Rui-Qin Zhang

List of Publications by Year
in descending order

374	11,212	31976 53	48315 88
papers	citations	h-index	g-index

385	385	385	12522
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The thermal and elastic properties of U3Si5 and their variations induced by incorporated aluminum. Journal of Nuclear Materials, 2022, 558, 153331.	2.7	1
2	Î”-Machine learning-driven discovery of double hybrid organicâ€“inorganic perovskites. Journal of Materials Chemistry A, 2022, 10, 1402-1413.	10.3	12
3	Volcano Plots of Reaction Yields in Cross-Coupling Catalysis. Journal of Physical Chemistry Letters, 2022, 13, 520-526.	4.6	3
4	Crystal growth engineering and origin of the weak ferromagnetism in antiferromagnetic matrix of orthochromates from t-e orbital hybridization. IScience, 2022, 25, 104111.	4.1	10
5	Role of the A-Element in the Structural, Mechanical, and Electronic Properties of Ti₃AC₂ MAX Phases. Inorganic Chemistry, 2022, 61, 2129-2140.	4.0	4
6	Biochemical analyses of a novel thermostable GH5 endo Î²-1,4-mannanase with minor Î²-1,4-glucosidic cleavage activity from Bacillus sp. KW1 and its synergism with a commercial Î±-galactosidase on galactomannan hydrolysis. International Journal of Biological Macromolecules, 2021, 166, 778-788.	7.5	12
7	An efficient Z-scheme (Cr, B) codoped g-C3N4/BiVO4 photocatalyst for water splitting: A hybrid DFT study. International Journal of Hydrogen Energy, 2021, 46, 247-261.	7.1	59
8	An ultra-sensitive gas sensor based on a two-dimensional manganese porphyrin monolayer. Physical Chemistry Chemical Physics, 2021, 23, 11852-11862.	2.8	13
9	Adenine ultrafast photorelaxation via electron-driven proton transfer. Physical Chemistry Chemical Physics, 2021, 23, 23090-23095.	2.8	2
10	Solution of two-electron SchrÃ¶dinger equations using a residual minimization method and one-dimensional basis functions. AIP Advances, 2021, 11, .	1.3	6
11	Strong Interaction between Cyclo[18]Carbon and Graphene. Advanced Theory and Simulations, 2021, 4, 2100022.	2.8	16
12	Solvents Hinder the Interlocking Rotation between Molecular Gears, as Revealed by Torque Calculations. Journal of Physical Chemistry C, 2021, 125, 17612-17621.	3.1	5
13	Revealing the tunability of electronic structures and optical properties of novel SWCNT derivatives, phenine nanotubes. Physical Chemistry Chemical Physics, 2021, 23, 24239-24248.	2.8	4
14	A machine learning approach using frequency descriptor for molecular property predictions. New Journal of Chemistry, 2021, 45, 20672-20680.	2.8	2
15	Crowding-induced polymer trapping in a channel. Physical Review E, 2021, 104, 054502.	2.1	2
16	Novel Two-Step Surface Boron Decoration of Graphitic Carbon Nitride Photoelectrodes for Efficient Charge Transport and Separation. Journal of Physical Chemistry C, 2021, 125, 25207-25216.	3.1	9
17	1/f Noise responses of Ultra-Thin Body and Buried oxide FD-SOI PMOSFETs under total ionizing dose irradiation. Radiation Effects and Defects in Solids, 2021, 176, 1202-1214.	1.2	0
18	Engineering the excited state of graphitic carbon nitride nanostructures by covalently bonding with graphene quantum dots. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	13

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19	Mo₂B, an MBene member with high electrical and thermal conductivities, and satisfactory performances in lithium ion batteries. Nanoscale Advances, 2020, 2, 347-355.	4.6	38
20	Recent developments in carbon nitride based films for photoelectrochemical water splitting. Sustainable Energy and Fuels, 2020, 4, 485-503.	4.9	68
21	In situ textured carbon nitride photoanodes with enhanced photoelectrochemical activity by band-gap state modulation. Journal of Materials Chemistry A, 2020, 8, 24005-24012.	10.3	9
22	Photoelectrochemical Performance Enhancement of ZnSe Nanorods versus Dots: Combined Experimental and Computational Insights. Journal of Physical Chemistry Letters, 2020, 11, 10414-10420.	4.6	5
23	A pseudo-metal-free strategy for constructing high performance photoelectrodes. Journal of Materials Chemistry A, 2020, 8, 12767-12773.	10.3	4
24	Atomic Sulfur Passivation Improves the Photoelectrochemical Performance of ZnSe Nanorods. Nanomaterials, 2020, 10, 1081.	4.1	5
25	Efficient degradation of industrial pollutants with sulfur (IV) mediated by LiCoO2 cathode powders of spent lithium ion batteries: A â€œtreating waste with wasteâ€•strategy. Journal of Hazardous Materials, 2020, 399, 123090.	12.4	19
26	High-Angular-Momentum Orbitals and Superatomic Characteristics of Boron-Nitrogen Cages. Journal of Physical Chemistry C, 2020, 124, 3881-3885.	3.1	9
27	Colorful carbon nitride based composite films. Applied Surface Science, 2020, 511, 145535.	6.1	11
28	Charge Transfer Boosting Moisture Resistance of Seminude Perovskite Nanocrystals via Hierarchical Alumina Modulation. Journal of Physical Chemistry Letters, 2020, 11, 3159-3165.	4.6	16
29	Numerical variational solution of hydrogen molecule and ions using one-dimensional hydrogen as basis functions. New Journal of Physics, 2020, 22, 093059.	2.9	8
30	Photocatalytic water splitting of (F, Ti) codoped heptazine/triazine based g-C3N4 heterostructure: A hybrid DFT study. Applied Surface Science, 2019, 463, 809-819.	6.1	39
31	Substrate-mediated and temperature-modulated long-range interactions between bromine adatom stripes on Cu(1â€¯1â€¯1). Applied Surface Science, 2019, 463, 253-260.	6.1	2
32	Photoinduced Waterâ€“Heptazine Electron-Driven Proton Transfer: Perspective for Water Splitting with g-C₃N₄. Journal of Physical Chemistry Letters, 2019, 10, 4310-4316.	4.6	33
33	The nature of small molecules adsorbed on defective carbon nanotubes. Royal Society Open Science, 2019, 6, 190727.	2.4	7
34	Nonradiative Excitedâ€State Decay via Conical Intersection in Graphene Nanostructures. ChemPhysChem, 2019, 20, 2754-2758.	2.1	7
35	A novel glycoside hydrolase family 42 enzyme with bifunctional Î²-galactosidase and Î±-L-arabinopyranosidase activities and its synergistic effects with cognate glycoside hydrolases in plant polysaccharides degradation. International Journal of Biological Macromolecules, 2019, 140, 129-139.	7.5	7
36	Periodicity-dependent long range coulomb on-site repulsion in hydrogen adsorbed graphene: A DFT+U study. Progress in Natural Science: Materials International, 2019, 29, 362-366.	4.4	0

