review Materials, 2020, 4, .	0.9	3
16919	Magnetic Anisotropy of Graphene-Coated Ultrathin Iron Layers on a Substrate of Hexagonal Boron Nitride Gr/Fe/h-BN. Physics of the Solid State, 2020, 62, 2203-2207.	0.2	0
16920	A computational study of the S <sub>N</sub> Ar reaction of 2-ethoxy-3,5-dinitropyridine and 2-methoxy-3,5-dinitropyridine with piperidine. ChemistrySelect, 2022, 7, 589-603.	0.7	0
16921	Effect of Sulfur Substitution on Charge Transport Ability of Benzopyrazine-Fused Tetracene Derivatives: A Theoretical Study. Applied Science and Convergence Technology, 2020, 29, 149-153.	0.3	0
16922	Design of Materials for Nuclear Energy Applications: First-Principles Calculations and Artificial Intelligence Methods. High Temperature, 2020, 58, 907-937.	0.1	3
16923	Study of Donor-Acceptor Bonds on the N-Coordinated Sn/Pb(II) Atoms in peri-Substituted Naphthalenes: Evidence of Pb <sup>+</sup> B Interaction. European Journal of Inorganic Chemistry, 2020, 2020, 3644-3653.	1.0	7
16925	Atomic-Scale Mechanism of Unidirectional Oxide Growth. Advanced Functional Materials, 2019, 30, .	7.8	2
16926	Metallic C <sub>5</sub> N monolayer as an efficient catalyst for accelerating redox kinetics of sulfur in lithium-sulfur batteries. Physical Chemistry Chemical Physics, 2021, 24, 180-190.	1.3	9
16927	Correction methods for first-principles calculations of the solution enthalpy of gases and compounds in liquid metals. Physical Chemistry Chemical Physics, 2022, 24, 757-770.	1.3	3
16928	Revealing the influence of Mo addition on interphase precipitation in Ti-bearing low carbon steels. Acta Materialia, 2022, 223, 117475.	3.8	22
16929	Theoretical studies on dicopper(II) complexes of phenoxido-bridged ligands: Magneto-structural correlations. Computational and Theoretical Chemistry, 2022, 1207, 113524.	1.1	6
16930	Plasma enhanced anti-coking performance of Pd/CeO <sub>2</sub> catalysts for the conversion of methane. Sustainable Energy and Fuels, 2021, 6, 98-109.	2.5	20
16931	A DFT computational prediction of 2H phase W <sub>2</sub> C monolayer and the effect of O functional groups. Physics Letters, Section A: General, Atomic and Solid State Physics, 2022, 424, 127842.	0.9	4
16932	Mechanism of ethanol steam reforming on B <sub>12</sub> N <sub>12</sub> and Al <sub>12</sub> N <sub>12</sub> nano-cages: A theoretical study. Materials Today Communications, 2022, 30, 103014.	0.9	2

#	ARTICLE	IF	CITATIONS
16933	First-principles and experimental investigations on ductility/brittleness of intermetallic compounds and joint properties in steel/aluminum laser welding. Transactions of Nonferrous Metals Society of China, 2021, 31, 2962-2977.	1.7	17
16934	Assessment of the van der Waals, Hubbard $U$ parameter and spin-orbit coupling corrections on the $2D/3D$ structures from metal gold congeners clusters. Journal of Computational Chemistry, 2022, 43, 230-243.	1.5	4
16935	Benchmarking isotropic hyperfine coupling constants using (QTP) DFT functionals and coupled cluster theory. Journal of Chemical Physics, 2022, 156, 094107.	1.2	5
16936	Theoretical Screening of Transition Metal Doped Defective $MoS_2$ as Efficient Electrocatalyst for CO Conversion to $CH_4$ . ChemPhysChem, 2022, 23, .	1.0	2
16937	Breaking the energy density limit of $LiNiO_2$ : $Li_2NiO_3$ or $Li_2NiO_2$ ?. Science China Materials, 2022, 65, 913-919.	3.5	6
16938	Exploring DFT+U parameter space with a Bayesian calibration assisted by Markov chain Monte Carlo sampling. Npj Computational Materials, 2021, 7, .	3.5	8
16939	Adsorption and Oxidation of CO on Ceria Nanoparticles Exposing Single-Atom Pd and Ag: A DFT Modelling. Materials, 2021, 14, 6888.	1.3	2
16940	Tunable CO/H <sub>2</sub> ratios of electrochemical reduction of CO <sub>2</sub> through the Zn-Ln dual atomic catalysts. Science Advances, 2021, 7, eabl4915.	4.7	82
16941	Revealing Size Dependent Structural Transitions in Supported Gold Nanoparticles in Hydrogen at Atmospheric Pressure. Small, 2021, 17, e2104571.	5.2	13
16942	Density Functional Theory Calculations on Electrocatalytic CO <sub>2</sub> Hydrogenation to C <sub>2</sub> -Based Products over Cu(100) Nanocubes. ACS Applied Nano Materials, 2021, 4, 11907-11919.	2.4	9
16943	Theoretical study of SnS <sub>2</sub> encapsulated in Graphene as a promising anode material for K <sup>+</sup> ion batteries. Journal of Physics Condensed Matter, 2021, , .	0.7	0
16944	Mechanism of Oxygen Reduction Reaction on Monolayer WTe <sub>2</sub> with and without S Dopant at Low Coverage. E-Journal of Surface Science and Nanotechnology, 2021, 19, 119-124.	0.1	0
16945	An inexpensive density functional theory based protocol to predict accurate <sup>19</sup> F NMR chemical shifts. Journal of Computational Chemistry, 2022, 43, 170-183.	1.5	5
16946	Accurate <sup>57</sup> Fe Mössbauer Parameters from General Gaussian Basis Sets. Journal of Chemical Theory and Computation, 2021, 17, 7724-7731.	2.3	3
16947	Highly Mesoporous Cobalt-Hybridized 2D Cu <sub>3</sub> P Nanosheet Arrays as Boosting Janus Electrocatalysts for Water Splitting. Inorganic Chemistry, 2021, 60, 18325-18336.	1.9	8
16948	Rashba-split surface state and spin-dependent photon emission from Re(0001) at $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML">\langle \text{mml:mover}>\langle \text{mml:mi mathvariant="normal">\hat{I}</mml:mi>\langle \text{mml:mo>\hat{A}</mml:mo>\langle \text{mml:mover}>\langle \text{mml:math}>$ . Physical Review B, 2021, 104, .	1.1	4
16949	Understanding the Role of Element Grain Boundary Diffusion Mechanism in Nd-Fe-B Magnets. Advanced Functional Materials, 2022, 32, 2109529.	7.8	49
16950	Rationalization of Nonlinear Adsorption Energy-Strain Relations and Brønsted-Evans-Polanyi and Transition State Scaling Relationships under Strain. Journal of Physical Chemistry Letters, 2021, 12, 11578-11584.	2.1	4

#	ARTICLE	IF	CITATIONS
16951	The influence of secondary interactions on the [Ni(O <sub>2</sub> )] <sup>+</sup> mediated aldehyde oxidation reactions. Journal of Inorganic Biochemistry, 2021, 227, 111668.	1.5	2
16952	Deep machine learning potentials for multicomponent metallic melts: Development, predictability and compositional transferability. Journal of Molecular Liquids, 2022, 349, 118181.	2.3	25
16953	Transition Metal-Modified Co <sub>4</sub> Clusters Supported on Graphdiyne as an Effective Nitrogen Reduction Reaction Electrocatalyst. Inorganic Chemistry, 2021, 60, 18251-18259.	1.9	21
16954	Dissociative Adsorption of H <sub>2</sub> S on Li(110) Surface Using Density Functional Theory Calculations and Car-Parrinello Molecular Dynamics Simulations. ChemPhysChem, 2022, 23, .	1.0	5
16955	Targeted Regulation of the Electronic States of Nickel Toward the Efficient Electrosynthesis of Benzonitrile and Hydrogen Production. ACS Applied Materials & Interfaces, 2021, 13, 56140-56150.	4.0	21
16956	First-Principles Study on the Effect of Strain on Single-Layer Molybdenum Disulfide. Nanomaterials, 2021, 11, 3127.	1.9	9
16957	Simulation of STM Images of Hematite $\hat{\pm}$ -Fe <sub>2</sub> O <sub>3</sub> (0001) Surfaces: Dependence on Distance and Bias. Journal of Physical Chemistry C, 2021, 125, 26711-26717.	1.5	3
16958	Benchmark calculations and error cancelations for bond dissociation enthalpies of X <sup>+</sup> NO <sub>2</sub> . Defence Technology, 2023, 22, 144-155.	2.1	6
16959	Influence of sulfur vacancy on pyrite oxidization by water and oxygen molecules. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 634, 127954.	2.3	11
16960	Diffusion Barriers for Carbon Monoxide on the Cu(001) Surface Using Many-Body Perturbation Theory and Various Density Functionals. Journal of Chemical Theory and Computation, 2021, 17, 7862-7872.	2.3	10
16961	Low loaded MoS <sub>2</sub> /Carbon cloth as a highly efficient electrocatalyst for hydrogen evolution reaction. International Journal of Hydrogen Energy, 2022, 47, 1579-1588.	3.8	9
16962	Radiation damage of MoAlB at elevated temperatures: Investigating MAB phases as potential neutron shielding materials. Journal of the European Ceramic Society, 2022, 42, 1311-1321.	2.8	8
16963	Inorganic gas sensing performance of $\hat{\pm}$ -borophene and the van der Waals heterostructure. Applied Surface Science, 2022, 581, 151906.	3.1	18
16964	Theoretical study of methanol synthesis from CO <sub>2</sub> hydrogenation on the surface of NiO supported In <sub>2</sub> O <sub>3</sub> (110) catalyst. Journal of Fuel Chemistry and Technology, 2021, 49, 1684-1692.	0.9	3
16965	An oxygen vacancy-rich ZnO layer on garnet electrolyte enables dendrite-free solid state lithium metal batteries. Chemical Engineering Journal, 2022, 433, 133665.	6.6	23
16966	Impact of magnetic transition on Mn diffusion in $\hat{\pm}$ -iron: Correlative state-of-the-art theoretical and experimental study. Physical Review B, 2021, 104, .	1.1	3
16967	Study of the electronic and opto-electronic properties of the perovskite KPbBr <sub>3</sub> by DFT and TDDFT methods. Computational Condensed Matter, 2022, 33, e00617.	0.9	15
16968	Analytic Alchemical Derivatives for the Analysis of Differential Acidity Assisted by the <i>h</i> Function. Journal of Physical Chemistry A, 2021, 125, 10463-10474.	1.1	4

#	ARTICLE	IF	CITATIONS
16969	Computational Screening of First-Row Transition-Metal Based Alloy Catalystsâ€™Ligand Induced N <sub>2</sub> Reduction Reaction Selectivity. ACS Physical Chemistry Au, 2022, 2, 125-135.	1.9	7
16970	Laser-fabricated channeled Cu <sub>6</sub> Sn <sub>5</sub> /Sn as electrocatalyst and gas diffusion electrode for efficient CO <sub>2</sub> electroreduction to formate. Applied Catalysis B: Environmental, 2022, 307, 120991.	10.8	26
16971	Interface features and electronic structure of Bi <sub>2</sub> SiO <sub>5</sub> /Bi <sub>2</sub> O <sub>3</sub> hetero-junction. , 2021, , .		0
16972	New mode of stress sensing in multicolor (Ca1-Sr) <sub>8</sub> Mg <sub>3</sub> Al <sub>2</sub> Si <sub>7</sub> O <sub>28</sub> :Eu <sup>2+</sup> solid-solution compounds. Nano Energy, 2022, 93, 106799.	8.2	14
16973	Heterogeneous Atoms Substituted Rock Salt Phase Mn <sub>1-x</sub> Fe <sub>x</sub> O Solid Solution with Rich Defects for Advanced Lithium-Ion Batteries. Small, 2022, 18, e2106273.	5.2	2
16974	Vapor-Phase Intercalation of Cesium into Black Phosphorous. Journal of Physical Chemistry C, 2021, 125, 27440-27448.	1.5	2
16975	Halogen-Ion-Induced Structural Phase Transition Giving a Polymorph of HgBr <sub>2</sub> with Balanced Nonlinear Optical Properties. Inorganic Chemistry, 2021, 60, 19297-19303.	1.9	5
16976	Elasticity, Mechanical and Thermal Properties of Polycrystalline Hafnium Carbide and Tantalum Carbide at High Pressure. SSRN Electronic Journal, 0, , .	0.4	0
16977	Calculations of the three-dimensional crystal structures consisting of 4-8 graphene layers functionalized with fluorine. AIP Conference Proceedings, 2021, , .	0.3	0
16978	The effect of organic cation dynamics on the optical properties in (PEA) <sub>2</sub> (MA)[Pb <sub>2</sub> I <sub>7</sub> ] perovskite dimorphs. Journal of Materials Chemistry C, 2021, 9, 17050-17060.	2.7	2
16979	Single-atom catalysts on supported silicomolybdc acid for CO <sub>2</sub> electroreduction: a DFT prediction. Journal of Materials Chemistry A, 2022, 10, 6178-6186.	5.2	25
16980	Approach for noncollinear GGA kernels in closed-shell systems. Physical Review B, 2022, 105, , .	1.1	3
16981	Hydrogen trapping and storage in the group IVB-VIB transition metal carbides. Materials and Design, 2022, 214, 110399.	3.3	20
16982	Solar fuels: research and development strategies to accelerate photocatalytic CO <sub>2</sub> conversion into hydrocarbon fuels. Energy and Environmental Science, 2022, 15, 880-937.	15.6	304
16983	First-Principles Study on Metal-Modified N <sub>2</sub> P <sub>6</sub> Nanoscale Layers for Adsorption Performance and Sensing Capability. ACS Applied Nano Materials, 2022, 5, 1102-1109.	2.4	3
16984	Unveiling the mechanism of high-performance hydrogen evolution reaction on noble-metal-free (113)-faceted Ni <sub>3</sub> C: <i>ab initio</i> calculations. RSC Advances, 2021, 12, 869-873.	1.7	1
16985	Adsorption studies of 2,3-butanedione and acetic acid on Î¶-phosphorene sheets based on the first-principles study. Computational and Theoretical Chemistry, 2022, 1208, 113548.	1.1	10
16986	First-principles calculations to investigate ultra-wide bandgap semiconductor behavior of NaMgF <sub>3</sub> fluoro-perovskite with external static isotropic pressure and its impact on optical properties. Optik, 2022, 252, 168532.	1.4	24

#	ARTICLE	IF	CITATIONS
16987	Structure, mechanical stability, lattice dynamics and thermodynamic properties of C15-Laves phase Mg <sub>2</sub> Ce. Solid State Communications, 2022, 342, 114641.	0.9	1
16988	New high-pressure monoclinic phase of Sn. Solid State Communications, 2022, 342, 114635.	0.9	1
16989	Compatibility of UN with refractory metals (V, Nb, Ta, Cr, Mo and W): An ab initio approach to interface reactions and diffusion behavior. Journal of Nuclear Materials, 2022, 560, 153482.	1.3	5
16990	The new stable phases of Fe <sub>2</sub> Pd crystal alloy and their properties. Computational Materials Science, 2022, 204, 111183.	1.4	1
16991	Ni/Li antite site induced disordered passivation layer for high-Ni layered oxide cathode material. Energy Storage Materials, 2022, 45, 720-729.	9.5	29
16992	Band gap controlling of doped bulk silicon carbide structure under the influence of tensile stress: DFT. Computational Condensed Matter, 2022, 30, e00624.	0.9	7
16993	Insight into the Sb(III) and Sb(V) removal mechanisms on porous Fe-Ti-chitosan composite: Experiment and DFT calculations. Chemical Engineering Journal, 2022, 432, 134420.	6.6	7
16994	Cathode electrochemically reconstructed V-doped CoO nanosheets for enhanced alkaline hydrogen evolution reaction. Chemical Engineering Journal, 2022, 432, 134331.	6.6	31
16995	A first principles investigation on the structural, elastic, and mechanical properties of MAX phase M <sub>3</sub> AlC <sub>2</sub> (M= Ta, Ti, V) as a function of pressure. Computational Condensed Matter, 2022, 30, e00638.	0.9	2
16996	First-principles study on stability, adhesion and fracture properties of ZrO <sub>2</sub> /W interface in composite materials. Journal of Nuclear Materials, 2022, 560, 153510.	1.3	3
16997	Single transition metal atom anchored on VSe <sub>2</sub> as electrocatalyst for nitrogen reduction reaction. Applied Surface Science, 2022, 580, 152272.	3.1	15
16998	Supercritical CO <sub>2</sub> assisted synthesis of highly accessible iron single atoms and clusters on nitrogen-doped carbon as efficient oxygen reduction electrocatalysts. Chemical Engineering Journal, 2022, 433, 134460.	0.8	5
16999	Supercritical CO <sub>2</sub> assisted synthesis of highly accessible iron single atoms and clusters on nitrogen-doped carbon as efficient oxygen reduction electrocatalysts. Chemical Engineering Journal, 2022, 433, 134460.	6.6	22
17000	Metal/antiperovskite metal nitride composites Ag/AgNNi <sub>3</sub> as novel efficient electrocatalysts for hydrogen evolution reaction in alkaline media. Journal of Materials Science and Technology, 2022, 112, 222-229.	5.6	8
17001	Ultrafine Co-MoS <sub>2</sub> monolayer catalyst derived from oil-soluble single-molecule polyoxometalates for slurry phase hydrocracking. Fuel, 2022, 315, 123134.	3.4	11
17002	Tuning the structural properties and chemical activities of graphene and hexagonal boron nitride for efficient adsorption of steroidal pollutants. Applied Surface Science, 2022, 580, 152110.	3.1	6
17004	Gas-Phase Thermochemistry of MX <sub>3</sub> and M <sub>2</sub> X <sub>6</sub> (M = Sc, Y; X = F, Cl). Tj ETQq0 0 0 rgBT /Overlocl Chemistry, 2020, 59, 17084-17095.	1.9	6
17005	Mo <sub>2</sub> CS <sub>2</sub> -Mxene Supported Single-Atom Catalysts for Efficient and Selective CO <sub>2</sub> Electrochemical Reduction. SSRN Electronic Journal, 0, , .	0.4	0

#	ARTICLE	IF	CITATIONS
17006	Structural, electronic, and thermodynamic properties of a rare earth dihydride TbH <sub>2</sub> , 2021, . , .		0
17007	Dipole Polarizability of C28 and its Counterparts Nb4B18 and Ta4B18. Insights from a Density Functional Theory (DFT) Endeavour. Journal of Physics: Conference Series, 2021, 2090, 012172.	0.3	0
17008	Investigation of the effect of surface phosphate ester dispersant on viscosity by coarse-grain modeling of BaTiO slurry. Journal of the American Ceramic Society, 2022, 105, 2791-2803.	1.9	0
17009	Laves Phase Formation in High Entropy Alloys. Metals, 2021, 11, 1962.	1.0	6
17010	Insight into the stacking and the species-ordering dependences of interlayer bonding in SiC/GeC polar heterostructures. Nanotechnology, 2022, 33, 155706.	1.3	5
17011	Two-dimensional CdS/SnS <sub>2</sub> heterostructure: a highly efficient direct Z-scheme water splitting photocatalyst. Physical Chemistry Chemical Physics, 2022, 24, 3826-3833.	1.3	18
17012	Impurity Controlled near Infrared Surface Plasmonic in AlN. Nanomaterials, 2022, 12, 459.	1.9	1
17013	Pb <sub>4</sub> SeBr <sub>6</sub> : A Congruently Melting Mid-Infrared Nonlinear Optical Material with Excellent Comprehensive Performance. Advanced Optical Materials, 2022, 10, .	3.6	21
17014	DFT study of crystal structure and electronic properties of metal-doped AlH <sub>3</sub> polymorphs. International Journal of Hydrogen Energy, 2022, 47, 6142-6153.	3.8	6
17015	Role of Mn-substitution towards the enhanced hydrogen storage performance in FeTi. International Journal of Hydrogen Energy, 2022, 47, 9357-9371.	3.8	4
17016	Catalytic reduction of 4-nitrophenol using CuO@Na <sub>2</sub> Ti(PO <sub>4</sub> ) <sub>2</sub> ·xH <sub>2</sub> O. Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering, 2022, 57, 65-79.	0.9	3
17017	Vacancy engineering of oxidized Nb <sub>2</sub> C <sub>x</sub> MXenes for a biased nitrogen fixation. Green Energy and Environment, 2023, 8, 1185-1194.	4.7	11
17018	On the Nature of the Bonding in Coinage Metal Halides. Molecules, 2022, 27, 490.	1.7	7
17019	Equation of state and strength of diamond in high-pressure ramp loading. Physical Review B, 2022, 105, .	1.1	4
17020	A polyoxometalate cluster-based single-atom catalyst for NH <sub>3</sub> synthesis <i>via</i> an enzymatic mechanism. Journal of Materials Chemistry A, 2022, 10, 6165-6177.	5.2	23
17021	Crystal Facet and Architecture Engineering of Metal Oxide Nanonetwork Anodes for High-Performance Potassium Ion Batteries and Hybrid Capacitors. ACS Nano, 2022, 16, 1486-1501.	7.3	63
17022	Heisenberg Spin Hamiltonian Derived from a Multiple Grand Canonical Spin Density Functional Theory with a Principal Nonlocal Exchange-Correlation Energy Functional. Journal of the Physical Society of Japan, 2022, 91, .	0.7	1
17023	GGA-SIC Calculations for Electronic and Magnetic Study of CdS Alloys. Journal of Superconductivity and Novel Magnetism, 2022, 35, 331-338.	0.8	1



#	ARTICLE	IF	CITATIONS
17024	Thermodynamic reassessment of Au-Pt-Sn system. <i>Materials Research Express</i> , 2022, 9, 016507.	0.8	0
17025	Radiation-doped SiC*/Si heterostructure formation and defects evolution. <i>Journal of Physics: Conference Series</i> , 2022, 2155, 012012.	0.3	0
17026	First Principles Study of Regulation of Monolayer ZnO and Vacancy Defects Equibiaxial Strain. <i>Journal of Superconductivity and Novel Magnetism</i> , 2022, 35, 925-934.	0.8	2
17027	Thermoelectric properties plus phonon and de Haas-van Alphen frequencies of hole/electron-doped $\text{CeIn}_3$ . <i>Scientific Reports</i> , 2022, 12, 663.	1.6	4
17028	DFT calculations for adsorption of H <sub>2</sub> S and other natural gas compounds on (Fe, Co, Ni, Cu and Zn)-Y zeolite clusters. <i>Microporous and Mesoporous Materials</i> , 2022, 331, 111643.	2.2	17
17029	Binding of As <sup>3+</sup> and As <sup>5+</sup> to Fe(III) Oxyhydroxide Clusters and the Influence of Aluminum Substitution: A Molecular Perspective. <i>Journal of Physical Chemistry A</i> , 2022, 126, 670-684.	1.1	2
17030	Clarification of the relative magnitude of exciton binding energies in ZnO and SnO <sub>2</sub> . <i>Applied Physics Letters</i> , 2022, 120, .	1.5	8
17031	Pressure-stabilized hexafluorides of first-row transition metals. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1736-1742.	1.3	4
17032	Novel Two-Dimensional Metal-Based $\pi$ -d Conjugated Nanosheets as Photocatalyst for Nitrogen Reduction Reaction: The First-Principle Investigation. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 5384-5394.	4.0	10
17033	Evidence of a Tetrahedrally Coordinated RuO <sub>4</sub> Surface Complex on RuO <sub>2</sub> (100): Density Functional Theory and Beyond. <i>Journal of Physical Chemistry C</i> , 2022, 126, 946-956.	1.5	4
17034	First-principles calculations of stable local structures and electronic structures of magnesium secondary battery cathode materials, MgCo <sub>2-x</sub> MnxO <sub>4</sub> (x=0, 0.5), in second charged state after first discharge. <i>Journal of Solid State Electrochemistry</i> , 2022, 26, 663-682.	1.2	3
17035	Ferromagnetic and nonmagnetic charge density wave states in transition metal dichalcogenides: Physical mechanisms and charge doping induced reversible transition. <i>Physical Review B</i> , 2022, 105, .	1.1	4
17036	High-Temperature Superconductivity in the Lanthanide Hydrides at Extreme Pressures. <i>Applied Sciences (Switzerland)</i> , 2022, 12, 874.	1.3	4
17037	Manipulation of current rectification in van der Waals ferroionic CuInP <sub>2</sub> S <sub>6</sub> . <i>Nature Communications</i> , 2022, 13, 574.	5.8	60
17038	Ab Initio Simulations of Water/Metal Interfaces. <i>Chemical Reviews</i> , 2022, 122, 10746-10776.	23.0	72
17039	Linear response calculation with nonlocal van der Waals density functionals. <i>Physical Review B</i> , 2022, 105, .	1.1	3
17040	Ultra-deep desulfurization of mercaptan by cyclic selective adsorption- reactive regeneration at room temperature. <i>AIChE Journal</i> , 2022, 68, .	1.8	3
17041	Giant Shift Photovoltaic Current in Group V Binary Nanosheets. <i>Advanced Theory and Simulations</i> , 0, 2100472.	1.3	3

#	ARTICLE	IF	CITATIONS
17042	Influence of strain and external electric field on the performance of PC6/MoSe2 heterostructure. Journal of Materials Science, 2022, 57, 477-488.	1.7	6
17043	Modification of Metal (Fe, Al) Doping on Reaction Properties of a NiO Oxygen Carrier with CO during Chemical Looping Combustion. ACS Omega, 2022, 7, 4381-4388.	1.6	5
17044	Engineering a heteroatom-doped multidimensional carbon network for dendrite-free lithium metal anode. Materials Today Energy, 2022, 24, 100949.	2.5	9
17045	Ultrathick MoS <sub>2</sub> Films with Exceptionally High Volumetric Capacitance. Advanced Energy Materials, 2022, 12, .	10.2	44
17046	Accurate Spectral Properties within Double-Hybrid Density Functional Theory: A Spin-Scaled Range-Separated Second-Order Algebraic-Diagrammatic Construction-Based Approach. Journal of Chemical Theory and Computation, 2022, 18, 865-882.	2.3	14
17047	Critical assessment of machine-learned repulsive potentials for the density functional based tight-binding method: A case study for pure silicon. Journal of Chemical Physics, 2022, 156, 064101.	1.2	4
17048	Electronic properties of zero-line modes in bilayer graphene: An <i>ab initio</i> study. Physical Review B, 2022, 105, .	1.1	2
17051	<i>In silico</i> design of dual-doped nitrogenated graphene (C <sub>2</sub> N) employed in electrocatalytic reduction of carbon monoxide to ethylene. Journal of Materials Chemistry A, 2022, 10, 4703-4710.	5.2	12
17052	Effect of cobalt phosphide (CoP) vacancies on its hydrogen evolution activity <i>via</i> water splitting: a theoretical study. Physical Chemistry Chemical Physics, 2022, 24, 4644-4652.	1.3	20
17053	Rational Design of Bimetallic Zeolitic Imidazolate Framework-Derived C, N Dual-Doped ZnO/Co for Boosting Lithium Storage. Advanced Sustainable Systems, 2022, 6, .	2.7	1
17054	Computation and Simulation. Modern Aspects of Electrochemistry, 2022, , 355-395.	0.2	1
17055	Stress-Strain Relations and Deformation Mechanisms of ZrN and HfN Superconductors. Crystal Growth and Design, 2022, 22, 1104-1109.	1.4	1
17056	Study on New High-Pressure Phases and Electronic Properties of Iodine Chloride Employing Ab Initio Calculations. Journal of Electronic Materials, 2022, 51, 1632-1638.	1.0	3
17057	Two-dimensional B7P2: Dual-purpose functional material for hydrogen evolution reaction/hydrogen storage. International Journal of Hydrogen Energy, 2022, 47, 8338-8347.	3.8	6
17058	The mechanism of MOF as a heterogeneous catalyst for propene hydroformylation: a DFT study. Reaction Chemistry and Engineering, 2022, 7, 1156-1167.	1.9	8
17059	B2O and B4N monolayers supported single-metal atom as highly efficient bifunctional electrocatalyst for OER and ORR. Journal of Materials Science, 2022, 57, 398-410.	1.7	4
17060	Atomically Thin Indium-Tin-Oxide Transistors Enabled by Atomic Layer Deposition. IEEE Transactions on Electron Devices, 2022, 69, 231-236.	1.6	20
17061	Theoretical studies on the two-photon absorption of II-VI semiconductor nano clusters. Scientific Reports, 2022, 12, 110.	1.6	3

#	ARTICLE	IF	CITATIONS
17062	A density functional theory investigation of the reaction of water with Ce <sub>2</sub> O <sub>3</sub> . Computational and Theoretical Chemistry, 2022, 1209, 113603.	1.1	0
17063	Unraveling the Mechanism of Palladium-Catalyzed Base-Free Cross-Coupling of Vinyl Carboxylates: Dual Role of Arylboronic Acids as a Reducing Agent and a Coupling Partner. ACS Catalysis, 2022, 12, 1809-1817.	5.5	3
17064	High-Throughput Screening of Efficient Biatom Catalysts Based on Monolayer Carbon Nitride for the Nitric Oxide Reduction Reaction. Journal of Physical Chemistry Letters, 2022, 13, 527-535.	2.1	35
17065	Pb <sub>0.8</sub> Sn <sub>0.2</sub> Se thin films: synthesis, sensitization, and properties evolution. Journal of Materials Science: Materials in Electronics, 2022, 33, 5564-5574.	1.1	2
17066	$\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \text{mathvariant="double-struck"} \rangle \langle \text{mml:mn} \rangle \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$ nontrivial topology of rare-earth binary oxide superconductor LaO. Physical Review B, 2022, 105, .	1.1	2
17067	Exploring the Compositional Space of High-Entropy Alloys for Cost-Effective High-Temperature Applications. Frontiers in Materials, 2022, 8, .	1.2	5
17068	Emergence of Magnetic Transition in Cobalt Oxide Nanowires on Vicinal Pt Substrate. IEEE Magnetics Letters, 2022, 13, 1-5.	0.6	1
17069	Methylcyclohexane and methyl methacrylate sensing studies using $\hat{\Gamma}^3$ -arsene nanoribbon – A first-principles investigation. Computational and Theoretical Chemistry, 2022, 1209, 113595.	1.1	12
17070	Spin transport characteristics and photoelectric properties of magnetic semiconductor NiBr <sub>2</sub> monolayer. Wuli Xuebao/Acta Physica Sinica, 2022, .	0.2	2
17071	Cation-Doping in Organic-Inorganic Perovskites to Improve the Structural Stability from Theoretical Prediction. Journal of Physical Chemistry Letters, 2022, 13, 1180-1186.	2.1	2
17072	High-ammonia selective metal-organic framework-derived Co-doped Fe <sub>2</sub> O <sub>3</sub> catalysts for electrochemical nitrate reduction. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	75
17073	The role of defects presenting in graphitic SiC sheets and their consequences in the exfoliation of layers – a first principles approach. Physical Chemistry Chemical Physics, 2022, 24, 4262-4269.	1.3	3
17074	High electrocatalytical performance of FeCoNiCuPd high-entropy alloy for nitrogen reduction reaction. Molecular Catalysis, 2022, 519, 112141.	1.0	13
17075	Exploring the heavy transition metal trihalide family: Two-dimensional magnetic materials with tunable band gap, huge magnetic anisotropy, and high-temperature magnetic ordering. Physical Review Materials, 2022, 6, .	0.9	6
17076	Rich activated edges of hexagonal boron nitride flakes in-situ triggered by nickel nanoparticles to achieve efficient reduction of friction and wear. Composites Part B: Engineering, 2022, 234, 109710.	5.9	9
17077	Two-Dimensional WO <sub>3</sub> -Transition-Metal Dichalcogenide Vertical Heterostructures for Nitrogen Fixation: A Photo(Electro) Catalysis Theoretical Strategy. Journal of Physical Chemistry C, 2022, 126, 3043-3053.	1.5	8
17078	Slater-Pauling behavior of interfacial magnetic properties of $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle \langle \text{mml:mn} \rangle \langle \text{mml:mi} \rangle \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$ transition metal alloy/Pt structures. Physical Review B, 2022, 105, .	4.1	35
17079	Z-scheme 2D/2D WS <sub>2</sub> /Bi <sub>2</sub> WO <sub>6</sub> heterostructures with enhanced photocatalytic performance. Applied Catalysis A: General, 2022, 631, 118485.	2.2	30

