Alessandro Fortunelli

List of Publications by Year
in descending order

298 papers	11,405 citations	34105 52 h-index	39675 94 g-index
310 all docs	310 docs citations	310 times ranked	10096 citing authors

#	Article	IF	Citations
1	Vertical Heterostructures between Transitionâ€Metal Dichalcogenidesâ€”A Theoretical Analysis of the NbS2/WSe2 Junction. Advanced Electronic Materials, 2022, 8, .	5.1	6
2	Reaction Mechanisms, Kinetics, and Improved Catalysts for Ammonia Synthesis from Hierarchical High Throughput Catalyst Design. Accounts of Chemical Research, 2022, 55, 1124-1134.	15.6	23
3	Ab Initio Modeling of the ZnO-Cu(111) Interface. Journal of Physical Chemistry C, 2022, 126, 764-771.	3.1	7
4	Plasmonic Circular Dichroism in Chiral Gold Nanowire Dimers. Molecules, 2022, 27, 93.	3.8	5
5	Exploring the materials space in the smallest particle size range: from heterogeneous catalysis to electrocatalysis and photocatalysis. Physical Chemistry Chemical Physics, 2022, 24, 12083-12115.	2.8	14
6	Adsorption and Activation of CO2 on a Au19Pt Subnanometer Cluster in Aqueous Environment. Computational and Theoretical Chemistry, 2022, , 113701.	2.5	2
7	Unfolding the structural stability of nanoalloys via symmetry-constrained genetic algorithm and neural network potential. Npj Computational Materials, 2022, 8, .	8.7	9
8	Experimental Sabatier plot for predictive design of active and stable Pt-alloy oxygen reduction reaction catalysts. Nature Catalysis, 2022, 5, 513-523.	34.4	57
9	Mechanisms of the Oxygen Evolution Reaction on NiFe₂O₄ and CoFe₂O₄ Inverse-Spinel Oxides. ACS Catalysis, 2022, 12, 9058-9073.	11.2	40
10	Pristine graphene covalent functionalization with aromatic aziridines and their application in the sensing of volatile amines â€“ an ab initio investigation. RSC Advances, 2021, 11, 7070-7077.	3.6	10
11	An augmented (multi-descriptor) grouping algorithm to optimize chemical ordering in nanoalloys. Physical Chemistry Chemical Physics, 2021, 23, 23075-23089.	2.8	2
12	Theoretical Investigation of Photoinduced Processes in Subnanometer Oxide-Supported Metal Catalysts. Journal of Physical Chemistry C, 2021, 125, 2022-2032.	3.1	4
13	Diverse Phases of Carbonaceous Materials from Stochastic Simulations. ACS Nano, 2021, 15, 6369-6385.	14.6	10
14	Predictions of Chemical Shifts for Reactive Intermediates in CO2 Reduction under Operando Conditions. ACS Applied Materials & Interfaces, 2021, 13, 31554-31560.	8.0	12
15	Circularly Polarized Plasmons in Chiral Gold Nanowires via Quantum-Mechanical Design. Journal of Physical Chemistry Letters, 2021, 12, 5829-5835.	4.6	4
16	Understanding Reaction Networks through Controlled Approach to Equilibrium Experiments Using Transient Methods. Journal of the American Chemical Society, 2021, 143, 10998-11006.	13.7	6
17	6 The use of hydrogen in ammonia synthesis, and in oxygen and carbon dioxide catalytic reduction â€“ the reaction mechanisms. , 2021, , 269-302.		0
18	Predictive optical photoabsorption of Ag24Au(DMBT)18â^' via efficient TDDFT simulations. Journal of Chemical Physics, 2021, 155, 084103.	3.0	12

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19	Nanomolecular Metallurgy: Transformation from Au₁₄₄(SCH₂CH₂Ph)₆₀ to Au₂₇₉(SPh-tBu)₈₄. Journal of Physical Chemistry C, 2021, 125, 20488-20502.	3.1	4
20	Discovering indium as hydrogen production booster for a Cu/SiO2 catalyst in steam reforming of methanol. Applied Catalysis B: Environmental, 2021, 297, 120398.	20.2	26
21	Design of a fluorescent and clickable Ag₃₈(SRN₃)₂₄ nanocluster platform: synthesis, modeling and self-assembling. Nanoscale Advances, 2021, 3, 2948-2960.	4.6	2
22	Controlling the Shapes of Nanoparticles by Dopant-Induced Enhancement of Chemisorption and Catalytic Activity: Application to Fe-Based Ammonia Synthesis. ACS Nano, 2021, 15, 1675-1684.	14.6	11
23	Optical Activity of Metal Nanoclusters Deposited on Regular and Doped Oxide Supports from First-Principles Simulations. Molecules, 2021, 26, 6961.	3.8	2
24	Density Functional Theory Investigation of Graphene Functionalization with Activated Carbenes and Its Application in the Sensing of Heavy Metallic Cations. Journal of Physical Chemistry C, 2021, 125, 26418-26428.	3.1	11
25	Vibrational Spectroscopy Signatures of Catalytically Relevant Configurations for N₂ Reduction to NH₃ on Fe Surfaces via Density Functional Theory. Journal of Physical Chemistry C, 2021, 125, 27919-27930.	3.1	1
26	Isomeric Thiolate Monolayer Protected Au₉₂ and Au₁₀₂ Nanomolecules. Journal of Physical Chemistry C, 2020, 124, 1655-1666.	3.1	9
27	Chiral Functionalization of an Atomically Precise Noble Metal Cluster: Insights into the Origin of Chirality and Photoluminescence. ACS Nano, 2020, 14, 9687-9700.	14.6	56
28	Discovery of Dramatically Improved Ammonia Synthesis Catalysts through Hierarchical High-Throughput Catalyst Screening of the Fe(211) Surface. Chemistry of Materials, 2020, 32, 9914-9924.	6.7	6
29	Theoretical Analysis of a 2D Metallic/Semiconducting Transitionâ€Metal Dichalcogenide NbS₂//WSe₂ Hybrid Interface. Advanced Theory and Simulations, 2020, 3, 2000164.	2.8	4
30	The Missing Link: Au191(SPh-tBu)66 Janus Nanoparticle with Molecular and Bulk-Metal-like Properties. Journal of the American Chemical Society, 2020, 142, 15799-15814.	13.7	48
31	An efficient hybrid scheme for time dependent density functional theory. Journal of Chemical Physics, 2020, 152, 184104.	3.0	10
32	Si-Doped Fe Catalyst for Ammonia Synthesis at Dramatically Decreased Pressures and Temperatures. Journal of the American Chemical Society, 2020, 142, 8223-8232.	13.7	28
33	Edge Defects Promoted Oxidation of Monolayer WS₂ Synthesized on Epitaxial Graphene. Journal of Physical Chemistry C, 2020, 124, 9035-9044.	3.1	22
34	Reactivity and Catalysis by Nanoalloys. , 2020, , 267-345.		2
35	Selectivity-Driven Design of the Agâ€“Cu Alloys for the Ethylene Epoxidation. Industrial & Engineering Chemistry Research, 2019, 58, 12996-13006.	3.7	5
36	Ultrathin WO₃ Bilayer on Ag(100): A Model for the Structure of 2D WO₃ Nanosheets. Journal of Physical Chemistry C, 2019, 123, 27584-27593.	3.1	11