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37	Thermal vacuum de-oxygenation and post oxidation of TiO₂ nanorod arrays for enhanced photoelectrochemical properties. Journal of Materials Chemistry A, 2019, 7, 5434-5441.	10.3	18
38	Revealing the trap emission in graphene-based nanostructures. Carbon, 2019, 150, 439-445.	10.3	6
39	Mechanism of the charge separation improvement in carbon-nanodot sensitized g-C3N4. Applied Surface Science, 2019, 487, 151-158.	6.1	27
40	Hydrogen-Location-Sensitive Modulation of the Redox Reactivity for Oxygen-Deficient TiO₂. Journal of the American Chemical Society, 2019, 141, 8407-8411.	13.7	59
41	n â†' Ï€* Interaction Promoted Charge Carrier Transfer between Helical SWNTs and a 4-(1-Pyrenyl)phenyl Group. Journal of Physical Chemistry C, 2019, 123, 13976-13982.	3.1	3
42	Unusual self-assembly of chloroaluminium phthalocyanine on graphite. Surface Science, 2019, 681, 104-110.	1.9	3
43	Formation Mechanism of Atmospheric Ammonium Bisulfate: HydrogenâCBondâCPromoted Nearly Barrierless Reactions of SO₃ with NH₃ and H₂O. ChemPhysChem, 2018, 19, 967-972.	2.1	18
44	Interlocking Mechanism between Molecular Gears Attached to Surfaces. ACS Nano, 2018, 12, 3020-3029.	14.6	21
45	Engineering the Band Gap States of the Rutile TiO₂(110) Surface by Modulating the Active Heteroatom. Angewandte Chemie - International Edition, 2018, 57, 8550-8554.	13.8	20
46	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>2</mml:mn><mml:mi>p</mml:mi></mml:mrow></mml:r -insulator heterointerfaces: Creation of half-metallicity and anionogenic ferromagnetism via double exchange. Physical Review B, 2018, 97, .	3.2	2
47	Selective interface transparency in graphene nanoribbon based molecular junctions. Nanoscale, 2018, 10, 4861-4864.	5.6	7
48	Electronic and optical performances of (Cu, N) codoped TiO2/g-C3N4 heterostructure photocatalyst: A spin-polarized DFTâ€+â€U study. Solar Energy, 2018, 162, 306-316.	6.1	23
49	Low-dimensional Mo:BiVO₄ photoanodes for enhanced photoelectrochemical activity. Journal of Materials Chemistry A, 2018, 6, 3602-3609.	10.3	86
50	Interlocking Molecular Gear Chains Built on Surfaces. Journal of Physical Chemistry Letters, 2018, 9, 2611-2619.	4.6	17
51	Engineering the Band Gap States of the Rutile TiO 2 (110) Surface by Modulating the Active Heteroatom. Angewandte Chemie, 2018, 130, 8686-8690.	2.0	9
52	Surface effects on the thermal conductivity of silicon nanowires. Chinese Physics B, 2018, 27, 036801.	1.4	7
53	Design of conjugated microporous polymer nanotubes for efficient benzene molecular adsorptions. International Journal of Quantum Chemistry, 2018, 118, e25492.	2.0	8
54	Intermolecular orbital interaction in Ï€ systems. Molecular Physics, 2018, 116, 978-986.	1.7	1