#	ARTICLE	IF	CITATIONS
17080	Ionically Conductive Tunnels in $\text{WVO}_3$ Enable High-Rate $\text{NH}_4^+$ Storage. <i>Advanced Science</i> , 2022, 9, e2105158.	5.6	46
17081	Water-Stable Nickel Metal-Organic Framework Nanobelts for Cocatalyst-Free Photocatalytic Water Splitting to Produce Hydrogen. <i>Journal of the American Chemical Society</i> , 2022, 144, 2747-2754.	6.6	109
17082	Computational Methods for Charge Density Waves in 2D Materials. <i>Nanomaterials</i> , 2022, 12, 504.	1.9	1
17083	Catalytic pyrolysis of biomass with Ni/Fe-CaO-based catalysts for hydrogen-rich gas: DFT and experimental study. <i>Energy Conversion and Management</i> , 2022, 254, 115246.	4.4	33
17084	CO <sub>2</sub> reduction reaction pathways on single-atom Co sites: Impacts of local coordination environment. <i>Chinese Journal of Catalysis</i> , 2022, 43, 832-838.	6.9	18
17085	A first principles study of the adsorption and hydrogenation of formic acid on a Cu <sub>3</sub> Zn material: Implication for bulk alloying effect on CO <sub>2</sub> hydrogenation reactivity of Cu/ZnO-based catalysts. <i>Computational Materials Science</i> , 2022, 205, 111222.	1.4	1
17086	Development of a physically-informed neural network interatomic potential for tantalum. <i>Computational Materials Science</i> , 2022, 205, 111180.	1.4	7
17087	Role of Ni on the helium diffusion, stability and energetics of vacancy-type clusters in Fe <sub>6.25</sub> Cr <sub>3.13</sub> Ni (at.%) ternary alloys: From first-principles. <i>Computational Materials Science</i> , 2022, 205, 111213.	1.4	1
17088	Improving performance of zinc-manganese battery via efficient deposition/dissolution chemistry. <i>Energy Storage Materials</i> , 2022, 46, 165-174.	9.5	32
17089	Theoretical investigation of the HgTe topological edge states with a Fe impurity. <i>Physica B: Condensed Matter</i> , 2022, 630, 413673.	1.3	0
17090	Empowering hydrogen storage performance of B <sub>4</sub> C <sub>3</sub> monolayer through decoration with lithium: A DFT study. <i>Surfaces and Interfaces</i> , 2022, 29, 101723.	1.5	15
17091	Electronic and magnetic properties of MAX phase Cr <sub>2</sub> SiC with GGA+U approximation. <i>Journal of Solid State Chemistry</i> , 2022, 308, 122870.	1.4	4
17092	The role of some triazoles on the corrosion inhibition of C1020 steel and copper in a desalination descaling solution. <i>Desalination</i> , 2022, 527, 115551.	4.0	25
17093	Ag modified Tb-doped double-phase In <sub>2</sub> O <sub>3</sub> for ultrasensitive hydrogen gas sensor. <i>Applied Surface Science</i> , 2022, 583, 152521.	3.1	25
17094	Fabrication of N, S co-doped carbon nanofiber matrix with cobalt sulfide nanoparticles enhancing lithium/sodium storage performance. <i>Journal of Alloys and Compounds</i> , 2022, 902, 163812.	2.8	11
17095	Study on microstructure and compressive properties of Fe-C-W-Cr-V-Nb coating with boron addition. <i>Journal of Alloys and Compounds</i> , 2022, 904, 163986.	2.8	3
17096	DFT insights into the adsorption mechanism of five-membered aromatic heterocycles containing N, O, or S on Fe(1 1 0) surface. <i>Applied Surface Science</i> , 2022, 583, 152524.	3.1	13
17097	Computational studies on the reactions of thiols, sulfides and disulfides with hydroperoxides. Relevance for jet fuel autoxidation. <i>Fuel</i> , 2022, 316, 123326.	3.4	2

#	ARTICLE	IF	CITATIONS
17098	A new salt-inclusion chalcogenide exhibiting distinctive [Cd <sub>11</sub> In <sub>9</sub> S <sub>26</sub> ] <sub>3</sub> host framework and decent nonlinear optical performances. <i>Journal of Alloys and Compounds</i> , 2022, 902, 163656.	2.8	7
17099	Second-order magnetoelastic effects: From the Dirac equation to the magnetic properties of ultrathin epitaxial films for magnetic thin-film applications. <i>International Journal of Materials Research</i> , 2022, 93, 970-973.	0.1	0
17100	A predictive model of surface adsorption in dissolution on transition metals and alloys. <i>Journal of Materials Chemistry A</i> , 2022, 10, 6731-6739.	5.2	7
17101	Perfect spin Seebeck effect, spin-valve, spin-filter and spin-rectification based on the heterojunction of sawtooth graphene and graphyne nanoribbons. <i>Nanoscale</i> , 2022, 14, 3818-3825.	2.8	17
17102	Pressure-induced phase transition of a series of energetic pentazolate anion salts: a DFT study. <i>New Journal of Chemistry</i> , 2022, 46, 5653-5662.	1.4	3
17103	The 2D or 3D morphology of sub-nanometer Cu <sub>5</sub> and Cu <sub>8</sub> clusters changes the mechanism of CO oxidation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 4504-4514.	1.3	3
17104	First-Principles Calculations to Investigate the Influence of Irradiation Defects on the Swelling Behavior of Fe-13Cr Alloys. <i>Materials</i> , 2022, 15, 1267.	1.3	0
17105	First principal calculation of electronic structure and magnetism property of transition metals (Mn, Tj). <i>ETQq1 1 0.784314 rgBT /Overload</i>	0.9	2
17106	A highly distorted ultraelastic chemically complex Elinvar alloy. <i>Nature</i> , 2022, 602, 251-257.	13.7	75
17107	Energies and structures of Cu/Nb and Cu/W interfaces from density functional theory and semi-empirical calculations. <i>Materialia</i> , 2022, 21, 101362.	1.3	13
17108	Photon energy dependent appearance and disappearance of magnetic dipole transition in Gd <sub>2</sub> Hf <sub>2</sub> O <sub>7</sub> :Sm <sup>3+</sup> nanophosphors. <i>Journal of Luminescence</i> , 2022, 245, 118789.	1.5	3
17109	Mechanism of Caspase-1 Inhibition by Four Anti-inflammatory Drugs Used in COVID-19 Treatment. <i>International Journal of Molecular Sciences</i> , 2022, 23, 1849.	1.8	6
17110	Weak intermolecular interactions of cysteine on BNNT, BNAINT and BC2NNT: a DFT investigation. <i>Bulletin of Materials Science</i> , 2022, 45, 1.	0.8	29
17111	Precise control of single-phenanthrene junction's conductance. <i>Journal of Computational Electronics</i> , 2022, 21, 71.	1.3	2
17112	Investigating the influence of nano film depositions on the metal surface on the solid-liquid interfacial work function. <i>Surfaces and Interfaces</i> , 2022, 29, 101789.	1.5	1
17113	Excellent high-temperature strength and ductility of the ZrC nanoparticles dispersed molybdenum. <i>Acta Materialia</i> , 2022, 227, 117725.	3.8	34
17114	Computational study of nanoscale mechanical properties of Fe-Cr-Ni alloy. <i>Molecular Simulation</i> , 2022, 48, 551-567.	0.9	6
17115	Novel modified BODIPY-C60 as photosensitizer in photodynamic therapy. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113632.	1.1	2

#	ARTICLE	IF	CITATIONS
17116	Functional gel cathode strategy to enhance the long-term cyclability of the lithium-polysulfide full cell. <i>Electrochimica Acta</i> , 2022, 410, 140052.	2.6	22
17117	Atmospheric growth of ZnO thin films doped and co-doped with Ni and Co via UMVD: experimental and theoretical study. <i>Journal of Materials Science: Materials in Electronics</i> , 2022, 33, 6999-7010.	1.1	4
17118	Viscosity of Fe-Ni Liquids up to Core Pressures and Implications for Dynamics of Planetary Cores. <i>Geophysical Research Letters</i> , 0, , .	1.5	2
17119	Interaction mechanism between lead species and activated carbon in MSW incineration flue gas: Role of different functional groups. <i>Chemical Engineering Journal</i> , 2022, 436, 135252.	6.6	8
17120	Thiotetrelates $\text{Li}_2\text{ZnXS}_4$ (X = Si, Ge, and Sn) As Potential Li-Ion Solid-State Electrolytes. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 9203-9211.	4.0	2
17121	Theoretical Study on the Electronic Structure and Magnetic Properties Regulation of Janus Structure of $\text{M}^{\text{TM}}\text{MCO}_2$ 2D MXenes. <i>Nanomaterials</i> , 2022, 12, 556.	1.9	6
17122	Effect of surface segregation on the oxidation resistance of $\text{Cu}_3\text{MnO}_7$ . <i>Physical Review Materials</i> , 2022, 6, .	3.2	2
17123	CARNOT: a Fragment-Based Direct Molecular Dynamics and Virtual Reality Simulation Package for Reactive Systems. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1297-1313.	2.3	10
17124	Quantum molecular modeling of oxazolidines as detergent-dispersant additives for gasoline: A valuable technological adviser. <i>Fuel</i> , 2022, 315, 122715.	3.4	3
17125	Structural Changes from Conventional $\text{SrSnO}_3$ to Ruddlesden-Popper $\text{Sr}_2\text{SnO}_4$ Perovskites and Its Implication on Photoluminescence and Optoelectronic Properties. <i>ACS Applied Electronic Materials</i> , 2022, 4, 878-890.	2.0	8
17126	Tetraphenyl Tetrel Molecules and Molecular Crystals: From Structural Properties to Nonlinear Optics. <i>Journal of Physical Chemistry C</i> , 2022, 126, 3713-3726.	1.5	4
17127	Hydroxylation and molecular adsorption behavior of $\text{SnO}_2$ (110) crystal plane. <i>Materials Research Bulletin</i> , 2022, 150, 111787.	2.7	5
17128	Structural evolution in TiZrHfNb high-entropy alloy. <i>Materialia</i> , 2022, 21, 101311.	1.3	11
17129	A long-standing polarized electric field in $\text{TiO}_2/\text{BaTiO}_3/\text{CdS}$ nanocomposite for effective photocatalytic hydrogen evolution. <i>Fuel</i> , 2022, 314, 122758.	3.4	20
17130	Density functional theory characterisation of cementite ( $\text{Fe}_3\text{C}$ ) molybdenum (Mo) atoms. <i>Physica B: Condensed Matter</i> , 2022, 631, 413669.	1.3	2
17131	New dislocation dissociation accompanied by anti-phase shuffling in the $\text{L}_{12}$ martensite phase of a Ti alloy. <i>Acta Materialia</i> , 2022, 227, 117705.	3.8	4
17132	Structural, elastic, mechanical, electronic, magnetic and optical properties of half-Heusler compounds $\text{CoFeZ}$ (Z = P, As, Sb): A GGA+U approximation. <i>Materials Science in Semiconductor Processing</i> , 2022, 143, 106445.	1.9	8
17133	Guanidinium Fluorooxoborates as Efficient Metal-free Short-Wavelength Nonlinear Optical Crystals. <i>Chemistry of Materials</i> , 2022, 34, 440-450.	3.2	67



#	ARTICLE	IF	CITATIONS
17134	Potential Solid-State Electrolytes with Good Balance between Ionic Conductivity and Electrochemical Stability: $\text{Li}_5\text{M}_2\text{O}_4$ ( $M = \text{Al}, \text{Ti}, \text{Zr}, \text{Hf}$ )	0.0	0
17135	Insights into the Mechanism of Methanol Steam Reforming for Hydrogen Production over Ni-Cu-Based Catalysts. <i>ACS Catalysis</i> , 2022, 12, 512-526.	5.5	31
17136	Few-Layer $\text{WS}_2/\text{WSe}_2$ Lateral Heterostructures: Influence of the Gas Precursor Selenium/Tungsten Ratio on the Number of Layers. <i>ACS Nano</i> , 2022, 16, 1198-1207.	7.3	16
17137	Assessing density functionals for describing methane dissociative chemisorption on Pt(110)-(2 $\times$ 1) surface. <i>Chinese Journal of Chemical Physics</i> , 2021, 34, 883-895.	0.6	2
17138	Microstructure Control and Strengthening Mechanism of Fine-Grained Cast Mg Alloys Based on Grain Boundary Segregation of Al Solute. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17139	Spatiotemporal Sonodynamic Therapy for the Treatment of Rheumatoid Arthritis Based on Z-Scheme Heterostructure Sonosensitizer of Ho-1 Inhibitor Jointed Bismuth Nanotriangle. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17140	Surface Spinel and Oxygen Vacancies Enhanced Lithium-Rich Layered Oxides with Excellent Electrochemical Performances. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17141	Biobr/Bi <sub>2</sub> S <sub>3</sub> Heterojunction with S-Scheme Structure and Oxygen Defects: In-Situ Construction and Photocatalytic Behavior for Reduction of CO <sub>2</sub> with H <sub>2</sub> O. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17142	In-Situ Construction of Cu-Co &N@CC Hierarchical Binder-Free Cathode for Advanced and Flexible Li-CO <sub>2</sub> Batteries: Electron Structure and Mass Transfer Modulation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17143	Electronic Structure of Graphene on Silicon Carbide Intercalated with Silicon and Cobalt Atoms. <i>Physics of the Solid State</i> , 2021, 63, 819-824.	0.2	0
17144	NbN nanodot decorated N-doped graphene as a multifunctional interlayer for high-performance lithium-sulfur batteries. <i>Journal of Materials Chemistry A</i> , 2022, 10, 8578-8590.	5.2	39
17145	Effects of transition metal doping on electronic structure of metastable $\text{Fe}_2\text{O}_3$ photocatalyst for solar-to-hydrogen conversion. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 6958-6963.	1.3	3
17146	Abnormal In-Plane Thermal Conductivity Anisotropy in Bilayer $\gamma$ -Phase Tellurene. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17147	Theoretical scheme of nonvolatile strain-switchable high/low resistance based on novel strain-tunable magnetic anisotropy in the $\text{Mn}_{2.25}\text{Co}_{0.75}\text{Ga}_{0.5}\text{Sn}_{0.5}/\text{MgO}$ superlattice. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7826-7835.	1.3	1
17148	Reaction Mechanism of NiO Supported on Inert Material for Chemical Looping Methane Reforming. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17149	Intrinsic Activity and Selectivity Enhancement of Single-Atom Rh in Syngas-to-C <sub>2</sub> Oxygenates by Engineering the Local Coordination Atom. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17150	Ab Initio Study of the Effects of Cr on Helium Behaviors in Fe-Ycr (Y = 9.38, 12.50 At.%) Austenitic Binary Alloys. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17151	Cohesive properties of $\text{PbBi}/\text{Fe}_3\text{O}_4$ and $\text{PbBi}/(\text{Fe,Cr})_3\text{O}_4$ interfaces. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 6732-6741.	1.3	4

#	ARTICLE	IF	CITATIONS
17152	Tuning the Activity and Selectivity of Nitrogen Reduction Reaction on Double-Atom Catalysts by B Doping: A Density Functional Theory Study. SSRN Electronic Journal, 0, , .	0.4	0
17153	Effects of vibrational and rotational excitations on dissociative chemisorption dynamics of N <sub>2</sub> on Fe(111). Chinese Journal of Chemical Physics, 2022, 35, 443-450.	0.6	2
17154	Ultrahigh-stability SnOX (X = S, Se) nanotubes with a built-in electric field as a highly promising platform for sensing NH <sub>3</sub> , NO and NO <sub>2</sub> : a theoretical investigation. Journal of Materials Chemistry A, 2022, 10, 7948-7959.	5.2	4
17155	Realizing Robust and Efficient Acidic Oxygen Evolution by Electronic Modulation of Od/2d Ceo <sub>2</sub> Quantum Dots Decorated Srro <sub>3</sub> Nanosheets. SSRN Electronic Journal, 0, , .	0.4	0
17156	Revisit the Vec Criterion in High Entropy Alloys (Heas) with High-Throughput Ab Initio Calculations: A Case Study with Al-Co-Cr-Fe-Ni System. SSRN Electronic Journal, 0, , .	0.4	0
17158	Pressure-stabilized graphene-like P layer in superconducting LaP <sub>2</sub> . Physical Chemistry Chemical Physics, 2022, 24, 6469-6475.	1.3	5
17159	3D porous spheroidal Na <sub>4</sub> Mn <sub>0.9</sub> Ce <sub>0.1</sub> V(PO <sub>4</sub> ) <sub>3</sub> @CeO <sub>2</sub> /C 5.2 cathode for high-energy Na ion batteries. Journal of Materials Chemistry A, 2022, 10, 10625-10637.	5.2	22
17160	Structural diversity and magnetic properties of copper(II) quinaldinate compounds with amino alcohols. New Journal of Chemistry, 2022, 46, 6899-6920.	1.4	3
17161	The Unusual Behaviors of Nox on Al. SSRN Electronic Journal, 0, , .	0.4	0
17163	Effect of O <sub>2</sub> on the Thermal Stability and Decomposition Process of C5F10O. IEEE Transactions on Dielectrics and Electrical Insulation, 2022, , 1-1.	1.8	0
17165	Nitric oxide reduction reaction for efficient ammonia synthesis on topological nodal-line semimetal Cu <sub>2</sub> Si monolayer. Journal of Materials Chemistry A, 2022, 10, 8568-8577.	5.2	21
17166	The Dynamical Stability, Electronic, Elastic Properties and Ideal Strength of Diamond-Like Cubic B <sub>2</sub> cn: A First-Principles Study. SSRN Electronic Journal, 0, , .	0.4	0
17167	Theoretical investigation of the Î±-substitution effect on Î³-C(sp <sup>3</sup> )â€“H arylation of amines: structureâ€“reactivity relationship (SRR) studies. Organic Chemistry Frontiers, 0, , .	2.3	0
17168	Single-, double-, and triple-atom catalysts on graphene-like C <sub>2</sub> N enable electrocatalytic nitrogen reduction: insight from first principles. Catalysis Science and Technology, 2022, 12, 2604-2617.	2.1	15
17169	Experimental and Theoretical Insight into Dsscs Mechanism Influenced by Different Doping Metal Ions. SSRN Electronic Journal, 0, , .	0.4	0
17170	Self-limiting nitrogen/hydrogen plasma radical chemistry in plasma-enhanced atomic layer deposition of cobalt. Nanoscale, 2022, 14, 4712-4725.	2.8	5
17171	Thermoelectric Properties and High Degree of Plastic Deformation in Zrrhbi Heusler Alloys. SSRN Electronic Journal, 0, , .	0.4	0
17172	Deep Insight into the Sb(II) and Sb(V) Removal Mechanism by Fe-Cu-Chitosan Material. SSRN Electronic Journal, 0, , .	0.4	0

#	ARTICLE	IF	CITATIONS
17173	The effect of different energy portions on the 2D/3D stability swapping for 13-atom metal clusters. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 6515-6524.	1.3	1
17174	Effects of Non-Local Exchange Functionals in the Density Functional Theories for the Description of Molecular Vibrations. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17175	Adsorption Behavior of Environmental Gas Molecules on Pristine and Defective MoSi <sub>2</sub> N <sub>4</sub> : Possible Application as Highly Sensitive and Reusable Gas Sensors. <i>ACS Omega</i> , 2022, 7, 8706-8716.	1.6	20
17176	Two-Dimensional Anisotropic Flexibility of Mechanically Responsive Crystalline Cadmium(II) Coordination Polymers. <i>Chemistry of Materials</i> , 2022, 34, 2439-2448.	3.2	14
17177	An efficient single atom catalysts Os/P3C sheet for ammonia borane dehydrogenation. <i>Chinese Chemical Letters</i> , 2022, 33, 3281-3286.	4.8	8
17178	Eu <sup>2+</sup> Doping Concentration-Induced Site-Selective Occupation and Photoluminescence Tuning in K <sub>2</sub> ScSi <sub>2</sub> O <sub>7</sub> :Eu <sup>2+</sup> Phosphor. <i>ACS Materials Au</i> , 2022, 2, 374-380.	2.6	24
17179	Assessment of Various Density Functional Theory Methods for Finding Accurate Structures of Actinide Complexes. <i>Molecules</i> , 2022, 27, 1500.	1.7	2
17180	Interfacial engineering manipulation of magnetic anisotropy evolution via orbital reconstruction in low-dimensional manganite superlattices. <i>Science China Materials</i> , 2022, 65, 1902-1911.	3.5	3
17181	Theoretical Investigation on the Hydrogen Evolution, Oxygen Evolution, and Oxygen Reduction Reactions Performances of Two-Dimensional Metal-Organic Frameworks Fe <sub>3</sub> (C <sub>2</sub> X) <sub>12</sub> (X = NH, O, S). <i>Molecules</i> , 2022, 27, 1528.	1.7	10
17182	Giant tunneling magnetoresistance and electroresistance in $\hat{I}_{\pm}$ -based van der Waals multiferroic tunnel junctions. <i>Physical Review B</i> , 2022, 105, .		
17183	Interface synergistic effects induced multi-mode luminescence. <i>Nano Research</i> , 2022, 15, 4457-4465.	5.8	21
17184	Universal p-Type Doping via Lewis Acid for 2D Transition-Metal Dichalcogenides. <i>ACS Nano</i> , 2022, 16, 4884-4891.	7.3	17
17185	Relativistic Effects in Platinum Nanocluster Catalysis: A Statistical Ensemble-Based Analysis. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1345-1359.	1.1	7
17186	Highly active Fe <sub>36</sub> Co <sub>44</sub> bimetallic nanoclusters catalysts for hydrolysis of ammonia borane: The first-principles study. <i>Chinese Chemical Letters</i> , 2023, 34, 107261.	4.8	46
17187	Effective Work Functions of the Elements. <i>Progress in Surface Science</i> , 2022, 97, 100583.	3.8	38
17188	Hirshfeld atom refinement based on projector augmented wave densities with periodic boundary conditions. <i>IUCr</i> , 2022, 9, 286-297.	1.0	9
17189	Solving oxygen embrittlement of refractory high-entropy alloy via grain boundary engineering. <i>Materials Today</i> , 2022, 54, 83-89.	8.3	72
17190	Towards dielectric relaxation at a single molecule scale. <i>Scientific Reports</i> , 2022, 12, 2865.	1.6	4

#	ARTICLE	IF	CITATIONS
17191	Updated Calibrated Model for the Prediction of Molecular Frontier Orbital Energies and Its Application to Boron Subphthalocyanines. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 829-840.	2.5	2
17192	Modeling the Binding Free Energy of Large Atmospheric Sulfuric Acid–Ammonia Clusters. <i>ACS Omega</i> , 2022, 7, 8077-8083.	1.6	6
17193	Modulating vectored non-covalent interactions for layered assembly with engineerable properties. <i>Bio-Design and Manufacturing</i> , 2022, 5, 529-539.	3.9	6
17194	Theoretical Analysis of Electronic Structure and Optical Properties of Potassium Dihydrogen Phosphate Crystal Affected by [011] Screw Dislocation. <i>Crystal Growth and Design</i> , 2022, 22, 1764-1769.	1.4	1
17195	Pressure-Induced Phase Transition and Compression Properties of HfO <sub>2</sub> Nanocrystals. <i>Inorganic Chemistry</i> , 2022, 61, 3498-3507.	1.9	4
17196	Revealing the Potential of Ternary Medium-Entropy Alloys as Exceptional Electrocatalysts toward Nitrogen Reduction: An Example of Heusler Alloys. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 15235-15242.	4.0	15
17197	Poly(ferrocenylsilane)s from planar-chiral sila[1]ferrocenophanes: How to twist a zig-zag chain into a helix. <i>Polymer</i> , 2022, 242, 124477.	1.8	4
17198	A First-Principles Study on Electronic and Magnetic Properties of Intrinsic Point Defects in SrO Crystals. <i>Journal of Electronic Materials</i> , 0, , 1.	1.0	0
17199	Controllable Growth of $\hat{1}\pm$ - and $\hat{1}^2$ -Antimonene by Interfacial Strain. <i>Journal of Physical Chemistry C</i> , 2022, 126, 5022-5027.	1.5	5
17200	Density functional theory study of nitrogen-doped black phosphorene doped with monatomic transition metals as high performance electrocatalysts for N <sub>2</sub> reduction reaction. <i>Nanotechnology</i> , 2022, 33, 245401.	1.3	9
17201	Co-segregation behavior and weakening effect of the major elements in Al-Zn-Mg-Cu series alloys on Al $\hat{1}\hat{3}(111)[110]$ symmetrical tilt grain boundary: a first-principles study. <i>Journal of Materials Research and Technology</i> , 2022, 18, 3158-3172.	2.6	6
17202	Simultaneously Regulating the Band Gap and Catalytic Activity of TiO <sub>2</sub> via Embedded MoO <sub>2</sub> Based on Interlaced CNT Carrier for Li-S Battery to Achieve Efficient Adsorption. <i>Journal of the Electrochemical Society</i> , 2022, 169, 030512.	1.3	1
17203	Improved adhesion of TiN coatings on Al <sub>2</sub> O <sub>3</sub> –carbide composites by DFT calculations and experimental arc-PVD synthesis. <i>Journal of the American Ceramic Society</i> , 2022, 105, 4859-4869.	1.9	2
17204	Insights into Interaction of CO( <sub>2</sub> ) with N and B-doped Graphenes. <i>Communications in Physics</i> , 2022, 32, .	0.0	0
17205	Phase Transition in Cobalt Selenide with a Greatly Improved Electrocatalytic Activity in Hydrogen Evolution Reactions. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 4022-4030.	3.2	33
17206	Effects of $\hat{1}\hat{1}$ -conjugation on the charge-transport properties of $\hat{1}\hat{1}$ -transporting materials featuring diphenylamine–quinacridone for perovskite solar cells: A theoretical study. <i>Bulletin of the Korean Chemical Society</i> , 0, , .	1.0	1
17207	Tetragonal-structure germanene van der Waals 2D crystal and its Raman spectra. <i>Applied Physics A: Materials Science and Processing</i> , 2022, 128, 1.	1.1	0
17208	Tetrahedral W <sub>4</sub> cluster confined in graphene-like C <sub>2</sub> N enables electrocatalytic nitrogen reduction from theoretical perspective. <i>Nanotechnology</i> , 2022, 33, 245706.	1.3	8

#	ARTICLE	IF	CITATIONS
17209	Valence energy correction for electron reactive force field. Journal of Computational Chemistry, 2022, 43, 870-878.	1.5	3
17210	Investigation of Nd <sup>3+</sup> incorporation in Ce-hydrophane: Insight from structural flexibility and occupation mechanism. Journal of the American Ceramic Society, 0, , .	1.9	4
17211	Mechanism of Preferential Hydrogenation of Hydroxymethyl Group to Aldehyde Group in 5-Hydroxymethylfurfural over W <sub>2</sub> C-Based Catalyst. ChemSusChem, 2022, 15, e202200174.	3.6	4
17212	Li decorated heteroborospherene C4B32 as high capacity and reversible hydrogen storage media: A DFT study. International Journal of Hydrogen Energy, 2022, 47, 11948-11954.	3.8	11
17213	Nonmetallic Active Sites on Nickel Phosphide in Oxygen Evolution Reaction. Nanomaterials, 2022, 12, 1130.	1.9	3
17214	A Theoretical Study on the Structural, Electronic, and Magnetic Properties of Bimetallic Pt <sub>13</sub> Ni <sub>n</sub> (N) Tj ETQq1 1 0.784314 rgBT /Oer Frontiers in Chemistry, 2022, 10, 852196.	1.8	0
17215	An assessment of density functionals for predicting CO <sub>2</sub> adsorption in diamine-functionalized metal-organic frameworks. Journal of Chemical Physics, 2022, 156, 154113.	1.2	7
17216	$\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{DFT} \langle \text{mml:mi} \rangle \langle \text{mml:mo} \rangle + \langle \text{mml:mq} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:math} \text{mathvariant="normal"} \rangle \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \text{method for electron correlation effects at transition metal surfaces. Physical Review B, 2022, 105, .}$	1.1	7
17217	Understanding the growth mechanism of SiO <sub>2</sub> on the surface of FeSi clusters: an MD and DFT simulation study. Journal of Sol-Gel Science and Technology, 2022, 102, 335-342.	1.1	2
17218	Photocatalytic Reduction of CO <sub>2</sub> with H <sub>2</sub> O Mediated by Ce-Tailored Bismuth Oxybromide Surface Frustrated Lewis Pairs. ACS Catalysis, 2022, 12, 4016-4025.	5.5	95
17219	Single-site Pt-doped RuO <sub>2</sub> hollow nanospheres with interstitial C for high-performance acidic overall water splitting. Science Advances, 2022, 8, eabl9271.	4.7	117
17220	SrAl <sub>5</sub> Pt <sub>3</sub> and Sr <sub>2</sub> Al <sub>16</sub> Pt <sub>9</sub> – two new strontium aluminum platinides. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2022, 77, 367-379.	0.3	2
17221	Three new Ag-based full-Heusler alloys: Ag <sub>2</sub> TiGa, Ag <sub>2</sub> VGa, and Ag <sub>2</sub> TiTi. ChemPhysMater, 2022, , .	1.4	0
17222	Niobium-doped cobalt phosphide nanowires realizing enhanced electrocatalytic activity for overall water splitting. International Journal of Hydrogen Energy, 2022, 47, 13251-13260.	3.8	17
17223	Multitask Quantum Study of the Curcumin-Based Complex Physicochemical and Biological Properties. International Journal of Molecular Sciences, 2022, 23, 2832.	1.8	3
17224	<i>Ab initio</i> investigation of the role of the <i>d</i> -states on the adsorption and activation properties of CO <sub>2</sub> on 3 <i>d</i> , 4 <i>d</i> , and 5 <i>d</i> transition-metal clusters. Journal of Chemical Physics, 2022, 156, 124106.	1.2	0
17225	Systematic study of phase transformation, wide-to-narrow electronic band transition and optical properties of barium zirconium Oxynitrate: <i>Ab initio</i> calculations. Molecular Physics, 2022, 120, .	0.8	0
17226	A top-down strategy for amorphization of hydroxyl compounds for electrocatalytic oxygen evolution. Nature Communications, 2022, 13, 1187.	5.8	63

#	ARTICLE	IF	CITATIONS
17227	Formation and local structure of framework Al Lewis sites in beta zeolites. <i>Journal of Chemical Physics</i> , 2022, 156, 104702.	1.2	2
17228	Superconducting ScP4 with a novel phosphorus framework. <i>Applied Physics A: Materials Science and Processing</i> , 2022, 128, 1.	1.1	2
17229	Kinetic Study of the Oxidative Addition Reaction between Methyl Iodide and [Rh(imino- $\eta^2$ -diketonato)(CO)(PPh) <sub>3</sub> ] Complexes, Utilizing UV-Vis, IR Spectrophotometry, NMR Spectroscopy and DFT Calculations. <i>Molecules</i> , 2022, 27, 1931.	1.7	1
17230	Relative Populations and IR Spectra of Cu <sub>38</sub> Cluster at Finite Temperature Based on DFT and Statistical Thermodynamics Calculations. <i>Frontiers in Chemistry</i> , 2022, 10, 841964.	1.8	3
17231	Existence of interfacial polaronic plasmon: A comparative study between FeSe and CoSe. <i>Physical Review B</i> , 2022, 105, .	1.1	0
17232	Computational materials discovery for lanthanide hydrides at high pressure for high temperature superconductivity. <i>Physical Review Research</i> , 2022, 4, .	1.3	2
17233	Exceptionally active and stable RuO <sub>2</sub> with interstitial carbon for water oxidation in acid. <i>CheM</i> , 2022, 8, 1673-1687.	5.8	52
17234	On the Origins of Stereo- and Regio-Selectivities in the Formation of Fullerene-Fluorene Dyads. <i>Journal of Organic Chemistry</i> , 2022, 87, 4702-4711.	1.7	2
17235	A comparison of water-gas shift reaction on ZnO $\left(\overline{100}\right)$ surface and 6Cu cluster deposited over ZnO $\left(\overline{100}\right)$ surface using density functional theory studies. <i>Journal of Molecular Modeling</i> , 2022, 28, 84.	0.8	4
17236	Dirac nodal-line semimetal zinc polynitride at high pressure. <i>Physical Review B</i> , 2022, 105, .	1.1	2
17237	Short-Range to Long-Range Ni/Mn Order in LiMn <sub>2</sub> xNi <sub>x</sub> O <sub>4</sub> (0.38 $\leq$ x $\leq$ 0.50) Positive Electrode Materials: A Gradual Temperature-Driven Sublattice Disorder through Antiphase Boundary Defects. <i>Chemistry of Materials</i> , 2022, 34, 3152-3167.	3.2	4
17238	Three-Dimensional Porous h-BC <sub>2</sub> N Based on BN Chains and Prismane C <sub>8</sub> Units for Alkali Metal Ion Battery Anodes. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2348-2355.	2.1	3
17239	Modulation of the B <sub>4</sub> N monolayer as an efficient electrocatalyst for hydrogen evolution reaction. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 11511-11519.	3.8	1
17240	Influence of Dimensionality on the Charge Density Wave Phase of 2H-TaSe <sub>2</sub> . <i>Advanced Theory and Simulations</i> , 0, , 2100329.	1.3	0
17241	Transition metal anchored on C <sub>9</sub> N <sub>4</sub> as a single-atom catalyst for CO <sub>2</sub> hydrogenation: A first-principles study. <i>Chinese Physics B</i> , 2022, 31, 107306.	0.7	3
17242	Synergy between Palladium Single Atoms and Nanoparticles via Hydrogen Spillover for Enhancing CO <sub>2</sub> Photoreduction to CH <sub>4</sub> . <i>Advanced Materials</i> , 2022, 34, e2200057.	11.1	162
17243	Regulating MoS <sub>2</sub> edge site for photocatalytic nitrogen fixation: A theoretical and experimental study. <i>Chemical Engineering Journal</i> , 2022, 442, 136211.	6.6	27
17244	Element segregation and thermal stability of Ni-Pd nanoparticles. <i>Journal of Materials Science</i> , 2022, 57, 7384-7399.	1.7	7