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37	Optical Properties and Chemical Ordering of Agâ€“Pt Nanoalloys: A Computational Study. Journal of Physical Chemistry C, 2019, 123, 25482-25491.	3.1	11
38	Laser-Beam-Patterned Topological Insulating States on Thin Semiconducting <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>MoS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></m Physical Review Letters, 2019, 123, 146803.	7.8	23
39	Effect of Co doping on mechanism and kinetics of ammonia synthesis on Fe(1â€¯1â€¯1) surface. Journal of Catalysis, 2019, 370, 364-371.	6.2	13
40	Highly Efficient Ni-Doped Iron Catalyst for Ammonia Synthesis from Quantum-Mechanics-Based Hierarchical High-Throughput Catalyst Screening. Journal of Physical Chemistry C, 2019, 123, 17375-17383.	3.1	16
41	2D oxides on metal materials: concepts, status, and perspectives. Physical Chemistry Chemical Physics, 2019, 21, 11510-11536.	2.8	37
42	Reaction mechanism and kinetics for ammonia synthesis on the Fe(211) reconstructed surface. Physical Chemistry Chemical Physics, 2019, 21, 11444-11454.	2.8	27
43	Reaction intermediates during operando electrocatalysis identified from full solvent quantum mechanics molecular dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 7718-7722.	7.1	70
44	Phonon-assisted carrier transport through a lattice-mismatched interface. NPG Asia Materials, 2019, 11, .	7.9	5
45	Crystal Structure of Au_{36-x}Ag_x(SPh-tBu)₂₄ Nanoalloy and the Role of Ag Doping in Excited State Coupling. Journal of Physical Chemistry C, 2019, 123, 29484-29494.	3.1	13
46	Ultralow Specific Contact Resistivity in Metalâ€“Graphene Junctions via Contact Engineering. Advanced Materials Interfaces, 2019, 6, 1801285.	3.7	41
47	Pd doping, conformational, and charge effects on the dichroic response of a monolayer protected Au₃₈(SR)₂₄ nanocluster. Physical Chemistry Chemical Physics, 2019, 21, 3585-3596.	2.8	6
48	Au₂₇₉(SR)₈₄: The Smallest Gold Thiolate Nanocrystal That Is Metallic and the Birth of Plasmon. Journal of Physical Chemistry Letters, 2018, 9, 1295-1300.	4.6	65
49	Principles of Optical Spectroscopy of Aromatic Alloy Nanomolecules: Au_{36â€“x}Ag_x(SPh-tBu)₂₄. Journal of Physical Chemistry C, 2018, 122, 4524-4531.	3.1	28
50	Bimetallic Agâ€Pt Subâ€nanometer Supported Clusters as Highly Efficient and Robust Oxidation Catalysts. Angewandte Chemie, 2018, 130, 1223-1227.	2.0	3
51	Reaction Mechanism and Kinetics for Ammonia Synthesis on the Fe(111) Surface. Journal of the American Chemical Society, 2018, 140, 6288-6297.	13.7	126
52	Perspective: Size selected clusters for catalysis and electrochemistry. Journal of Chemical Physics, 2018, 148, 110901.	3.0	93
53	Empirical-potential global minima and DFT local minima of trimetallic Ag Au Pt (l+m+n= 13, 19, 33, 38) clusters. Computational Materials Science, 2018, 141, 30-40.	3.0	29
54	Bimetallic Agâ€Pt Subâ€nanometer Supported Clusters as Highly Efficient and Robust Oxidation Catalysts. Angewandte Chemie - International Edition, 2018, 57, 1209-1213.	13.8	47

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55	Atomically precise Au₁₄₄(SR)₆₀ nanoclusters (R = Et, Pr) are capped by 12 distinct ligand types of 5-fold equivalence and display gigantic diastereotopic effects. Chemical Science, 2018, 9, 8796-8805.	7.4	30
56	QM-Mechanism-Based Hierarchical High-Throughput in Silico Screening Catalyst Design for Ammonia Synthesis. Journal of the American Chemical Society, 2018, 140, 17702-17710.	13.7	32
57	Electronic Structure of Oxide Ultrathin Layers on Metal Surfaces. , 2018, , 86-96.		0
58	TDDFT Study of the Optical Spectra of Free and Supported Binary Coinage Metal Hexamers: Effect of Doping and Support. Journal of Physical Chemistry C, 2018, 122, 23143-23152.	3.1	5
59	Chirality in bare and ligand-protected metal nanoclusters. Advances in Physics: X, 2018, 3, 1509727.	4.1	21
60	Stacking and interlayer electron transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mm Physical Review B, 2018, 98, .	3.2	10
61	Timeâ€dependent densityâ€functional study of the photoabsorption spectrum of Au₂₅(SC₂H₄C₆H₅)₁₈ anion: Validation of the computational protocol. International Journal of Quantum Chemistry, 2018, 118, e25769.	2.0	9
62	Au₃₆(SePh)₂₄ nanomolecules: synthesis, optical spectroscopy and theoretical analysis. Physical Chemistry Chemical Physics, 2018, 20, 13255-13262.	2.8	10
63	Ligand Structure Determines Nanoparticles' Atomic Structure, Metal-Ligand Interface and Properties. Frontiers in Chemistry, 2018, 6, 330.	3.6	58
64	Hydrogen evolution reaction (HER) on Au@Ag ultrananoclusters as electro-catalysts. Nanoscale, 2018, 10, 17730-17737.	5.6	21
65	Individual Component Map of Rotatory Strength and Rotatory Strength Density Plots As Analysis Tools of Circular Dichroism Spectra of Complex Systems. Journal of Chemical Theory and Computation, 2018, 14, 3703-3714.	5.3	13
66	Optical Properties of Metal Nanoclustersâ€”Theory. , 2018, , 534-545.		4
67	Highâ€Performance 2D pâ€Type Transistors Based on GaSe Layers: An Ab Initio Study. Advanced Electronic Materials, 2017, 3, 1600399.	5.1	20
68	Alumina-supported sub-nanometer Pt₁₀ clusters: amorphization and role of the support material in a highly active CO oxidation catalyst. Journal of Materials Chemistry A, 2017, 5, 4923-4931.	10.3	72
69	Ligand-Enhanced Optical Response of Gold Nanomolecules and Its Fragment Projection Analysis: The Case of Au₃₀(SR)₁₈. Journal of Physical Chemistry C, 2017, 121, 10832-10842.	3.1	21
70	Au₂₁S(SAdm)₁₅: Crystal Structure, Mass Spectrometry, Optical Spectroscopy, and First-Principles Theoretical Analysis. Journal of Physical Chemistry C, 2017, 121, 10865-10869.	3.1	29
71	Growthâ€Induced Strain in Chemical Vapor Deposited Monolayer MoS₂: Experimental and Theoretical Investigation. Advanced Materials Interfaces, 2017, 4, 1700031.	3.7	50
72	Magnetic Ordering in Gold Nanoclusters. ACS Omega, 2017, 2, 2607-2617.	3.5	69