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55	Excited state dynamics study of the self-trapped exciton formation in silicon nanosheets. Physical Chemistry Chemical Physics, 2018, 20, 29299-29305.	2.8	3
56	Actinide embedded nearly planar gold superatoms: structural properties and applications in surface-enhanced Raman scattering (SERS). Physical Chemistry Chemical Physics, 2018, 20, 27523-27527.	2.8	14
57	How Does the Flexibility of Molecules Affect the Performance of Molecular Rotors?. Journal of Physical Chemistry C, 2018, 122, 25067-25074.	3.1	15
58	Theoretical and Experimental Methods for Determining the Thermal Conductivity of Nanostructures. SpringerBriefs in Physics, 2018, , 11-40.	0.7	0
59	Intramolecular Torque Study of a Molecular Rotation Stimulated by Electron Injection and Extraction. Journal of Physical Chemistry A, 2018, 122, 7614-7619.	2.5	6
60	Phonon Thermal Transport in Silicene and Its Defect Effects. SpringerBriefs in Physics, 2018, , 67-80.	0.7	0
61	Thermal Stability and Phonon Thermal Transport in Spherical Silicon Nanoclusters. SpringerBriefs in Physics, 2018, , 41-51.	0.7	0
62	Phonon Thermal Transport in Silicon Nanowires and Its Surface Effects. SpringerBriefs in Physics, 2018, , 53-66.	0.7	0
63	A scheme of numerical solution for threeâ€dimensional isoelectronic series of hydrogen atom using oneâ€dimensional basis functions. International Journal of Quantum Chemistry, 2018, 118, e25694.	2.0	8
64	Crystalâ€Face Tailored Graphitic Carbon Nitride Films for Highâ€Performance Photoelectrochemical Cells. ChemSusChem, 2018, 11, 2497-2501.	6.8	34
65	Collaborative enhancement of photon harvesting and charge carrier dynamics in carbon nitride photoelectrode. Applied Catalysis B: Environmental, 2018, 237, 783-790.	20.2	38
66	Exciton Self-Trapping in sp² Carbon Nanostructures Induced by Edge Ether Groups. Journal of Physical Chemistry Letters, 2018, 9, 4857-4864.	4.6	55
67	Fragment motion in motor molecules: basic concepts and application to intra-molecular rotations. Physical Chemistry Chemical Physics, 2018, 20, 21487-21497.	2.8	5
68	Mechanism of Charge Separation and Frontier Orbital Structure in Graphitic Carbon Nitride and Graphene Quantum Dots. ChemPhysChem, 2018, 19, 2534-2539.	2.1	9
69	Spin-orbit torque in a completely compensated synthetic antiferromagnet. Physical Review B, 2018, 97, .	3.2	73
70	Tuning the optical properties of graphene quantum dots by selective oxidation: a theoretical perspective. Journal of Materials Chemistry C, 2018, 6, 6875-6883.	5.5	59
71	Na₂C monolayer: a novel 2p Dirac half-metal with multiple symmetry-protected Dirac cones. Nanoscale, 2018, 10, 13645-13651.	5.6	38
72	The electronic structure, optical absorption and photocatalytic water splitting of (FeÂ+ÂNi)-codoped TiO2: A DFT +U study. International Journal of Hydrogen Energy, 2017, 42, 4966-4976.	7.1	22

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73	The electronic structure and optical absorption of rutile TiO 2 with La and N dopants from first-principles calculation. Computational Materials Science, 2017, 131, 178-186.	3.0	12
74	C=C Ï€ Bond Modified Graphitic Carbon Nitride Films for Enhanced Photoelectrochemical Cell Performance. Chemistry - an Asian Journal, 2017, 12, 1005-1012.	3.3	35
75	A <scp>G</scp>reen's function approach to the nonrelativistic radial wave equation of hydrogen atom. International Journal of Quantum Chemistry, 2017, 117, e25360.	2.0	2
76	Energetics of hexagonal boron nitride nanostructures: edge dependence and truncation effects. Nanoscale, 2017, 9, 6734-6740.	5.6	22
77	Enhanced optical absorption and photocatalytic activity of anatase TiO 2 through C Nd-codoped: A DFT+ U calculations. Journal of Physics and Chemistry of Solids, 2017, 109, 70-77.	4.0	6
78	Enhanced optical absorption and photocatalytic H2 production activity of g-C3N4/TiO2 heterostructure by interfacial coupling: A DFT+U study. International Journal of Hydrogen Energy, 2017, 42, 9903-9913.	7.1	50
79	Beyond the electrostatic model: the significant roles of orbital interaction and the dispersion effect in aqueousâ€“Ï€ systems. Physical Chemistry Chemical Physics, 2017, 19, 1298-1302.	2.8	7
80	Donor/Acceptor Properties of Aromatic Molecules in Complex Metalâ€“Molecule Interfaces. Langmuir, 2017, 33, 451-458.	3.5	13
81	Evaluating frontier orbital energy and HOMO/LUMO gap with descriptors from density functional reactivity theory. Journal of Molecular Modeling, 2017, 23, 3.	1.8	75
82	Bonding reactivity descriptor from conceptual density functional theory and its applications to elucidate bonding formation. Journal of Chemical Physics, 2017, 147, 134303.	3.0	10
83	DFT study of benzyl alcohol/TiO2 interfacial surface complex: reaction pathway and mechanism of visible light absorption. Journal of Molecular Modeling, 2017, 23, 285.	1.8	3
84	Tunneling lifetimes of electrons escaping from atoms under a static electric field. Journal of Chemical Physics, 2017, 147, 064109.	3.0	2
85	Role of Cl Ion Desorption in Photocurrent Enhancement of the Annealed Rutile Single-Crystalline TiO₂ Nanorod Arrays. Journal of Physical Chemistry C, 2017, 121, 18892-18899.	3.1	15
86	A Thermodynamic Model of Diameter- and Temperature-dependent Semiconductor Nanowire Growth. Scientific Reports, 2017, 7, 15029.	3.3	7
87	Structural Asymmetry-Facilitated Tunability of Spin Distribution in the (10, 0) Carbon Nanotube Induced by Charging. Journal of Electronic Materials, 2017, 46, 3857-3861.	2.2	2
88	Chemical Coupling SERS Properties of Pyridine on Silver-Caged Metal Clusters M@Ag12 (MÂ=ÂVâ˜, Nbâ˜,) Tj ETQq0 0 0 rgBT /Overlock	2.2	4
89	Improved projected Green's function approach to electron tunneling lifetime calculations in quantum wells. Physical Review B, 2017, 96, .	3.2	1
90	Electronic structure and properties of highly ordered C₆₀ nano arrays on Au (111): STM & DFT study. Journal of Physics: Conference Series, 2017, 864, 012076.	0.4	0