#	ARTICLE	IF	CITATIONS
17245	The exclusive surface and electronic effects of Ni on promoting the activity of Pt towards alkaline hydrogen oxidation. <i>Nano Research</i> , 2022, 15, 5865-5872.	5.8	12
17246	Interrelationship of bonding strength with structural stability of ternary oxide phases of MgSnO <sub>3</sub> : A first-principles study. <i>Physica B: Condensed Matter</i> , 2022, 637, 413896.	1.3	7
17247	Metal-organic framework derived dual-metal sites for electroreduction of carbon dioxide to HCOOH. <i>Applied Catalysis B: Environmental</i> , 2022, 311, 121377.	10.8	40
17248	Mo <sub>2</sub> CS <sub>2</sub> -MXene supported single-atom catalysts for efficient and selective CO <sub>2</sub> electrochemical reduction. <i>Applied Surface Science</i> , 2022, 592, 153339.	3.1	20
17249	Accounting for Dispersion Effects in the DFT Framework of Electrocatalysis: A Hybrid Solvation Model-Based Case Study of the Oxygen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2022, 126, 6171-6188.	1.5	3
17250	Bonding character of intermediates in on- $\epsilon$ -surface Ullmann reactions revealed with energy decomposition analysis. <i>Journal of Computational Chemistry</i> , 2023, 44, 179-189.	1.5	2
17251	Hydrogen adsorption behavior on AXenes Na <sub>2</sub> N and K <sub>2</sub> N: a first-principles study. <i>Materials Research Express</i> , 2022, 9, 045501.	0.8	4
17252	Black phosphorus incorporated cobalt oxide: Biomimetic channels for electrocatalytic water oxidation. <i>Chinese Journal of Catalysis</i> , 2022, 43, 1123-1130.	6.9	5
17253	Enhanced thermoelectric performance based on special micro-configuration of graphene-ZnO induced by high-pressure and high-temperature. <i>Ceramics International</i> , 2022, 48, 9014-9023.	2.3	5
17254	Towards reconciling experimental and computational determinations of Earth's core thermal conductivity. <i>Earth and Planetary Science Letters</i> , 2022, 584, 117466.	1.8	10
17255	Hydrogenolysis Cleavage of the C <sub>sp<sup>2</sup></sub> -C <sub>sp<sup>3</sup></sub> Bond over a Metal-Free NbOPO <sub>4</sub> Catalyst. <i>ACS Catalysis</i> , 2022, 12, 4806-4812.	5.5	14
17256	Origin of the Enhanced Hydrogen Evolution Reaction Activity of Grain Boundaries in MoS <sub>2</sub> Monolayers. <i>Journal of Physical Chemistry C</i> , 2022, 126, 6215-6222.	1.5	5
17257	Theoretical study on the influence of Cr, Mo, and W alloying additions on the helium behavior in nickel. <i>Journal of Nuclear Materials</i> , 2022, 565, 153720.	1.3	5
17258	A Mixed-Ligand Strategy to Modulate P3HT Regioregularity for High-Efficiency Solar Cells. <i>Macromolecules</i> , 2022, 55, 3078-3086.	2.2	26
17259	Spin transport properties and nanodevice simulations of NiI <sub>2</sub> monolayer. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 142, 115262.	1.3	9
17260	B <sub>3</sub> O <sub>3</sub> monolayer with dual application in sensing of COVID-19 biomarkers and drug delivery for treatment purposes: A periodic DFT study. <i>Journal of Molecular Liquids</i> , 2022, 354, 118855.	2.3	19
17261	Unusual structure and properties of germanium under pressure. <i>Computational Materials Science</i> , 2022, 207, 111310.	1.4	2
17262	Ferromagnetism in V and Cr doped ScN diluted magnetic semiconductor in B <sub>3</sub> phase: A DFT study. <i>Solid State Communications</i> , 2022, 347, 114724.	0.9	3

#	ARTICLE	IF	CITATIONS
17263	Homogeneous transformation of the grain boundary phase and Tb grain boundary diffusion optimization in sintered Nd-Fe-B magnet. <i>Intermetallics</i> , 2022, 144, 107490.	1.8	11
17264	Effect of the local chemical environment on oxidation resistance mechanisms in AlNbTiZr refractory high entropy alloys: A first-principles study. <i>Scripta Materialia</i> , 2022, 213, 114624.	2.6	4
17265	First-principles study on the solute-induced low diffusion and self-trapping of helium in fcc iron. <i>Journal of Nuclear Materials</i> , 2022, 563, 153613.	1.3	1
17266	Enhanced electrochemical properties of W-doped Na <sub>3</sub> V <sub>2</sub> (PO <sub>4</sub> ) <sub>2</sub> F <sub>3</sub> @C as cathode material in sodium ion batteries. <i>Electrochimica Acta</i> , 2022, 415, 140256.	2.6	12
17267	Structural evolution, electronic properties and spectra of titanium clusters. <i>Physica B: Condensed Matter</i> , 2022, 633, 413783.	1.3	4
17268	Theoretical study about adsorbed oxygen reduction over $\gamma$ -Fe <sub>5</sub> C <sub>2</sub> : formation of H <sub>2</sub> O and CO <sub>2</sub> . <i>Molecular Catalysis</i> , 2022, 524, 112236.	1.0	3
17269	Monoclinic mC28 carbon: A sp <sup>2</sup> -sp <sup>3</sup> hybridized carbon allotrope with superhard and metallic properties. <i>Chemical Physics</i> , 2022, 558, 111503.	0.9	0
17270	Determination of thermodynamic growth conditions for a high-efficiency Cu <sub>10</sub> Si <sub>10</sub> alloy. <i>Journal of Applied Physics</i> , 2022, 123, 105301.		

#	ARTICLE	IF	CITATIONS
17281	Element segregation and thermal stability of Ni-Rh nanoparticles. <i>Journal of Solid State Chemistry</i> , 2022, 311, 123096.	1.4	8
17282	Cookies-like Ag <sub>2</sub> S/Bi <sub>4</sub> NbO <sub>8</sub> Cl heterostructures for high efficient and stable photocatalytic degradation of refractory antibiotics utilizing full-spectrum solar energy. <i>Separation and Purification Technology</i> , 2022, 292, 120969.	3.9	12
17283	Tetragonal transition metal selenide for hydrogen evolution. <i>Applied Surface Science</i> , 2022, 591, 153249.	3.1	19
17284	High-Throughput computational screening of Single-atom embedded in defective BN nanotube for electrocatalytic nitrogen fixation. <i>Applied Surface Science</i> , 2022, 591, 153130.	3.1	13
17285	The effect of bulk conversion into surface on physical properties of HfO <sub>2</sub> : First principle study. <i>Materials Science in Semiconductor Processing</i> , 2022, 146, 106650.	1.9	4
17286	Engineering surface oxygenated functionalities on commercial hard carbon toward superior sodium storage. <i>Chemical Engineering Journal</i> , 2022, 441, 135899.	6.6	18
17287	A dynamic Ni(OH) <sub>2</sub> -NiOOH/NiFeP heterojunction enabling high-performance E-upgrading of hydroxymethylfurfural. <i>Applied Catalysis B: Environmental</i> , 2022, 311, 121357.	10.8	75
17288	Benchmark Study of Computational Methods for Predicting Partition Coefficient of Chlormethiazole. <i>El-Cezeri Journal of Science and Engineering</i> , 0, , .	0.1	0
17289	The Doping Effect on the Electronic Properties of the Titanium Dioxide TiO <sub>2</sub> : A DFT Study. <i>Integrated Ferroelectrics</i> , 2021, 221, 199-214.	0.3	3
17290	Ni-Catalyzed Dearomative Cycloaddition of Alkynes to 10- <i>l</i> -Aromatic Benzothiophenes: Elucidation of Reaction Mechanism. <i>Bulletin of the Chemical Society of Japan</i> , 2021, 94, 2727-2738.	2.0	0
17291	First-Principles Density Functional Theory Study of Modified Germanene-Based Electrode Materials. <i>Materials</i> , 2022, 15, 103.	1.3	11
17292	Effects of Co-adsorbed Water on Different Bond Cleavages of Oxygenates on Pd (111). <i>ACS Catalysis</i> , 2022, 12, 789-798.	5.5	4
17293	Density Functional Theory Study of CO Adsorption on the CaFe <sub>2</sub> O <sub>4</sub> (001) Surface. <i>ISIJ International</i> , 2021, 61, 2937-2943.	0.6	0
17294	Effects of electric field and biaxial strain on the (NO <sub>2</sub> , NO, O <sub>2</sub> , and SO <sub>2</sub> ) gas adsorption properties of Sc <sub>2</sub> CO <sub>2</sub> monolayer. <i>Superlattices and Microstructures</i> , 2022, 163, 107135.	1.4	15
17295	Stability and electronic structure of magnesium hydride and magnesium deuteride under high pressure. <i>Journal of Physics: Conference Series</i> , 2021, 2145, 012026.	0.3	1
17296	Ternary Mg-Nb-H polyhydrides under high pressure. <i>Physical Review B</i> , 2021, 104, .	1.1	23
17297	A DFT study of the effect of stacking on the quantum capacitance of bilayer graphene materials. <i>New Carbon Materials</i> , 2021, 36, 1062-1070.	2.9	10
17298	Potential application of XC <sub>3</sub> (X = B, N) nanosheets in drug delivery of hydroxyurea anticancer drug: a comparative DFT study. <i>Molecular Physics</i> , 2022, 120, .	0.8	19





#	ARTICLE	IF	CITATIONS
17335	First-principles study of interface stability and behaviors of He at the W/Y2O3 interface. <i>Materials Today Communications</i> , 2022, , 103520.	0.9	0
17336	Rare-earth defects in GaN: A systematic investigation of the lanthanide series. <i>Physical Review Materials</i> , 2022, 6, .	0.9	6
17337	Noncentrosymmetric Rare-Earth Borate Fluoride $\text{La}_{22}\text{B}_{59}\text{O}_{93}\text{F}_3$ : A New Ultraviolet Nonlinear Optical Crystal with Enhanced Linear and Nonlinear Performance. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 18704-18712.	4.0	28
17338	Evolution of Discharge Products on Carbon Nanotube Cathodes in $\text{Li}^{\ominus}\text{O}_2$ Batteries Unraveled by Molecular Dynamics and Density Functional Theory. <i>ACS Catalysis</i> , 2022, 12, 5048-5059.	5.5	13
17339	Comprehensive Understanding of H Adsorption on $\text{MoO}_3$ from Systematic <i>Ab Initio</i> Simulations. <i>Journal of Physical Chemistry C</i> , 0, , .	1.5	1
17340	Electroreduction of nitrogen to ammonia by single-atom catalysis with synergistic boron-carbon nitrogen nanotubes. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 107752.	3.3	5
17341	Density Functional Theory-Based Calculations for 2D Hexagonal Lanthanide Metals. <i>Advanced Theory and Simulations</i> , 0, , 2200057.	1.3	5
17342	Removal of mercury(II) from aqueous solution by partially reduced graphene oxide. <i>Scientific Reports</i> , 2022, 12, 6326.	1.6	25
17343	The self-complementary effect through strong orbital coupling in ultrathin high-entropy alloy nanowires boosting pH-universal multifunctional electrocatalysis. <i>Applied Catalysis B: Environmental</i> , 2022, 312, 121431.	10.8	40
17344	Intensifying bismuth concentration in tin chalcogenide for solar cell applications. <i>International Journal of Modern Physics B</i> , 2022, 36, .	1.0	3
17345	Tracing the Primordial Chemical Life of Glycine: A Review from Quantum Chemical Simulations. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4252.	1.8	12
17346	Oriented external electric fields act as a "switch" of Pt-M/BC <sub>3</sub> N <sub>2</sub> diatomic catalysts activate pristine ammonia borane dehydrogenation: A DFT study. <i>Materials Today Communications</i> , 2022, 31, 103544.	0.9	2
17347	Molecular insight into iron corrosion induced by chloride and sulphate. <i>Computational Materials Science</i> , 2022, 209, 111429.	1.4	16
17348	Abnormal in-plane thermal conductivity anisotropy in bilayer $\Gamma$ -phase tellurene. <i>International Journal of Heat and Mass Transfer</i> , 2022, 192, 122908.	2.5	2
17349	Bifunctional integrated electrode for high-efficient hydrogen production coupled with 5-hydroxymethylfurfural oxidation. <i>Applied Catalysis B: Environmental</i> , 2022, 312, 121400.	10.8	63
17350	Metal-organic framework-derived three-dimensional $\text{CoSe}_2/\text{Cd}_{0.8}\text{Zn}_{0.2}\text{S}$ Schottky junction for highly efficient photocatalytic H <sub>2</sub> evolution. <i>Applied Surface Science</i> , 2022, 593, 153420.	3.1	14
17351	In-situ construction of $\text{Cu}^{\ominus}\text{Co}_4\text{N}@CC$ hierarchical binder-free cathode for advanced and flexible $\text{Li}^{\ominus}\text{CO}_2$ batteries: Electron structure and mass transfer modulation. <i>Journal of Power Sources</i> , 2022, 535, 231446.	4.0	9
17352	$\text{BiOBr}/\text{Bi}_2\text{S}_3$ heterojunction with S-scheme structure and oxygen defects: In-situ construction and photocatalytic behavior for reduction of CO <sub>2</sub> with H <sub>2</sub> O. <i>Journal of Colloid and Interface Science</i> , 2022, 620, 407-418.	5.0	56



#	ARTICLE	IF	CITATIONS
17353	Atomically dispersed ruthenium in carbon aerogels as effective catalysts for pH-universal hydrogen evolution reaction. <i>Chemical Engineering Journal</i> , 2022, 442, 136337.	6.6	27
17354	Theoretical insight on mechanically robust graphene-nickel interfaces using chromium-substituted nickel and boron-doped graphene. <i>Applied Surface Science</i> , 2022, 593, 153356.	3.1	2
17355	Ab Initio Study of Mechanical Deformation. , 2005, , 439-448.		0
17361	Alkali Metal Doping in B-C <sub>3</sub> N <sub>4</sub> Extends Carrier Lifetime and Increases the CO <sub>2</sub> Adsorption: Dft Study and Time-Domain Ab Initio Analysis. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17362	Screening of transition metal single-atom catalysts supported by a WS <sub>2</sub> monolayer for electrocatalytic nitrogen reduction reaction: insights from activity trend and descriptor. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 13384-13398.	1.3	10
17363	New Insights of Heterogeneous Nucleation Induced by Submicron Scaled Y <sub>2</sub> O <sub>3</sub> in H13 Die Steel: A Mutual Diffusion Behaviour. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17364	The Mechanism of Nitrogen Reduction Reaction on Defective Bn Monolayer with Monatomic Co, Ni, and Mo Doped-A First Principles Study. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17365	Phase transition induced by an external electric field as a buffer to facilitate the initial decomposition of a series of catenated nitrogen energetic systems: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 12488-12500.	1.3	3
17366	Reaction surfaces and interfaces of metal sulfides: cryo-XPS meets HAXPES and DFT. <i>Faraday Discussions</i> , 2022, , .	1.6	3
17368	Towards the rational design of Pt-based alloy catalysts for the low-temperature water-gas shift reaction: from extended surfaces to single atom alloys. <i>Chemical Science</i> , 2022, 13, 6385-6396.	3.7	9
17369	Aluminum, an Efficient Gas Sensor and Scavenger for SF <sub>6</sub> Decomposition Products. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17370	Two-Dimensional Cds/SiO <sub>2</sub> Heterostructure with Low Carrier Recombination as a Promising Photocatalyst for Water Splitting. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17371	Three Co-Based Tartratoborates with Fundamental Building Blocks [B(C <sub>4</sub> H <sub>2</sub> O <sub>6</sub> ) <sub>2</sub> ] <sup>5-</sup> from Facile Condensation Reactions. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17372	Theoretical description of water from single-molecule to condensed phase: Recent progress on potential energy surfaces and molecular dynamics. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 227-241.	0.6	2
17373	Electronic, Optical and Thermoelectric Properties of the Csmf <sub>3</sub> (M= Si or Ge) Fluoro-Perovskites. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17374	Influence of Intercalated Gd Atoms on Graphene-4h-SiC(0001) Properties. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17375	Two-dimensional ordering governs the overpotential of Li intercalation and plating on graphene and its variants. <i>Journal of Applied Physics</i> , 2022, 131, .	1.1	1
17376	Magnetocaloric Effect in ScGdHo Medium-Entropy Alloy. <i>Journal of Superconductivity and Novel Magnetism</i> , 2022, 35, 1539-1545.	0.8	7

#	ARTICLE	IF	CITATIONS
17377	Electronic and optical properties of layered Van der Waals heterostructures based on blue phosphorus and zinc oxide. , 2022, , .		0
17378	New stable structures of OsN <sub>4</sub> predicted using first-principles calculations. Phase Transitions, 0, , 1-11.	0.6	0
17379	Van der Waals Heterostructures Based on Porous Graphene for Photocatalytic Water Splitting. Journal of Physical Chemistry C, 2022, 126, 7849-7858.	1.5	7
17380	Lone Pair-Driven Enhancement of Birefringence in Polar Alkali Metal Antimony Phosphates. Chemistry of Materials, 2022, 34, 4224-4231.	3.2	19
17381	The role of silver in 13-atom palladium-silver bimetallic clusters: nucleation and growth, structural evolution, electron interaction. Journal of Materials Science, 2022, 57, 8180-8194.	1.7	3
17382	In Situ Electrochemically Formed Ag/NiOOH/Ni <sub>3</sub> S <sub>2</sub> Heterostructure Electrocatalysts with Exceptional Performance toward Oxygen Evolution Reaction. ACS Sustainable Chemistry and Engineering, 2022, 10, 5976-5985.	3.2	15
17383	Modulation Doping Enables Ultrahigh Power Factor and Thermoelectric ZT in n-Type Bi <sub>2</sub> Te <sub>2.7</sub> Se <sub>0.3</sub> . Advanced Science, 2022, 9, e2201353.	5.6	19
17384	Self-Poisoning by C <sub>2</sub> Products in CO <sub>2</sub> Photoreduction Using a Phosphorus-Doped Carbon Nitride with Nitrogen Vacancies. ACS Sustainable Chemistry and Engineering, 2022, 10, 5758-5769.	3.2	14
17385	Influence of doping Sn direction and concentration on vanadium pentoxide based on density functional theory. Functional Materials Letters, 2022, 15, .	0.7	0
17386	Theoretical study of transition metal doped $\hat{1}\pm$ -borophene nanosheet as promising electrocatalyst for electrochemical reduction of N <sub>2</sub> . Computational and Theoretical Chemistry, 2022, 1213, 113732.	1.1	8
17387	Distribution Pattern of Metal Atoms in Bimetal-Doped Pyridinic N <sub>4</sub> Pores Determines Their Potential for Electrocatalytic N <sub>2</sub> Reduction. Journal of Physical Chemistry A, 2022, 126, 3080-3089.	1.1	0
17388	Quantum Chemical Approaches to the Calculation of NMR Parameters: From Fundamentals to Recent Advances. Magnetochemistry, 2022, 8, 50.	1.0	20
17389	Molecular Dynamics Study of the Photodegradation of Polymeric Chains. Journal of Physical Chemistry Letters, 2022, 13, 4374-4380.	2.1	2
17390	Pt-based intermetallic compounds with tunable activity and selectivity toward hydrogen production from formic acid. Applied Surface Science, 2022, 597, 153530.	3.1	7
17391	New quaternary sulfide LiGaSiS <sub>4</sub> : Synthesis, structure and optical properties. Journal of Solid State Chemistry, 2022, , 123230.	1.4	0
17392	Revisiting the Performance of Time-Dependent Density Functional Theory for Electronic Excitations: Assessment of 43 Popular and Recently Developed Functionals from Rungs One to Four. Journal of Chemical Theory and Computation, 2022, 18, 3460-3473.	2.3	61
17393	Structural, Electronic, and Transport Properties of Phosphorene-Graphene Lateral Heterostructure Anodes: Insights from First-Principles Calculations. Journal of Physical Chemistry C, 2022, 126, 8928-8937.	1.5	7
17394	Surface functionalization of Linde F (K) nano-zeolite and its application for photocatalytic wastewater treatment and hydrogen production. Applied Physics A: Materials Science and Processing, 2022, 128, 1.	1.1	7

#	ARTICLE	IF	CITATIONS
17395	Computational design of ternary NiO/MPt interface active sites for H <sub>2</sub> O dissociation. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 20040-20048.	3.8	2
17396	A New Enthalpy of Formation Test Set Designed for Organic Fluorine Containing Compounds. <i>Advanced Theory and Simulations</i> , 0, , 2200093.	1.3	1
17397	Exploration of potassium silicide compounds under high pressure. <i>Physica B: Condensed Matter</i> , 2022, , 414013.	1.3	0
17398	Superconducting Li <sub>10</sub> Se electride under pressure. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	8
17399	First-Principles Study on Optoelectronic Properties of Fe-Doped Montmorillonite Clay. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 4257-4262.	2.1	2
17400	Experimental and theoretical insight into DSSCs mechanism influenced by different doping metal ions. <i>Applied Surface Science</i> , 2022, 597, 153607.	3.1	4
17401	High-Performance Blue Quantum-Dot Light-Emitting Diodes by Alleviating Electron Trapping. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	14
17402	Strategic design and fabrication of MXenes-Ti <sub>3</sub> CNCl <sub>2</sub> @CoS <sub>2</sub> core-shell nanostructure for high-efficiency hydrogen evolution. <i>Nano Research</i> , 2022, 15, 5977-5986.	5.8	61
17403	Insight into the mechanism of the key step for the production of 1,4-butanediol on Ni(111) surface: A DFT study. <i>Molecular Catalysis</i> , 2022, 524, 112335.	1.0	1
17404	Fast Transformation of CO <sub>2</sub> into CO Via a Hydrogen Bond Network on the Cu Electro-catalysts. <i>Journal of Physical Chemistry C</i> , 2022, 126, 7841-7848.	1.5	8
17405	Large negative differential resistance in triangular and square cyclopropyllithium derivative molecule. <i>Physica B: Condensed Matter</i> , 2022, , 413989.	1.3	0
17406	Experimental study and thermodynamic modeling of the Ti-Cu-B system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2022, 77, 102431.	0.7	0
17407	Correlation governs the impurity (Ti, Zr, Hf) diffusion in face-centered cubic iridium through first-principles calculation. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2022, 77, 102433.	0.7	1
17408	Suppressing disorder-order phase transition of Gd <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> pyrochlore by Dy <sup>3+</sup> doping and their impact on luminescence. <i>Materials Today Chemistry</i> , 2022, 24, 100931.	1.7	3
17409	The role of entropy and enthalpy in high entropy carbides. <i>Computational Materials Science</i> , 2022, 210, 111474.	1.4	8
17410	A permselective and multifunctional 3D N-doped carbon nanotubes interlayer for high-performance lithium-sulfur batteries. <i>Electrochimica Acta</i> , 2022, 421, 140430.	2.6	15
17411	Influence of doping Fe on performance of calcium-based doped materials for thermochemical energy storage: A DFT study. <i>Physica B: Condensed Matter</i> , 2022, 638, 413956.	1.3	2
17412	Pressure-induced metallization and robust superconductivity in pristine 1T-HfSe <sub>2</sub> . <i>Materials Today Physics</i> , 2022, 25, 100698.	2.9	11

#	ARTICLE	IF	CITATIONS
17413	Mechanical properties of the novel L12-Ir3Z ultra-high temperature alloys (Z =Ti, V, Zr, Nb, Hf and Ta). Journal of Alloys and Compounds, 2022, 912, 165244.	2.8	6
17414	W coordinated with unsymmetrical S1N3 (W-S1N3) as an electrocatalyst for efficient ammonia synthesis. Materials Letters, 2022, 320, 132381.	1.3	1
17415	Oxidation mechanism of arsenopyrite under alkaline conditions: Experimental and theoretical analyses. Journal of Cleaner Production, 2022, 358, 131987.	4.6	9
17416	The trapping effects of silicon and phosphorus on point defects in $\hat{3}$ -Fe. Computational Materials Science, 2022, 210, 111488.	1.4	1
17417	Locating the rate-limiting step of hydrogen conversion on Sr2Fe1.5Mo0.5O6 (0 0 1) surface: Implications for efficient SOFC anode design. Applied Surface Science, 2022, 595, 153513.	3.1	6
17418	Nonmetallic surface plasmon resonance coupling with pyroelectric effect for enhanced near-infrared-driven CO2 reduction. Chemical Engineering Journal, 2022, 445, 136739.	6.6	14
17419	Laser fabrication of Pt anchored Mo2C micropillars as integrated gas diffusion and catalytic electrode for proton exchange membrane water electrolyzer. Applied Catalysis B: Environmental, 2022, 314, 121455.	10.8	18
17420	Synthesis, microstructure, and formation mechanism of a potential neutron shielding material: WAIB. Journal of Materials Science and Technology, 2022, 126, 127-131.	5.6	7
17421	Tuning the activity and selectivity of nitrogen reduction reaction on double-atom catalysts by B doping: A density functional theory study. Nano Energy, 2022, 99, 107363.	8.2	21
17422	Effects of surface microtopography on material removal and ultra-smooth surface creation processes in ultraviolet-induced nanoparticle colloid jet machining. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 648, 129161.	2.3	2
17423	The dynamical stability, electronic, elastic properties and ideal strength of diamond-like cubic B2CN: A first-principles study. Solid State Communications, 2022, 352, 114805.	0.9	3
17424	Electroreduction of N <sub>2</sub> to NH <sub>3</sub> catalyzed by a Mn/Re(111) single-atom alloy catalyst with high activity and selectivity: a new insight from a first-principles study. Catalysis Science and Technology, 2022, 12, 4074-4085.	2.1	6
17425	Investigation of the W/Y <sub>2</sub> O <sub>3</sub> heterogeneous interface properties and its effect on hydrogen behavior using first-principles calculations. Nuclear Fusion, 2022, 62, 086015.	1.6	2
17426	A DFT study of adsorption properties of SO2, SOF2, and SO2F2 on ZnO/CuO doped graphene. Diamond and Related Materials, 2022, 126, 109103.	1.8	15
17427	Tailoring Oxygen Reduction Reaction Pathway on Spinel Oxides via Surficial Geometrical Site Occupation Modification Driven by the Oxygen Evolution Reaction. Advanced Materials, 2022, 34, e2202874.	11.1	52
17428	Structural analysis and magnetic properties of cobalt-doped nanotitania. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2022, 282, 115761.	1.7	3
17429	The Na-H system: from first-principles calculations to thermodynamic modeling. International Journal of Materials Research, 2022, 97, 845-853.	0.1	5
17430	Thermodynamic modeling of the sodium alanates and the Na-Al-H system. International Journal of Materials Research, 2022, 97, 1484-1494.	0.1	4



#	ARTICLE	IF	CITATIONS
17449	Revisit the VEC criterion in high entropy alloys (HEAs) with high-throughput ab initio calculations: A case study with Al-Co-Cr-Fe-Ni system. <i>Journal of Alloys and Compounds</i> , 2022, 916, 165477.	2.8	14
17450	Synergy of nitrogen vacancies and Fe <sub>2</sub> P cocatalyst on graphitic carbon nitride for boosting photocatalytic CO <sub>2</sub> conversion. <i>Chemical Engineering Journal</i> , 2022, 446, 137096.	6.6	19
17451	Electronic, Optical and Thermoelectric Properties of WSe <sub>2</sub> -Inn 2d Interface: A Dft Study. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17452	Complex Segregation and Fracture Mechanisms at Interfaces in Liquid Metal Embrittlement and Corrosion. <i>SSRN Electronic Journal</i> , 0, , .	0.4	1
17453	Bimetallic Mmos <sub>4</sub> (M = Ni, Co, Cu) Cocatalysts Architected CDS Nanoflowers for Synergistically Boosting Visible-Light-Driven Photocatalytic H <sub>2</sub> Evolution from Water and Benzyl Alcohol. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17454	Ultrathin Znti-Ldh Nanosheet: A Bifunctional Lewis and Bronsted Acid Photocatalyst for Synthesis of N-Benzylideneaniline Via a Tandem Reaction. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17455	Molecular Adsorption Behavior of Zn <sub>2</sub> sno <sub>4</sub> (111) Crystal Surface. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17457	First Principles Calculations of Charge Shift Photocurrent in Vdws Slide Double Layered 2d H-Bn and P̂-Ges Homostructures. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17458	First-principles design of hetero CoM (M = 3d, 4d, 5d block metals) double-atom catalysts for oxygen evolution reaction under alkaline conditions. <i>Nanoscale Advances</i> , 2022, 4, 2913-2921.	2.2	3
17459	Insights into Cation-Disorder Effect on Stability, Electronic Structure and Defect Properties of Zn-iv-Nitrides: The Case of Zngen <sub>2</sub> . <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17460	Controlling the Cation Exsolution of Perovskite to Customize Heterostructure Active Site for Oxygen Evolution Reaction. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 25638-25647.	4.0	26
17461	Three-dimensionally ordered mesoporous Co <sub>3</sub> O <sub>4</sub> decorated with Mg as bifunctional oxygen electrocatalysts for high-performance zinc-air batteries. <i>Nano Energy</i> , 2022, 100, 107425.	8.2	39
17462	Cu-Doping Effect on the Electrocatalytic Properties of Self-Supported Cu-Doped Ni <sub>3</sub> S <sub>2</sub> Nanosheets for Hydrogen Production via Efficient Urea Oxidation. <i>Industrial &amp; Engineering Chemistry Research</i> , 2022, 61, 7777-7786.	1.8	23
17463	Mechanism Insight into Catalytic Performance of Ni <sub>12</sub> P <sub>5</sub> over Ni <sub>2</sub> P toward the Catalytic Deoxygenation of Butyric Acid. <i>Catalysts</i> , 2022, 12, 569.	1.6	1
17464	Effects of uniaxial strain on structural, electronic, and optical properties of LiNbO <sub>3</sub> : Ab-initio calculations. <i>Computational Condensed Matter</i> , 2022, 33, e00694.	0.9	0
17465	Microstructure Formation of Cast and Directionally Solidified Mo-Ti-B Alloys. <i>Metals</i> , 2022, 12, 916.	1.0	0
17466	Unusual mechanical properties of ice VIII: Auxetic potential in a high pressure polymorph of ice. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 169, 110755.	1.9	1
17467	Orbital and electronic responses in the GaN/AlN quantum structures constructed on different crystal planes. <i>Applied Physics Express</i> , 2022, 15, 071002.	1.1	1



#	ARTICLE	IF	CITATIONS
17468	Atomic Layer Deposition of Intermetallic Fe <sub>4</sub> Zn <sub>9</sub> Thin Films from Diethyl Zinc. <i>Chemistry of Materials</i> , 2022, 34, 5241-5248.	3.2	2
17469	Jacutingaite family: An efficient platform for coexistence of spin valley Hall effects, valley spin-valve realization, and layer spin crossover. <i>Physical Review B</i> , 2022, 105, .	1.1	8
17470	Boosting the Electrocatalytic Oxygen Evolution of Perovskite LaCo <sub>1-x</sub> Fe <sub>x</sub> O <sub>3</sub> by the Construction of Yolk-shell Nanostructures and Electronic Modulation. <i>Small</i> , 2022, 18, .	5.2	31
17471	High Curie Temperature in (Fe/Cr)-doped Zincblende SnC Half-metal Ferromagnet: First-principles Study. <i>Journal of Superconductivity and Novel Magnetism</i> , 0, , .	0.8	1
17472	Unveiling the role of C60-supported vanadium single atoms for catalytic overall water splitting. <i>Cell Reports Physical Science</i> , 2022, 3, 100910.	2.8	7
17473	Implementation of self-consistent MCGA functionals in augmented plane wave based methods. <i>Physical Review B</i> , 2022, 105, .	1.1	4
17474	Nickel and Palladium Complexes of a PP(O)P Pincer Ligand Based upon a <i>peri</i> -Substituted Acenaphthyl Scaffold and a Secondary Phosphine Oxide. <i>Inorganic Chemistry</i> , 2022, 61, 8406-8418.	1.9	3
17475	Electronic, optical and thermoelectric properties of the CsMF <sub>3</sub> (M= Si or Ge) fluoro-perovskites. <i>Computational Condensed Matter</i> , 2022, 32, e00699.	0.9	37
17476	Theoretical insights on designing of difluoramino compounds. <i>FirePhysChem</i> , 2022, , .	1.5	0
17477	Adamantanes as White-Light Emitters: Controlling the Arrangement and Functionality by External Coulomb Forces. <i>Journal of Physical Chemistry C</i> , 0, , .	1.5	2
17478	Cluster of Hexamolybdenum [Mo <sub>6</sub> Cl <sub>14</sub> ] <sup>2+</sup> for Sensing Nitroaromatic Compounds. <i>ACS Omega</i> , 0, , .	1.6	2
17479	Mn <sub>2</sub> NO <sub>2</sub> MXene as a promising anode material for metal ion batteries: A first-principles study. <i>Surfaces and Interfaces</i> , 2022, , 102091.	1.5	5
17480	Explore the underlying mechanism of graphitic C <sub>3</sub> N <sub>5</sub> -hosted single-atom catalyst for electrocatalytic nitrogen fixation. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 22035-22044.	3.8	15
17481	Elucidation of the reaction mechanism of indirect oxidative carbonylation of methanol to dimethyl carbonate on Pd/NaY catalyst: Direct identification of reaction intermediates. <i>Journal of Catalysis</i> , 2022, 412, 30-41.	3.1	16
17482	DFT and TDDFT studies of structural, electronic and optical properties of the inorganic solar perovskites XPbBr <sub>3</sub> (X=Li or Na). <i>Phase Transitions</i> , 2022, 95, 501-514.	0.6	17
17483	Molecular Modeling in Anion Exchange Membrane Research: A Brief Review of Recent Applications. <i>Molecules</i> , 2022, 27, 3574.	1.7	6
17484	Three Co-based tartratoborates with fundamental building blocks [B(C <sub>4</sub> H <sub>2</sub> O <sub>6</sub> ) <sub>2</sub> ] <sup>5-</sup> from facile condensation reactions. <i>Journal of Solid State Chemistry</i> , 2022, , 123304.	1.4	1
17485	Investigation on the correlation between ferrous ion and the floatability of pyrite with different oxidation degrees. <i>Minerals Engineering</i> , 2022, 184, 107636.	1.8	4