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73	Au₃₈(SPh)₂₄: Au₃₈ Protected with Aromatic Thiolate Ligands. Journal of Physical Chemistry Letters, 2017, 8, 1530-1537.	4.6	33
74	Au₂₁S(SAdm)₁₅: An Anisotropic Gold Nanomolecule. Optical and Photoluminescence Spectroscopy and First-Principles Theoretical Analysis. Journal of Physical Chemistry Letters, 2017, 8, 457-462.	4.6	8
75	Intense fluorescence of Au20. Journal of Chemical Physics, 2017, 147, 074301.	3.0	18
76	Core-Size Conversion of Au₃₈(SCH₂CH₂Ph)₂₄ to Au₃₀(Sâ€“tBu)₁₈ Nanomolecules. Journal of Physical Chemistry C, 2017, 121, 14929-14935.	3.1	22
77	Electrical properties of graphene-metal contacts. Scientific Reports, 2017, 7, 5109.	3.3	119
78	Transistor Concepts Based on Lateral Heterostructures of Metallic and Semiconducting Phases of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>MoS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review Applied, 2017, 8, .	3.8	38
79	Core Size Interconversions of Au₃₀(S-tBu)₁₈ and Au₃₆(SPhX)₂₄. Journal of Physical Chemistry C, 2017, 121, 14914-14919.	3.1	38
80	A new timeâ€dependent densityâ€functional method for molecular plasmonics: Formalism, implementation, and the Au₁₄₄(SH)₆₀ case study. International Journal of Quantum Chemistry, 2016, 116, 1603-1611.	2.0	24
81	Nanoscale Domain Structure and Defects in a 2-D WO₃ Layer on Pd(100). Journal of Physical Chemistry C, 2016, 120, 28682-28693.	3.1	21
82	Optical absorption of (Ag-Au)133(SCH3)52 bimetallic monolayer-protected clusters. Progress in Natural Science: Materials International, 2016, 26, 467-476.	4.4	2
83	Two-dimensional transistors based on MoS<inf>2</inf> lateral heterostructures. , 2016, , .		2
84	Photoabsorption of Icosahedral Noble Metal Clusters: An Efficient TDDFT Approach to Large-Scale Systems. Journal of Physical Chemistry C, 2016, 120, 12773-12782.	3.1	57
85	Atomistic and Electronic Structure Methods for Nanostructured Oxide Interfaces. Springer Series in Materials Science, 2016, , 39-90.	0.6	4
86	Oxide Materials at the Two-Dimensional Limit. Springer Series in Materials Science, 2016, , .	0.6	24
87	Gate-Tunable Atomically Thin Lateral MoS₂ Schottky Junction Patterned by Electron Beam. Nano Letters, 2016, 16, 3788-3794.	9.1	99
88	Extension of the Time-Dependent Density Functional Complex Polarizability Algorithm to Circular Dichroism: Implementation and Applications to Ag₈ and Au₃₈(SC₂H₄C₆H₅)₂₄. Journal of Physical Chemistry C, 2016, 120, 24335-24345.	3.1	14
89	Editorial: Nanocatalysis. Catalysis Science and Technology, 2016, 6, 6763-6765.	4.1	5
90	Ultrafine jagged platinum nanowires enable ultrahigh mass activity for the oxygen reduction reaction. Science, 2016, 354, 1414-1419.	12.6	1,292

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91	All-atom molecular dynamics simulations of multiphase segregated polyurea under quasistatic, adiabatic, uniaxial compression. Polymer, 2016, 106, 100-108.	3.8	16
92	Catalytic activity of Pt₃₈ in the oxygen reduction reaction from first-principles simulations. Catalysis Science and Technology, 2016, 6, 6901-6909.	4.1	23
93	The quantum mechanics derived atomistic mechanism underlying the acceleration of catalytic CO oxidation on Pt(110) by surface acoustic waves. Journal of Materials Chemistry A, 2016, 4, 12036-12045.	10.3	7
94	Two-dimensional iron oxide bi-and trilayer structures on Pd(100). Surface Science, 2016, 645, 13-22.	1.9	10
95	Two-Dimensional Iron Tungstate: A Ternary Oxide Layer With Honeycomb Geometry. Journal of Physical Chemistry C, 2016, 120, 7629-7638.	3.1	28
96	Lattice Strain Defects in a Ceria Nanolayer. Journal of Physical Chemistry Letters, 2016, 7, 1303-1309.	4.6	17
97	Crystal Structure and Theoretical Analysis of Green Gold Au₃₀(S-tBu)₁₈ Nanomolecules and Their Relation to Au₃₀S(S-tBu)₁₈. Journal of Physical Chemistry C, 2016, 120, 6256-6261.	3.1	72
98	Nanoalloy Simulation. , 2016, , 2293-2305.		1
99	Simulation of Supported Metal Clusters. , 2016, , 3680-3692.		0
100	Does enhanced oxygen activation always facilitate <scp>CO</scp> oxidation on gold clusters?. Journal of Computational Chemistry, 2015, 36, 2177-2187.	3.3	10
101	Designing ligand-enhanced optical absorption of thiolated gold nanoclusters. Chemical Communications, 2015, 51, 7935-7938.	4.1	31
102	Transformation of Au₁₄₄(SCH₂CH₂Ph)₆₀ to Au₁₃₃(SPh-tBu)₅₂ Nanomolecules: Theoretical and Experimental Study. Journal of Physical Chemistry Letters, 2015, 6, 2134-2139.	4.6	58
103	Au₁₃₃(SPh-tBu)₅₂ Nanomolecules: X-ray Crystallography, Optical, Electrochemical, and Theoretical Analysis. Journal of the American Chemical Society, 2015, 137, 4610-4613.	13.7	265
104	Understanding the nature of metal-graphene contacts: A theoretical and experimental study. , 2015, , .		3
105	Analogy between homogeneous and heterogeneous catalysis by subnanometer metal clusters: Ethylene oxidation on Ag trimers supported on MgO(1 0 0). Inorganica Chimica Acta, 2015, 431, 150-155.	2.4	11
106	Optimizing the oxygen evolution reaction for electrochemical water oxidation by tuning solvent properties. Nanoscale, 2015, 7, 4514-4521.	5.6	20
107	The atomistic origin of the extraordinary oxygen reduction activity of Pt₃Ni₇fuel cell catalysts. Chemical Science, 2015, 6, 3915-3925.	7.4	53
108	Chemical properties of two-dimensional oxide systems: Adsorption of (WO3)3 clusters on CuWO4. Surface Science, 2015, 640, 96-103.	1.9	9