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91	Hydrogen-terminated silicon quantum dots. , 2017, , 413-432.		1
92	Hydrogen-terminated silicon quantum dots. Series in Materials Science and Engineering, 2017, , 413-432.	0.1	0
93	Efficiency Enhancement of Carbon Nitride Photoelectrochemical Cells via Tailored Monomers Design. Advanced Energy Materials, 2016, 6, 1600263.	19.5	116
94	Roles of the active species involved in the photocatalytic oxidation of benzyl alcohol into benzaldehyde on TiO 2 under UV light: Experimental and DFT studies. Journal of Molecular Catalysis A, 2016, 420, 82-87.	4.8	29
95	Dual response of graphene-based ultra-small molecular junctions to defect engineering. Nano Research, 2016, 9, 1480-1488.	10.4	10
96	Intramolecular torque, an indicator of the internal rotation direction of rotor molecules and similar systems. Physical Chemistry Chemical Physics, 2016, 18, 29665-29672.	2.8	13
97	Aggregation of metal-free organic sensitizers on TiO 2 (1 0 1) surface for use in dye-sensitized solar cells: A computational investigation. Computational and Theoretical Chemistry, 2016, 1093, 1-8.	2.5	10
98	A new insight into Ï€â€“Ï€ stacking involving remarkable orbital interactions. Physical Chemistry Chemical Physics, 2016, 18, 25452-25457.	2.8	48
99	Graphitic Carbon Nitride Film: An Emerging Star for Catalytic and Optoelectronic Applications. ChemSusChem, 2016, 9, 2723-2735.	6.8	96
100	Molecular orbital analysis of the hydrogen bonded water dimer. Scientific Reports, 2016, 6, 22099.	3.3	45
101	Strong orbital interaction in a weak CH-Ï€ hydrogen bonding system. Scientific Reports, 2016, 6, 22304.	3.3	19
102	Nonresonant chemical mechanism in surface-enhanced Raman scattering of pyridine on M@Au₁₂clusters. Nanoscale, 2016, 8, 4086-4093.	5.6	30
103	Facet-Controlling Agents Free Synthesis of Hematite Crystals with High-Index Planes: Excellent Photodegradation Performance and Mechanism Insight. ACS Applied Materials & Interfaces, 2016, 8, 142-151.	8.0	37
104	Composition dependent reactivity of titanium oxide clusters. Physical Chemistry Chemical Physics, 2016, 18, 10594-10599.	2.8	9
105	Computational prediction of optimal metal ions to induce coordinated polymerization of muscle-like [c2]daisy chains. Physical Chemistry Chemical Physics, 2016, 18, 7419-7426.	2.8	6
106	Chirality dependent spin polarization of carbon nanotubes. New Journal of Physics, 2016, 18, 023029.	2.9	8
107	A durable surface-enhanced Raman scattering substrate: ultrathin carbon layer encapsulated Ag nanoparticle arrays on indium-tin-oxide glass. Physical Chemistry Chemical Physics, 2015, 17, 14849-14855.	2.8	6
108	A novel electrolyte additive for improving the interfacial stability ofÂhigh voltage lithium nickel manganese oxide cathode. Journal of Power Sources, 2015, 293, 71-77.	7.8	84

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109	Enhancement of spin polarization induced by Coulomb on-site repulsion between localized pz electrons in graphene embedded with line defects. Physical Chemistry Chemical Physics, 2015, 17, 30744-30750.	2.8	5
110	Reproducible and recyclable SERS substrates: Flower-like Ag structures with concave surfaces formed by electrodeposition. Applied Surface Science, 2015, 333, 126-133.	6.1	30
111	Self-doping and magnetic ordering induced by extended line defects in graphene. Physical Review B, 2015, 91, .	3.2	15
112	Electronic delocalization in small water rings. Physical Chemistry Chemical Physics, 2015, 17, 2987-2990.	2.8	18
113	Efficient Emission Facilitated by Multiple Energy Level Transitions in Uniform Graphitic Carbon Nitride Films Deposited by Thermal Vapor Condensation. ChemPhysChem, 2015, 16, 954-959.	2.1	72
114	Correlation between electron delocalization and structural planarization in small water rings. International Journal of Quantum Chemistry, 2015, 115, 817-819.	2.0	5
115	Revealing highly unbalanced energy barriers in the extension and contraction of the muscle-like motion of a [c2]daisy chain. Physical Chemistry Chemical Physics, 2015, 17, 18318-18326.	2.8	17
116	Tunable dipole induced hydrogen bonds between a hydrogen molecule and alkali halides. Physical Chemistry Chemical Physics, 2015, 17, 20361-20367.	2.8	3
117	Strong Core@Shell Dependence in Surface-Enhanced Raman Scattering of Pyridine on Stable 13-Atom Silver-Caged Bimetallic Clusters. Journal of Physical Chemistry C, 2015, 119, 17429-17437.	3.1	19
118	Theoretical study on catalyzed selective photoreduction mechanism for 4-bromobenzaldehyde in two different solvents. Physical Chemistry Chemical Physics, 2015, 17, 19997-20005.	2.8	2
119	Economical basis sets and their uses in ab initio calculations. International Journal of Quantum Chemistry, 2015, 115, 570-577.	2.0	10
120	Dynamic crystallography reveals early signalling events in ultraviolet photoreceptor UVR8. Nature Plants, 2015, 1, .	9.3	48
121	Physisorption of benzene derivatives on graphene: critical roles of steric and stereoelectronic effects of the substituent. Physical Chemistry Chemical Physics, 2015, 17, 12185-12193.	2.8	29
122	The role of tryptophans in the UV-B absorption of a UVR8 photoreceptor â€“ a computational study. Physical Chemistry Chemical Physics, 2015, 17, 10786-10794.	2.8	15
123	Water Clusters on Graphitic Carbon Surfaces. Journal of Cluster Science, 2015, 26, 361-373.	3.3	2
124	Thermal vapor condensation of uniform graphitic carbon nitride films with remarkable photocurrent density for photoelectrochemical applications. Nano Energy, 2015, 15, 353-361.	16.0	208
125	Tris(trimethylsilyl)borate as an electrolyte additive for improving interfacial stability of high voltage layered lithium-rich oxide cathode/carbonate-based electrolyte. Journal of Power Sources, 2015, 285, 360-366.	7.8	118
126	Charging-induced asymmetric spin distribution in an asymmetric (9,0) carbon nanotube. Physical Chemistry Chemical Physics, 2015, 17, 28860-28865.	2.8	6