#	ARTICLE	IF	CITATIONS
17486	First-Principles Study of Electronic and Optical Properties of Tri-Layered van der Waals Heterostructures Based on Blue Phosphorus and Zinc Oxide. <i>Journal of Composites Science</i> , 2022, 6, 163.	1.4	0
17487	Isolation, characterization, molecular electronic structure investigation, and in-silico modeling of the anti-inflammatory potency of trihydroxystilbene. <i>Journal of Molecular Structure</i> , 2022, 1266, 133418.	1.8	16
17488	Doping Effects in the Thiolate-protected Gold Nanoclusters from the Perspective of Balance between Ligands and the Core. <i>Journal of Computational Biophysics and Chemistry</i> , 0, , .	1.0	0
17489	Intercalation-driven ferroelectric-to-ferroelastic conversion in a layered hybrid perovskite crystal. <i>Nature Communications</i> , 2022, 13, .	5.8	27
17490	Terahertz Spectroscopy and Density Functional Theory Analysis of the Molecular Interactions in Crystalline Orotic Acid Monohydrate. <i>Journal of Applied Spectroscopy</i> , 0, , .	0.3	0
17491	Simultaneously Enhancing Catalytic Performance and Increasing Density of Bifunctional CuN <sub>3</sub> Active Sites in Dopant-Free 2D C <sub>3</sub> N <sub>3</sub> Cu for Oxygen Reduction/Evolution Reactions. <i>ACS Omega</i> , 2022, 7, 19794-19803.	1.6	4
17492	Density functional theory study of hydrogen as reducing agent of hematite (̂±-Fe2O3) in ironmaking process. <i>Thin Solid Films</i> , 2022, 754, 139321.	0.8	0
17493	Anticorrosion mechanism of Al-modified phosphate ceramic coating in the high-temperature marine atmosphere. <i>Surface and Coatings Technology</i> , 2022, 441, 128572.	2.2	6
17494	DFT investigation of carbon-expanded ̂± phase with different alloying element. <i>Vacuum</i> , 2022, 202, 111199.	1.6	1
17495	Recent progress in nanocrystalline Sm̂€“Co based magnets. <i>Materials Today Chemistry</i> , 2022, 25, 100983.	1.7	4
17496	Theoretical study on CO2 reduction to methanol catalyzed by highly stable single-atom transition metal riveted bilayer 2D material. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 648, 129365.	2.3	2
17497	Quantum spin Hall effect in two-dimensional transition-metal chalcogenides MX <sub>2</sub> (M = Zr, Hf and X = S, Se). <i>Tj ETQq1 1 0.784314 rgB</i>	1.3	2
17498	Realizing robust and efficient acidic oxygen evolution by electronic modulation of 0D/2D CeO2 quantum dots decorated SrIrO3 nanosheets. <i>Applied Catalysis B: Environmental</i> , 2022, 315, 121579.	10.8	28
17499	One-Pot Synthesis and Characterization of Three Chromotropic Supramolecular Isomeric Cu(II) Coordination Polymers as 1-D Zigzag or Helical Chains with Homochiral or Heterochiral Cu(II) Coordination Centres. <i>Journal of Molecular Structure</i> , 2022, 1265, 133422.	1.8	1
17500	Thermodynamic stability of niobium-doped ceria surfaces. <i>Journal of Molecular Structure</i> , 2022, 1265, 133416.	1.8	2
17504	Adsorption Selectivity of TiCl4 Precursor on Pt Surfaces for Atomic Layer Deposition by Density Functional Theory. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17505	Solvent Controlled Excited State Intramolecular Proton Transfer (Esipt) Behavior and Luminescent Property of a Novel Phthalimide-Based Fluorophore: A Td-Dft Study. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17506	Atmospheric atomic layer deposition of SnO <sub>2</sub> thin films with tin(acetylacetonate) and water. <i>Dalton Transactions</i> , 2022, 51, 9278-9290.	1.6	15

#	ARTICLE	IF	CITATIONS
17507	Photocatalytic hydrogen production and storage in carbon nanotubes: a first-principles study. RSC Advances, 2022, 12, 17029-17035.	1.7	6
17508	A <sub>3</sub> Ga <sub>8</sub> Se <sub>14</sub> (A = Rb, Cs): second-harmonic generation responses realized through the parallel arrangement of AgSe <sub>4</sub> and GaSe <sub>4</sub> tetrahedrons. Dalton Transactions, 2022, 51, 11048-11053.	1.6	2
17509	Symmetric Spiroenes: Promising Building Blocks for New Generation Opto-Electronic Materials. Physical Chemistry Chemical Physics, 0, , .	1.3	0
17510	Electronic and Optical Properties of C <sub>16</sub> S <sub>8</sub> and C <sub>16</sub> S <sub>4</sub> Se <sub>4</sub> Molecules and Crystals. New Journal of Chemistry, 0, , .	1.4	1
17511	Small Palladium Clusters and Their Adducts With Atomic Oxygen. SSRN Electronic Journal, 0, , .	0.4	0
17512	A comparative DFT+U study of CO oxidation on Pd- and Zr-doped ceria. Journal of Rare Earths, 2023, 41, 1042-1048.	2.5	2
17513	Turning on photoelectric activity by cation exchange within an anionic pyrene-based hydrogen-bonded organic framework. Dyes and Pigments, 2022, 205, 110506.	2.0	6
17514	Formation of $N\text{H}_3$ compound at the extreme condition of planetary interiors. Physical Review B, 2022, 105, .	1.1	5
17515	Phase-Dependent Epitaxy for Antimonene Growth on Silver Substrate. Frontiers in Physics, 0, 10, .	1.0	4
17516	Stable structures and superconducting properties of Ca-La-H compounds under pressure. Journal of Physics Condensed Matter, 0, , .	0.7	1
17517	Elasticity, mechanical and thermal properties of polycrystalline hafnium carbide and tantalum carbide at high pressure. Journal of the European Ceramic Society, 2022, 42, 5220-5228.	2.8	6
17518	Boron nanostructure formation on Mo(112) surface. Surface Science, 2022, 724, 122145.	0.8	5
17519	Identification of a Robust and Durable Fe <sub>4</sub> C Catalyst for ORR in PEM Fuel Cells and the Role of the Fifth Ligand. ACS Catalysis, 2022, 12, 7541-7549.	5.5	30
17520	Enhancing the bifunctional activity of CoSe <sub>2</sub> nanocubes by surface decoration of CeO <sub>2</sub> for advanced zinc-air batteries. Journal of Colloid and Interface Science, 2022, 625, 839-849.	5.0	14
17522	Carbonate-Ion-Mediated Photogenerated Hole Transfer to Boost Hydrogen Production. Journal of Physical Chemistry C, 2022, 126, 10367-10377.	1.5	4
17523	Determining Repulsion in Cyclophane Cages. Molecules, 2022, 27, 3969.	1.7	5
17524	Computational studies of structural, energetic, and electronic properties of pure Pt and Mo and mixed Pt/Mo clusters: Comparative analysis of characteristics and trends. Journal of Chemical Physics, 2022, 157, .	1.2	3
17525	Novel Van Der Waals Heterostructures Based on Borophene, Graphene-like GaN and ZnO for Nanoelectronics: A First Principles Study. Materials, 2022, 15, 4084.	1.3	9

#	ARTICLE	IF	CITATIONS
17526	High-entropy hydrides for fast and reversible hydrogen storage at room temperature: Binding-energy engineering via first-principles calculations and experiments. <i>Acta Materialia</i> , 2022, 236, 118117.	3.8	30
17527	Homogeneous nitrogen-doped (111)-type layered Sr <sub>5</sub> Nb <sub>4</sub> O <sub>15</sub> ~ <sup>x</sup> N <sub>x</sub> as a visible-light-responsive photocatalyst for water oxidation. <i>Nano Research</i> , 2022, 15, 9976-9984.	5.8	8
17528	Probing the Intermediates of Catalyzed Dehydration Reactions of Primary Amide to Nitrile in Plasmonic Junctions. <i>ACS Catalysis</i> , 2022, 12, 7737-7747.	5.5	13
17529	Study of the reversible hydrogen storage performance of Ti-decorated hexagonal B36 by DFT calculations with van der Waals corrections. <i>International Journal of Hydrogen Energy</i> , 2022, , .	3.8	10
17530	The Fe <sub>2</sub> O <sub>3</sub> (0001) Surface Under Electroreduction Conditions: A DFT Study of L-Cysteine Adsorption. <i>Journal of the Electrochemical Society</i> , 2022, 169, 064513.	1.3	1
17531	New pecS- <i>n</i> ( <i>n</i> = 1, 2) basis sets for quantum chemical calculations of the NMR chemical shifts of H, C, N, and O nuclei. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	6
17532	Centimeter-scale perovskite SrTaO <sub>2</sub> N single crystals with enhanced photoelectrochemical performance. <i>Science Bulletin</i> , 2022, 67, 1458-1466.	4.3	6
17533	Effects of order-disorder transition on phase relationship, elastic strength, and mechanical anisotropy of Al-Li alloys. <i>Materialia</i> , 2022, 24, 101483.	1.3	0
17534	Computational complexity of the ground state energy density problem. , 2022, , .		3
17535	Regulating iron species compositions by Fe-Al interaction in CO <sub>2</sub> hydrogenation. <i>Journal of Catalysis</i> , 2022, 413, 331-341.	3.1	17
17536	Leucine on Silica: A Combined Experimental and Modeling Study of a System Relevant for Origins of Life, and the Role of Water Coadsorption. <i>Langmuir</i> , 2022, 38, 8038-8053.	1.6	4
17537	Enhancing Conversion of Polysulfides via Porous Carbon Nanofiber Interlayer with Dual-Active Sites for Lithium-Sulfur Batteries. <i>Journal of Colloid and Interface Science</i> , 2022, , .	5.0	5
17538	High-throughput screening of dual-atom doped PC6 electrocatalysts for efficient CO <sub>2</sub> electrochemical reduction to CH <sub>4</sub> by breaking scaling relations. <i>Electrochimica Acta</i> , 2022, 426, 140764.	2.6	13
17539	Spin-polarized electrons in atomic layer materials formed on solid surfaces. <i>Progress in Surface Science</i> , 2022, 97, 100665.	3.8	1
17540	Effects of non-local exchange functionals in the density functional theories for the description of molecular vibrations. <i>Journal of Chemical Sciences</i> , 2022, 134, .	0.7	2
17541	Fully exposed nickel clusters with electron-rich centers for high-performance electrocatalytic CO <sub>2</sub> reduction to CO. <i>Science Bulletin</i> , 2022, 67, 1477-1485.	4.3	13
17542	Direct electro-synthesis of valuable C=N compound from NO. <i>Chem Catalysis</i> , 2022, 2, 1807-1818.	2.9	21
17543	Tunable green syngas generation from CO <sub>2</sub> and H <sub>2</sub> O with sunlight as the only energy input. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	16

#	ARTICLE	IF	CITATIONS
17544	Design of frustrated Lewis pair in defective TiO <sub>2</sub> for photocatalytic non-oxidative methane coupling. Chem Catalysis, 2022, 2, 1775-1792.	2.9	12
17545	High Anisotropic Optoelectronics in Monolayer Binary M <sub>8</sub> X <sub>12</sub> (M = Mo, W; X =) Tj ETQq <sub>4.0</sub> 1.0.784314 rgBT	1.0	0
17546	Optical Properties of Graphene-like Be <sub>3</sub> C <sub>2</sub> Monolayer by First-Principles Calculations. Journal of the Physical Society of Japan, 2022, 91, .	0.7	2
17547	Prediction of new stable phases of FePd <sub>2</sub> crystal alloy. Journal of Solid State Chemistry, 2022, 313, 123328.	1.4	0
17548	Insight into ideal shear strength of Ni-based dilute alloys using first-principles calculations and correlational analysis. Computational Materials Science, 2022, 212, 111564.	1.4	1
17549	Mechanical and thermal properties of zirconium claddings after doping niobium: Understanding from first-principles calculations. Journal of Nuclear Materials, 2022, 568, 153876.	1.3	3
17550	MSSe-N <sub>2</sub> CO <sub>2</sub> (M=Mo, W and N=Zr, Hf) van der Waals heterostructures; A first principles study. Chemical Physics, 2022, 561, 111607.	0.9	1
17551	How do the available density functionals perform on the calculation of eigenvalues of frontier to deeper orbitals? A metric space evaluation of experimental and quantum chemical findings. Chemical Physics, 2022, 561, 111600.	0.9	1
17552	CO conversion over LaFeO <sub>3</sub> perovskite during chemical looping processes: Influences of Ca-doping and oxygen species. Applied Catalysis B: Environmental, 2022, 316, 121598.	10.8	20
17553	Prussian blue analogue/KB-derived Ni/Co/KB composite as a superior adsorption-catalysis separator modification material for Li-S batteries. Journal of Colloid and Interface Science, 2022, 625, 425-434.	5.0	7
17554	Electrocatalytic activity of a $\hat{1}^2$ -Sb two-dimensional surface for the hydrogen evolution reaction. Physical Chemistry Chemical Physics, 2022, 24, 17832-17840.	1.3	2
17555	Strain tunable nanoporous r-N-GDY membrane for efficient seawater desalination. Journal of Materials Chemistry A, 2022, 10, 16533-16540.	5.2	7
17556	Coordination/cation exchangeable dual sites intercalated multilayered T <sub>3</sub> C <sub>2</sub> T <sub>x</sub> MXene for selective and ultrafast removal of thallium( <sup>+</sup> ) from water. Environmental Science: Nano, 2022, 9, 3385-3396.	2.2	1
17557	Rb <sub>2</sub> MGe <sub>3</sub> S <sub>8</sub> (M=Zn, Cd): Non-Centrosymmetry Transformation Led by Structure Change of [MGe <sub>3</sub> S <sub>8</sub> ] <sup>2-</sup> Unit <sup>+</sup> . Acta Chimica Sinica, 2022, 80, 633.	0.5	2
17558	Modulation of intrinsic defect in vertically grown ZnO nanorods by ion implantation. Physical Chemistry Chemical Physics, 0, , .	1.3	1
17559	Insights into Cation-Disorder Effect on Stability, Electronic Structure and Defect Properties of Zn-IV-Nitrides: The Case of Zngen <sub>2</sub> . SSRN Electronic Journal, 0, , .	0.4	0
17560	Theoretical insights into the electroreduction of nitrate to ammonia on graphene-based single-atom catalysts. Nanoscale, 2022, 14, 10862-10872.	2.8	57
17561	Cu segregation in Au@Cu nanoparticles exposed to hydrogen atmospheric pressure: how is fcc symmetry maintained?. Faraday Discussions, 0, 242, 375-388.	1.6	4





#	ARTICLE	IF	CITATIONS
17580	External Electric Field-Induced Phase Transition of a Series of Energetic Pentazole Crystals: A First-Principles Study. <i>Crystal Growth and Design</i> , 0, , .	1.4	0
17581	3D Hierarchical Grapheneâ€CNT Anode for Sodiumâ€Ion Batteries: a Firstâ€Principles Assessment. <i>Advanced Theory and Simulations</i> , 2022, 5, .	1.3	1
17582	An Ab-initio study of the Y decorated 2D holey graphyne for hydrogen storage application. <i>Nanotechnology</i> , 2022, 33, 405406.	1.3	11
17583	<sc>Ultralowâ€Energyâ€Barrier H<sub>2</sub>O<sub>2</sub></sc> Dissociation on Coordinatively Unsaturated Metal Centers in Binary <sc>Ceâ€Fe</sc> Prussian Blue Analogue for Efficient and Stable <sc>Photoâ€Fenton</sc> Catalysis. <i>Energy and Environmental Materials</i> , 2023, 6, .	7.3	3
17584	Magnetoâ€Optical Properties of Oxidized Co Nanowires on Pt Substrate. <i>Physica Status Solidi (B): Basic Research</i> , 2022, 259, .	0.7	4
17585	Cation-selective two-dimensional polyimine membranes for high-performance osmotic energy conversion. <i>Nature Communications</i> , 2022, 13, .	5.8	49
17586	ĐšĐ¼Đ½Ń†ĐµĐ½Ń,ŃĐ°Ń†Ń–Đ½Đ½Ń– Đ·Đ°Đ»ĐµĐ†Đ½Đ¼ŃŃ,Ń– ĐŃ–ĐµĐ»ĐµĐ°Ń,ŃĐ,Ń†Đ½Đ,Ń... Đ;Đ°ŃĐ½Đ¼ĐµŃ,ŃŃ–Đ²		
17587	Intercalation of Small Organic Molecules into Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene Cathodes for Flexible Highâ€Volumeâ€Capacitance Znâ€Ion Microsupercapacitor. <i>Advanced Materials Technologies</i> , 2022, 7, .	3.0	11
17588	O-terminated interface for thickness-insensitive transport properties of aluminum oxide Josephson junctions. <i>Scientific Reports</i> , 2022, 12, .	1.6	2
17589	Delocalization error: The greatest outstanding challenge in densityâ€functional theory. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2023, 13, .	6.2	43
17590	Transformation of ZnS microspheres to ZnO, their computational (DFT) validation and dye-sensitized solar cells application. <i>AIP Advances</i> , 2022, 12, 075001.	0.6	1
17591	Formation of solid <math>\text{SiO}_2</math> compound at high pressure and high temperature. <i>Physical Review B</i> , 2022, 106, .		
17592	Bonding-unsaturation-dependent superconductivity in P-rich sulfides. <i>Matter and Radiation at Extremes</i> , 2022, 7, .	1.5	10
17593	Converting inert ALOOH into efficient electrocatalyst for oxygen evolution reaction via structural/electronic modulation. <i>Journal of Colloid and Interface Science</i> , 2022, 627, 532-540.	5.0	4
17594	Alkali metal doping in Bâ€C3N4 extends carrier lifetime and increases the CO2 adsorption: DFT study and time-domain Ab initio analysis. <i>Journal of Physics and Chemistry of Solids</i> , 2022, , 110905.	1.9	2
17595	Tunable electronic properties of two-dimensional C<sub>3</sub>N/antimonene van der Waals heterostructure. <i>Journal Physics D: Applied Physics</i> , 2022, 55, 404001.	1.3	2
17596	Understanding the Anisotropy in the Electrical Conductivity of CuPt<sub>B</sub>-type Ordered GaInP Thin Films by Combining <i>In Situ</i> TEM Biasing and First Principles Calculations. <i>ACS Applied Electronic Materials</i> , 2022, 4, 3478-3485.	2.0	3
17597	Vibronic Excitonâ€Phonon States in Stack-Engineered van der Waals Heterojunction Photodiodes. <i>Nano Letters</i> , 2022, 22, 5751-5758.	4.5	6

#	ARTICLE	IF	CITATIONS
17598	Phosphorus-induced electronic structure reformation of hollow NiCo <sub>2</sub> Se <sub>4</sub> nanoneedle arrays enabling highly efficient and durable hydrogen evolution in all-pH media. <i>Nano Research</i> , 2022, 15, 8771-8782.	5.8	11
17599	Unraveling the capacitive effect in the vacancy-heterostructure WTe <sub>2</sub> /MoTe <sub>2</sub> for hydrogen evolution reaction by the grand canonical potential kinetics. <i>International Journal of Hydrogen Energy</i> , 2022, , .	3.8	0
17600	Universal Principle for Large-Scale Production of a High-Quality Two-Dimensional Monolayer via Positive Charge-Driven Exfoliation. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 6597-6603.	2.1	6
17601	Billiard Catalysis at Ti <sub>3</sub> C <sub>2</sub> MXene/MAX Heterostructure for Efficient Nitrogen Fixation. <i>Applied Catalysis B: Environmental</i> , 2022, 317, 121755.	10.8	17
17602	Cluster-Glass for Low-Cost White-Light Emission. <i>Advanced Materials</i> , 2022, 34, .	11.1	8
17603	Effect of vacancy modification on the quantum capacitance of silicene- based electrode in efficient supercapacitors. <i>Thin Solid Films</i> , 2022, 756, 139378.	0.8	1
17604	Understanding the optoelectronic properties of interface between Cs <sub>2</sub> TiBr <sub>6</sub> and TiO <sub>2</sub> for solar cell applications. <i>Materials Today Communications</i> , 2022, 32, 103963.	0.9	0
17605	Furthering the understanding of product formation in monoethanolamine degradation: A mechanistic DFT study. <i>International Journal of Greenhouse Gas Control</i> , 2022, 119, 103732.	2.3	2
17606	Umbrella sampling with machine learning potentials applied for solid phase transition of GeSbTe. <i>Chemical Physics Letters</i> , 2022, 803, 139813.	1.2	2
17607	Synergetic enhancement of activity and selectivity for reverse water gas shift reaction on Pt-Re/SiO <sub>2</sub> catalysts. <i>Journal of CO<sub>2</sub> Utilization</i> , 2022, 63, 102128.	3.3	12
17608	First principles calculations of charge shift photocurrent in vdWs slide double layered 2D h-BN and $\beta$ -GeS homostructures. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 169, 110887.	1.9	1
17609	Solution processed edge activated Ni-MoS <sub>2</sub> nanosheets for highly sensitive room temperature NO <sub>2</sub> gas sensor applications. <i>Applied Surface Science</i> , 2022, 600, 154086.	3.1	26
17610	Enhanced electrocatalytic full water-splitting reaction by interfacial electric field in 2D/2D heterojunction. <i>Chemical Engineering Journal</i> , 2022, 450, 137789.	6.6	27
17611	Insight into the elemental mercury immobilization mechanism with carbon and sulfur over the mackinawite (FeS) surface via density functional theory. <i>Chemical Engineering Journal</i> , 2022, 450, 137934.	6.6	6
17612	Feasible Structure Manipulation of Vanadium Selenide into VSe <sub>2</sub> on Au(111). <i>Nanomaterials</i> , 2022, 12, 2518.	1.9	2
17613	Prediction of Core Electron Reactivity and High Oxidation States in Radium under High Pressure. <i>Journal of Physical Chemistry C</i> , 0, , .	1.5	2
17614	Probing Copper and Copper-Gold Alloy Surfaces with Space-Quantized Oxygen Molecular Beam. <i>Jacs Au</i> , 0, , .	3.6	2
17615	First-principles studies of monolayers MoSi <sub>2</sub> N <sub>4</sub> decorated with transition metal single-atom for visible light-driven high-efficient CO <sub>2</sub> reduction by strain and electronic engineering. <i>Chemical Engineering Journal</i> , 2022, 450, 138198.	6.6	11

#	ARTICLE	IF	CITATIONS
17616	Effect of alloying elements on liquid metal embrittlement of pure BCC Fe in contact with liquid lead-bismuth eutectic: Experiments and first principles calculation. <i>Corrosion Science</i> , 2022, 208, 110522.	3.0	6
17617	Microstructure control and strengthening mechanism of fine-grained cast Mg alloys based on grain boundary segregation of Al solute. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2022, 851, 143665.	2.6	10
17618	Fullerenes Pose a Strain on Hybrid Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4709-4720.	1.1	5
17619	NO <sub>x</sub> on Al: The Unusual Adsorption Site Preference and the Attraction among Adsorbates. <i>Journal of Physical Chemistry C</i> , 2022, 126, 11971-11980.	1.5	2
17620	Ammonia: the molecule for establishing <sup>14</sup> N and <sup>15</sup> N absolute shielding scales and a source of information on nuclear magnetic moments. <i>Journal of Chemical Physics</i> , 0, .	1.2	1
17621	Ab initio calculations for the transport properties of metals within Boltzmann transport theory: From equilibrium to nonequilibrium heating regime. <i>Physical Review B</i> , 2022, 106, .	1.1	6
17622	Enhancing effect of vanadium releasing efficiently from lattice in black shale by thermal activation. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 651, 129773.	2.3	6
17623	Effects of Mg doping on physical properties of zinc-blende mercury selenide HgSe compound. <i>Physica B: Condensed Matter</i> , 2022, 644, 414204.	1.3	8
17624	Energy and mechanical properties predictions in Fe-Ni binary system by ab initio calculations. <i>Materials Today Communications</i> , 2022, 33, 104118.	0.9	1
17625	Stability of oxidized states of freestanding and ceria-supported PtOx particles. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	4
17626	Enhanced charge storage performance of MXene based all-solid-state supercapacitor with vertical graphene arrays as the current collector. <i>Journal of Energy Storage</i> , 2022, 54, 105355.	3.9	19
17627	Pressure-induced YSe <sub>3</sub> and Y <sub>3</sub> Se with charming structures and properties. <i>Journal of Alloys and Compounds</i> , 2022, 923, 166465.	2.8	0
17628	Synthesis, X-ray diffraction and anti-proliferative biological activity of hispolon derivatives and their (1-6-p-cymene)(Hispolonato)Ruthenium[II] chloride complexes. <i>Inorganica Chimica Acta</i> , 2022, 542, 121099.	1.2	2
17629	Selectivity of volatile organic compounds on the surface of zinc oxide nanosheets for gas sensors. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 20491-20505.	1.3	2
17630	Predicted crystal structures of xenon and alkali metals under high pressures. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18119-18123.	1.3	2
17631	Physical insights into the Au growth on the surface of a LaAlO <sub>3</sub> /SrTiO <sub>3</sub> heterointerface. <i>RSC Advances</i> , 2022, 12, 24146-24155.	1.7	1
17632	On-purpose design of dual active sites in single V atom anchored C <sub>2</sub> N nanosheets for propane dehydrogenation catalysis. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 5517-5526.	3.0	2
17633	Molecular adsorption of Al <sup>3+</sup> -doped ZnO (002) crystal plane and its effect on electrical properties. <i>Journal of Materials Science: Materials in Electronics</i> , 2022, 33, 19107-19118.	1.1	1

#	ARTICLE	IF	CITATIONS
17634	First principles DFT analysis on the diffusion kinetics of hydrogen isotopes through bcc iron (Fe): Role of temperature and surface coverage. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 31481-31498.	3.8	6
17635	Discovery of Polythioplattinate(II) [Pt <sub>3</sub> S <sub>2</sub> (SO <sub>3</sub> ) <sub>6</sub> ] <sup>10+</sup> and Study of Its Solution and Catalytic Properties. <i>Inorganic Chemistry</i> , 2022, 61, 11529-11538.	1.9	3
17636	Difluoro(oxalato)borates as Short-Wavelength Optical Crystals with Bifunctional [BF <sub>2</sub> CO <sub>4</sub> ] Units. <i>Chemistry of Materials</i> , 2022, 34, 7516-7525.	3.2	15
17637	Generalized quasiharmonic approximation via space group irreducible derivatives. <i>Physical Review B</i> , 2022, 106, .	1.1	8
17638	Probing Dynamic Self-Reconstruction on Perovskite Fluorides toward Ultrafast Oxygen Evolution. <i>Advanced Science</i> , 2022, 9, .	5.6	19
17639	Stability and Rupture of an Ultrathin Ionic Wire. <i>Physical Review Letters</i> , 2022, 129, .	2.9	1
17640	A prospectus for thickness dependent electronic properties of two-dimensional metals using density functional theory calculation. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	3
17641	Rigid Body Approximation for the Anharmonic Description of Molecule Surface Vibrations. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 5618-5635.	2.3	6
17642	Defect Engineered Ternary Spinel: An Efficient Cathode for an Aqueous Rechargeable Zinc-Ion Battery of Long-Term Cyclability. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 37577-37586.	4.0	12
17643	Conformational change-modulated spin transport at the single-molecule level in carbon systems. Invited for the Third Carbon Special Topic. <i>Chinese Physics B</i> , 0, , .	0.7	0
17644	Discovery of New Plasmonic Metals via High-Throughput Machine Learning. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	2
17645	Effects of thermal, elastic, and surface properties on the stability of SiC polytypes. <i>Physical Review B</i> , 2022, 106, .	1.1	6
17646	Density functional theory computation of the binding free energies between various mutations of SARS-CoV-2 RBD and human ACE2: molecular level roots of the contagiousness. <i>Heliyon</i> , 2022, 8, e10128.	1.4	2
17647	Intramolecular force field for carboxylate Pt(II)-complexes. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	1
17648	Mechanism of improved crystallinity by defect-modification in proton-irradiated GaAsPN photovoltaics: Experimental and first-principle calculations approach. <i>Journal of Applied Physics</i> , 2022, 132, .	1.1	1
17649	Hydrolysis of Acetamide on Low-Index CeO <sub>2</sub> Surfaces: Ceria as a Deamidation and General De-esterification Catalyst. <i>ACS Catalysis</i> , 2022, 12, 10222-10234.	5.5	5
17650	Boosting Nitrogen Reduction Activity by Defect Engineering in 2D Iron Monochalcogenides FeX (X=S, Tj ETQq0 0 0 rgBT /Overlock 10 T	6.9	6
17651	Computational Prediction of Tc-99 NMR Chemical Shifts in Technetium Complexes with Radiopharmaceutical Applications. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5434-5448.	1.1	3

#	ARTICLE	IF	CITATIONS
17653	Anisotropic Thermal Expansion and Electronic Structure of LiInSe <sub>2</sub> . <i>Molecules</i> , 2022, 27, 5078.	1.7	10
17654	Ultralow Thermal Conductivity and High Thermoelectric Performance of $\hat{\Gamma}^3$ -GeSe: Effects of Dimensionality and Thickness. <i>ACS Applied Energy Materials</i> , 2022, 5, 9914-9928.	2.5	11
17655	Transition metal atoms anchored on nitrogen-doped $\hat{\Gamma}^3$ -arsenene as efficient electrocatalysts for nitrogen electroreduction reaction. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 29781-29793.	3.8	7
17656	MOF-Transformed In <sub>2</sub> O <sub>3</sub> -x@C Nanocorn Electrocatalyst for Efficient CO <sub>2</sub> Reduction to HCOOH. <i>Nano-Micro Letters</i> , 2022, 14, .	14.4	35
17657	Nickel dual-atom sites for electrochemical carbon dioxide reduction. , 2022, 1, 719-728.		83
17659	Density Functional Theory Studies of Earth-Abundant Late Transition Metal-Substituted Surface + Subsurface Iron Alloys for Selective Electrocatalytic N <sub>2</sub> Reduction. <i>ACS Applied Nano Materials</i> , 2022, 5, 11648-11655.	2.4	4
17660	High-capacity hydrogen storage in yttrium-decorated $\hat{\Gamma}^3$ -graphene: Acumen from density functional theory. <i>Journal of Applied Physics</i> , 2022, 132, .	1.1	7
17661	Asymmetric Coupled Dual-Atom Sites for Selective Photoreduction of Carbon Dioxide to Acetic Acid. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	46
17662	The stability and properties of the PtFe <sub>2</sub> Laves phases. <i>Physica B: Condensed Matter</i> , 2022, , 414268.	1.3	0
17663	DFT-1/2 and shell DFT-1/2 methods: electronic structure calculation for semiconductors at LDA complexity. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 403001.	0.7	17
17664	Photocatalytic degradation of tetracycline wastewater through heterojunction based on 2D rhombic ZrMo <sub>2</sub> O <sub>8</sub> nanosheet and nano-TiO <sub>2</sub> . <i>Journal of Nanoparticle Research</i> , 2022, 24, .	0.8	5
17665	High capacity hydrogen storage on zirconium decorated $\hat{\Gamma}^3$ -graphyne: A systematic first-principles study. <i>International Journal of Hydrogen Energy</i> , 2023, 48, 37834-37846.	3.8	6
17667	Thermal stability and selective nitridation of Cr <sub>2</sub> AlC in nitrogen at elevated temperatures. <i>Ceramics International</i> , 2022, 48, 33151-33159.	2.3	8
17668	Inhibition Mechanism of Class D $\hat{\Gamma}^2$ -Lactamases by Avibactam. <i>ACS Catalysis</i> , 2022, 12, 10338-10352.	5.5	5
17669	Effect of Re and Ta on self-trapping of helium in tungsten: a first-principles calculation. <i>Nuclear Fusion</i> , 2022, 62, 096017.	1.6	1
17670	Metal-Support Interaction and Charge Distribution in Ceria-Supported Au Particles Exposed to CO. <i>Chemistry of Materials</i> , 0, , .	3.2	6
17671	Strain dependences of electronic properties, band alignments and thermal properties of bilayer WX <sub>2</sub> (X = Se, Te). <i>Philosophical Magazine</i> , 2022, 102, 2323-2343.	0.7	3
17672	Pressure effects on structural, electronic and anisotropic elastic properties of Si doped RuGe compound with different concentrations by first-principles calculations. <i>Materials Chemistry and Physics</i> , 2022, , 126695.	2.0	3