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109	Temperature and Doping Effect on Thermal Conductivity of Copperâ€“Gold Icosahedral Bimetallic Nanoclusters and Bulk Structures. Journal of Physical Chemistry C, 2015, 119, 7922-7932.	3.1	14
110	Optical properties of nanoalloys. Physical Chemistry Chemical Physics, 2015, 17, 27952-27967.	2.8	45
111	Organosoluble Au₁₀₂(SPh)₄₄ Nanomolecules: Synthesis, Isolation, Compositional Assignment, Core Conversion, Optical Spectroscopy, Electrochemistry, and Theoretical Analysis. Journal of Physical Chemistry C, 2015, 119, 25077-25084.	3.1	24
112	Exploring the energy landscape of Pt Au115â^' nanoalloys. Computational and Theoretical Chemistry, 2015, 1074, 150-156.	2.5	4
113	Comment on â€œ(Auâ€“Ag)₁₄₄(SR)₆₀alloy nanomoleculesâ€•by C. Kumara and A. Dass, Nanoscale, 2011,3, 3064. Nanoscale, 2015, 7, 8166-8167.	5.6	17
114	Simulation of Supported Metal Clusters. , 2015, , 1-14.		1
115	Nanoalloy Simulation. , 2015, , 1-13.		0
116	Ligand/cluster/support catalytic complexes in heterogeneous ultrananocatalysis: NO oxidation on Ag₃/MgO(100). Physical Chemistry Chemical Physics, 2014, 16, 26570-26577.	2.8	10
117	Concepts in theoretical heterogeneous ultrananocatalysis. Comptes Rendus Chimie, 2014, 17, 625-633.	0.5	26
118	Tuning the catalytic activity of Auâ€“Pd nanoalloys in CO oxidation via composition. Journal of Catalysis, 2014, 314, 47-55.	6.2	33
119	Dramatic Increase in the Oxygen Reduction Reaction for Platinum Cathodes from Tuning the Solvent Dielectric Constant. Angewandte Chemie - International Edition, 2014, 53, 6669-6672.	13.8	33
120	Metal Tungstates at the Ultimate Two-Dimensional Limit: Fabrication of a CuWO₄ Nanophase. ACS Nano, 2014, 8, 3947-3954.	14.6	53
121	Au₂₄(SAdm)₁₆ Nanomolecules: X-ray Crystal Structure, Theoretical Analysis, Adaptability of Adamantane Ligands to Form Au₂₃(SAdm)₁₆ and Au₂₅(SAdm)₁₆, and Its Relation to Au₂₅(SR)₁₈. Journal of the American Chemical Society, 2014, 136, 14933-14940.	13.7	139
122	Optical Properties of Pt and Agâ€“Pt Nanoclusters from TDDFT Calculations: Plasmon Suppression by Pt Poisoning. Journal of Physical Chemistry C, 2014, 118, 28101-28108.	3.1	18
123	Probing the atomic structure of metallic nanoclusters with the tip of a scanning tunneling microscope. Nanoscale, 2014, 6, 2170-2176.	5.6	20
124	Optical Properties of Silver Nanoshells from Time-Dependent Density Functional Theory Calculations. Journal of Physical Chemistry C, 2014, 118, 12450-12458.	3.1	38
125	A grouping approach to homotop global optimization in alloy nanoparticles. Physical Chemistry Chemical Physics, 2014, 16, 24256-24265.	2.8	34
126	Composition-dependent melting behaviour of NaxK55â€“xcoreâ€“shell nanoalloys. Molecular Physics, 2014, 112, 2933-2944.	1.7	2

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127	Experimental and Theoretical Scanning Tunneling Spectroscopy Analysis of an Ultrathin Titania Film and Adsorbed Au Nanoparticles. Journal of Physical Chemistry C, 2014, 118, 14640-14646.	3.1	2
128	Redox processes at a nanostructured interface under strong electric fields. Nanoscale, 2014, 6, 10589-10595.	5.6	4
129	Atomistic Quantum Plasmonics of Gold Nanowire Arrays. ACS Photonics, 2014, 1, 315-322.	6.6	13
130	Communication: Striking dependence of diffusion kinetics in Agâ€“Cu nanoalloys upon composition and quantum effects. Journal of Chemical Physics, 2014, 141, 041108.	3.0	10
131	Influence of temperature and H2 adsorption on the structure of silica-supported gold subnanometer clusters. Computational and Theoretical Chemistry, 2013, 1021, 222-228.	2.5	10
132	Reactivity and catalysis by nanoalloys. , 2013, , 283-344.		1
133	Structure and Electronic Properties of CoO Nanostructures on a Vicinal Pd(100) Surface. Journal of Physical Chemistry C, 2013, 117, 18464-18474.	3.1	12
134	Effect of CO and H adsorption on the compositional structure of binary nanoalloys via DFT modeling. European Physical Journal D, 2013, 67, 1.	1.3	13
135	Electronic excited states at ultrathin dielectric-metal interfaces. Physical Review B, 2013, 88, .	3.2	5
136	Alloys on the Nanoscale. , 2013, , 409-472.		1
137	Global Minimum Pt₁₃M₂₀ (M = Ag, Au, Cu, Pd) Dodecahedral Coreâ€“Shell Clusters. Journal of Physical Chemistry A, 2013, 117, 14261-14266.	2.5	32
138	Study of two dimensional anisotropic Ising models via a renormalization group approach. Physica A: Statistical Mechanics and Its Applications, 2013, 392, 5604-5614.	2.6	3
139	Communication: Kinetics of chemical ordering in Ag-Au and Ag-Ni nanoalloys. Journal of Chemical Physics, 2013, 139, 111102.	3.0	29
140	Direct atomic imaging and density functional theory study of the Au24Pd1 cluster catalyst. Nanoscale, 2013, 5, 9620.	5.6	37
141	DFT study of the structures and energetics of 98-atom AuPd clusters. Nanoscale, 2013, 5, 646-652.	5.6	56
142	Adsorptionâ€Induced Restructuring and Early Stages of Carbonâ€Nanotube Growth on Ni Nanoparticles. Chemistry - A European Journal, 2013, 19, 406-413.	3.3	2
143	Nanostripe Pattern of NaCl Layers on Cu(110). Physical Review Letters, 2013, 110, 216101.	7.8	18
144	Density-Functional Theory of Free and Supported Metal Nanoclusters and Nanoalloys. Nanostructure Science and Technology, 2013, , 29-79.	0.1	7