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127	Tailoring the transmission lineshape spectrum of zigzag graphene nanoribbon based heterojunctions via controlling their width and edge protrusions. Nanoscale, 2015, 7, 20003-20008.	5.6	11
128	Strong orbital deformation due to CHâ€“Ï€ interaction in the benzeneâ€“methane complex. Physical Chemistry Chemical Physics, 2015, 17, 29489-29491.	2.8	13
129	New insight into the spin-conserving excitation of the negatively charged nitrogen-vacancy center in diamond. Scientific Reports, 2015, 4, 5144.	3.3	12
130	Intermolecular Ï€/Ï€ and H/Ï€ interactions in dimers researched by different computational methods. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450057.	1.8	2
131	Symmetry-dependent band gap opening in graphene induced by g-C₃N₄ substrates. RSC Advances, 2014, 4, 64577-64582.	3.6	7
132	Stabilizing reconstruction induced by O protrusions of the ZnO (0001) polar surface. RSC Advances, 2014, 4, 54249-54255.	3.6	2
133	Environmental-Confinement-Induced Stability Enhancement of Chiral Molecules. ChemPhysChem, 2014, 15, 2672-2675.	2.1	0
134	A unique feature of chiral transition of a difluorobenzo[c]phenanthrene molecule confined in a boron-nitride nanotube based on molecular dynamics simulations. Chemical Physics Letters, 2014, 591, 265-267.	2.6	5
135	Synthesis of Carbon Materialsâ€“TiO₂ Hybrid Nanostructures and Their Visibleâ€Light Photoâ€catalytic Activity. ChemPlusChem, 2014, 79, 454-461.	2.8	16
136	The structure, electronic, and optical properties of (Sm,N)-codoped anatase TiO2 photocatalyst: A density functional study. Journal of Catalysis, 2014, 309, 115-120.	6.2	21
137	Growth Mechanisms and Novel Properties of Silicon Nanostructures from Quantum-Mechanical Calculations. Springer Briefs in Molecular Science, 2014, , .	0.1	12
138	Point defect weakened thermal contraction in monolayer graphene. Journal of Chemical Physics, 2014, 141, 064705.	3.0	11
139	Selective adsorption ofl-serine functional groups on the anatase TiO2(101) surface in benthic microbial fuel cells. Physical Chemistry Chemical Physics, 2014, 16, 20806-20817.	2.8	7
140	Strong slip-induced anomalous enhancement and red-shifts in wide-range optical absorption of graphite under uniaxial pressure. Nanoscale, 2014, 6, 8943-8948.	5.6	3
141	The mechanism of Nâ€“Ag bonding determined tunability of surface-enhanced Raman scattering of pyridine on MAg (M = Cu, Ag, Au) diatomic clusters. Physical Chemistry Chemical Physics, 2014, 16, 20665-20671.	2.8	21
142	Anomalous effect of hydrogenation on phonon thermal conductivity in thin silicon nanowires. Europhysics Letters, 2014, 105, 56003.	2.0	21
143	Boundary and Symmetry Determined Exciton Distribution in Two Dimensional Silicon Nanosheets. Journal of Physical Chemistry C, 2014, 118, 20070-20076.	3.1	24
144	Structural Evolution of Cu/ZnO Active Sites: From Reactive Environment to Ultrahigh Vacuum. ChemCatChem, 2014, 6, 2322-2326.	3.7	5