#	ARTICLE	IF	CITATIONS
17673	Lewis Superacidic Divalent Bis( <i>m</i> -terphenyl)element Cations [(2,6-Mes <sub>2</sub> C <sub>6</sub> H <sub>3</sub> ) <sub>2</sub> E] <sup>+</sup> of Group 13 Revisited and Extended (E=B, Al, Ga, In, Tl). European Journal of Inorganic Chemistry, 2023, 26, .	1.0	2
17674	Application of two-component neural network for exchange-correlation functional interpolation. Scientific Reports, 2022, 12, .	1.6	2
17675	Identification of a Unique Pyridinic FeN <sub>4</sub> C Electro-catalyst for N <sub>2</sub> Reduction: Tailoring the Coordination and Carbon Topologies. Journal of Physical Chemistry C, 2022, 126, 14460-14469.	1.5	1
17676	Efficient band structure tuning of single-layer group IV-N semiconductors for visible-light-driven water splitting. International Journal of Hydrogen Energy, 2022, 47, 28869-28878.	3.8	1
17677	High activity and selectivity of single palladium atom for oxygen hydrogenation to H <sub>2</sub> O <sub>2</sub> . Nature Communications, 2022, 13, .	5.8	39
17678	Single-atom nanozymes catalytically surpassing naturally occurring enzymes as sustained stitching for brain trauma. Nature Communications, 2022, 13, .	5.8	72
17679	Surface functionalization effect on physical properties and quantum capacitance of Ca <sub>2</sub> C MXenes. FlatChem, 2022, 35, 100414.	2.8	9
17680	First-principles study on electronic properties and lattice configurations of Ni <sub>3</sub> S <sub>2</sub> /LiAlO <sub>2</sub> interface towards lithium ions storage. Solid State Ionics, 2022, 384, 115995.	1.3	0
17681	Bimetal defects boost efficient photocatalytic H <sub>2</sub> O <sub>2</sub> in-situ production of Cu <sub>1-x</sub> Co <sub>2-y</sub> O <sub>4-z</sub> for contaminant degradation. Journal of Cleaner Production, 2022, 369, 133245.	4.6	5
17682	Mechanism of germanium doping in sphalerite on copper ion activation: A DFT study. Chemical Physics, 2022, 562, 111667.	0.9	5
17683	High sensitivity of 2D covalent triazine framework for recognition of NO, NO <sub>2</sub> , and HO <sub>2</sub> radicals: A periodic DFT study. Chemical Physics Letters, 2022, 805, 139940.	1.2	3
17684	Electronic, optical and thermoelectric properties of WSe <sub>2</sub> /InN 2D interface: A DFT study. Solid State Communications, 2022, 354, 114889.	0.9	3
17685	Atomic scale insight into the mechanisms of chloride induced steel corrosion in concrete. Construction and Building Materials, 2022, 351, 128811.	3.2	4
17686	Stability and electronic properties of five new ternary tantalum carbonitrides. Computational Materials Science, 2022, 214, 111728.	1.4	2
17687	Ordered double transition metal MBene: the hexagonal ScTiB <sub>2</sub> monolayer as a superior anode material for lithium-ion batteries. Computational Materials Science, 2022, 214, 111736.	1.4	2
17688	Effect of 3.7Åt% F doping on the atomic structure and reducibility of CeO <sub>2</sub> (111) surface: A first principles calculation. Current Applied Physics, 2022, 43, 9-14.	1.1	3
17689	A strain-engineered self-intercalation Ta <sub>9</sub> Se <sub>12</sub> based bifunctional single atom catalyst for oxygen evolution and reduction reactions. Applied Surface Science, 2022, 602, 154378.	3.1	3
17690	Vacancy defect assisted enhanced nitrogen fixation in boron nitride nanomaterials. Applied Surface Science, 2022, 602, 154406.	3.1	3



#	ARTICLE	IF	CITATIONS
17691	Influence mechanism of inert carrier on the anti-carbon deposition effect of nickel-based oxygen carrier in chemical looping methane reforming process. <i>Applied Surface Science</i> , 2022, 602, 154373.	3.1	6
17692	Bimetallic MMoS <sub>4</sub> (M = Ni, Co, Cu) cocatalysts architected CdS nanoflowers for synergistically boosting visible-light-driven photocatalytic H <sub>2</sub> evolution from water and benzyl alcohol. <i>Journal of Alloys and Compounds</i> , 2022, 924, 166645.	2.8	6
17693	High-throughput screening of protective layers to stabilize the electrolyte-anode interface in solid-state Li-metal batteries. <i>Nano Energy</i> , 2022, 102, 107640.	8.2	12
17694	Ab initio study of the effects of Cr on helium behaviors in Fe- $\gamma$ Cr (Y = 9.38, 12.50 at%) austenitic binary alloys. <i>Materials Today Communications</i> , 2022, 33, 104207.	0.9	0
17695	Two simple hole-transporting materials for perovskite solar cells: A DFT calculation and experimental study. <i>Applied Surface Science</i> , 2022, 604, 154603.	3.1	10
17696	The extended Ising model Hamiltonian for order-disorder phase transition on the clean Si (001) surface. <i>Surface Science</i> , 2022, 726, 122163.	0.8	0
17697	In-situ N-defect and single-metal atom synergetic engineering of high-efficiency Ag-Na-C electrocatalysts for CO <sub>2</sub> reduction. <i>Applied Catalysis B: Environmental</i> , 2022, 318, 121826.	10.8	16
17698	First-principles study of Co <sub>21</sub> W <sub>18</sub> with pressure effect: The structural, mechanical, electronic properties and Debye temperature. <i>Materials Today Communications</i> , 2022, 33, 104276.	0.9	2
17699	Indirect learning and physically guided validation of interatomic potential models. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	3
17700	Pronounced inhibitory mechanism of Cr on vacancy-like defects in Fe <sub>9</sub> Cr alloy irradiation with helium ions. <i>Nuclear Materials and Energy</i> , 2022, 33, 101235.	0.6	0
17701	Synergize curvature and confinement effects for Fe-, Co-, Ni- N <sub>2</sub> sites on graphene nanobuds towards eNRR. <i>Molecular Catalysis</i> , 2022, 531, 112656.	1.0	0
17702	Piezoelectricity and optical properties of janus MXY (M = Sb, As; X = Te, Se; Y = Br, I) monolayers. , 2022, 170, 207396.		4
17703	Transition metal atom anchored by defective WSe monolayer as bifunctional single atom catalyst for ORR and OER. <i>Journal of Electroanalytical Chemistry</i> , 2022, 922, 116731.	1.9	5
17704	Superalkali NLi <sub>4</sub> cluster decorated $\hat{1}^3$ -graphyne as a promising hydrogen storage material: A density functional theory simulation. <i>FlatChem</i> , 2022, 36, 100429.	2.8	5
17705	Selective penetration mechanism of hydrogen isotope through graphene membrane. <i>Carbon</i> , 2022, 200, 430-436.	5.4	3
17706	The adsorption mode and evolution of O <sub>2</sub> molecules on the SnO <sub>2</sub> (221) crystal plane. <i>Materials Chemistry and Physics</i> , 2022, 291, 126692.	2.0	2
17707	Thermodynamic assessment of the Ga-Lu system by the combination of ab-initio calculations and the CALPHAD approach. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2022, 79, 102464.	0.7	2
17708	Two-Dimensional metal-free compounds of BC <sub>4</sub> N and BC <sub>6</sub> N <sub>2</sub> with boron atoms as highly efficient catalytic centers toward sulfur redox in lithium-sulfur batteries. <i>Applied Surface Science</i> , 2022, 606, 154773.	3.1	3

#	ARTICLE	IF	CITATIONS
17709	Activation energy of homogeneous nucleation of Zr hydride: Density functional theory calculation. Computational Materials Science, 2022, 215, 111769.	1.4	1
17710	Fast Li <sup>+</sup> migration in LiPON electrolytes doped by multi-valent Fe ions. Journal of Energy Chemistry, 2022, 75, 349-359.	7.1	5
17711	Interaction mechanism between cadmium species and Fe/Mn-doped carbon materials in municipal solid waste incineration flue gas: A density functional theory study. Applied Surface Science, 2022, 605, 154824.	3.1	3
17712	Adsorption selectivity of TiCl <sub>4</sub> precursor on Pt surfaces for atomic layer deposition via density functional theory. Applied Surface Science, 2022, 606, 154695.	3.1	1
17713	Effect of vacancy defects and co-doping on the quantum capacitance of silicene-based electrode materials. Applied Surface Science, 2022, 605, 154673.	3.1	9
17714	Electronic structure and thermoelectric properties of uniaxial strained SnSe from first-principles calculations. Physica B: Condensed Matter, 2022, 646, 414334.	1.3	5
17715	Chemical interactions of solute atoms during L12 cluster formation in Mg-Zn-Gd alloys with long-period stacking ordered structure. Journal of Alloys and Compounds, 2022, 928, 167101.	2.8	6
17716	First-principles calculations to investigate mechanical, thermodynamic and electronic properties of Al <sub>2</sub> CuMg intermetallic compound under pressure effect. Computational Condensed Matter, 2022, 33, e00738.	0.9	3
17717	Adjustable electronic properties of PtSe <sub>2</sub> /HfS <sub>2</sub> heterostructures via strain engineering. Applied Surface Science, 2022, 606, 154838.	3.1	4
17718	Effects of short-range order on phase equilibria and opto-electronic properties of ternary alloy Zn <sub>x</sub> Cd <sub>1-x</sub> Te. Solar Energy Materials and Solar Cells, 2022, 248, 111971.	3.0	1
17719	Insights into Cation-disorder effect on stability, electronic structure and defect properties of Zn-IV-nitrides: The case of ZnGeN <sub>2</sub> . Materials Today Communications, 2022, 33, 104385.	0.9	0
17720	First-principles study of the effect of N on the $\sqrt{5}$ (210) [001] grain boundary of $\hat{\Gamma}^3$ -Fe. Materials Today Communications, 2022, 33, 104496.	0.9	1
17721	V <sub>8</sub> SiB <sub>4</sub> "A new ternary phase in the V-Si-B system. Intermetallics, 2022, 151, 107691.	1.8	0
17722	Magnetocaloric effect in ScGdTbDyHo high-entropy alloy: Impact of synthesis route. Intermetallics, 2022, 151, 107678.	1.8	9
17723	Multi-methodological study of temperature trends in Mössbauer effect in Sn. Computational Materials Science, 2022, 215, 111780.	1.4	2
17724	Nanoscale surface modification to suppress capacity fade of Ni-Rich layered oxide material at high cut-off voltage. Chemical Engineering Journal, 2023, 451, 138911.	6.6	12
17725	Solvent controlled excited state intramolecular proton transfer (ESIPT) behavior and luminescent property of a novel phthalimide-based fluorophore: A TD-DFT Study. Journal of Molecular Structure, 2023, 1272, 134123.	1.8	5
17726	Efficient removal of antimony by a facile liquid-controlled strategy reinforced hematite-spinel (Fe <sub>2</sub> O <sub>3</sub> -MnFe <sub>2</sub> O <sub>4</sub> ) composite: construction, simulation and practical evaluation. Chemical Engineering Journal, 2023, 451, 138974.	6.6	5

#	ARTICLE	IF	CITATIONS
17727	Theoretical investigations of Sc <sub>2</sub> C based functionalized MXenes for applications in nanoelectromechanical systems. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2023, 145, 115491.	1.3	5
17728	Dual-doping NiMoO <sub>4</sub> with multi-channel structure enable urea-assisted energy-saving H <sub>2</sub> production at large current density in alkaline seawater. <i>Applied Catalysis B: Environmental</i> , 2023, 320, 121977.	10.8	67
17729	Atomic-structure and charge redistribution modified by intrinsic strain in $\hat{I}\pm$ -fe/TMN (TM=Ti/Zr/Hf/V/Nb/Ta) interfaces. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2023, 145, 115495.	1.3	3
17730	Predicting Dislocation Density in Martensite Ab-Initio. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17731	Ab initio simulation of graphane polymorphs. <i>AIP Conference Proceedings</i> , 2022, , .	0.3	0
17732	Pericyclic reaction benchmarks: hierarchical computations targeting CCSDT(Q)/CBS and analysis of DFT performance. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18028-18042.	1.3	14
17733	Electronic structure, magnetoresistance and spin filtering in graphene   2 monolayer-CrI <sub>3</sub>   graphene van der Waals magnetic tunnel junctions. <i>RSC Advances</i> , 2022, 12, 28533-28544.	1.7	4
17734	A DFT prediction of two-dimensional MB <sub>3</sub> (M = V, Nb, and Ta) monolayers as excellent anode materials for lithium-ion batteries. <i>RSC Advances</i> , 2022, 12, 28525-28532.	1.7	6
17735	First Principles Study on the Adsorption of Hydrogen Atoms on the Surface of Plutonium-Aluminum Systems. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17736	Li-Free ternary sulphide Cs <sub>5</sub> Ga <sub>9</sub> S <sub>16</sub> with excellent nonlinear optical performance similar to classic LiGaS <sub>2</sub> . <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 4624-4631.	3.0	4
17737	A carbon capture and storage technique using gold nanoparticles coupled with Cu-based composited thin film catalysts. <i>Sustainable Energy and Fuels</i> , 2022, 6, 4765-4778.	2.5	1
17738	A coordination environment effect of single-atom catalysts on their nitrogen reduction reaction performance. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18854-18859.	1.3	6
17739	Studies on the photoelectronic properties of a manganese (Mn)-doped lead-free double perovskite. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 25648-25655.	1.3	5
17740	Efficient direct conversion of methane into methanol on CuZn hetero-diatomic catalysts with certain coordination spheres: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 24264-24270.	1.3	3
17741	Three-dimensional porous platinum-tellurium-rhodium surface/interface achieve remarkable practical fuel cell catalysis. <i>Energy and Environmental Science</i> , 2022, 15, 3877-3890.	15.6	32
17742	Constructing Interstitial Pillar to Manipulating Interlamination Interaction Force: Towards High Sodium-Content P <sub>2</sub> /O <sub>3</sub> Intergrowth Cathodes. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17743	Dual-Atom Cu <sub>2</sub> /N-Doped Carbon Catalyst for Electroreduction of Co <sub>2</sub> to C <sub>2</sub> H <sub>4</sub> . <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17744	In-Depth Insight into the Mechanism on Photocatalytic Selective Co <sub>2</sub> Reduction Coupled with Tetracycline Oxidation Over Bio <sub>1</sub> -X Br/G-C <sub>3</sub> N <sub>4</sub> . <i>SSRN Electronic Journal</i> , 0, , .	0.4	0

#	ARTICLE	IF	CITATIONS
17745	Revealing the promotion of carbonyl groups on vacancy stabilized Pt <sub>4</sub> /nanocarbons for propane dehydrogenation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 23236-23244.	1.3	2
17746	<i>In silico</i> activation of dinitrogen with a light atom molecule. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 20953-20967.	1.3	3
17747	Structure and electronic properties of 5-7c graphyne polymorphs. <i>AIP Conference Proceedings</i> , 2022, , .	0.3	1
17748	Two-dimensional covalent triazine frameworks as superior nanocarriers for the delivery of thioquinine anti-cancer drugs: a periodic DFT study. <i>New Journal of Chemistry</i> , 2022, 46, 15635-15644.	1.4	5
17749	Emergent superconductivity in K <sub>2</sub> ReH <sub>9</sub> under pressure. <i>Journal of Materials Chemistry C</i> , 2022, 10, 14626-14632.	2.7	2
17750	Engineering Ni(OH)X/(Ni, Cu)Se <sub>2</sub> Heterostructure Nanosheet Arrays for Highly-Efficient Water Oxidation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17751	Water reduction on the facets of Fe(OH) <sub>2</sub> : an experimental and DFT study. <i>Environmental Science: Nano</i> , 2022, 9, 3407-3416.	2.2	2
17752	First principles study of hydrogen adsorption and dissociation behavior on <sup>137</sup> U (100)/Mo surface. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2022, 71, 226601.	0.2	1
17753	<i>In silico</i> capture of noble gas atoms with a light atom molecule. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 20968-20979.	1.3	2
17754	Quantum Capacitance Modulation of Mxenes by Metal Atoms Adsorption. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17755	The Chemical Environments Around Cu in Amorphous FeSiCuNb Alloy. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17756	Computational Screening of Bimetallene for the Composite Lithium Metal Anode. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
17757	Advanced DFT Atomistic Approaches for Electronic, Optical, and Structural Properties of Semiconductor Oxides. <i>Engineering Materials</i> , 2022, , 255-265.	0.3	0
17758	Stereodynamics of adiabatic and non-adiabatic energy transfer in a molecule surface encounter. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 19753-19760.	1.3	4
17759	Monitoring MgCl <sub>2</sub> hydrate formation from aqueous solutions using terahertz time-domain spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 23490-23496.	1.3	0
17760	Valence engineering at the interface of MoS <sub>2</sub> /Mo <sub>2</sub> C heterostructure for bionic nitrogen reduction. <i>Chemical Engineering Journal</i> , 2023, 452, 139515.	6.6	9
17761	Investigation of electronic and photocatalytic properties of AgTi <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> NASICON-type phosphate: Combining experimental data and DFT calculations. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 435, 114289.	2.0	9
17762	Dynamical mean-field theory for spin-dependent electron transport in spin-valve devices. <i>Physical Review B</i> , 2022, 106, .	1.1	4

#	ARTICLE	IF	CITATIONS
17763	Revealing enhanced thermoelectric performance of tin-bismuth-telluride materials. Bulletin of Materials Science, 2022, 45, .	0.8	4
17764	Discovery of Efficient Visible-Light Driven Oxygen Evolution Photocatalysts: Automated High-Throughput Computational Screening of MA <sub>2</sub> Z <sub>4</sub> . Advanced Functional Materials, 2022, 32, .	7.8	19
17765	Enhancement of Photoactivity of TiO <sub>2</sub> for Potential Applications in CO <sub>2</sub> Conversion and Water Splitting: A Hybrid Density Functional Theory Study. Journal of Physical Chemistry C, 2022, 126, 15080-15093.	1.5	3
17767	Anchor single atom in h-BN assist NO synthesis NH <sub>3</sub> : a computational view. Rare Metals, 2022, 41, 3456-3465.	3.6	23
17768	Theoretical Study on the Electrochemical Water Splitting of Two-Dimensional Metal-Organic Frameworks TM <sub>3</sub> C <sub>12</sub> O <sub>12</sub> (TM = Mn, Fe, Co, Ni). Crystals, 2022, 12, 1289.	1.0	5
17769	Unraveling the Effect of A-Site Sr-Doping in Double Perovskites Ca <sub>2-x</sub> Sr <sub>x</sub> ScRuO <sub>6</sub> (x = 0 and 1): Structural Interpretation and Mechanistic Investigations of Trifunctional Electrocatalytic Effects. ACS Applied Energy Materials, 2022, 5, 11632-11645.	2.5	7
17770	Dehydrogenation of Ammonia Borane Impacts Valence and Core Electrons: A Photoemission Spectroscopic Study. ACS Omega, 0, .	1.6	4
17771	Hydrogen bond network connectivity in the electric double layer dominates the kinetic pH effect in hydrogen electrocatalysis on Pt. Nature Catalysis, 2022, 5, 900-911.	16.1	134
17772	Molecular adsorption behavior and photoelectric properties of SnO <sub>2</sub> (221) crystal plane. Sensors and Actuators B: Chemical, 2023, 374, 132753.	4.0	4
17773	Molecular Dynamics Simulations of the Interactions between a Hydrolyzed Polyacrylamide with the Face and Edge Surfaces of Molybdenite. Polymers, 2022, 14, 3680.	2.0	0
17774	Inner Co Synergizing Outer Ru Supported on Carbon Nanotubes for Efficient pH-Universal Hydrogen Evolution Catalysis. Nano-Micro Letters, 2022, 14, .	14.4	39
17775	Ultrasmall SnS <sub>2</sub> quantum dot-based photodetectors with high responsivity and detectivity. Nanophotonics, 2022, 11, 4781-4792.	2.9	5
17776	Inspection the potential of B <sub>3</sub> O <sub>3</sub> monolayer as a carrier for flutamide anticancer delivery system. Computational and Theoretical Chemistry, 2022, 1217, 113886.	1.1	3
17777	Electronic Transport Properties and Nanodevice Designs for Monolayer $\text{MoSi}_2\text{P}_4$ . Physical Review Applied, 2022, 18, .		
17778	Synthesis of Porous Hierarchical In <sub>2</sub> O <sub>3</sub> Nanostructures with High Methane Sensing Property at Low Working Temperature. Nanomaterials, 2022, 12, 3081.	1.9	2
17779	Niobium and Tantalum Halocyanide Clusters: The Complete Family. Inorganic Chemistry, 0, .	1.9	2
17780	Dynamic Stability of Copper Single-Atom Catalysts under Working Conditions. Journal of the American Chemical Society, 2022, 144, 17140-17148.	6.6	79
17781	Relativistic correction of the Coulomb interaction in the local density approximation for energies and radii in doubly-magic nuclei. Progress of Theoretical and Experimental Physics, 2022, 2022, .	1.8	0

#	ARTICLE	IF	CITATIONS
17782	Balanced Crystallinity and Nanostructure for SnS <sub>2</sub> Nanosheets through Optimized Calcination Temperature toward Enhanced Pseudocapacitive Na <sup>+</sup> Storage. ACS Nano, 2022, 16, 14745-14753.	7.3	21
17783	Crystal structures, effective masses, electronic and optical properties of KTa <sub>5</sub> O <sub>13</sub> and KTaO <sub>3</sub> : A density functional theory study. Physica B: Condensed Matter, 2022, 647, 414372.	1.3	1
17784	Theoretical investigation on yttrium clustering in tungsten grain boundary region and strengthening effect. Journal of Applied Physics, 2022, 132, .	1.1	2
17785	Rapid 3D roll-up of gas-phase planar gold clusters and affinity and alienation for Mg and Ge: A theoretical study of MgGeAun (n=1-12) clusters. IScience, 2022, 25, 105215.	1.9	5
17786	Tuning lattice strain in biphenylene for enhanced electrocatalytic oxygen reduction reaction in proton exchange membrane fuel cells. International Journal of Hydrogen Energy, 2022, 47, 36294-36305.	3.8	4
17787	Modeling the Potential-Dependent Kinetics of CO <sub>2</sub> Electroreduction on Single-Nickel Atom Catalysts with Explicit Solvation. ACS Catalysis, 2022, 12, 11380-11390.	5.5	19
17788	Intrinsic hard magnetism and thermal stability of a ThMn <sub>12</sub> -type permanent magnet. Npj Computational Materials, 2022, 8, .	3.5	4
17789	Orbital Hall effect in crystals: Interatomic versus intra-atomic contributions. Physical Review B, 2022, 106, .	1.1	8
17790	Chemical interaction, self-ordering and corrosion inhibition properties of 2-mercaptobenzothiazole monolayers: DFT atomistic modeling on metallic copper. Corrosion Science, 2022, 209, 110658.	3.0	8
17791	One-dimensional electronic states in a natural misfit structure. Physical Review Materials, 2022, 6, .	0.9	4
17792	Tantalum Diboride: The Superhard and Metallic Boride. Crystal Growth and Design, 2022, 22, 6201-6206.	1.4	5
17793	A Review on MXene Synthesis, Stability, and Photocatalytic Applications. ACS Nano, 2022, 16, 13370-13429.	7.3	142
17794	Tuning the Coordination Microenvironment to Boost the Electrocatalytic HER Activity of M <sub>3</sub> (C <sub>6</sub> O <sub>3</sub> S <sub>3</sub> ) <sub>2</sub> . Journal of Physical Chemistry C, 2022, 126, 16606-16614.	1.5	1
17795	Density functional theory: The evaluation of structural, electronic, optical, and mechanical properties of WO <sub>3</sub> . Computational Condensed Matter, 2022, 33, e00752.	0.9	4
17796	How Computations Can Assist the Rational Design of Drugs for Photodynamic Therapy: Photosensitizing Activity Assessment of a Ru(II)-BODIPY Assembly. Molecules, 2022, 27, 5635.	1.7	4
17797	Subsystem density-functional theory: A reliable tool for spin-density based properties. Journal of Chemical Physics, 2022, 157, .	1.2	6
17798	Role of Si in the Oxide Nucleation and Growth Mechanisms of 60Si2Mn Spring Steel: Experimental and First-Principles Study. Oxidation of Metals, 0, , .	1.0	2
17799	Integrated As <sub>2</sub> O <sub>3</sub> /SeO <sub>2</sub> capture mechanism by Mn-Fe binary oxide in coal-fired flue gas. Journal of Cleaner Production, 2022, 377, 134547.	4.6	4



#	ARTICLE	IF	CITATIONS
17800	D-band center optimization of iron carbide via Cr substitution for enhanced alkaline hydrogen evolution. <i>Materials Today Energy</i> , 2022, 29, 101133.	2.5	9
17801	How good are recent density functionals for ground and excited states of one-electron systems?. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	6
17802	A green and sustainable strategy toward lithium resources recycling from spent batteries. <i>Science Advances</i> , 2022, 8, .	4.7	26
17803	Selective synthesis of olefins via CO <sub>2</sub> hydrogenation over transition-metal-doped iron-based catalysts. <i>Applied Catalysis B: Environmental</i> , 2023, 321, 122050.	10.8	38
17804	Metal-organic coordination polymers-derived ultra-small MoC nanodot/N-doped carbon combined with CdS: A hollow Z-type catalyst for stable and efficient H <sub>2</sub> production/CO <sub>2</sub> reduction. <i>Applied Surface Science</i> , 2023, 608, 155176.	3.1	5
17805	Boosting the solar conversion efficiency of MoSe <sub>2</sub> /PtX <sub>2</sub> (X=O, S) vdW heterostructure by strain and electric field engineering. <i>Physica Scripta</i> , 2022, 97, 115801.	1.2	5
17806	Systematic Mapping of Electrocatalytic Descriptors for Hybrid and Non-Hybrid Molybdenum Dichalcogenides with Graphene Support for Cathodic Hydrogen Generation. <i>Journal of Physical Chemistry C</i> , 2022, 126, 17011-17024.	1.5	6
17807	Sensitivity of coupled cluster electronic properties on the reference determinant: Can Kohn-Sham orbitals be more beneficial than Hartree-Fock orbitals?. <i>Journal of Computational Chemistry</i> , 0, , .	1.5	4
17808	O- or/and S-functionalized Cr <sub>2</sub> C as electrode material for metal-ion (Li, Na, K, and Mg) batteries: A first principles study. <i>Computational and Theoretical Chemistry</i> , 2022, 1217, 113892.	1.1	4
17809	Crystalline aluminum silicides with electride state and superconductivity under high pressure. <i>Materials Today Physics</i> , 2022, 28, 100853.	2.9	4
17810	Constructing interstitial pillar to manipulating interlamination interaction force: Towards high sodium-content P <sub>2</sub> /O <sub>3</sub> intergrowth cathodes. <i>Electrochimica Acta</i> , 2022, 433, 141253.	2.6	3
17811	Theoretical Screening of Lead-Free Hybrid Organic-Inorganic Halide Double Perovskites for Solar Cells. <i>Journal of Materials Chemistry C</i> , 0, , .	2.7	1
17812	SnSe <sub>2</sub> monolayer with square lattice structure: a promising p-type thermoelectric material with an indirect bandgap and low lattice thermal conductivity. <i>Journal of Materials Chemistry C</i> , 2022, 10, 16116-16125.	2.7	11
17813	Incorporated O-CoP nanosheets with an O-P interpenetrated interface as electrocatalytic cathodes for rechargeable Li-CO <sub>2</sub> batteries. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
17814	ThC <sub>2</sub> @C <sub>82</sub> versus Th@C <sub>84</sub> : unexpected formation of triangular thorium carbide cluster inside fullerenes. <i>Chemical Science</i> , 2022, 13, 12980-12986.	3.7	6
17815	Thermodynamic properties of high energy amine borane adducts. <i>Annual Reports in Computational Chemistry</i> , 2022, , 169-201.	0.9	0
17816	Structure Effect on the Response of ZnGa <sub>2</sub> O <sub>4</sub> Gas Sensor for Nitric Oxide Applications. <i>Nanomaterials</i> , 2022, 12, 3759.	1.9	4
17817	Reciprocal space study of Heisenberg exchange interactions in ferromagnetic metals. <i>Physical Review B</i> , 2022, 106, .	1.1	1

#	ARTICLE	IF	CITATIONS
17818	Stabilizing $Ti_{3}C_{2}T_x$ in a Water Medium under Multiple Environmental Conditions by Scavenging Oxidative Free Radicals. <i>Chemistry of Materials</i> , 2022, 34, 9517-9526.	3.2	7
17820	Investigation of the physical properties and Mulliken charge distribution of the cube perovskite $BiGaO_3$ is calculated by GGA-PBE. <i>Digest Journal of Nanomaterials and Biostructures</i> , 2022, 17, 1181-1190.	0.3	1
17821	Constructing Air-Stable and Reconstruction-Inhibited Transition Metal Sulfide Catalysts via Tailoring Electron-Deficient Distribution for Water Oxidation. <i>ACS Catalysis</i> , 2022, 12, 13234-13246.	5.5	37
17822	Fabricating PdCe/OMS-2 catalysts with boosted low-temperature activity for toluene deep degradation. <i>Journal of Rare Earths</i> , 2023, 41, 839-849.	2.5	6
17823	Attenuating metal-substrate conjugation in atomically dispersed nickel catalysts for electroreduction of $CO_2$ to $CO$ . <i>Nature Communications</i> , 2022, 13, .	5.8	71
17824	$Ni_3B$ as p-Block Element-Modulated Cocatalyst for Efficient Photocatalytic $CO_2$ Reduction. <i>Inorganic Chemistry</i> , 2022, 61, 17268-17277.	1.9	4
17825	Finding a Deep-UV Borate $BaZnB_4O_8$ with Edge-sharing $[BO_4]$ Tetrahedra and Strong Optical Anisotropy. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	6
17826	Effect of structural iron on nanoscroll formation via exfoliation of a high iron-content kaolin. <i>Journal of Materials Research</i> , 0, , .	1.2	0
17827	Machine learning interatomic potentials for aluminium: application to solidification phenomena. <i>Journal of Physics Condensed Matter</i> , 2023, 35, 035402.	0.7	3
17828	Computational Design of a Strain-Induced 2D/2D g- $C_3N_4$ /ZnO S-Scheme Heterostructured Photocatalyst for Water Splitting. <i>ACS Applied Energy Materials</i> , 2022, 5, 13997-14007.	2.5	16
17829	Many recent density functionals are numerically ill-behaved. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	14
17830	Enhanced Oxide Reduction by Hydrogen at Cuprous Oxide-Copper Interfaces near Ascending Step Edges. <i>Journal of Physical Chemistry C</i> , 2022, 126, 18645-18651.	1.5	1
17831	Correlation between the activity of Fe@ (N, S, and P) doped graphene catalysts and the coordination environment: A density functional theory study. <i>International Journal of Hydrogen Energy</i> , 2023, 48, 171-179.	3.8	5
17832	V (Nb) Single Atoms Anchored by the Edge of a Graphene Armchair Nanoribbon for Efficient Electrocatalytic Nitrogen Reduction: A Theoretical Study. <i>Inorganic Chemistry</i> , 2022, 61, 17864-17872.	1.9	9
17833	Reliable Isotropic Electron-Paramagnetic-Resonance Hyperfine Coupling Constants from the Frozen-Density Embedding Quasi-Diabatic Approach. <i>Journal of Physical Chemistry A</i> , 2022, 126, 8358-8368.	1.1	1
17834	Aromatic Polyphenol $\pi$ - $\pi$ Interactions with Superoxide Radicals Contribute to Radical Scavenging and Can Make Polyphenols Mimic Superoxide Dismutase Activity. <i>Current Issues in Molecular Biology</i> , 2022, 44, 5209-5220.	1.0	10
17835	Theoretical and Comparative Analysis of Graphdiyne and Confined Flexible Nitrogen-Doped Graphdiyne-Supported Single-Atom Catalysts for Electrochemical Nitrogen Reduction. <i>Journal of Physical Chemistry C</i> , 2022, 126, 18282-18291.	1.5	4
17836	Two-Dimensional Electron Gas in $MoSi_2N_4/VSi_2N_4$ Heterojunction by First Principles Calculation. <i>Chinese Physics Letters</i> , 2022, 39, 127301.	1.3	1