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145	Modelling the metal-on-top effect for Pd clusters on the MgO{100} substrate. Journal of Chemical Physics, 2013, 138, 224703.	3.0	11
146	Computational Approaches to the Chemical Conversion of Carbon Dioxide. ChemSusChem, 2013, 6, 944-965.	6.8	144
147	Structureâ€“Property Relationship and Chemical Aspects of Oxideâ€“Metal Hybrid Nanostructures. Chemical Reviews, 2013, 113, 4314-4372.	47.7	160
148	Structural Motifs of Bimetallic Pt_{101â€“x}Au_x Nanoclusters. Journal of Physical Chemistry C, 2013, 117, 20967-20974.	3.1	12
149	Kinetic asymmetry in the growth of two-dimensional Mn oxide nanostripes. Physical Review B, 2013, 88, .	3.2	14
150	Ordered Arrays of Size-Selected Oxide Nanoparticles. Physical Review Letters, 2012, 108, 195507.	7.8	21
151	Au<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>N</mml:mi></mml:msub></mml:math>clusters (<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML") Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 502 Td (display="in on MgO(100) surfaces: Effect of exact exchange and dispersion interactions on adhesion energies. Physical Review B, 2012, 85, .	3.2	35
152	Dependence of self-diffusion coefficient, surface energy, on size, temperature, and Debye temperature on size for aluminum nanoclusters. Fluid Phase Equilibria, 2012, 335, 26-31.	2.5	18
153	Building Principles and Structural Motifs in TiO_x Ultrathin Films on a (111) Substrate. Journal of Physical Chemistry C, 2012, 116, 13302-13306.	3.1	30
154	Scanning tunneling microscopy imaging of NiO(100)(1Ã—1) islands embedded in Ag(100). Surface Science, 2012, 606, 803-807.	1.9	23
155	Theoretical study of AuCu nanoalloys adsorbed on MgO(001). Surface Science, 2012, 606, 938-944.	1.9	11
156	CO Oxidation by Subnanometer Ag_xAu_{3â€“x} Supported Clusters via Density Functional Theory Simulations. ACS Catalysis, 2012, 2, 1860-1864.	11.2	57
157	Growth of carbon clusters on a Ni(111) surface. Computational Materials Science, 2012, 63, 303-311.	3.0	13
158	Theoretical Modelling of Oxide-Supported Metal Nanoclusters and Nanoalloys. Frontiers of Nanoscience, 2012, , 159-211.	0.6	2
159	Kinetics of chemical ordering in a Ag-Pt nanoalloy particle via first-principles simulations. Journal of Chemical Physics, 2012, 137, 194302.	3.0	21
160	Spin coupling and magnetic field effects on the finite-size free energy and its non-extensivity for 1-D Ising model with nearest and next-nearest neighbor interactions in nanosystem. Phase Transitions, 2012, 85, 577-591.	1.3	1
161	Work Function of Oxide Ultrathin Films on the Ag(100) Surface. Journal of Chemical Theory and Computation, 2012, 8, 629-638.	5.3	24
162	A first-principles theoretical approach to heterogeneous nanocatalysis. Nanoscale, 2012, 4, 1208-1219.	5.6	47

#	Article	IF	Citations
163	Tracking thermally-activated transformations in a nanostructured metal/oxide/metal system. Physical Chemistry Chemical Physics, 2011, 13, 17171.	2.8	6
164	Homogeneous Nucleation of Graphitic Nanostructures from Carbon Chains on Ni(111). Journal of Physical Chemistry C, 2011, 115, 10537-10543.	3.1	68
165	Interplay between Layer-Resolved Chemical Composition and Electronic Structure in a Sn/Pt(110) Surface Alloy. Journal of Physical Chemistry C, 2011, 115, 14264-14269.	3.1	14
166	Alloying Effects on the Optical Properties of Agâ€“Au Nanoclusters from TDDFT Calculations. Journal of Physical Chemistry C, 2011, 115, 24085-24091.	3.1	61
167	Structure and Bonding of Tungsten Oxide Clusters on Nanostructured Cu-O Surfaces. Journal of Physical Chemistry C, 2011, 115, 23480-23487.	3.1	30
168	On the existence of an analytic solution to the 1-D Ising model with nearest and next-nearest neighbor interactions in the presence of a magnetic field. Phase Transitions, 2011, 84, 77-84.	1.3	5
169	Optimization of chemical ordering in AgAu nanoalloys. Physical Chemistry Chemical Physics, 2011, 13, 10232.	2.8	55
170	Optical Properties of Au Nanoclusters from TD-DFT Calculations. Journal of Physical Chemistry C, 2011, 115, 6277-6282.	3.1	100
171	Interface Effects on the Magnetism of CoPt-Supported Nanostructures. Nano Letters, 2011, 11, 5542-5547.	9.1	27
172	Investigation of magnetic field effect on surface and finite-site free energy in one-dimensional Ising model of nanosystems. Phase Transitions, 2011, 84, 613-623.	1.3	1
173	Patchy Multishell Segregation in Pdâ^'Pt Alloy Nanoparticles. Nano Letters, 2011, 11, 1766-1769.	9.1	94
174	Investigation of size effects on the physical properties of one-dimensional Ising models in nanosystems. Molecular Physics, 2011, 109, 385-395.	1.7	3
175	Size-dependent selectivity and activity of silver nanoclusters in the partial oxidation of propylene to propylene oxide and acrolein: A joint experimental and theoretical study. Catalysis Today, 2011, 160, 116-130.	4.4	115
176	Template-assisted assembly of transition metal nanoparticles on oxide ultrathin films. Progress in Surface Science, 2011, 86, 59-81.	8.3	38
177	Structures of AgPd nanoclusters adsorbed on MgO(100): A computational study. Surface Science, 2011, 605, 483-488.	1.9	24
178	Structures of small Au clusters on MgO(001) studied by density-functional calculations. Physical Review B, 2011, 83, .	3.2	29
179	Metamorphosis of ultrathin Ni oxide nanostructures on Ag(100). Physical Review B, 2011, 84, .	3.2	24
180	The two-dimensional cobalt oxide (9 Ã— 2) phase on Pd(100). Journal of Chemical Physics, 2011, 134, 184706.	3.0	24