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145	Oxygen vacancy diffusion in bare ZnO nanowires. Nanoscale, 2014, 6, 11882-11886.	5.6	29
146	Carbon Dot Loading and TiO₂ Nanorod Length Dependence of Photoelectrochemical Properties in Carbon Dot/TiO₂ Nanorod Array Nanocomposites. ACS Applied Materials & Interfaces, 2014, 6, 4883-4890.	8.0	169
147	Stable electronic structures of a defective uranofullerene. Carbon, 2014, 78, 19-25.	10.3	11
148	Two-dimensional topological insulators with binary honeycomb lattices:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Si</mml:mi><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>siligraphene and its analogs. Physical Review B, 2014, 89, .	3.2	83
149	Tuning thermal expansions of zinc oxide sheets by varying the layer thickness. Europhysics Letters, 2014, 107, 26007.	2.0	7
150	Electronic and Vibrational Properties of Stable Isomers of (SiO)_n^(0,Â±) (n = 2â€“7) Clusters. Journal of Physical Chemistry A, 2014, 118, 8893-8900.	2.5	9
151	Remarkable Thermal Contraction in Small Size Single-Walled Boron Nanotubes. Communications in Computational Physics, 2014, 16, 201-212.	1.7	4
152	Rectifying Properties of Oligo(Phenylene Ethynylene) Heterometallic Molecular Junctions: Molecular Length and Side Group Effects. Scientific Reports, 2014, 4, 6357.	3.3	23
153	Novel Electronic Properties of Silicon Nanostructures. Springer Briefs in Molecular Science, 2014, , 31-63.	0.1	0
154	Growth Mechanism of Silicon Nanowires. Springer Briefs in Molecular Science, 2014, , 7-12.	0.1	0
155	Stability of Silicon Nanostructures. Springer Briefs in Molecular Science, 2014, , 13-30.	0.1	0
156	Anomalous stability of graphene containing defects covered by a water layer. Nanoscale, 2013, 5, 6767.	5.6	12
157	Excited State Relaxation and Stabilization of Hydrogen Terminated Silicon Quantum Dots. Journal of Cluster Science, 2013, 24, 381-397.	3.3	9
158	Basis set effect on defect induced spin polarization of a carbon nanotube in density functional theory calculations. Chemical Physics Letters, 2013, 585, 107-111.	2.6	4
159	Signatures in vibrational and UV-visible absorption spectra for identifying cyclic hydrocarbons by graphene fragments. Nanoscale, 2013, 5, 12178.	5.6	15
160	New superhard carbon allotropes based on C20 fullerene. Carbon, 2013, 63, 571-573.	10.3	17
161	Strong Adsorption Between Uranium Dicarbide and Graphene Surface Induced by f Electrons. Journal of Physical Chemistry C, 2013, 117, 26849-26857.	3.1	14
162	Zwitterions are the most stable form for neutral arginylglycine in gas phase: Clear theoretical evidence. Computational and Theoretical Chemistry, 2013, 1008, 96-102.	2.5	9

#	Article	IF	Citations
163	Engineering of Facets, Band Structure, and Gasâ€Sensing Properties of Hierarchical Sn²⁺â€Doped SnO₂ Nanostructures. Advanced Functional Materials, 2013, 23, 4847-4853.	14.9	108
164	Chemical Mechanism and Tunability of Surface-Enhanced Raman Scattering of Pyridine on Heteronuclear Coinage Metal Diatomic Clusters: A Density Functional Study. Journal of Physical Chemistry C, 2013, 117, 12544-12551.	3.1	16
165	Size dependent catalytic effect of TiO2 clusters in water dissociation. Journal of Molecular Catalysis A, 2013, 366, 163-170.	4.8	8
166	Cooperative Modulation of Electronic Structures of Aromatic Molecules Coupled to Multiple Metal Contacts. Physical Review Letters, 2013, 110, 046802.	7.8	31
167	Size-dependent structural characteristics and phonon thermal transport in silicon nanoclusters. AIP Advances, 2013, 3, 082114.	1.3	6
168	Defect Induced Electronic Structure of Uranofullerene. Scientific Reports, 2013, 3, 1341.	3.3	30
169	STABLE STRUCTURES AND CHARACTERISTIC VIBRATIONAL SPECTRA OF Ti_nO_m (n = 2â€“4; m = 1â€“2n) CLUSTERS. Journal of Theoretical and Computational Chemistry, 2013, 12, 1250094.	1.8	5
170	Inducing novel electronic properties in âŒ©112âŒª Ge nanowires by means of variations in their size, shape and strain: a first-principles computational study. Journal of Physics Condensed Matter, 2012, 24, 015301.	1.8	6
171	Adsorbate-induced reconstruction by C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>60</mml:mn></mml:msub></mml:math>on close-packed metal surfaces: Mechanism for Detailed low-energy electron diffraction analysis of the (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 402 Td (xmlns:mml="http://w	3.2	22
172	surface structure of C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>60</mml:mn></mml:msub></mml:math>on Cu(111): Seven-atom-vacancy reconstruction. Physical Review B, 2012, 86, .	3.2	27
173	A COMPARATIVE STUDY ON INTERMOLECULAR HYDROGEN BOND INTERACTIONS IN MOLECULAR DIMERS USING DIFFERENT LEVELS OF COMPUTATIONAL METHODS. Journal of Theoretical and Computational Chemistry, 2012, 11, 1237-1259.	1.8	7
174	CHARACTERISTIC VIBRATIONAL MODES OF H2O ADSORBED MOLECULARLY AND DISSOCIATIVELY ON TITANIUM OXIDE CLUSTERS. Journal of Theoretical and Computational Chemistry, 2012, 11, 1289-1295.	1.8	1
175	Inducing extended line defects in graphene by linear adsorption of C and N atoms. Applied Physics Letters, 2012, 101, .	3.3	7
176	Possible cage-like nanostructures formed by amino acids. Organic and Biomolecular Chemistry, 2012, 10, 5049.	2.8	9
177	Strong interactions and charge transfers between a charged benzene molecule and multilayer graphenes. Journal of Materials Chemistry, 2012, 22, 23380.	6.7	19
178	Vacancy-defectâ€“induced diminution of thermal conductivity in silicene. Europhysics Letters, 2012, 99, 36001.	2.0	101
179	Structural, Electronic, Dynamical, and Superconducting Properties in Dense GeH₄(H₂)₂. Journal of Physical Chemistry C, 2012, 116, 5225-5234.	3.1	55
180	Interactions between Organics and Metal Surfaces in the Intermediate Regime between Physisorption and Chemisorption. Journal of Physical Chemistry C, 2012, 116, 23603-23607.	3.1	19