#	ARTICLE	IF	CITATIONS
17837	Point Defects Stability, Hydrogen Diffusion, Electronic Structure, and Mechanical Properties of Defected Equiatomic $\text{I}^3(\text{U,Zr})$ from First-Principles. <i>Materials</i> , 2022, 15, 7452.	1.3	2
17838	Nucleation and Growth of Dendritic Islands during Platinum Oxidation-Reduction Cycling. <i>Journal of the Electrochemical Society</i> , 2022, 169, 112506.	1.3	3
17839	Strong modulation of carrier effective mass in $\text{WTe}_2$ via coherent lattice manipulation. <i>Npj 2D Materials and Applications</i> , 2022, 6, .	3.9	2
17840	Black phosphorus nanodot incorporated tin oxide hollow-spherical heterojunction for enhanced properties of room-temperature gas sensors. <i>Ceramics International</i> , 2023, 49, 8248-8258.	2.3	6
17841	Unraveling Electroreductive Mechanisms of Biomass-Derived Aldehydes via Tailoring Interfacial Environments. <i>ACS Catalysis</i> , 2022, 12, 14072-14085.	5.5	15
17842	A Mechanistic Study of the Cobalt(I)-Catalyzed Amination of Aryl Halides: Effects of Metal and Ligand. <i>Inorganic Chemistry</i> , 2022, 61, 18019-18032.	1.9	4
17843	Tunable activity of electrocatalytic CO dimerization on strained Cu surfaces: Insights from ab initio molecular dynamics simulations. <i>Chinese Journal of Catalysis</i> , 2022, 43, 2898-2905.	6.9	4
17844	The Accuracy of Semi-Empirical Quantum Chemistry Methods on Soot Formation Simulation. <i>International Journal of Molecular Sciences</i> , 2022, 23, 13371.	1.8	1
17845	Synergy of yolk-shelled structure and tunable oxygen defect over $\text{CdS/CdCO}_3\text{-CoS}_2$ : Wide band-gap semiconductors assist in efficient visible-light-driven $\text{H}_2$ production and $\text{CO}_2$ reduction. <i>Chemical Engineering Journal</i> , 2023, 454, 140113.	6.6	8
17846	$\text{Sn}_3\text{B}_{10}\text{O}_{17}\text{Cl}_2$ Achieving Birefringence Enhancement by Stereochemical Activity Lone Pair. <i>Inorganic Chemistry</i> , 2022, 61, 18238-18244.	1.9	7
17847	First-principles study of non-radiative carrier capture by defects at amorphous- $\text{SiO}_2/\text{Si}(100)$ interface. <i>Chinese Physics B</i> , 0, , .	0.7	0
17848	Theoretical study of CO adsorption and activation on $\text{h-Fe/C}_3$ for Fischer-Tropsch synthesis. <i>Molecular Catalysis</i> , 2022, 532, 112732.	1.0	1
17849	Theoretical study on site preference of Mn in B-containing $\text{Ni}_3\text{Al}$ alloys and elastic properties. <i>Materials Today Communications</i> , 2022, 33, 104816.	0.9	0
17850	Regulating on photocatalytic overall water splitting performance of gallium thiophosphate based on transition metal doping: A first-principles study. <i>Molecular Catalysis</i> , 2022, 533, 112765.	1.0	0
17851	Comparative study of the structural, electronic, optical and thermoelectric properties of $\text{LaNi}_2$ ( $Z=$ )	0.9	0
17852	Effects of electric fields along different directions on the sensitivity and decomposition of TKX-50. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 171, 111035.	1.9	1
17853	First principles calculations of the inorganic halide perovskite $\text{RbSnBr}_3$ : Optical and thermoelectric properties of its three phases. <i>Computational Condensed Matter</i> , 2022, 33, e00761.	0.9	1
17854	The chemical environments around Cu in amorphous $\text{FeSiBCuNb}$ alloy. <i>Journal of Non-Crystalline Solids</i> , 2022, 598, 121961.	1.5	1

#	ARTICLE	IF	CITATIONS
17855	Computational screening of bimetallic for the composite lithium metal anode. Applied Surface Science, 2023, 609, 155403.	3.1	1
17856	Local coordination atom and metal types of single-atom catalysts to regulate catalytic performance of C <sub>2</sub> H <sub>2</sub> selective hydrogenation. Chemical Engineering Science, 2023, 265, 118242.	1.9	5
17857	Spin regulation for efficient electrocatalytic N <sub>2</sub> reduction over diatomic Fe-Mo catalyst. Journal of Colloid and Interface Science, 2023, 630, 215-223.	5.0	17
17858	Influence of intercalated Gd atoms on graphene-4H-SiC(0001) properties. Applied Surface Science, 2023, 609, 155365.	3.1	1
17859	Effects of strain and Al doping on monolayer h-BN: First-principles calculations. Physica E: Low-Dimensional Systems and Nanostructures, 2023, 146, 115546.	1.3	4
17860	Insight into the effect of surface coverage of carbon support on selective CO <sub>2</sub> electroreduction to C <sub>2</sub> H <sub>4</sub> over copper-based catalyst. Applied Surface Science, 2023, 609, 155394.	3.1	6
17861	Metallic bismuth nanoclusters confined in micropores for efficient electrocatalytic reduction of carbon dioxide with long-term stability. Journal of Colloid and Interface Science, 2023, 630, 81-90.	5.0	8
17862	Hydrogen trapping, desorption and clustering in heterophase interfaces of W-ZrC alloy. Acta Materialia, 2023, 242, 118469.	3.8	7
17863	Efficient polyselenides anchoring and conversion by functionalized Mo <sub>2</sub> B <sub>2</sub> MBene for advanced Li-Se battery. Journal of Alloys and Compounds, 2023, 932, 167722.	2.8	6
17864	Experimental study of covalent Cr <sub>3</sub> C <sub>2</sub> with high ionicity: Sound velocities, elasticity, and mechanical properties under high pressure. Scripta Materialia, 2023, 224, 115146.	2.6	2
17865	Deep eutectic solvent induced ultrathin Co <sub>4</sub> N/N-doped carbon nanosheets self-supporting electrode for boosting hydrogen evolution integrated with biomass electrooxidation. Applied Surface Science, 2023, 608, 155283.	3.1	8
17866	Stable nanoparticles dispersion induced an unprecedented high strength in a bulk W-TiC alloy. Scripta Materialia, 2023, 224, 115136.	2.6	2
17867	Synergistic effect of copper and vanadium species on Hg <sup>0</sup> removal of Cu-SCR catalyst: A DFT and experimental study. Fuel, 2023, 333, 126527.	3.4	3
17868	Exploration of the physical properties of the newly synthesized kagome superconductor La <sub>1-x</sub> Ga <sub>2x</sub> using different exchange-correlation functionals. Physical Chemistry Chemical Physics, 2022, 24, 29640-29654.	1.3	5
17869	Decoration of defective graphene with MoS <sub>2</sub> enabling enhanced anchoring and catalytic conversion of polysulfides for lithium-sulfur batteries: A first-principles study. Physical Chemistry Chemical Physics, 0, , .	1.3	2
17870	Ammonia Sensing Properties of SnS <sub>2</sub> /SnO <sub>2</sub> , Nanocomposite-Based Gas Sensor by SnS <sub>2</sub> , Annealing. IEEE Sensors Journal, 2022, 22, 23456-23463.	2.4	1
17871	Reaction mechanism for the Zn-MnO <sub>2</sub> cathode in aqueous Zn ion batteries revisited: elucidating the irreversible transformation of Zn-MnO <sub>2</sub> into Zn <sub>2</sub> (OH) <sub>2</sub> SO <sub>4</sub> . Journal of Materials Chemistry A, 2022, 10, 25620-25632.	5.2	10
17872	Effect of oxygen coordination on the electrocatalytic nitrogen fixation of a vanadium single-atom catalyst embedded in graphene. New Journal of Chemistry, 2022, 46, 22936-22943.	1.4	5

#	ARTICLE	IF	CITATIONS
17873	Carbon-based frustrated Lewis pairs mediate hydrogenation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 28895-28902.	1.3	5
17874	Trends in opto-electronic properties of $Mg_xZn_{1-x}Sn_2$ using first principles methods. <i>Materials Chemistry and Physics</i> , 2023, 294, 126995.	2.0	1
17875	Construction mechanisms of a new generation of high-energy all- and high-nitrogen materials under extreme conditions: Ab initio molecular dynamics simulations from pentazole compounds. <i>Chemical Engineering Journal</i> , 2023, 454, 140359.	6.6	2
17876	Engineering $Ni(OH)_x/(Ni, Cu)Se_2$ heterostructure nanosheet arrays for highly-efficient water oxidation. <i>Journal of Alloys and Compounds</i> , 2023, 933, 167730.	2.8	2
17877	Understanding the catalytic ozonation process on ceria nanorods: Efficacy, Frenkel-type oxygen vacancy as a key descriptor and mechanism insight. <i>Applied Catalysis B: Environmental</i> , 2023, 323, 122152.	10.8	14
17878	Quantitative decorating Ni-sites for water-oxidation with the synergy of electronegative sites and high-density spin state. <i>Applied Catalysis B: Environmental</i> , 2023, 323, 122167.	10.8	9
17879	Predicting dislocation density in martensite ab-initio. <i>Acta Materialia</i> , 2023, 243, 118500.	3.8	10
17880	Mass-zero constrained dynamics for simulations based on orbital-free density functional theory. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	1
17881	Synergistic effect of diatomic $Mo\delta\delta B$ site confined in graphene-like $C_2N$ enables electrocatalytic nitrogen reduction via novel mechanism. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	6
17882	Adsorption Properties of $NF_3$ and $N_2O$ on Al- and Ga-Doped Graphene Surface: A Density Functional Theory Study. <i>Adsorption Science and Technology</i> , 2022, 2022, .	1.5	0
17883	The first-principles study of structural and electronic properties of two-dimensional SiC/GeC lateral polar heterostructures. <i>Journal of Applied Physics</i> , 2022, 132, 184301.	1.1	0
17884	Machine learning prediction of the mechanical properties of refractory multicomponent alloys based on a dataset of phase and first principles simulation. , 0, 1, .		0
17885	Second-order topological insulator in van der Waals heterostructures of $CoBr_2$ . <i>Physical Review B</i> , 2022, 106, .		
17886	Macro superlubricity of two-dimensional disulphide/amorphous carbon heterogeneous via tribochemistry. <i>Materials Today Nano</i> , 2023, 21, 100286.	2.3	7
17887	Molecular and periodic DFT calculations of the corrosion protection of Fe(1 1 0) by individual components of <i>Aerva lanata</i> flower as a green corrosion inhibitor. <i>Journal of Saudi Chemical Society</i> , 2022, 26, 101566.	2.4	6
17888	Decoherence of a spin-valley qubit in a $MoS_2$ , quantum dot. <i>Journal of Physics Communications</i> , 0, , .	0.5	0
17889	Electronic and optical properties of phosphorus doped InI crystal: Ab Initio Study. , 2022, , .		0
17890	Blue Light-Excitable Broadband Yellow Emission in a Zero-Dimensional Hybrid Bismuth Halide with Type-II Band Alignment. <i>Inorganic Chemistry</i> , 2022, 61, 19483-19491.	1.9	7

#	ARTICLE	IF	CITATIONS
17891	Evaluation of phase relationship in W-Fe-C ternary system through symmetry principles and first-principles calculation. <i>Materials and Design</i> , 2022, 224, 111376.	3.3	2
17892	A Tour of Soft Atomic Motions: Chemical Pressure Quadrupoles Across Transition Metalâ€“Main Group 1:2 Structure Types. <i>Chemistry of Materials</i> , 2022, 34, 10011-10024.	3.2	8
17893	Theory-driven designed TiO <sub>2</sub> @MoO <sub>2</sub> heterojunction: Balanced crystallinity and nanostructure toward desirable kinetics and high-rate sodium-ion storage. <i>Nano Research</i> , 2023, 16, 4941-4949.	5.8	4
17894	Machine learning approach for screening alloy surfaces for stability in catalytic reaction conditions. <i>JPhys Energy</i> , 2023, 5, 015002.	2.3	2
17895	Electronic effects on the radiation damage in high-entropy alloys. <i>Acta Materialia</i> , 2023, 244, 118511.	3.8	7
17896	Interaction between peptides and an MoS <sub>2</sub> monolayer containing a nanopore: First-principles calculations. <i>Chinese Journal of Physics</i> , 2023, 84, 486-499.	2.0	0
17897	Stabilization of Dinuclear Rhodium and Iridium Clusters on Layered Titanate and Niobate Supports. <i>Inorganic Chemistry</i> , 2023, 62, 1113-1121.	1.9	0
17899	Self-standing hollow porous Co/a-WO <sub>x</sub> nanowire with maximum Mott-Schottky effect for boosting alkaline hydrogen evolution reaction. <i>Nano Research</i> , 2023, 16, 4603-4611.	5.8	7
17900	First Principles Study on the Adsorption of Hydrogen Atoms on the Surface of Plutonium-Aluminum Systems. <i>Crystals</i> , 2022, 12, 1592.	1.0	0
17901	Structural and electronic properties of Na-B-H compounds at high pressure. <i>Physical Review B</i> , 2022, 106, .	1.1	2
17902	TiO <sub>2</sub> /Cu <sub>2</sub> O heterostructure enabling selective and uniform lithium deposition towards stable lithium metal anodes. <i>Nano Research</i> , 2023, 16, 4917-4925.	5.8	6
17903	Bismuth nanosheets with rich grain boundaries for efficient electroreduction of CO <sub>2</sub> to formate under high pressures. <i>Chinese Journal of Catalysis</i> , 2022, 43, 3161-3169.	6.9	10
17904	Sensing behavior of porous B <sub>6</sub> N <sub>6</sub> boron nitride covalent organic framework toward cationic drugs: A DFT study. <i>Inorganic Chemistry Communication</i> , 2022, 146, 110205.	1.8	8
17905	Influence of carbon on hydrogen retention in molybdenum for nuclear material application: A first-principles investigation. <i>Nuclear Materials and Energy</i> , 2022, 33, 101311.	0.6	0
17906	Revealing the Origin of Heterogeneous Phase Transition and Deformation Behavior in Au-Ag-Cu-Based Multicomponent Alloys. <i>Metals</i> , 2022, 12, 1966.	1.0	1
17907	Preventing Sudden Death of High-Energy Lithium-Ion Batteries at Elevated Temperature Through Interfacial Ion-Flux Rectification. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	4
17908	Cellulose hydrogen bond detection using terahertz time-domain spectroscopy to indicate deterioration of oilâ€“paper insulation. <i>Cellulose</i> , 2023, 30, 727-740.	2.4	3
17909	Aln <sub>3</sub> Si <sub>4</sub> P <sub>9</sub> (A = Ca, Sr): quaternary phosphides with double-helix structures exhibiting high laser-induced damage thresholds. <i>Inorganic Chemistry Frontiers</i> , 2023, 10, 1112-1118.	3.0	3



#	ARTICLE	IF	CITATIONS
17910	Hydrogenated V <sub>2</sub> O <sub>5</sub> with fast Zn-ion migration kinetics as high-performance cathode material for aqueous zinc-ion batteries. <i>Electrochimica Acta</i> , 2023, 439, 141717.	2.6	11
17911	Magnetic-field-regulated Ni-Fe-Mo ternary alloy electrocatalysts with enduring spin polarization enhanced oxygen evolution reaction. <i>Chemical Engineering Journal</i> , 2023, 455, 140821.	6.6	16
17912	Two-dimensional magnetic Janus monolayers and their van der Waals heterostructures: a review on recent progress. <i>Materials Horizons</i> , 2023, 10, 788-807.	6.4	7
17913	ToF-SIMS, XPS and DFT study of the adsorption of 2-mercaptobenzothiazole on copper in neutral aqueous solution and corrosion protection in chloride solution. <i>Corrosion Science</i> , 2023, 210, 110854.	3.0	14
17914	Catalytic active centers beyond transition metals: atomically dispersed alkaline-earth metals for the electroreduction of nitrate to ammonia. <i>Journal of Materials Chemistry A</i> , 2023, 11, 1817-1828.	5.2	51
17915	Exploring a novel class of Janus MXenes by first principles calculations: structural, electronic and magnetic properties of Sc <sub>2</sub> CXT, X = O, F, OH; T = C, S, N. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 1881-1888.	1.3	5
17916	Catalysis of dinitrogen activation and reduction by a single Fe <sub>13</sub> cluster and its doped systems. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 1196-1204.	1.3	1
17917	First-principles calculations to investigate magnetic, electronic, mechanical and dynamical properties of the bimetallic M-Pt (M: Mn Co and Ni) alloys. <i>Journal of Magnetism and Magnetic Materials</i> , 2023, 565, 170298.	1.0	2
17918	Biaxial strain induced tunable electronic properties study of ZnO nanoparticles via first-principles density functional theory. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2023, 288, 116186.	1.7	5
17919	New strategies to improve two-electron oxygen reduction reaction selectivity of polypyrrole-based catalysts. <i>Journal of Materials Chemistry A</i> , 2023, 11, 2168-2177.	5.2	6
17920	Magneto-structural correlations of dinickel(II) complexes with phenoxido/azido coligands: A theoretical investigation. <i>Chemical Physics Letters</i> , 2023, 811, 140241.	1.2	2
17921	Coupled effect of Cr and Al on interactions between a prismatic interstitial dislocation loop and an edge dislocation line in Fe-Cr-Al alloy. <i>Acta Materialia</i> , 2023, 245, 118651.	3.8	7
17922	Density functional theory study of formation and diffusion of hydrogen, deuterium, and tritium in Pd-V intermetallic compounds. <i>Computational Materials Science</i> , 2023, 218, 111976.	1.4	2
17923	First-principles study on interfacial performance of Cl, Br and O-doped Li <sub>3</sub> PS <sub>4</sub> against lithium for all-solid-state batteries. <i>Journal of Solid State Chemistry</i> , 2023, 318, 123771.	1.4	1
17924	Modeling assisted synthesis of Zr-doped Li <sub>3-x</sub> In <sub>1-x</sub> Zr <sub>x</sub> Cl <sub>6</sub> with ultrahigh ionic conductivity for lithium-ion batteries. <i>Journal of Power Sources</i> , 2023, 556, 232465.	4.0	4
17925	Selectivity of Mo N C sites for electrocatalytic N <sub>2</sub> reduction: A function of the single atom position on the surface and local carbon topologies. <i>Applied Surface Science</i> , 2023, 612, 155908.	3.1	3
17926	Electrospray ion beam deposition of small peptides on solid surfaces: A molecular level description of the glutathione/copper interface. <i>Applied Surface Science</i> , 2023, 612, 155895.	3.1	2
17927	A comparative analysis of different van der Waals treatments for molecular adsorption on the basal plane of 2H-MoS <sub>2</sub> . <i>Surface Science</i> , 2023, 729, 122226.	0.8	5

#	ARTICLE	IF	CITATIONS
17928	A dual defect co-modified S-scheme heterojunction for boosting photocatalytic CO <sub>2</sub> reduction coupled with tetracycline oxidation. <i>Applied Catalysis B: Environmental</i> , 2023, 324, 122232.	10.8	25
17929	The low symmetry 1Tâ€²-MoS <sub>2</sub> enabling the lithium directional diffusion through ferroelastic domain switching. <i>Applied Surface Science</i> , 2023, 612, 155761.	3.1	2
17930	Site-selective photocoupled electrocatalytic CO <sub>2</sub> reduction over efficient Al-oxo chain based-porphyrin framework. <i>Applied Catalysis B: Environmental</i> , 2023, 325, 122315.	10.8	5
17931	Structural and mechanical properties of monazite type LnPO <sub>4</sub> (Ln = La, Ce, Pr and Nd). <i>MATEC Web of Conferences</i> , 2022, 370, 09008.	0.1	1
17932	Density Functional Theory Investigation on the Molecular Structure and Vibrational Spectra of Triclosan. <i>Spectroscopy (Santa Monica)</i> , 2022, , 23-32.	0.3	0
17933	Adsorption behaviors of the Sc <sub>2</sub> C(OH) <sub>2</sub> monolayer for small gas molecules: A first-principles study. <i>Computational and Theoretical Chemistry</i> , 2023, 1221, 113936.	1.1	0
17934	Comment on "Multiple locations of boron atoms in the exohedral and endohedral C <sub>60</sub> fullerene". <i>Physical Review A</i> , 2022, 106, .	1.0	3
17935	Simultaneously Constructing Active Sites and Regulating Mn-O Strength of Ru-Substituted Perovskite for Efficient Oxidation and Hydrolysis Oxidation of Chlorobenzene. <i>Advanced Science</i> , 2023, 10, .	5.6	13
17936	Atomic Magnetic Heating Effect Enhanced Hydrogen Evolution Reaction of Gd@MoS <sub>2</sub> Single-Atom Catalysts. <i>Small</i> , 2023, 19, .	5.2	12
17937	Rational Design of Fe/Co-based Diatomic Catalysts for Li-S Batteries by First-principles Calculations. <i>Chinese Physics B</i> , 0, , .	0.7	0
17938	Protocols for Understanding the Redox Behavior of Copper-Containing Systems. <i>ACS Omega</i> , 2022, 7, 45057-45066.	1.6	2
17939	Experimental and Theoretical Correlation of Modulated Architectures of Î²-Ag <sub>2</sub> MoO <sub>4</sub> Microcrystals: Effect of Different Synthesis Routes on the Morphology, Optical, Colorimetric, and Photocatalytic Properties. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2023, 33, 424-450.	1.9	9
17940	Density functional theory study of the enhancement of quantum capacitance of graphene by phosphorous doping. <i>International Journal of Quantum Chemistry</i> , 2023, 123, .	1.0	2
17941	Tailoring Rational Crystal Orientation and Tunable Sulfur Vacancy on Metal-Sulfides toward Advanced Ultrafast Ion-Storage Capability. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	16
17942	Propelling polysulfide redox by Fe <sub>3</sub> C-FeN heterostructure@nitrogen-doped carbon framework towards high-efficiency Li-S batteries. <i>Journal of Energy Chemistry</i> , 2023, 78, 105-114.	7.1	31
17943	Topological corner states in graphene by bulk and edge engineering. <i>Physical Review B</i> , 2022, 106, .	1.1	4
17944	Dual Pt-Ni atoms dispersed on N-doped carbon nanostructure with novel (NiPt)-N <sub>4</sub> C <sub>2</sub> configurations for synergistic electrocatalytic hydrogen evolution reaction. <i>Science China Materials</i> , 2023, 66, 1389-1397.	3.5	14
17945	Ambimodal Bispericyclic [6 + 4]/[4 + 6] Transition State Competes with Diradical Pathways in the Cycloheptatriene Dimerization: Dynamics and Experimental Characterization of Thermal Dimers. <i>Journal of the American Chemical Society</i> , 2022, 144, 22251-22261.	6.6	8

#	ARTICLE	IF	CITATIONS
17946	Massive Assessment of the Binding Energies of Atmospheric Molecular Clusters. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 7373-7383.	2.3	11
17947	Conversion of CO <sub>2</sub> to Methanol and Ethanol on Pt/CeO <sub>x</sub> /TiO <sub>2</sub> (110): Enabling Role of Water in C–C Bond Formation. <i>ACS Catalysis</i> , 2022, 12, 15097-15109.	5.5	8
17948	Performance Limit of Gate-All-Around $\langle \text{Si} \rangle$ Nanowire Field-Effect Transistors: An Ab Initio Quantum Transport Simulation. <i>Physical Review Applied</i> , 2022, 18, .	1.5	9
17949	Rational Design of Dynamic Bimetallic NiCoSe <sub>2</sub> /2D Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> MXene Hybrids for a High-Performance Flexible Supercapacitor and Hydrogen Evolution Reaction. <i>Energy &amp; Fuels</i> , 2022, 36, 15066-15079.	2.5	8
17950	Testing of Exchange-Correlation Functionals of DFT for a Reliable Description of the Electron Density Distribution in Organic Molecules. <i>International Journal of Molecular Sciences</i> , 2022, 23, 14719.	1.8	7
17951	On the Nature of Three-Atom Metal Cluster Catalysis for N <sub>2</sub> Reduction to Ammonia. <i>ACS Catalysis</i> , 2022, 12, 14964-14975.	5.5	21
17952	Performance of Screened-Exchange Functionals for Band Gaps and Lattice Constants of Crystals. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 311-323.	2.3	1
17953	An ab-initio perspective on the electronic and optical characteristics of MoSe <sub>2</sub> nanosheet: Role of external electric field. <i>Physica B: Condensed Matter</i> , 2023, 651, 414574.	1.3	0
17954	Origin of the nucleation preference of coherent and semicoherent nanoprecipitates in Al–Cu alloys based on atomistically informed classical nucleation theory. <i>Journal of Alloys and Compounds</i> , 2022, , 168559.	2.8	0
17955	Effects of B and P Doping on Electronic Structure and Lithium Diffusion Properties of Si(100) Surface. <i>Advanced Theory and Simulations</i> , 0, , 2200724.	1.3	0
17956	First Principles Study of Double Boron Atoms Supported on Graphitic Carbon Nitride (g-C <sub>3</sub> N <sub>4</sub> ) for Nitrogen Electoreduction. <i>Crystals</i> , 2022, 12, 1744.	1.0	0
17957	Electronic Tuning of Active Sites in Bifunctional Covalent Organic Frameworks for Photoassisted CO <sub>2</sub> Electrochemical Full Reaction. <i>Chemistry of Materials</i> , 2022, 34, 10752-10760.	3.2	6
17958	SBH17: Benchmark Database of Barrier Heights for Dissociative Chemisorption on Transition Metal Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 245-270.	2.3	8
17959	Density Functional Theory Analysis Identifying the Mechanism for Ignition Sensitivity of Ammonium Periodate Compared with Ammonium Perchlorate. <i>Journal of Physical Chemistry C</i> , 2022, 126, 21723-21733.	1.5	1
17960	Graphite Nanoflake-Modified Mo <sub>2</sub> C with Ameliorated Interfacial Interaction as an Electrocatalyst for Hydrogen Evolution Reaction. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 56407-56415.	4.0	3
17961	Double-layer stretching broadens the absorption range of the solar spectrum in XSi <sub>2</sub> N <sub>4</sub> . <i>Physica B: Condensed Matter</i> , 2023, 651, 414583.	1.3	1
17962	TM <sub>2</sub> B <sub>2</sub> Quadruple Active Sites Supported on a Defective C <sub>3</sub> N Monolayer as Catalyst for the Electrochemical CO <sub>2</sub> Reduction: A Theoretical Perspective. <i>ChemSusChem</i> , 2023, 16, .	3.6	3
17963	Role of vacancies and transition metals on the thermodynamic properties of MgH <sub>2</sub> : Ab-initio study. <i>International Journal of Hydrogen Energy</i> , 2023, 48, 8179-8188.	3.8	5

#	ARTICLE	IF	CITATIONS
17965	High-temperature oxidation of 60Si2Mn spring steel in dry air and wet air: Insights from an experimental and first-principles study. <i>Steel Research International</i> , 0, , .	1.0	1
17966	Rational design of nitrogen-doped carbon nanotubes by defect engineering for Zn-air batteries with high performance. <i>Carbon</i> , 2023, 204, 411-426.	5.4	11
17967	DFT study of methanethiol (CH3SH) adsorptions on the Fe(110) surface. <i>Pramana - Journal of Physics</i> , 2023, 97, .	0.6	1
17968	A detailed computational study to investigate the influence of metals (Bi, Sn, Tl) substitution on phase transition, electronic band structure and their implications on optical, elastic, anisotropic and mechanical properties of PbHfO3. <i>Optical and Quantum Electronics</i> , 2023, 55, .	1.5	4
17969	Universal Synthesized Strategy for Amorphous Pd-Based Nanosheets Boosting Ambient Ammonia Electrosynthesis. <i>Small Methods</i> , 2023, 7, .	4.6	4
17970	Defect-Induced Atomic Arrangement in CoFe Bimetallic Heterostructures with Boosted Oxygen Evolution Activity. <i>Small</i> , 2023, 19, .	5.2	11
17971	Ab Initio Study of High-Capacity Hydrogen Storage in Lithium-Shrouded Honeycomb Borophene Oxide Nanosheet. <i>Journal of Physical Chemistry C</i> , 2022, 126, 20762-20772.	1.5	2
17972	Molecular dynamics simulations of fluoroethylene carbonate and vinylene carbonate as electrolyte additives for Li-ion batteries. <i>Molecular Simulation</i> , 2023, 49, 271-283.	0.9	0
17973	Superconductivity in Th-H and Pu-H Compounds under High-Pressure Conditions: A First-Principles Study. <i>Physica Status Solidi (B): Basic Research</i> , 2023, 260, .	0.7	1
17974	Geometrical configuration modulation via iron doping and defect engineering in spinel oxides for enhanced oxygen evolution activity. <i>Chemical Engineering Journal</i> , 2023, 456, 140975.	6.6	5
17975	Computational investigation to explore the effects of metals (Mg, Ca, Sr) doping on phase transition, electronic band structure and their repercussions on optical, elastic and mechanical properties of BaThO <sub>3</sub> . <i>Physica Scripta</i> , 2023, 98, 015814.	1.2	0
17976	Structural defects in a Janus MoSSe monolayer: A density functional theory study. <i>Physical Review B</i> , 2022, 106, .	1.1	2
17977	Single atom catalysts supported on metallic C5N monolayers for oxygen reduction/evolution reactions with more active sites than loaded metal atoms. <i>Applied Surface Science</i> , 2023, 614, 156048.	3.1	4
17978	Insights into molecular cluster materials with adamantane-like core structures by considering dimer interactions. <i>Journal of Computational Chemistry</i> , 2023, 44, 843-856.	1.5	1
17979	Evolution of the Fe-Co magnetism and magnetic proximity effects in alternate Fe/Co monolayers on nonmagnetic $\text{Cu}_3\text{N}$ . <i>Physical Review B</i> , 2022, 106, .	1.1	0
17980	In-depth insight into the mechanism on photocatalytic selective CO2 reduction coupled with tetracycline oxidation over BiO1-Br/g-C3N4. <i>Applied Surface Science</i> , 2023, 614, 156017.	3.1	5
17981	<i>In-Silico</i> Partial N <sub>2</sub> to NH <sub>3</sub> Conversion with a Light Atom Molecule. <i>ChemPhysChem</i> , 2023, 24, .	1.0	1
17982	First-principles investigation of TiC(001)/TiAl(100) interface: atomic structure, stability and electronic property. <i>Journal of Materials Science</i> , 2022, 57, 21339-21351.	1.7	3

#	ARTICLE	IF	CITATIONS
17983	Grain Refinement via Changing the Shuffling Motion of the Grain Boundary by Traces of Ce and Lu in Gold Alloys. <i>Journal of Physical Chemistry C</i> , 2022, 126, 21864-21870.	1.5	0
17984	Valley-polarized quantum anomalous Hall effect in van der Waals heterostructures based on monolayer jacutingaite family materials. <i>Frontiers of Physics</i> , 2023, 18, .	2.4	5
17985	B3O3 monolayer an emerging 2D material in as a carrier for anticancer delivery system. <i>Materials Chemistry and Physics</i> , 2023, 296, 127158.	2.0	3
17986	Enabling Efficient Photocatalytic Hydrogen Evolution via In Situ Loading of Ni Single Atomic Sites on Red Phosphorus Quantum Dots. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	7
17987	Kinetically Stabilized Diarylpnictogenium Ions. <i>ChemPlusChem</i> , 2023, 88, .	1.3	1
17988	The subsystem quantum chemistry program <scp>Serenity</scp>. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2023, 13, .	6.2	11
17989	Influence of the surface states on the nonlinear Hall effect in Weyl semimetals. <i>Physical Review B</i> , 2022, 106, .	1.1	4
17990	Predicted High-Temperature Superconductivity in Rare Earth Hydride ErH <sub>2</sub> at Moderate Pressure. <i>Chinese Physics Letters</i> , 2022, 39, 127403.	1.3	4
17991	Atomic-Scale Insights into the Interfacial Polarization Effect in the InGaN/GaN Heterostructure for Solar Cells. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 55762-55769.	4.0	5
17992	Impact of magnetic and antisite disorder on the vibrational densities of states in $NiMn_2Sn$ Heusler alloys. <i>Physical Review B</i> , 2022, 106, .	1.1	7
17993	Band Gap Opening in Borophene/GaN and Borophene/ZnO Van der Waals Heterostructures Using Axial Deformation: First-Principles Study. <i>Materials</i> , 2022, 15, 8921.	1.3	2
17994	3D Artificial Array Interface Engineering Enabling Dendrite-Free Stable Zn Metal Anode. <i>Nano-Micro Letters</i> , 2023, 15, .	14.4	20
17995	Designing heterostructured FeP-CoP for oxygen evolution reaction: Interface engineering to enhance electrocatalytic performance. <i>Nano Research</i> , 2023, 16, 6601-6607.	5.8	21
17996	Aerophilic Triphase Interface Tuned by Carbon Dots Driving Durable and Flexible Rechargeable Zn-Air Batteries. <i>Nano-Micro Letters</i> , 2023, 15, .	14.4	26
17997	Role of Fluxionality and Metastable Isomers in the ORR Activity: A Case Study. <i>Journal of Physical Chemistry C</i> , 2023, 127, 217-228.	1.5	3
17998	Bicontinuous oxide heteroepitaxy with enhanced photoconductivity. <i>Nature Communications</i> , 2023, 14, .	5.8	0
17999	Fe-doped SnSe monolayer: A promising 2D material for reusable SO <sub>2</sub> gas sensor with high sensitivity. <i>Journal of Alloys and Compounds</i> , 2023, 940, 168919.	2.8	14
18000	Mechanism of <scp>NO</scp> removal in selective catalytic reduction based on <scp>Î³-Fe <sub>2</sub> O <sub>3</sub> </scp> catalyst doped with <scp>Mg</scp> element. <i>Canadian Journal of Chemical Engineering</i> , 2023, 101, 4683-4691.	0.9	0