#	Article	IF	Citations
181	Kondo versus magnetic coupling of cobalt dimers in a Cuâ€“O (2 Ã— 1) reconstruction. Journal of Physics Condensed Matter, 2010, 22, 222202.	1.8	3
182	Analysis of the electronic structure of ultrathin NiO/Ag(100) films. European Physical Journal B, 2010, 75, 5-13.	1.5	14
183	Simulation of vacancy diffusion in a silver nanocluster. Chemical Physics Letters, 2010, 498, 312-316.	2.6	14
184	Kondo effect of cobalt adatoms on nanostructured Cu-O surfaces: Scanning tunneling spectroscopy experiments and first-principles calculations. Physical Review B, 2010, 81, .	3.2	23
185	Validation of density-functional versus density-functional+U approaches for oxide ultrathin films. Journal of Chemical Physics, 2010, 132, 124703.	3.0	47
186	Growth and Surface Structure of Zinc Oxide Layers on a Pd(111) Surface. Journal of Physical Chemistry C, 2010, 114, 15432-15439.	3.1	153
187	Exotic Supported CoPt Nanostructures: From Clusters to Wires. Journal of Physical Chemistry Letters, 2010, 1, 111-115.	4.6	41
188	The Effect of CO and H Chemisorption on the Chemical Ordering of Bimetallic Clusters. Journal of Physical Chemistry C, 2010, 114, 19678-19686.	3.1	47
189	Prediction of the structures of free and oxide-supported nanoparticles by means of atomistic approaches: the benchmark case of nickel clusters. Physical Chemistry Chemical Physics, 2010, 12, 8564.	2.8	11
190	Structures of gas-phase Agâ€“Pd nanoclusters: A computational study. Journal of Chemical Physics, 2010, 132, 234703.	3.0	44
191	Preparation, characterisation and structure of Ti and Al ultrathin oxide films on metals. International Reviews in Physical Chemistry, 2009, 28, 517-576.	2.3	75
192	Surface-Supported Gold Cages. Physical Review Letters, 2009, 102, 216102.	7.8	34
193	Structures of metal nanoparticles adsorbed on MgO(001). II. Pt and Pd. Journal of Chemical Physics, 2009, 130, 174703.	3.0	48
194	Structural and electronic properties of small platinum metallorganic complexes. Theoretical Chemistry Accounts, 2009, 123, 317-325.	1.4	7
195	Chemisorption of CO and H on Pd, Pt and Au nanoclusters: a DFT approach. European Physical Journal D, 2009, 52, 131-134.	1.3	37
196	Cooperative Phase Transformation in Self-Assembled Metal-on-Oxide Arrays. Journal of Physical Chemistry C, 2009, 113, 1143-1146.	3.1	13
197	Structure of Reduced Ultrathin TiO_x Polar Films on Pt(111). Journal of Physical Chemistry C, 2009, 113, 5721-5729.	3.1	64
198	Diffusion of adatoms and small clusters on magnesium oxide surfaces. Journal of Physics Condensed Matter, 2009, 21, 264001.	1.8	22

#	Article	IF	Citations
199	Theoretical Studies of Palladiumâ^'Gold Nanoclusters: Pdâ^'Au Clusters with up to 50 Atoms. Journal of Physical Chemistry C, 2009, 113, 9141-9152.	3.1	152
200	Adsorption and Diffusion of Fe on a Titania Ultrathin Film. Journal of Physical Chemistry A, 2009, 113, 14860-14866.	2.5	12
201	Directed assembly of Au and Fe nanoparticles on a TiOx/Pt(111) ultrathin template: the role of oxygen affinity. Physical Chemistry Chemical Physics, 2009, 11, 11305.	2.8	19
202	Au nanoparticles on a templating TiOx/Pt(111) ultrathin polar film: a photoemission and photoelectron diffraction study. Physical Chemistry Chemical Physics, 2009, 11, 2177.	2.8	17
203	Structures of metal nanoparticles adsorbed on MgO(001). I. Ag and Au. Journal of Chemical Physics, 2009, 130, 174702.	3.0	75
204	Small Au clusters on a defective MgO(100) surface. Chemical Physics Letters, 2008, 457, 143-147.	2.6	15
205	Searching for the optimum structures of alloy nanoclusters. Physical Chemistry Chemical Physics, 2008, 10, 640-649.	2.8	185
206	Structural motifs, mixing, and segregation effects in 38-atom binary clusters. Journal of Chemical Physics, 2008, 128, 134517.	3.0	147
207	Interface-Stabilized Phases of Metal-on-Oxide Nanodots. ACS Nano, 2008, 2, 1849-1856.	14.6	58
208	A study of bimetallic Cuâ€“Ag, Auâ€“Ag and Pdâ€“Ag clusters adsorbed on a double-vacancy-defected MgO(100) terrace. Faraday Discussions, 2008, 138, 37-47.	3.2	27
209	Metal adsorption on oxide polar ultrathin films. Physical Chemistry Chemical Physics, 2008, 10, 1876.	2.8	24
210	Mobility of Au on TiO_x Substrates with Different Stoichiometry and Defectivity. Journal of Physical Chemistry C, 2008, 112, 3187-3190.	3.1	25
211	Simulations of Lipid Adsorption on TiO₂ Surfaces in Solution. Langmuir, 2008, 24, 10145-10154.	3.5	35
212	Defect evolution in oxide nanophases: The case of a zigzag-like<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:mrow></mml:math>phase on Pt(111). Physical Review B, 2008, 77, .	3.2	43
213	Derivation of an empirical potential for gold with angular corrections. Physical Review B, 2008, 77, .	3.2	18
214	Structure and diffusion of small Ag and Au clusters on the regular MgO (100) surface. New Journal of Physics, 2007, 9, 22-22.	2.9	64
215	Epitaxy, Truncations, and Overhangs in Palladium Nanoclusters Adsorbed on MgO(001). Physical Review Letters, 2007, 98, 156101.	7.8	38
216	Constitutive model for plasticity in an amorphous polycarbonate. Physical Review E, 2007, 76, 041806.	2.1	8