#	Article	IF	Citations
181	Atomic nitrogen chemisorption on graphene with extended line defects. Journal of Materials Chemistry, 2012, 22, 21167.	6.7	14
182	Survey of structural and electronic properties of C60 on close-packed metal surfaces. Journal of Materials Science, 2012, 47, 7341-7355.	3.7	41
183	Energetics and dynamics of a new type of extended line defects in graphene. Nanoscale, 2012, 4, 2580.	5.6	15
184	A Strategy of Enhancing the Photoactivity of g-C₃N₄ via Doping of Nonmetal Elements: A First-Principles Study. Journal of Physical Chemistry C, 2012, 116, 23485-23493.	3.1	590
185	Adsorption and properties of aromatic amino acids on single-walled carbon nanotubes. Nanoscale, 2012, 4, 1146-1153.	5.6	45
186	A random rotor molecule: Vibrational analysis and molecular dynamics simulations. Journal of Chemical Physics, 2012, 137, 234302.	3.0	3
187	Excited state properties of Si quantum dots. Physica Status Solidi (B): Basic Research, 2012, 249, 401-412.	1.5	24
188	Characteristic Vibrational Modes and Electronic Structures of Carbon Nanotubes Containing Defects. Journal of Physical Chemistry C, 2012, 116, 292-297.	3.1	14
189	Modeling Silicon Nanostructure Surface Functionalization for Biological Detections. , 2012, , 33-51.		0
190	C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>60</mml:mn></mml:msub></mml:math>on the Pt(111) surface: Structural tuning of electronic properties. Physical Review B, 2011, 84, .	3.2	24
191	Electron Transport Suppression from Tipâ^Ï€ State Interaction on Si(100)-2 Ã— 1 Surfaces. Journal of Chemical Theory and Computation, 2011, 7, 707-712.	5.3	4
192	Spin-polarized transport through ZnMnSe/ZnSe/ZnBeSe heterostructures. Journal of Applied Physics, 2011, 110, 093717.	2.5	16
193	Intramolecular Torsion Based Molecular Switch Functionality Enhanced in Ï€-Conjugated Oligomolecules by a Ï€-Conjugated Pendant Group. Journal of Physical Chemistry C, 2011, 115, 13911-13918.	3.1	6
194	Strain Induced Band Dispersion Engineering in Si Nanosheets. Journal of Physical Chemistry C, 2011, 115, 23682-23687.	3.1	54
195	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î²</mml:mi><mml:mtext mathvariant="normal">â^'</mml:mtext><mml:mi>tin</mml:mi><mml:mo>â†'</mml:mo><mml:mi>I</mml:mi><mml:mi>m</mml:mi> Transitions of Germanium. Physical Review Letters, 2011, 106, 135502.	7.8	38
196	Moleculeâ€“substrate interaction channels of metal-phthalocyanines on graphene on Ni(111) surface. Journal of Chemical Physics, 2011, 134, 094705.	3.0	74
197	DFT calculations on structural and electronic properties of Bi2MO6 (M = Cr, Mo, W). Rare Metals, 2011, 30, 166-172.	7.1	60
198	Interactions between free radicals and a graphene fragment: Physical versus chemical bonding, charge transfer, and deformation. Journal of Computational Chemistry, 2011, 32, 3264-3268.	3.3	33

#	Article	IF	Citations
199	Surface-nitrogenationâ€“induced thermal conductivity attenuation in silicon nanowires. Europhysics Letters, 2011, 96, 56007.	2.0	15
200	Stabilizing and activating dopants in âŸ¨112âŸ© silicon nanowires by alkene adsorptions: A first-principles study. Applied Physics Letters, 2011, 98, 073115.	3.3	8
201	Size effects on formation energies and electronic structures of oxygen and zinc vacancies in ZnO nanowires: A first-principles study. Journal of Applied Physics, 2011, 109, 044306-044306-5.	2.5	17
202	Silicon nanowires for high-specificity and high-selectivity sensors under low-frequency scanning. Applied Physics Letters, 2011, 98, 043108.	3.3	5
203	Tunable optical and electronic properties of Si nanowires by electric bias. Journal of Applied Physics, 2011, 109, 083106.	2.5	6
204	Tuning Electronic Structures of ZnO Nanowires by Surface Functionalization: A First-Principles Study. Journal of Physical Chemistry C, 2010, 114, 8861-8866.	3.1	34
205	Superconductivity in Hydrogen-rich Material: GeH4. Journal of Superconductivity and Novel Magnetism, 2010, 23, 717-719.	1.8	22
206	Size Dependence of Nanoscale Confinement on Chiral Transformation. Chemistry - A European Journal, 2010, 16, 6482-6487.	3.3	6
207	Surface Passivationâ€Induced Strong Ferromagnetism of Zinc Oxide Nanowires. Chemistry - A European Journal, 2010, 16, 13072-13076.	3.3	7
208	N-doped ZnO nanowires: Surface segregation, the effect of hydrogen passivation and applications in spintronics. Physica Status Solidi (B): Basic Research, 2010, 247, 2195-2201.	1.5	22
209	Structural transitions of solid germane under pressure. Europhysics Letters, 2010, 90, 66006.	2.0	22
210	Barrier dependent electron tunneling lifetime in one-dimensional device structures. Journal of Applied Physics, 2010, 108, .	2.5	3
211	Ï€â€“Ï€ INTERACTION IN BENZENE DIMER STUDIED USING DENSITY FUNCTIONAL THEORY AUGMENTED WITH AN EMPIRICAL DISPERSION TERM. Journal of Theoretical and Computational Chemistry, 2010, 09, 109-123.	1.8	5
212	Prospects for Resolving Chemical Structure by Atomic Force Microscopy: A First-Principles Study. Langmuir, 2010, 26, 16271-16277.	3.5	22
213	Theoretical Exploration of the Structural, Electronic, and Magnetic Properties of ZnO Nanotubes with Vacancies, Antisites, and Nitrogen Substitutional Defects. Journal of Physical Chemistry C, 2010, 114, 5760-5766.	3.1	39
214	Tunable Electrical Properties of Silicon Nanowires via Surface-Ambient Chemistry. ACS Nano, 2010, 4, 3045-3052.	14.6	72
215	Chemical Trend of Pressure-Induced Metallization in Alkaline Earth Hydrides. Journal of Physical Chemistry C, 2010, 114, 14614-14617.	3.1	20
216	Structural Analysis and Electronic Properties of Negatively Charged TCNQ: 2D Networks of (TCNQ)2Mn Assembled on Cu(100). Journal of Physical Chemistry C, 2010, 114, 17197-17204.	3.1	28