#	ARTICLE	IF	CITATIONS
18001	The adsorption of single Au atom and nucleation on $\gamma$ -Al <sub>2</sub> O <sub>3</sub> surfaces. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	2
18002	Electrocatalysis Mechanism and Structure-Activity Relationship of Atomically Dispersed Metal-Nitrogen-Carbon Catalysts for Electrocatalytic Reactions. <i>Small Methods</i> , 2023, 7, .	4.6	7
18003	Halogen-Doped Chevrel Phase Janus Monolayers for Photocatalytic Water Splitting. <i>Nanomaterials</i> , 2023, 13, 368.	1.9	1
18004	Insight into Nitrogen Doped Waste-Tire Carbon for Radical and Nonradical Oxidation via a Probe-Based Kinetic Model. <i>ACS ES&amp;T Water</i> , 2023, 3, 129-138.	2.3	1
18005	The structure and optical properties of semiconductor nitrides MgSiN <sub>2</sub> , MgGeN <sub>2</sub> , ZnSiN <sub>2</sub> , ZnGeN <sub>2</sub> . <i>Proceedings of the National Academy of Sciences of Belarus Physics and Mathematics Series</i> , 2023, 58, 424-430.	0.1	0
18006	Blocking the reverse reactions of overall water splitting on a Rh/GaN-ZnO photocatalyst modified with Al <sub>2</sub> O <sub>3</sub> . <i>Nature Catalysis</i> , 2023, 6, 80-88.	16.1	41
18007	Enhanced toluene oxidation by photothermal synergetic catalysis on manganese oxide embedded with Pt single-atoms. <i>Journal of Colloid and Interface Science</i> , 2023, 636, 577-587.	5.0	7
18008	Oxygen vacancy-engineered titanium-based perovskite for boosting H <sub>2</sub> O activation and lower-temperature hydrolysis of organic sulfur. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2023, 120, .	3.3	12
18009	Coupled oxygen desorption and structural reconstruction accompanying reduction of copper oxide. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	2
18010	Octahedral rotations and defect-driven metallicity at the (001) surface of CaTiO <sub>3</sub> . <i>Physical Review B</i> , 2023, 107, .	1.1	3
18011	Reasonable design of ZnO decorated hollow porous carbon nanofibers for stable lithium metal anode. <i>Electrochimica Acta</i> , 2023, 443, 141904.	2.6	2
18012	Renormalizing Antiferroelectric Nanostripes in $\text{In}_2\text{Se}_3$ via Optomechanics. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 677-684.	2.1	4
18013	Synthesis and Characterization of Benzene- and Triazine-Based Azo-Bridged Porous Organic Polymers. <i>Polymers</i> , 2023, 15, 229.	2.0	7
18014	Highly efficient hydrogen storage of a Sc decorated biphenylene monolayer near ambient temperature: <i>ab initio</i> simulations. <i>Sustainable Energy and Fuels</i> , 2023, 7, 996-1010.	2.5	7
18015	A customized strategy to design intercalation-type Li-free cathodes for all-solid-state batteries. <i>National Science Review</i> , 2023, 10, .	4.6	6
18016	Structural characteristics and thermal stability of Pt-Ni nanoparticles. <i>Applied Physics A: Materials Science and Processing</i> , 2023, 129, .	1.1	0
18017	Study of the solar perovskites: XZnF <sub>3</sub> (X = Ag, Li or Na) by DFT and TDDFT methods. <i>Journal of the Korean Ceramic Society</i> , 2023, 60, 424-433.	1.1	6
18018	Structure, stability, and electronic and optical properties of TMDC-coinage metal composites: vertical atomically thin self-assembly of Au clusters. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 4177-4192.	1.3	3



#	ARTICLE	IF	CITATIONS
18019	Pressure-Induced Structural Transformations and Electronic Transitions in TeO <sub>2</sub> Glass by Raman Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 387-394.	2.1	2
18020	Atomically Dispersed Alkaline-Earth Metals as Active Centers for CO <sub>2</sub> Electroreduction to Exclusively Produce Formate. <i>Small Structures</i> , 2023, 4, .	6.9	23
18021	<i>Ab initio</i> study on structural, magnetic phase and helium migration behaviour of FCC Fe 6.25 at.% Cr binary alloys. <i>Philosophical Magazine</i> , 0, , 1-24.	0.7	0
18022	Bifunctional Photoassisted Li-O <sub>2</sub> Battery with Ultrahigh Rate-Cycling Performance Based on Siloxene Size Regulation. <i>ACS Nano</i> , 2023, 17, 1713-1722.	7.3	11
18023	Corrosion inhibition at emergent grain boundaries studied by DFT for 2-mercaptobenzothiazole on bi-crystalline copper. <i>Npj Materials Degradation</i> , 2023, 7, .	2.6	4
18024	Uncovering Structure-Activity Relationships in Pt/CeO <sub>2</sub> Catalysts for Hydrogen-Borrowing Amination. <i>ACS Catalysis</i> , 2023, 13, 1207-1220.	5.5	9
18025	Multi-high valence state metal doping in NiFe hydroxide toward superior oxygen evolution reaction activity. <i>Journal of Materials Chemistry A</i> , 2023, 11, 2985-2995.	5.2	5
18026	Relativistic Effects from Heavy Main Group p-Elements on the NMR Chemical Shifts of Light Atoms: From Pioneering Studies to Recent Advances. <i>Magnetochemistry</i> , 2023, 9, 24.	1.0	9
18027	Site-Selective Atomic Layer Deposition on Rutile TiO <sub>2</sub> : Selective Hydration as a Route to Target Point Defects. <i>Journal of Physical Chemistry C</i> , 0, , .	1.5	4
18028	Predicting and accessing metastable phases. <i>Materials Advances</i> , 2023, 4, 1101-1112.	2.6	0
18029	Simple and efficient synthesis methods for fabricating anode materials of sodium-ion batteries and their sodium-ion storage mechanism study. <i>Journal of Materials Chemistry A</i> , 2023, 11, 2920-2932.	5.2	6
18030	Is Structural Precision of Platonic Micelles Controlled Solely by Close-Packed Head Groups or Also by Hydrophobic Tail Packing? A DFT Exploration. <i>Langmuir</i> , 0, , .	1.6	2
18031	Decagonal Sn clathrate on $d$ -Al-Ni-Co. <i>Physical Review B</i> , 2023, 107, .	1.1	4
18032	Electronic $K\alpha$ x rays emitted from muonic atoms: An application of relativistic density-functional theory. <i>Physical Review A</i> , 2023, 107, .	1.0	0
18033	Single atomic ruthenium in WO <sub>3</sub> boosted hydrogen evolution stability at Ampere-level current density in whole pH range. <i>Chemical Engineering Journal</i> , 2023, 458, 141414.	6.6	12
18034	Insight at the atomic scale of corrosion inhibition: DFT study of 8-hydroxyquinoline on oxidized aluminum surfaces. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 4284-4296.	1.3	4
18035	Revealing the Selective Bifunctional Electrocatalytic Sites via In Situ Irradiated X-Ray Photoelectron Spectroscopy for Lithium-Sulfur Battery. <i>Advanced Science</i> , 2023, 10, .	5.6	19
18036	Effect of the oxide layer structure on the decarburization behavior of 60Si2Mn spring steel in dry air: Experimental and first-principle study. <i>Materials Characterization</i> , 2023, 196, 112651.	1.9	1

#	ARTICLE	IF	CITATIONS
18037	Biphenylene with doping B/N as promising metal-free single-atom catalysts for electrochemical oxygen reduction reaction. <i>Journal of Power Sources</i> , 2023, 558, 232613.	4.0	14
18038	High-entropy alloy metallene for highly efficient overall water splitting in acidic media. <i>Chinese Journal of Catalysis</i> , 2023, 45, 174-183.	6.9	14
18039	Volatile organic compounds gas molecule adsorption on Fe-MoS <sub>2</sub> monolayer: The first-principles study. <i>Chemical Physics Letters</i> , 2023, 813, 140298.	1.2	0
18040	Evaluation of oxygen vacancy and carbon deposition effect at the perovskite on methane adsorption. <i>Computational Materials Science</i> , 2023, 219, 112020.	1.4	0
18041	Highly efficient photocatalytic hydrogen production by platinum modified ferroelectric SrBi <sub>4</sub> Ti <sub>4</sub> O <sub>15</sub> . <i>Separation and Purification Technology</i> , 2023, 309, 123058.	3.9	6
18042	Nonlinear elastic behavior of 2D materials using molecular statics and comparisons with first principles calculations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2023, 148, 115633.	1.3	2
18043	Prussian blue analogues derived Fe-NiCoP reveals the cooperation of Fe doping and phosphating for enhancing OER activity. <i>Applied Surface Science</i> , 2023, 615, 156378.	3.1	18
18044	An atomic/molecular-level strategy for the design of a preferred nitrogen-doped carbon nanotube cathode for Li-O <sub>2</sub> batteries. <i>Applied Surface Science</i> , 2023, 615, 156367.	3.1	2
18045	Facile Synthesis of Gram-Scale Mesoporous Ag/TiO <sub>2</sub> Photocatalysts for Pharmaceutical Water Pollutant Removal and Green Hydrogen Generation. <i>ACS Omega</i> , 2023, 8, 1249-1261.	1.6	5
18046	Binding Energy and Diffusion Barrier of Formic Acid on Pd(111). <i>Journal of Physical Chemistry A</i> , 2023, 127, 142-152.	1.1	0
18047	Symmetry Breaking with the SCAN Density Functional Describes Strong Correlation in the Singlet Carbon Dimer. <i>Journal of Physical Chemistry A</i> , 2023, 127, 384-389.	1.1	10
18048	Magneto-volume effect in Fe <sub>x</sub> Ti <sub>13-x</sub> clusters during thermal expansion. <i>Chinese Physics B</i> , 0, , .	0.7	0
18049	Pseudo-structural Transition and Thermal Stress-Induced Microcracking in the NdCu Intermetallic. <i>Journal of Phase Equilibria and Diffusion</i> , 0, , .	0.5	0
18051	Stable Multifunctional Aluminum Phosphides at High Pressures. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
18052	<i>In silico</i> capture and activation of methane with light atom molecules. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 5656-5662.	1.3	1
18053	Segregation and Oxidation Behavior in Be {101̄...1} Grain Boundary by First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2023, 127, 2648-2656.	1.5	1
18054	The Predictive Power of Exact Constraints and Appropriate Norms in Density Functional Theory. <i>Annual Review of Physical Chemistry</i> , 2023, 74, 193-218.	4.8	22
18055	Self-consistent implementation of locally scaled self-interaction-correction method. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	6

#	ARTICLE	IF	CITATIONS
18056	Spectroscopic and DFT Study of Alizarin Red S Complexes of Ga(III) in Semi-Aqueous Solution. Photochem, 2023, 3, 61-81. <a href="#">Using ferroelastic variant switching to tune ferromagnetic properties of</a>	1.3	0

18057 [Using ferroelastic variant switching to tune ferromagnetic properties of](#)  $T$   $\epsilon^2$   $CrX_2$

#	ARTICLE	IF	CITATIONS
18076	Selective semi-hydrogenation of alkynes on palladium-selenium nanocrystals. <i>Journal of Catalysis</i> , 2023, 418, 247-255.	3.1	5
18077	Quantum capacitance modulation of MXenes by metal atoms adsorption. <i>Applied Surface Science</i> , 2023, 618, 156586.	3.1	10
18078	Controllable contact types of Janus MoSH and WSi <sub>2</sub> N <sub>4</sub> van der Waals heterostructures via biaxial strain and external electric field. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2023, 149, 115668.	1.3	3
18079	Experimental and theoretical investigation of the damage evolution of irradiated MoAlB and WAlB MAB phases. <i>Journal of Alloys and Compounds</i> , 2023, 942, 169099.	2.8	3
18080	Understanding the influence of bending on OER activity in metal phthalocyanines: A first-principles study. <i>Applied Surface Science</i> , 2023, 618, 156582.	3.1	6
18081	Covalent organic framework films grown on spongy g-C <sub>3</sub> N <sub>4</sub> for efficient photocatalytic hydrogen production. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 439, 114590.	2.0	2
18082	Unveiling the key intermediates in electrocatalytic synthesis of urea with CO <sub>2</sub> and N <sub>2</sub> coupling reactions on double transition-metal MXenes. <i>Journal of Materials Chemistry A</i> , 2023, 11, 6428-6439.	5.2	5
18083	One-Dimensional TeSe Nano-Heterojunction: Formation, Calculations, Carrier Dynamics, and Application in Broad-Spectrum Photodetectors. <i>Nanoscale</i> , 0, , .	2.8	0
18084	Insights into the ruthenium-catalysed selective reduction of cardanol derivatives <i>via</i> transfer hydrogenation: a density functional theory study. <i>Catalysis Science and Technology</i> , 0, , .	2.1	0
18085	Combined experimental and theoretical studies of conformationally diverse (thio)semicarbazone-based semiconducting materials. <i>CrystEngComm</i> , 2023, 25, 2133-2143.	1.3	1
18086	Anomalous Local Lattice Softening around Kink Boundaries in a Mille-Feuille Structured Dilute Mg <sub>1-x</sub> Zn <sub>x</sub> Y Alloy. <i>Materials Transactions</i> , 2023, 64, 1065-1071.	0.4	1
18087	Performance evaluation of free hole-transport layer CsPbI <sub>3</sub> perovskite solar cells. <i>Journal of Materials Science: Materials in Electronics</i> , 2023, 34, .	1.1	1
18088	First-principles phonon calculations of neodymium-magnet compounds. <i>Journal of Applied Physics</i> , 2023, 133, .	1.1	1
18089	Structural, half-metallic, electronic, magnetic and pressure-induced elastic changes of PdVSi, PdVGe, PdVSn, and PdVSb alloys. <i>Journal of Materials Science</i> , 2023, 58, 5349-5361.	1.7	0
18090	Tailoring the Electronic Structure of Ir Alloy Electrocatalysts through Lanthanide (La, Ce, Pr, and) Tj ETQq0 0 0 rgBT /Qverlock <sub>3</sub> 10 Tf 50 1	2.8	3
18091	Investigation of the electronic, optical, elastic, mechanical and vibrational properties of CuI using HSE03. <i>Modern Physics Letters B</i> , 0, , .	1.0	0
18092	Interface alloying design to improve the stability and cohesion of W/HfC interface by first-principles study. <i>Journal of Nuclear Materials</i> , 2023, 577, 154320.	1.3	3
18093	In-situ construction of hierarchical 2D MoS <sub>2</sub> /1D Te hybrid for supercapacitor applications. <i>Journal of Energy Storage</i> , 2023, 60, 106703.	3.9	9

#	ARTICLE	IF	CITATIONS
18094	Adsorption and activation of CO on perfect and defective h-Fe7C3 surfaces for Fischer-Tropsch synthesis. <i>Molecular Catalysis</i> , 2023, 541, 113081.	1.0	1
18095	The effect of alkyl chain length on imidazole chloroaluminate ionic liquid/Pt(1 1 1) interface and aluminum deposition: A DFT-D3 study. <i>Chemical Physics</i> , 2023, 568, 111842.	0.9	1
18096	Enhanced strength and plasticity in a Nb2MoWC0.5 alloy via eutectic dilute carbide. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2023, 872, 144920.	2.6	1
18097	Directed synthesis of nylon 5X key monomer cadaverine with alkaline metal modified Ru@FAU catalysts. <i>Applied Catalysis A: General</i> , 2023, 658, 119172.	2.2	2
18098	Electronic and optical properties of transition-metal (TM=Sc, Ni, Cu, Zn) adsorbed monolayer SnSe2., 2023, 177, 207548.		1
18099	Transfer learning aided high-throughput computational design of oxygen evolution reaction catalysts in acid conditions. <i>Journal of Energy Chemistry</i> , 2023, 80, 744-757.	7.1	7
18100	Built-in electric field-assisted W-C3/X-C3 van der Waals heterogeneous single-atom catalysts for enhanced electrocatalytic nitrogen reduction. <i>Applied Surface Science</i> , 2023, 619, 156790.	3.1	4
18101	Monolayer black phosphorus: Tunable band gap and optical properties. <i>Physica B: Condensed Matter</i> , 2023, 657, 414780.	1.3	4
18102	Synergistic effects of Ta and Mo on the hydrogen embrittlement resistance in ultra-high strength hot stamping steel. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2023, 872, 144956.	2.6	5
18103	The carrier transport properties of zigzag carbon nanotubes with intrinsic defects: An investigation from first principles. <i>Diamond and Related Materials</i> , 2023, 135, 109801.	1.8	0
18104	States of Pt/CeO2 catalysts for CO oxidation below room temperature. <i>Journal of Catalysis</i> , 2023, 421, 285-299.	3.1	9
18105	Lithium-decorated SiB monolayer for reversible hydrogen storage: High-capacity realization through strain engineering. <i>Applied Surface Science</i> , 2023, 618, 156707.	3.1	9
18106	Density functional theory studies of Pt2Ga and Pd2Ga monolayers as multifunctional electrocatalytic materials. <i>Computational Materials Science</i> , 2023, 224, 112164.	1.4	0
18107	First-principles calculations of the viscosity in multicomponent metallic melts: Al-Cu-Ni as a test case. <i>Journal of Molecular Liquids</i> , 2023, 380, 121751.	2.3	4
18108	Design of catalyst for syngas conversion to C2 oxygenates via confining diatomic metal within the framework of 2D carbon-based materials. <i>Fuel</i> , 2023, 342, 127858.	3.4	1
18109	Theoretical investigation on oxygen source for selective oxidation of glycerol at Au/CeO2 and Pt/CeO2 interfaces. <i>Fuel</i> , 2023, 342, 127884.	3.4	4
18110	Heteroatom substitution controlled luminescent property and excited state intramolecular proton transfer (ESIPT) process of novel benzothiazole-based fluorophore: A TD-DFT investigation. <i>Journal of Molecular Structure</i> , 2023, 1281, 135132.	1.8	2
18111	Theoretical study on surface stability, distortion and oxygen adsorption behavior of TiZrHfNb high entropy alloys. <i>Surface Science</i> , 2023, 732, 122273.	0.8	0

#	ARTICLE	IF	CITATIONS
18112	A comparative study of cubic methylammonium lead iodide (CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> ) perovskite by using density functional theory. <i>Materials Today Communications</i> , 2023, 35, 105814.	0.9	1
18113	Electron-stimulated desorption of potassium atoms from the surface of intermetallic compounds KxAu <sub>y</sub> . <i>Vacuum</i> , 2023, 212, 112050.	1.6	1
18114	Nanodevice design and electronic transport properties of Ge <sub>2</sub> Sb <sub>2</sub> -based monolayers. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2023, 150, 115681.	1.3	3
18115	Role of oxygen vacancy in spinel (FeCoNiCrMn) <sub>3</sub> O <sub>4</sub> high entropy oxides prepared via two different methods for the selective C-H bond oxidation of p-chlorotoluene. <i>Journal of Colloid and Interface Science</i> , 2023, 640, 359-371.	5.0	5
18116	The adjustable electronic and photoelectric properties of the WS <sub>2</sub> /WSe <sub>2</sub> and WSe <sub>2</sub> /WTe <sub>2</sub> van der Waals heterostructures. <i>Vacuum</i> , 2023, 212, 112020.	1.6	7
18117	Assimilation of electronic, elastic, mechanical, optical, and thermal profiles in metal halide perovskite CsPbCl <sub>3</sub> , for optoelectronic applications. <i>Computational Condensed Matter</i> , 2023, 35, e00804.	0.9	1
18118	An MD-based physical characteristics analysis on the PI/EP duo-layer composites, impacting of diamino groups. <i>Materials Today Communications</i> , 2023, 35, 105482.	0.9	1
18119	Heterogeneous nucleation of carbides attached to Y <sub>2</sub> O <sub>3</sub> in Y-modified H13 steel. <i>Materials Characterization</i> , 2023, 200, 112891.	1.9	5
18120	Metronidazole photodegradation under solar light with UiO-66-NH <sub>2</sub> photocatalyst: Mechanisms, pathway, and toxicity assessment. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109744.	3.3	0
18121	Synthesis, experimental, theoretical, and molecular dynamic studies of 1-(2,5-dimethoxy-4-methylphenyl)ethan-1-thiosemicarbazone as green inhibitor for carbon steel corrosion. <i>Journal of Molecular Structure</i> , 2023, 1282, 135228.	1.8	8
18122	Unrevealing the phase transition of high-performing high-nitrogen energetic material 1,5-diaminotetrazole-4: N-oxide via first-principles studies. <i>Materials Today Communications</i> , 2023, 35, 105940.	0.9	0
18123	Boosted Z-scheme photocatalytic overall water splitting with faceted Bi <sub>4</sub> TaO <sub>8</sub> Cl crystals as water oxidation photocatalyst. <i>Applied Catalysis B: Environmental</i> , 2023, 328, 122541.	10.8	6
18124	Zn-doped nickel iron (oxy)hydroxide nanocubes passivated by polyanions with high catalytic activity and corrosion resistance for seawater oxidation. <i>Journal of Energy Chemistry</i> , 2023, 81, 82-92.	7.1	6
18125	The hinge morphology of SnO <sub>2</sub> as multifunctional semiconductor: What we can learn from simulations, theory, and experiments. <i>Applied Surface Science</i> , 2023, 622, 156904.	3.1	3
18126	Theoretical study on structural transformation and mechanical properties of Ni <sub>3</sub> Ti <sub>1-x</sub> Nbx. <i>Results in Materials</i> , 2023, 18, 100387.	0.9	0
18127	Simultaneous enhancement of coercivity and electric resistivity of Nd-Fe-B magnets by Pr-Tb-Al-Cu synergistic grain boundary diffusion toward high-temperature motor rotors. <i>Journal of Materials Science and Technology</i> , 2023, 154, 54-64.	5.6	13
18128	Subphase exploration for SmFe <sub>12</sub> -based permanent magnets by Gibbs energies obtained with first-principles cluster-expansion method. <i>Journal of Alloys and Compounds</i> , 2023, 950, 169849.	2.8	0
18129	Electron self-sufficient core-shell BiOCl@Fe-BiOCl nanosheets boosting Fe(III)/Fe(II) recycling and synergetic photocatalysis-Fenton for enhanced degradation of phenol. <i>Applied Catalysis B: Environmental</i> , 2023, 330, 122642.	10.8	30



#	ARTICLE	IF	CITATIONS
18130	Design, synthesis and investigating the interaction of novel s-triazine collector with pyrite surface: A DFT-D3+U and experimental studies. <i>Surfaces and Interfaces</i> , 2023, 38, 102820.	1.5	1
18131	Synergetic effect of the interface electric field and the plasmon electromagnetic field in Au-Ag alloy mediated Z-type heterostructure for photocatalytic hydrogen production and CO <sub>2</sub> reduction. <i>Applied Catalysis B: Environmental</i> , 2023, 331, 122700.	10.8	5
18132	Lattice softness regulates recombination and lifetime of carrier in Germanium doped CsPbI <sub>2</sub> Br perovskite: First principles DFT and NAMD simulations. <i>Journal of Solid State Chemistry</i> , 2023, 322, 123981.	1.4	0
18133	Facilitating interface charge transfer via constructing NiO/NiCo <sub>2</sub> O <sub>4</sub> heterostructure for oxygen evolution reaction under alkaline conditions. <i>Journal of Colloid and Interface Science</i> , 2023, 643, 214-222.	5.0	10
18134	Unveiling anion induced surface reconstruction of perovskite oxide for efficient water oxidation. <i>Applied Catalysis B: Environmental</i> , 2023, 330, 122661.	10.8	10
18135	Emerging Trends of Computational Chemistry and Molecular Modeling in Froth Flotation: A Review. <i>ACS Engineering Au</i> , 2023, 3, 128-164.	2.3	4
18136	Screening Multi-layered Two-dimensional Cd chalcogenide Structures as Potential Candidates for Photocatalysis. <i>ChemPhysChem</i> , 0, . . .	1.0	0
18137	Topological Semimetal Phases in a Family of monolayer X <sub>3</sub> YZ <sub>6</sub>	1.3	0
18138	Challenging Structure Elucidation of Lumnitzeralactone, an Ellagic Acid Derivative from the Mangrove <i>Lumnitzera racemosa</i> . <i>Marine Drugs</i> , 2023, 21, 242.	2.2	0
18139	Synergistic double-atom catalysts of metal-boron anchored on g-C <sub>3</sub> N <sub>4</sub> for electrochemical nitrogen reduction: Mechanistic insight and catalyst screening. <i>Journal of Energy Chemistry</i> , 2023, 80, 350-360.	7.1	13
18140	Computational design of one FeCoNiCuZn high-entropy alloy for high-performance electrocatalytic nitrate reduction. <i>Applied Surface Science</i> , 2023, 626, 157246.	3.1	2
18141	Heterojunction material BiYO <sub>3</sub> /g-C <sub>3</sub> N <sub>4</sub> modified with cellulose nanofibers for photocatalytic degradation of tetracycline. <i>Carbohydrate Polymers</i> , 2023, 312, 120829.	5.1	16
18142	Effects of trace elements on mechanical properties of the TiZrHfNb high-entropy alloy. <i>Journal of Materials Science and Technology</i> , 2023, 152, 135-147.	5.6	5
18143	Regulating the solvation chemistry of non-flammable high voltage electrolyte through salt-solvent ratio modulation. <i>Journal of Colloid and Interface Science</i> , 2023, 642, 820-828.	5.0	1
18144	Revealing the effects of transition metal doping on CoSe cocatalyst for enhancing photocatalytic H <sub>2</sub> production. <i>Applied Catalysis B: Environmental</i> , 2023, 328, 122503.	10.8	24
18145	Intrinsic electrochemical activity modulation of MOF-derived C/N-NiCoMn-LDH/Ag electrode for low temperature hybrid supercapacitors. <i>Journal of Materials Science and Technology</i> , 2023, 150, 145-158.	5.6	19
18146	Density functional theory study on the effect of germanium doping in sphalerite on the adsorption mechanism of butyl xanthate. <i>Chemical Physics</i> , 2023, 571, 111907.	0.9	1
18147	Biochar-derived flower-like Co-Mo <sub>2</sub> C spheres/g-C <sub>3</sub> N <sub>4</sub> photocatalyst: Engineering morphology configuration and electronic structure tuning. <i>Separation and Purification Technology</i> , 2023, 316, 123808.	3.9	5

#	ARTICLE	IF	CITATIONS
18148	Fabrication and characterization of PEG-In <sub>2</sub> O <sub>3</sub> modified PbO <sub>2</sub> anode for electrochemical degradation of metronidazole. <i>Electrochimica Acta</i> , 2023, 442, 141919.	2.6	1
18149	Efficient electrocatalytic CO <sub>2</sub> reduction on Ti <sub>3</sub> C <sub>2</sub> O <sub>2</sub> surfaces: The effect of single-atom TM anchoring on product selectivity. <i>Applied Surface Science</i> , 2023, 616, 156492.	3.1	5
18150	Enhancement of the magnetic and mechanical properties by introducing element carbon for Ti-based alloy. <i>Journal of Magnetism and Magnetic Materials</i> , 2023, 568, 170438.	1.0	2
18151	Structural features, thermal stability and catalytic implication of Fe@Ni nanoparticles. <i>Journal of Solid State Chemistry</i> , 2023, 320, 123863.	1.4	1
18152	Boron Nitride-Graphene (BN-G) Bilayer as a Channel of Graphene Based Field Effect Transistor. <i>ECS Journal of Solid State Science and Technology</i> , 2023, 12, 021001.	0.9	0
18153	Phytochemical components of Allium Jesdianum flower as effective corrosion-resistant materials for Fe(1 1 0), Al(1 1 1), and Cu(1 1 1): DFT study. <i>Arabian Journal of Chemistry</i> , 2023, 16, 104625.	2.3	12
18154	Phase transition-induced initial decomposition of nitrogen-rich binary CN compound 2,2-azobis(5-azidotetrazole) and its precursor 2-amino-5-azidotetrazole via tetrazole ring opening under external electric fields: a comparative DFT-D study. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 6481-6490.	1.3	1
18155	The OER/ORR activities of copper oxyhydroxide series electrocatalysts. <i>Molecular Catalysis</i> , 2023, 537, 112942.	1.0	4
18156	Theoretical study of M <sub>2</sub> CO <sub>2</sub> MXenes stability and adsorption properties for heavy metals ions removal from water. <i>Computational Materials Science</i> , 2023, 220, 112042.	1.4	2
18157	Topological and nodal superconductor kagome magnesium triboride. <i>Physical Review Materials</i> , 2023, 7, .	0.9	3
18158	Room temperature d <sup>0</sup> ferromagnetism in carbon doped LaH <sub>3</sub> : insights from density functional theory simulations. <i>Journal Physics D: Applied Physics</i> , 2023, 56, 095001.	1.3	0
18159	Sulfide-Bridged Covalent Quinoxaline Frameworks for Lithium-Organosulfide Batteries. <i>Advanced Materials</i> , 2023, 35, .	11.1	12
18160	Insight into the hydrodenitrogenation mechanism of quinoline on the MoP(010) surface with and without the effect of sulfur. <i>Molecular Catalysis</i> , 2023, 538, 112970.	1.0	1
18161	Iron behavior during the continuous phase transition of iron-doped titanium dioxide determined via high-temperature in-situ X-ray diffraction, rietveld refinement, and density functional theory studies. <i>Journal of Materials Research and Technology</i> , 2023, 23, 2426-2439.	2.6	2
18162	Novel Boron-rich Phosphides with High Hardness, Large Strain, and Magnetism. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 1310-1317.	2.1	3
18163	Chiral Magnetic Interactions in Small Fe Clusters Triggered by Symmetry-Breaking Adatoms. <i>Symmetry</i> , 2023, 15, 397.	1.1	0
18164	Coupling a Main-Group Metal with a Transition Metal to Create Biatom Catalysts for Nitric Oxide Reduction. <i>Physical Review Applied</i> , 2023, 19, .	1.5	4
18166	Probing the affinity of noble metal nanoparticles to the segments of the SARS-CoV-2 spike protein. <i>IScience</i> , 2023, 26, 106110.	1.9	0