#	Article	IF	Citations
217	Magic silver cluster on a MgO(100) terrace with defects. Physical Review B, 2007, 76, .	3.2	27
218	A Magic Pdâ^'Ag Binary Cluster on the Fs-Defected MgO(100) Surface. Journal of Physical Chemistry C, 2007, 111, 11384-11389.	3.1	60
219	A Mixed Structural Motif in 34-Atom Pdâ^'Pt Clusters. Journal of Physical Chemistry C, 2007, 111, 2936-2941.	3.1	90
220	Structure of a TiOx Zigzag-Like Monolayer on Pt(111). Journal of Physical Chemistry C, 2007, 111, 6095-6102.	3.1	45
221	Structures and energetics of 98 atom Pdâ€"Pt nanoalloys: potential stability of the Leary tetrahedron for bimetallic nanoparticles. Physical Chemistry Chemical Physics, 2007, 9, 5202.	2.8	84
222	Structure of Ag Clusters Grown on Fs-Defect Sites of an MgO(1â€‰0â€‰0) Surface. Chemistry - A European Journal, 2007, 13, 6408-6418.	3.3	46
223	A comparison between the absorption properties of the regular and F s -defected MgO (100) surface. Theoretical Chemistry Accounts, 2007, 118, 807-812.	1.4	16
224	Density-functional global optimization of gold nanoclusters. Physical Review B, 2006, 73, .	3.2	106
225	Electronic and Structural Shell Closure in AgCu and AuCu Nanoclusters. Journal of Physical Chemistry B, 2006, 110, 23197-23203.	2.6	90
226	Rotational Invariance and Double Frustration in the Structures of Gold Clusters Growing around the Fs-Defected MgO (100) Surface. Journal of Physical Chemistry B, 2006, 110, 21021-21027.	2.6	22
227	Quantum effects on the structure of pure and binary metallic nanoclusters. Physical Review B, 2005, 72, .	3.2	174
228	Diffusion of Palladium Clusters on Magnesium Oxide. Physical Review Letters, 2005, 95, 246103.	7.8	62
229	The Interaction of Coinage Metal Clusters with the MgO(100) Surface. Journal of Chemical Theory and Computation, 2005, 1, 972-985.	5.3	114
230	Global optimization of bimetallic cluster structures. I. Size-mismatched Agâ€"Cu, Agâ€"Ni, and Auâ€"Cu systems. Journal of Chemical Physics, 2005, 122, 194308.	3.0	307
231	Global optimization of bimetallic cluster structures. II. Size-matched Ag-Pd, Ag-Au, and Pd-Pt systems. Journal of Chemical Physics, 2005, 122, 194309.	3.0	192
232	Simulation of the plastic behavior of amorphous glassy bis-phenol-A-polycarbonate. Journal of Chemical Physics, 2004, 121, 4941-4950.	3.0	16
233	Tight-binding parameterization of transition and noble metal clusters. International Journal of Quantum Chemistry, 2004, 99, 654-666.	2.0	9
234	Separability between valence and conduction bands in transition metal clusters. International Journal of Quantum Chemistry, 2004, 100, 277-287.	2.0	5

#	Article	IF	Citations
235	Magic Polyicosahedral Core-Shell Clusters. Physical Review Letters, 2004, 93, 105503.	7.8	361
236	Amorphization Mechanism of Icosahedral Metal Nanoclusters. Physical Review Letters, 2004, 93, 065502.	7.8	113
237	Density-Functional Calculations on Platinum Nanoclusters:â€‰ Pt13, Pt38, and Pt55. Journal of Physical Chemistry A, 2003, 107, 2934-2942.	2.5	96
238	NWChem for materials science. Computational Materials Science, 2003, 28, 209-221.	3.0	25
239	Crossover among structural motifs in transition and noble-metal clusters. Journal of Chemical Physics, 2002, 116, 3856-3863.	3.0	431
240	A theoretical study of the catalytic properties of Pt/Fe nanoclusters. Computational and Theoretical Chemistry, 2002, 586, 17-27.	1.5	19
241	Mechanism of Protonation of [Pt3(Î¼-PBut2)3(H)(CO)2], Yielding the Hydride-Bridged [Pt3(Î¼-PBut2)2(Î¼-H)(PBut2H)(CO)2]OTf (Tf = CF3SO2), and the Spectroscopic and Theoretical Characterization of a Kinetic Intermediate. Inorganic Chemistry, 2001, 40, 3055-3060.	4.0	17
242	Symmetrized mean-field description of magnetic instabilities inÎºâˆ’(BEDTâˆ’TTF)2Cu[N(CN)]2Ysalts. Physical Review B, 2001, 64, .	3.2	8
243	Density-functional study of Pt 13 and Pt 55 cuboctahedral clusters. Computational and Theoretical Chemistry, 2000, 501-502, 251-259.	1.5	48
244	Local properties of PT/FE nanoclusters from EHT calculations. Computational and Theoretical Chemistry, 2000, 528, 1-12.	1.5	8
245	Ab Initio Study of the Intra- and Intermolecular Bonding in AuCl(CO)â€. Journal of Physical Chemistry A, 2000, 104, 10834-10841.	2.5	16
246	Structural and electronic properties of Pt/Fe nanoclusters from EHT calculations. Computational and Theoretical Chemistry, 1999, 487, 251-266.	1.5	48
247	Density functional calculations on small platinum clusters: Pt n q (n =1â€“4, q =0,Â±1). Computational and Theoretical Chemistry, 1999, 493, 233-240.	1.5	44
248	The Îº-(BEDT-TTF)2Cu[N(CN)]2X family: A mean field view. Synthetic Metals, 1999, 103, 1993-1994.	3.9	1
249	Îº-Phase organic superconductors: the dimer model. Synthetic Metals, 1999, 103, 1995.	3.9	0
250	Experimental and Theoretical Study of the Kinetic and Thermodynamic Sites of Protonation in (CO)Pt(Î¼-PBut2)2Pt(PBut2H). Inorganic Chemistry, 1999, 38, 5257-5265.	4.0	14
251	Perturbation-response theory as a basis for the continuum models of solvation Inclusion of the polarization. Computational and Theoretical Chemistry, 1998, 428, 9-25.	1.5	1
252	Oxidant-Induced Hydride Abstraction from [Pt(Î¼-PBut2)(H)(PBut2H)]2Yielding [Pt2(Î¼-PBut2)2(H)(PBut2H)2]C3(CN)5. Spectroscopic, Crystallographic, and Theoretical Comparison of the Structures of Two â€œTautomersâ€• Journal of the American Chemical Society, 1998, 120, 9564-9573.	13.7	49

#	Article	IF	Citations
253	The dimer model for Î²-phase organic superconductors. Europhysics Letters, 1998, 42, 467-472.	2.0	22
254	Ab initio estimate of Hubbard model parameters:mA simple procedure appliedto BEDT-TTF salts. Physical Review B, 1997, 55, 16088-16095.	3.2	44
255	On theab initioevaluation of Hubbard parameters. II. The Î²-(BEDT-TTF)2Cu[N(CN)2]Br crystal. Journal of Chemical Physics, 1997, 106, 8051-8058.	3.0	31
256	On theab initioevaluation of Hubbard parameters. I. The analytical approach in the absence of orbital relaxation. Journal of Chemical Physics, 1997, 106, 8041-8050.	3.0	14
257	BEDT-TTF salts: microscopic parameters from ab-initio calculations. Synthetic Metals, 1997, 85, 1631-1632.	3.9	2
258	Synthesis, molecular and electronic structure of the first homoleptic complex of platinum with a secondary phosphine. Inorganica Chimica Acta, 1997, 264, 185-191.	2.4	13
259	On the solvation of (quasi-)degenerate solutes: a continuum analysis based on perturbation-response theory. Chemical Physics Letters, 1996, 248, 50-56.	2.6	4
260	Simplifications in the Theoretical Treatment of Solvation Effects Based on the Quadratic Expansion of the Energy. The Journal of Physical Chemistry, 1995, 99, 9056-9061.	2.9	10
261	Enthalpies of formation from theoretical methods: a new approach based on density functional theory plus semiempirical corrections. Computational and Theoretical Chemistry, 1995, 337, 25-30.	1.5	15
262	A study of the MBPT correlation corrections within the polarizable continuum model for solvation. Computational and Theoretical Chemistry, 1995, 357, 117-124.	1.5	8
263	Validation of selfâ€consistent hybrid density functionals for the study of structural and electronic characteristics of organic Ï€ radicals. Journal of Chemical Physics, 1995, 102, 384-393.	3.0	138
264	Ab initio calculations of isotropic hyperfine coupling constants in ?-ketoenolyl radicals. International Journal of Quantum Chemistry, 1994, 52, 97-108.	2.0	11
265	An analysis of the integrand occurring in correlation energy functionals. International Journal of Quantum Chemistry, 1994, 52, 705-710.	2.0	0
266	Density functional calculations on hydrocarbon isodesmic reactions. Chemical Physics Letters, 1994, 223, 390-396.	2.6	13
267	The implementation of density functional theory within the polarizable continuum model for solvation. Chemical Physics Letters, 1994, 231, 34-39.	2.6	81
268	The orbital relaxation: A possible origin of t - J model with large J. Solid State Communications, 1994, 89, 771-773.	1.9	3
269	Density Functional Calculations of Isotropic Hyperfine Coupling Constants in .beta.-Ketoenolyl Radicals. The Journal of Physical Chemistry, 1994, 98, 8648-8652.	2.9	29
270	Interacting electrons in the solid state: the role of orbital relaxation. Chemical Physics Letters, 1993, 214, 402-408.	2.6	10

#	Article	IF	Citations
271	A numerical integration scheme for the evaluation of correlation energy functionals. International Journal of Quantum Chemistry, 1993, 47, 135-144.	2.0	5
272	Recurrence relations for the evaluation of electron repulsion integrals over spherical Gaussian functions. International Journal of Quantum Chemistry, 1993, 48, 257-265.	2.0	12
273	Ab initio calculations of isotropic hyperfine coupling constants in Î²-ketoenolyl radicals. Computational and Theoretical Chemistry, 1993, 287, 89-92.	1.5	8
274	Alternative basis functions forL2calculations on the molecular continuum. II. Integrals with higher-order functions. Physical Review A, 1992, 45, 4438-4451.	2.5	5
275	Alternative basis functions forL2calculations on the molecular continuum. I. The basic prototype integrals. Physical Review A, 1992, 45, 4426-4437.	2.5	2
276	Valence-space-only calculations on molecules: polarization effects. Molecular Physics, 1992, 75, 1191-1202.	1.7	1
277	Algebraic formulae of matrix elements between valence-bond determinants for periodic systems: The one-band linear case. International Journal of Quantum Chemistry, 1992, 43, 281-300.	2.0	1
278	Cluster Simulations of Amorfous Silicon, with and without an Impurity Boron Atom. NATO ASI Series Series B: Physics, 1992, , 595-603.	0.2	1
279	Chemisorption of Ag on the Si(111) surface: a theoretical study. Surface Science, 1991, 244, 355-361.	1.9	15
280	Theoretical investigation of the ground and the lowest excited states of Co(SB) complexes (SB =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	4.0	4
281	Overlapping and non-overlapping integrals in molecular calculations. Chemical Physics Letters, 1991, 186, 372-378.	2.6	14
282	A simplified representation of the potential produced by Gaussian charge distributions. Journal of Computational Chemistry, 1991, 12, 36-41.	3.3	19
283	Single-centre expansion and angular decomposition of the overlap integral for Hermite Gaussian functions. Journal of Physics B: Atomic, Molecular and Optical Physics, 1990, 23, 1945-1949.	1.5	0
284	Test applications of a new SCF method for excited states. Theoretica Chimica Acta, 1989, 75, 323-331.	0.8	12
285	On the evaluation of matrix elements between slater determinants orthogonal among themselves. Chemical Physics Letters, 1988, 144, 493-496.	2.6	1
286	The Lippmann-Schwinger equation for obtaining the continuum orbital in Auger problems: Application to the KLL spectrum of atomic neon. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1988, 10, 355-360.	0.4	4
287	Hermite Gaussian functions modulated by plane waves: a general basis set for bound and continuum states. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1988, 10, 805-818.	0.4	16
288	A theoretical investigation of the ground and a few excited states of the lithium cobalt-Schiff base complexes. Journal of the American Chemical Society, 1988, 110, 8016-8022.	13.7	9

#	Article	IF	Citations
289	Correlation correction to the Hartree-Fock total energy of solids. II. Physica Scripta, 1988, 38, 194-198.	2.5	31
290	Hartree-Fock plus correlation energy in the valence space. The Journal of Physical Chemistry, 1988, 92, 921-924.	2.9	2
291	Correlation correction to the Hartree-Fock total energy of solids. Physical Review B, 1987, 36, 891-897.	3.2	75
292	An SCF technique for excited states. Theoretica Chimica Acta, 1987, 71, 467-478.	0.8	32
293	A mixed basis set of Slater and Gaussian functions. Integrals with modified Gaussian functions. International Journal of Quantum Chemistry, 1987, 31, 893-901.	2.0	3
294	A mixed basis set of plane waves and Hermite Gaussian functions. Analytic expressions of prototype integrals. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1987, 9, 969-977.	0.4	19
295	A valence-space-only approach to the calculation of the electronic structure of many electron systems. Molecular Physics, 1986, 57, 1305-1316.	1.7	12
296	Analysis of valence orbitals in the â€œcoreâ€•regions. Chemical Physics Letters, 1986, 127, 84-87.	2.6	5
297	A mixed basis set of slater and gaussian functions for molecular calculations. International Journal of Quantum Chemistry, 1986, 29, 1825-1837.	2.0	3
298	Atoms in molecules. I. A charge conservation rule for taking into account the â€˜â€˜orthogonality holeâ€™â€™. Journal of Chemical Physics, 1984, 80, 2654-2659.	3.0	18