#	ARTICLE	IF	CITATIONS
18167	Light Absorption by Cinnamaldehyde Constituents of Biomass Burning Organic Aerosol Modeled Using Time-Dependent Density Functional Theory. <i>ACS Earth and Space Chemistry</i> , 2023, 7, 490-500.	1.2	2
18168	Quantum-corrected thickness-dependent thermal conductivity in amorphous silicon predicted by machine learning molecular dynamics simulations. <i>Physical Review B</i> , 2023, 107, .	1.1	16
18169	Computational and experimental studies on spectra and bonding of cyclohexane linked tris-hydroxyquinoline flexible tripodal chelator and its complexes. <i>Chemical Papers</i> , 0, , .	1.0	0
18170	Modification of the Cu/W Interface Cohesion by Segregation. <i>Metals</i> , 2023, 13, 346.	1.0	2
18171	Elemental Doping Boosts Charge-Transfer Excitonic States in Polymeric Photocatalysts for Selective Oxidation Reaction. , 2023, 1, 40-48.		2
18172	Two-Dimensional Octuple-Atomic-Layer M <sub>2</sub> Si <sub>2</sub> N <sub>4</sub> (M = Al, Ga and In) with Long Carrier Lifetime. <i>Micromachines</i> , 2023, 14, 405.	1.4	0
18173	Interfacial interaction between graphene and ferromagnets: First principles study. <i>Physica B: Condensed Matter</i> , 2023, 655, 414740.	1.3	1
18174	First-Principles Calculation and Kink-Dislocation Dynamics Simulation on Dislocation Plasticity in TiZr-Based Concentrated Solid-Solution Alloys. <i>Metals</i> , 2023, 13, 351.	1.0	0
18176	Atomistic Origins of Reversible Noncatalytic Gas-Solid Interfacial Reactions. <i>Journal of the American Chemical Society</i> , 0, , .	6.6	1
18177	Combined experimental and DFT investigation of temozolomide sensing properties of 2D-2D interface of rich oxygen vacancies of WO <sub>3-x</sub> and sulfur-doped g-C <sub>3</sub> N <sub>4</sub> nanosheets hybrids composites. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109459.	3.3	0
18178	Positron trapping at the effective open volume in FeCr alloy containing hydrogen/helium atoms. , 2023, 9, 011001-011001.		0
18179	Partial substitution induced structural transformation and enhanced nonlinear optical properties of Na <sub>2</sub> GaxIn <sub>6-x</sub> Se <sub>10</sub> (x = 3, 3.76). <i>Materials Today Physics</i> , 2023, 32, 101007.	2.9	10
18180	Organic Eutectic Mixture Incorporated with Graphene Oxide Sheets as Lithiophilic Artificial Protective Layer for Dendrite-Free Lithium Metal Batteries. <i>Advanced Energy Materials</i> , 2023, 13, .	10.2	8
18181	Tunable band gap by chemical functionalization of the Sr <sub>2</sub> S monolayer from first-principles calculations. <i>Inorganic Chemistry Communication</i> , 2023, 150, 110529.	1.8	1
18182	Scavenging of Superoxide in Aprotic Solvents of Four Isoflavones That Mimic Superoxide Dismutase. <i>International Journal of Molecular Sciences</i> , 2023, 24, 3815.	1.8	4
18183	Facile Synthesis of Palladium-Silver Dilute Alloy Catalyst for Acetylene Hydrogenation. <i>ChemCatChem</i> , 2023, 15, .	1.8	4
18184	Strategies to Improve the Oxygen Reduction Reaction Activity on Pt-Bi Bimetallic Catalysts: A Density Functional Theory Study. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 1990-1998.	2.1	4
18185	Theoretical study of hydrogen adsorption kinetics: Mg <sub>17</sub> Al <sub>12</sub> vs pure Mg. <i>International Journal of Hydrogen Energy</i> , 2023, , .	3.8	0

#	ARTICLE	IF	CITATIONS
18186	Study of the perovskites CaZrO <sub>3-x</sub> Sx (x=0, 1, 2 and 3) for photovoltaic applications. Solid State Communications, 2023, 363, 115105.	0.9	7
18187	Phase Transitions, Mechanical and Dynamic Stability, and Electronic Properties of SnO Polymorphs under High Pressure. Physica Status Solidi (B): Basic Research, 2023, 260, .	0.7	1
18188	On the Nature of Hydrophobic Organic Compound Adsorption to Smectite Minerals Using the Example of Hexachlorobenzene-Montmorillonite Interactions. Minerals (Basel, Switzerland), 2023, 13, 280.	0.8	2
18189	USc <sub>2</sub> C <sub>2</sub> and USc <sub>2</sub> NC Clusters with U≡C Triple Bond Character Stabilized Inside Fullerene Cages. Journal of the American Chemical Society, 2023, 145, 5645-5654.	6.6	7
18190	Dynamic crystallography reveals spontaneous anisotropy in cubic GeTe. Nature Materials, 2023, 22, 311-315.	13.3	9
18191	A first-principles study of doping effect on enhancing ORR performance of Sr≡Ni≡Nb co-doped LaFeO <sub>3</sub> perovskite. International Journal of Hydrogen Energy, 2023, 48, 18744-18752.	3.8	3
18192	Supercritical CO <sub>2</sub> -induced New Chemical Bond of C≡Si in Graphdiyne to Achieve Robust Room-temperature Ferromagnetism. ChemPhysChem, 0, , .	1.0	1
18194	Charge Density Evolution Governing Interfacial Friction. Journal of the American Chemical Society, 2023, 145, 5536-5544.	6.6	12
18195	Dual Co <sub>x</sub> S <sub>y</sub> -Modified Tungsten Disulfide Double-Heterojunction Electrocatalyst for Efficient Hydrogen Evolution in All-pH Media. ACS Applied Materials & Interfaces, 2023, 15, 11765-11776.	4.0	8
18196	Single Ru(II) Ions on Ceria as a Highly Active Catalyst for Abatement of NO. Journal of the American Chemical Society, 2023, 145, 5029-5040.	6.6	21
18197	Atomically dispersed indium and cerium sites for selectively electroreduction of CO <sub>2</sub> to formate. Nano Research, 2023, 16, 8757-8764.	5.8	9
18198	Controllable p-type doping of 2D MoS <sub>2</sub> via Sodium intercalation for optoelectronics. Journal of Materials Chemistry C, 2023, 11, 3386-3394.	2.7	0
18199	Mechanistic Insight into Favorable Aldehyde Hydrogenation over Hydroxymethyl Hydrogenolysis in 5-Hydroxymethylfurfural by Formic Acid over Single-Atom Co-N <sub>3</sub> /C. Journal of Physical Chemistry C, 2023, 127, 4535-4543.	1.5	4
18200	Coordination Inversion of the Tetrahedrally Coordinated Ru <sub>4f</sub> Surface Complex on RuO <sub>2</sub> (100) and Its Decisive Role in the Anodic Corrosion Process. ACS Catalysis, 2023, 13, 3433-3443.	5.5	8
18201	Effect of Co substitution on ferrimagnetic Heusler compound Mn <sub>3</sub> Ga. Current Applied Physics, 2023, 49, 78-82.	1.1	0
18202	Analysis of XGaO <sub>3</sub> (X = Ba and Cs) cubic based perovskite materials for photocatalytic water splitting applications: a DFT study. Heliyon, 2023, 9, e14112.	1.4	7
18203	Large magnetoresistance and spin-polarized photocurrent in Mn <sub>2.25</sub> Co <sub>0.75</sub> Ga <sub>0.5</sub> Sn <sub>0.5</sub> /MgO/Mn <sub>2.25</sub> Co <sub>0.75</sub> Ga <sub>0.5</sub> Sn <sub>0.5</sub> magnetic tunnel junctions. Computational Materials Science, 2023, 221, 112086.	1.4	0
18204	Mechanism of tungsten strengthening hydrogen transportation in Nb <sub>48</sub> Ti <sub>27</sub> Co <sub>25</sub> hydrogen permeable alloy membrane. Journal of Materials Research and Technology, 2023, 23, 5413-5422.	2.6	2

#	ARTICLE	IF	CITATIONS
18205	Theoretical and Experimental Assessments of Elementary Steps and Bound Intermediates in Catalytic $H_2$ – $O_2$ Reactions on Dispersed Pt Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2023, 127, 4553-4569.	1.5	1
18206	Sila[1]ruthenocenophanes: Long Sought-After Family Members. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	1
18207	Scalable synthesis of Cu clusters for remarkable selectivity control of intermediates in consecutive hydrogenation. <i>Nature Communications</i> , 2023, 14, .	5.8	10
18208	Incommensurately Modulated Structure in AgCuSe-Based Thermoelectric Materials for Intriguing Electrical, Thermal, and Mechanical Properties. <i>Small</i> , 2023, 19, .	5.2	7
18209	Conductivities in Yttrium-Doped Barium Zirconate: A First-Principles Study. <i>Crystals</i> , 2023, 13, 401.	1.0	4
18210	A Coverage Self-Consistent Microkinetic Model for Vapor-Phase Formic Acid Decomposition over Pd/C Catalysts. <i>ACS Catalysis</i> , 2023, 13, 3655-3667.	5.5	5
18211	Creating and Stabilizing an Oxidized Pd Surface under Reductive Conditions for Photocatalytic Hydrogenation of Aromatic Carbonyls. <i>Journal of the American Chemical Society</i> , 2023, 145, 5353-5362.	6.6	6
18212	First-principle calculations of stable configurations and electronic structures of pristine and discharged spinel $Mg_{1.31}V_{1.67-x}Ni_xO_4$ ( $x=0, 0.13$ ) as cathode materials for magnesium secondary batteries. <i>Computational Materials Science</i> , 2023, 221, 112087.	1.4	1
18213	Restricted multicanonical sampling for machine learning potential construction. <i>Physical Review B</i> , 2023, 107, .	1.1	1
18214	Antioxidant Properties of Thymoquinone, Thymohydroquinone and Black Cumin ( <i>Nigella sativa</i> L.) Seed Oil: Scavenging of Superoxide Radical Studied Using Cyclic Voltammetry, DFT and Single Crystal X-ray Diffraction. <i>Antioxidants</i> , 2023, 12, 607.	2.2	5
18215	Theoretical Evaluation of Highly Efficient Nitrate Reduction to Ammonia on InBi. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 2410-2415.	2.1	4
18216	Structures of Sm–Cu intermetallics with Fe as subphase candidates in $SmFe_{12}$ -based permanent magnets studied by first-principles thermodynamics. <i>Japanese Journal of Applied Physics</i> , 2023, 62, 030902.	0.8	1
18217	Spin filters based on two-dimensional materials $Co_2Si$ and $Cu_2Si$ . <i>Journal of Physics Condensed Matter</i> , 2023, 35, 195001.	0.7	0
18218	Iron-Based Active Sites Encapsulated in Carbon Nanotubes for an Efficient Hydride Process. <i>ACS Applied Nano Materials</i> , 2023, 6, 3218-3225.	2.4	3
18219	Spontaneously enhanced visible-light-driven photocatalytic water splitting of type II PG/AlAs <sub>5</sub> van der Waal heterostructure: A first-principles study. <i>Chinese Chemical Letters</i> , 2023, 34, 108270.	4.8	8
18220	Kinetic Understanding of Catalytic Selectivity and Product Distribution of Electrochemical Carbon Dioxide Reduction Reaction. <i>Jacs Au</i> , 2023, 3, 905-918.	3.6	8
18221	Atomic reconstruction and oxygen adsorption behavior of the pyrite (100) surface: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 8826-8835.	1.3	0
18222	Molybdenum based 2D conductive Metal-Organic frameworks as efficient single-atom electrocatalysts for $N_2$ reduction: A density functional theory study. <i>International Journal of Hydrogen Energy</i> , 2023, 48, 19972-19983.	3.8	8

#	ARTICLE	IF	CITATIONS
18223	First-principles-based simulation of the electrocaloric effect. , 2023, , 63-91.		0
18224	Atomic-scale Revealing the Structure Distribution between $\text{LiMO}_2$ and $\text{Li}_2\text{MnO}_3$ in Li-Rich and Mn-Based Oxide Cathode Materials. <i>Advanced Energy Materials</i> , 2023, 13, .	10.2	19
18225	First-principles study on the interfacial bonding strength and segregation at Mg/MgZn <sub>2</sub> matrix interface. <i>Journal of Magnesium and Alloys</i> , 2023, , .	5.5	1
18226	Performance of Density Functionals and Semiempirical 3c Methods for Small Gold-Thiolate Clusters. <i>Journal of Physical Chemistry A</i> , 2023, 127, 2242-2257.	1.1	1
18227	DELTA50: A Highly Accurate Database of Experimental <sup>1</sup> H and <sup>13</sup> C NMR Chemical Shifts Applied to DFT Benchmarking. <i>Molecules</i> , 2023, 28, 2449.	1.7	6
18228	$\text{Eu}_4\text{Al}_{13}\text{Pt}_9$ – a coloring variant of the $\text{Ho}_4\text{Ir}_{13}\text{Ge}_9$ type structure. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2023, 78, 147-156.	0.3	0
18229	The Inducement and “Rejuvenation” of Li Dendrites by Space Confinement and Positive Fe/Co Sites. <i>Small</i> , 2023, 19, .	5.2	4
18230	Fluids and Electrolytes under Confinement in Single-Digit Nanopores. <i>Chemical Reviews</i> , 2023, 123, 2737-2831.	23.0	32
18231	A DFT study of structural and electronic properties of some $\text{B}_{12}$ -based compounds under hydrostatic pressure. <i>Physica Scripta</i> , 2023, 98, 045907.	1.2	0
18232	Stable all-solid-state Li-Te battery with $\text{Li}_3\text{TbBr}_6$ superionic conductor. <i>Nano Research</i> , 2023, 16, 9344-9351.	5.8	1
18233	Theoretically Predicted CO Adsorption and Activation on the Co-Doped hcp-Fe <sub>7</sub> C <sub>3</sub> Catalyst. <i>Catalysts</i> , 2023, 13, 564.	1.6	1
18234	Visible-light-responsive Photocatalyst Based on Nitrogen-doped Bulk Oxide $\text{YTaO}_4\text{N}_x$ for Z-scheme Overall Water Splitting. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	4
18235	Importance of Adatom on Pure Iron Catalyst Towards Electrocatalytic $\text{N}_2$ Reduction Reaction. <i>Chemistry - an Asian Journal</i> , 0, , .	1.7	0
18236	Theoretical Research Methods Involved in This Book. <i>Springer Theses</i> , 2023, , 19-43.	0.0	0
18237	$\text{Co}_2\text{CrAl}$ Heuslerene: Mechanical, Thermodynamic and Electronic Properties. <i>Metals</i> , 2023, 13, 582.	1.0	0
18238	Crystal plane dependent dispersion of cobalt metal on metastable aluminas. <i>Journal of Catalysis</i> , 2023, 421, 210-220.	3.1	1
18239	Eliminating over-oxidation of ruthenium oxides by niobium for highly stable electrocatalytic oxygen evolution in acidic media. <i>Joule</i> , 2023, 7, 558-573.	11.7	64
18240	The Bulk van der Waals Layered Magnet $\text{CrSBr}$ is a Quasi-1D Material. <i>ACS Nano</i> , 2023, 17, 5316-5328.	7.3	26



#	ARTICLE	IF	CITATIONS
18241	Single-atom vibrational spectroscopy with chemical-bonding sensitivity. <i>Nature Materials</i> , 2023, 22, 612-618.	13.3	10
18242	2D carbon nitrides: Regulating non-metal boron-doped C <sub>3</sub> N <sub>5</sub> for elucidating the mechanism of wide pH range photocatalytic hydrogen evolution reaction. <i>Chinese Journal of Catalysis</i> , 2023, 47, 150-160.	6.9	15
18243	Atomistic mechanisms for catalytic transformations of NO to NH <sub>3</sub> , N <sub>2</sub> O, and N <sub>2</sub> by Pd. <i>Chinese Journal of Chemical Physics</i> , 2023, 36, 94-102.	0.6	0
18244	Phosphorous/Fluorine Co-doped Biomass-derived Carbon for Enhanced Sodium-ion and Lithium-ion Storage. <i>ChemNanoMat</i> , 2023, 9, .	1.5	3
18246	Thermodynamics of phase stability and disorder in Inter-Lanthanide ternary ABO <sub>3</sub> oxides from first principles. <i>Materials and Design</i> , 2023, 228, 111830.	3.3	1
18247	Genesis of Active Pt/CeO <sub>2</sub> Catalyst for Dry Reforming of Methane by Reduction and Aggregation of Isolated Platinum Atoms into Clusters. <i>Small</i> , 2023, 19, .	5.2	6
18248	Transition-Metal-Free, Pure p-Block Alloy Electrocatalysts for the Highly Efficient Nitrate Reduction to Ammonia. <i>Chemistry of Materials</i> , 2023, 35, 2884-2891.	3.2	3
18249	Understanding the fundamentals of TiO <sub>2</sub> surfaces Part II. Reactivity and surface chemistry of TiO <sub>2</sub> single crystals. <i>Surface Engineering</i> , 2022, 38, 846-906.	1.1	0
18250	RuS <sub>2</sub> @CN-x with exposed (200) facet as a high-performance photocatalyst for selective C-C bond cleavage of biomass coupling with H <sub>2</sub> O bond cleavage of water to co-produce chemicals and H <sub>2</sub> . <i>Green Chemistry</i> , 2023, 25, 3236-3246.	4.6	5
18251	Li self-diffusion and ion conductivity in congruent $\text{LiNbO}_3$ and $\text{LiTaO}_3$ single crystals. <i>Physical Review Materials</i> , 2023, 7, .	0.9	6
18252	Energies Exploration for the Troponine Molecule Supported on Carbon Nanomaterials: DFT Study. <i>ACS Omega</i> , 2023, 8, 12334-12338.	1.6	1
18253	Electronic and strain-elimination effects of solute-vacancy interaction in molybdenum. <i>Journal of Applied Physics</i> , 2023, 133, 125106.	1.1	0
18254	Passivating Oxygen Evolution Activity of NiFe-LDH through Heterostructure Engineering to Realize High-Efficiency Electrocatalytic Formate and Hydrogen Co-Production. <i>Small</i> , 2023, 19, .	5.2	10
18255	Electronic band structure and density of state modulation of amphetamine and ABW type zeolite adsorption system: DFT-CASTEP analysis. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	4
18256	Noncollinear and Spin-Flip TDDFT in Multicollinear Approach. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 2270-2281.	2.3	2
18257	Physicochemical Properties of Organic Molecular Ferroelectric Diisopropylammonium Chloride Thin Films. <i>Nanomaterials</i> , 2023, 13, 1200.	1.9	0
18258	Stimulating the Intrinsic Activities of the MoS <sub>2</sub> Nanosheet Coated on S,N-Graphene for Efficient Membrane Electrofiltration. <i>ACS ES&amp;T Water</i> , 0, , .	2.3	0
18259	In or on, a study of the influence of the binding site for TiO <sub>2</sub> and MIL-101(Cr). <i>Dalton Transactions</i> , 0, , .	1.6	0

#	ARTICLE	IF	CITATIONS
18260	Zr <sub>3</sub> C <sub>2</sub> O <sub>2</sub> MXene as promising candidate for NH <sub>3</sub> sensor with high sensitivity and selectivity at room temperature. Applied Surface Science, 2023, 624, 157125.	3.1	3
18261	Intersite Coulomb Interactions in Charge-Ordered Systems. Physical Review Letters, 2023, 130, .	2.9	3
18262	Highly Selective N <sub>2</sub> Electroreduction to NH <sub>3</sub> Using a Boron- $\delta$ -Vacancy-Rich Diatomic Nb $\delta$ B Catalyst. Small, 2023, 19, .	5.2	10
18263	Quasi-periodic scattering of topological edge states induced by the vacancies in chloridized gallium bismuthide nanoribbons. Journal of Physics Condensed Matter, 2023, 35, 255302.	0.7	1
18264	Plasmons in a two-dimensional nonsymmorphic nodal-line semimetal. Physical Review B, 2023, 107, .	1.1	3
18265	Polaron-induced metal-to-insulator transition in vanadium oxides from density functional theory calculations. Physical Review B, 2023, 107, .	1.1	1
18266	Hydrophobicity Tailoring of Ferric Covalent Organic Framework/MXene Nanosheets for High-Efficiency Nitrogen Electroreduction to Ammonia. Advanced Science, 2023, 10, .	5.6	8
18267	A ten-fold coordinated high-pressure structure in hafnium dihydrogen with increasing superconducting transition temperature induced by enhance pressure. Chinese Physics B, 2023, 32, 097402.	0.7	1
18269	Experimental and computational investigation on the charge storage performance of a novel Al <sub>2</sub> O <sub>3</sub> -reduced graphene oxide hybrid electrode. Scientific Reports, 2023, 13, .	1.6	10
18270	In situ engineering 3D conductive core-shell nano-networks and electronic structure of bismuth alloy nanosheets for efficient electrocatalytic CO <sub>2</sub> reduction. Science China Materials, 2023, 66, 2266-2273.	3.5	5
18271	Tracking Atomic Diffusion in Surface and Bulk CuO via Neural Network-Based Molecular Dynamics. Journal of Physical Chemistry C, 2023, 127, 6948-6958.	1.5	1
18272	Heteroatom-Driven Coordination Fields Altering Single Cerium Atom Sites for Efficient Oxygen Reduction Reaction. Advanced Materials, 2023, 35, .	11.1	39
18273	Detailed Mechanical Characterization of LiCo <sub>2</sub> and LiNi <sub>0.33</sub> Co <sub>0.33</sub> Mn <sub>0.33</sub> O <sub>2</sub> Cathode Materials Using DFT Calculations. Chemistry Letters, 2023, 52, 317-321.	0.7	0
18274	Improving the hydrogen storage properties of lithium hydride (LiH) by lithium vacancy defects: Ab initio calculations. Solid State Communications, 2023, 371, 115167.	0.9	5
18275	Ultrafast Quantum Processes at the Nanoscale: Insights from Modeling. Springer Series in Optical Sciences, 2023, , 139-171.	0.5	0
18276	Enhancing the electrochemical reduction of carbon dioxide to multi-carbon products on copper nanosheet arrays via cation-catalyst interaction. Cell Reports Physical Science, 2023, 4, 101366.	2.8	7
18277	Synergistic effect of phosphorus doping and MoS <sub>2</sub> co-catalysts on g-C <sub>3</sub> N <sub>4</sub> photocatalysts for enhanced solar water splitting. Journal of Materials Science and Technology, 2023, 158, 171-179.	5.6	21
18278	Improvement of hydrogen storage performance and gravimetric density of $M\delta H_2$ by transition metals and vaca	0.9	3

#	ARTICLE	IF	CITATIONS
18279	Elucidating the Role of Noncovalent Interactions in Favipiravir, a Drug Active against Various Human RNA Viruses; a 1H-14N NQDR/Periodic DFT/QTAIM/RDS/3D Hirshfeld Surfaces Combined Study. <i>Molecules</i> , 2023, 28, 3308.	1.7	4
18280	Enhancing ferromagnetic coupling in CrXY (X = O, S, Se; Y = Cl, Br, I) monolayers by turning the covalent character of Cr-X bonds. <i>Npj Computational Materials</i> , 2023, 9, .	3.5	3
18281	Comprehensive Mechanism and Microkinetic Model-Driven Rational Screening of 3N-Modulated Single-Atom Catalysts for Propane Dehydrogenation. <i>ACS Catalysis</i> , 2023, 13, 5529-5537.	5.5	6
18282	Uniform Zinc Deposition Regulated by a Nitrogen- $\delta$ -Doped MXene Artificial Solid Electrolyte Interlayer. <i>Small</i> , 2023, 19, .	5.2	7
18283	An investigation into the Brønsted acidity of the perfluorinated alkoxy silanes $\{(F_{3-x}C)_3CO\}_3SiH$ and $\{(F_{6-x}C)_5CO\}_2Si(Cl)H$ . <i>Dalton Transactions</i> , 2023, 52, 5918-5925.	1.6	2
18285	Designing ternary superconducting hydrides with A15-type structure at moderate pressures. <i>Materials Today Physics</i> , 2023, 34, 101086.	2.9	6
18286	Investigation of electronic and magnetic properties in vacancy incorporated monolayer magnesium bromide for spintronics application: an ab-initio study. <i>Physica Scripta</i> , 2023, 98, 055937.	1.2	1
18287	Coverage-dependent adsorption and dissociation of H <sub>2</sub> O on Al surfaces. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	1
18288	Basal plane activation of two-dimensional transition metal dichalcogenides <i>via</i> alloying for the hydrogen evolution reaction: first-principles calculations and machine learning prediction. <i>Journal of Materials Chemistry A</i> , 2023, 11, 9964-9975.	5.2	4
18289	Magnetic transitions of hydrogenated H <sub>x</sub> CrO <sub>2</sub> (x = 0 $\leq$ 2) monolayer from a ferromagnetic half-metal to antiferromagnetic insulator. <i>Journal of Physics Condensed Matter</i> , 0, , .	0.7	0
18290	Exploration of reaction mechanism of LaFeO <sub>3</sub> oxygen carrier for chemical-looping steam methane reforming: A DFT study. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
18291	Theoretical investigation on NO reduction electro-catalyzed by transition-metal-anchored SnOSe nanotubes. <i>Nano Research</i> , 2023, 16, 8533-8541.	5.8	3
18292	Study of structural, magnetic and electronic properties of a new off-stoichiometric series of full-Heusler alloy Co <sub>2</sub> Nb <sub>1+x</sub> Z <sub>1-x</sub> (Z = As, In, Ga): Ab initio approach. <i>Journal of Alloys and Compounds</i> , 2023, 955, 170117.	2.8	2
18293	On the Strengthening Mechanisms and Interfacial Characteristics of TiB <sub>2</sub> /Hypoeutectic Al-Si Ceramic Composites. <i>Journal of Materials Engineering and Performance</i> , 2024, 33, 2623-2634.	1.2	0
18294	<sup>13</sup> C CPMAS NMR as an Alternative Method to Verify the Quality of Dietary Supplements Containing Curcumin. <i>Molecules</i> , 2023, 28, 3442.	1.7	2
18295	The electronic and optical properties of silicon doped on arsenic and antimony nanotubes: a first-principles study. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
18296	Dimensionality engineering dependence of vertical magnetization shift and magnetic anisotropy evolution in manganite superlattices. <i>Journal of Magnetism and Magnetic Materials</i> , 2023, 575, 170739.	1.0	0
18297	Comparison of the Performance of Density Functional Methods for the Description of Spin States and Binding Energies of Porphyrins. <i>Molecules</i> , 2023, 28, 3487.	1.7	3

#	ARTICLE	IF	CITATIONS
18298	Room-temperature fabrication of defective CoO <sub>x</sub> H <sub>y</sub> nanosheets with abundant oxygen vacancies and high porosity as efficient 5-hydroxymethylfurfural oxidation electrocatalysts. <i>Green Chemistry</i> , 2023, 25, 4674-4684.	4.6	5
18299	Evaluating thermal expansion in fluorides and oxides: Machine learning predictions with connectivity descriptors. <i>Chinese Physics B</i> , 2023, 32, 056302.	0.7	3
18300	Open metal sites in bimetallic vanadium/chromium-organic framework for enhancing adsorptive desulfurization performance. <i>Chemical Engineering Journal</i> , 2023, 465, 142989.	6.6	4
18301	Copper lattice tension boosts full-cell CO electrolysis to multi-carbon olefins and oxygenates. <i>Chem</i> , 2023, 9, 2161-2177.	5.8	14
18302	Hydrogen production from ammonia decomposition catalyzed by Ru nano-particles in alkaline molecular sieves under photothermal conditions. <i>Molecular Catalysis</i> , 2023, 543, 113160.	1.0	1
18303	Thermochemistry of the Smallest Hyperbolic Paraboloid Hydrocarbon: A High-Level Quantum Chemical Perspective. <i>Journal of Carbon Research</i> , 2023, 9, 41.	1.4	0
18304	Theoretical study of Li-ion migration in perovskite-type AVO <sub>3</sub> (A = Ca, La, Ce, and La <sub>0.75</sub> Ca <sub>0.25</sub> ) with DFT+U methods. <i>Materials Today Communications</i> , 2023, 35, 106029.	0.9	0
18305	In-Plane Anomalous Hall Effect in $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"> \langle \text{mml:mrow} \langle \text{mml:mi mathvariant="script">PT} \langle \text{mml:mi} \langle \text{mml:mrow} \langle \text{mml:math} \rangle \rangle \rangle \rangle \rangle$ -Symmetric Antiferromagnetic Materials. <i>Physical Review Letters</i> , 2023, 130, .	2.9	13
18306	Effects of Co Addition on Microstructure Evolution and Efficient Hydrogen Evolution of Self-Supported Fe@P@Cu Immiscible Alloy. , 0, , .		0
18307	DFT Study of Structural, Electronic, Thermoelectric and Elastic Properties of KPdX <sub>3</sub> (X = F, Cl, Br, and I) $\frac{1}{2} \text{ETQq1} \frac{1}{2} \frac{0.784314}{1.2} \text{rgBT} / \text{Over}$		0
18308	Strong ferromagnetism of g-C <sub>3</sub> N <sub>4</sub> achieved by atomic manipulation. <i>Nature Communications</i> , 2023, 14, .	5.8	20
18309	Density functional theoretical assessment of titanium metal for adsorption of hydrogen, deuterium and tritium isotopes. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	0
18310	Magneto-structural maps and bridged-ligand effect for dichloro-bridged dinuclear copper( <i>sc</i> ) complexes: a theoretical perspective. <i>RSC Advances</i> , 2023, 13, 12430-12437.	1.7	0
18311	Improved Mechanical Characterization of LiCoO <sub>2</sub> Cathode Material by <i>Ab-Initio</i> Calculations Using Density Functional Theory. <i>Bulletin of the Chemical Society of Japan</i> , 2023, 96, 475-483.	2.0	0
18312	DFT based comparative analysis of the physical properties of some binary transition metal carbides XC (X = Nb, Ta, Ti). <i>Journal of Materials Research and Technology</i> , 2023, 24, 4808-4832.	2.6	8
18313	Design and computational studies on energetic compounds composing bridged bis triazolo-triazine framework. <i>Chemical Physics</i> , 2023, 571, 111939.	0.9	2
18314	Experimental and theoretical studies of natural mineral attapulgite supported iron-based oxygen carriers in chemical looping hydrogen production. <i>Fuel</i> , 2023, 347, 128439.	3.4	2
18315	Sb <sub>4</sub> O <sub>3</sub> (TeO <sub>3</sub> ) <sub>2</sub> (HSO <sub>4</sub> ) <sub>2</sub> (OH): An Antimony Tellurite Sulfate Exhibiting Large Optical Anisotropy Activated by Lone Pair Stereoactivity. <i>Inorganic Chemistry</i> , 2023, 62, 7123-7129.	1.9	13

#	ARTICLE	IF	CITATIONS
18316	DFT study on termination stabilities of Mg17Al12 (110) surface. Transactions of Nonferrous Metals Society of China, 2023, 33, 755-764.	1.7	1
18317	Graphdiyne supported single-cluster catalysts catalyzed electrochemical nitrogen reduction reaction: A first-principles investigation. FlatChem, 2023, 39, 100507.	2.8	1
18318	Electronic, Optical, piezoelectric properties and photocatalytic water splitting performance of Two-dimensional group IV-V compounds. Applied Surface Science, 2023, 627, 157317.	3.1	4
18319	High graphitized N-doping porous carbon combined with bifunctional separator for the synergistic adsorption/conversion of polysulfides in Li-S batteries. Composites Part B: Engineering, 2023, 259, 110760.	5.9	2
18341	Comparative study of structural, electronic and magnetic properties of XBi (X = Gd, Tb, Dy, Ho, Er) alloys. AIP Conference Proceedings, 2023, , .	0.3	0
18345	Computational Approaches for Organic Semiconductors: From Chemical and Physical Understanding to Predicting New Materials. Chemical Reviews, 2023, 123, 7498-7547.	23.0	11
18379	Components of density functional reactivity theory-based stabilization energy: descriptors for thermodynamic and kinetic reactivity. , 2023, , 181-226.		1
18409	Modern Density Functionals Derived From First Principles. , 2024, , 69-77.		0
18430	Theoretical Approaches. , 2023, , 41-75.		0
18436	Template-free scalable growth of vertically-aligned MoS <sub>2</sub> nanowire array <i>meta</i>-structural films towards robust superlubricity. Materials Horizons, 2023, 10, 4148-4162.	6.4	1
18474	Density-Derived Electrostatic and Chemical Methods. , 2024, , 362-405.		1
18530	Optoelectronic and Thermoelectric Properties of the Perovskites: NaSnX <sub>3</sub> (X = Br or I) A DFT Study. Journal of Inorganic and Organometallic Polymers and Materials, 2023, 33, 3049-3059.	1.9	2
18555	Review of Approximations for the Exchange-Correlation Energy in Density-Functional Theory. , 2023, , 1-90.		3
18595	Quantum Chemistry of d- and f-Block Elements. , 2024, , 177-192.		1
18604	Analyzing barium titanate TiO <sub>2</sub> surface interactions with tert-butylphosphonic acid using density functional theory. MRS Communications, 0, , .	0.8	0
18620	Graphene-Sandwiched Van der Waals Heterostructures for Photodetectors. , 2023, , .		0
18696	Computational Insights of Dimensional Organic Materials. , 2023, , 382-473.		2
18708	Recent Mechanistic Insights into Some Enzyme Mimetic Functions of Ceria. Challenges and Advances in Computational Chemistry and Physics, 2024, , 201-229.	0.6	0

#	ARTICLE	IF	CITATIONS
18829	A covalency-aided electrochemical mechanism for CO <sub>2</sub> reduction: the synergistic effect of copper and boron dual active sites drives the formation of a high-efficiency ethanol product. <i>Nanoscale</i> , 2023, 15, 17776-17784.	2.8	1
18939	Phonon vortices at heavy impurities in two-dimensional materials. <i>Nanoscale Horizons</i> , 0, , .	4.1	0
18950	Single-atom catalysts supported on a hybrid structure of boron nitride/graphene for efficient nitrogen fixation <i>via</i> synergistic interfacial interactions. <i>Nanoscale</i> , 0, , .	2.8	0
19095	Investigation of Bulk,ÂElectronicÂand Transport Properties of Armchair Silicene Nanoribbon as Liquefied Petroleum Gas Combustion Indicator: A DFT Study. <i>Lecture Notes in Electrical Engineering</i> , 2024, , 273-287.	0.3	0
19100	Engineering a hollow bowl-like porous carbon-confined Ruâ€MgO hetero-structured nanopair as a high-performance catalyst for ammonia borane hydrolysis. <i>Materials Horizons</i> , 0, , .	6.4	1
19105	Hydrogen Storage Materialsâ€Background and Significance. <i>Green Energy and Technology</i> , 2024, , 263-302.	0.4	0