#	Article	IF	Citations
217	Possible Reaction Paths of Small Silicon Clusters with Oxygen Explored with Density Functional Theory. Journal of Physical Chemistry C, 2010, 114, 13196-13203.	3.1	3
218	Firstâ€principles calculations of atomic and electronic properties of ZnO nanostructures. Physica Status Solidi (B): Basic Research, 2010, 247, 2581-2593.	1.5	7
219	Surface modification of TiO<inf>2</inf> and ZnO nanosurfaces and applications. , 2010, , .		1
220	Interaction of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>O</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>H</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:mtext>O</mml:mtext></mml:mte xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>N</mml:mtext><mml:mn>2</mml:m. Physical Revi	3.2	24
221	The Stability and Mechanical Properties of Boron Nanotubes Explored through Density Functional Calculations. International Journal for Multiscale Computational Engineering, 2010, 8, 245-250.	1.2	2
222	First-principles study of silicon bulk and nanowire (111) surfaces terminated with trihydrides: Symmetric, rotated, and tilted. Physical Review B, 2009, 80, .	3.2	1
223	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, .	3.2	41
224	Stacking of polycyclic aromatic hydrocarbons as prototype for graphene multilayers, studied using density functional theory augmented with a dispersion term. Journal of Chemical Physics, 2009, 131, 194702.	3.0	46
225	Prediction of surface passivation doping of silicon nanowires with phosphorus. Applied Physics Letters, 2009, 95, .	3.3	10
226	An energetic stability predictor of hydrogen-terminated Si nanostructures. Applied Physics Letters, 2009, 95, .	3.3	14
227	Significant negative differential resistance predicted in scanning tunneling spectroscopy for a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>C</mml:mtext><mml:mrow><mml:mn>60</mml:mn></mml:mrow></mml:m on a metal surface. Physical Review B, 2009, 80, .	3.2	7
228	Metallization induced by nitrogen atom adsorption on silicon nanofilms and nanowires. Applied Physics Letters, 2009, 94, 113101.	3.3	6
229	Prediction of energetically optimal single-walled carbon nanotubes for hydrogen physisorption. Applied Physics Letters, 2009, 95, 013116.	3.3	23
230	APPLICATIONS OF DISCRETE SINGULAR CONVOLUTION ALGORITHM IN ONE-ELECTRON SYSTEMS: HYDROGEN ATOM. Journal of Theoretical and Computational Chemistry, 2009, 08, 813-826.	1.8	2
231	A NONSELF-CONSISTENT METHOD FOR THE NONEQUILIBRIUM GREEN'S FUNCTION TECHNIQUE. Journal of Theoretical and Computational Chemistry, 2009, 08, 423-431.	1.8	0
232	SENSITIVITY OF HYDROGENATED SILICON NANODOT ON SMALL POLAR MOLECULES. Journal of Theoretical and Computational Chemistry, 2009, 08, 299-316.	1.8	6
233	Surface Passivation and Transfer Doping of Silicon Nanowires. Angewandte Chemie - International Edition, 2009, 48, 9896-9900.	13.8	57
234	Single-electron tunneling and Coulomb blockade in carbon-based quantum dots. Frontiers of Physics in China, 2009, 4, 315-326.	1.0	2

#	Article	IF	Citations
235	Hydrogen and oxygen adsorption on ZnO nanowires: A first-principles study. Physical Review B, 2009, 79, .	3.2	51
236	External Electric Field Modulated Electronic and Structural Properties of ã€˜111ã€‰ Si Nanowires. Journal of Physical Chemistry C, 2009, 113, 10384-10389.	3.1	29
237	Adsorptions of Tetrafluorotetracyanoquinodimethane on Entirely and Partially Hydrogenated C(100)-2Ã—1 Surfaces. Journal of Physical Chemistry C, 2009, 113, 8829-8835.	3.1	3
238	Ab Initio Study on Thermal and Chemical Stabilities of Silicon Monoxide Clusters. Journal of Physical Chemistry C, 2009, 113, 12736-12741.	3.1	13
239	Quantum Mechanical Quantification of Weakly Interacting Complexes of Peptides with Single-Walled Carbon Nanotubes. Journal of Chemical Theory and Computation, 2009, 5, 2879-2885.	5.3	38
240	Resonance and antiresonance effects in electronic transport through several-quantum-dot combinations. Journal of Applied Physics, 2009, 105, 043706.	2.5	16
241	Band gap engineering of GaN nanowires by surface functionalization. Applied Physics Letters, 2009, 94, .	3.3	27
242	Stable calcium adsorbates on carbon nanostructures: Applications for high-capacity hydrogen storage. Physical Review B, 2009, 79, .	3.2	74
243	Al doped graphene: A promising material for hydrogen storage at room temperature. Journal of Applied Physics, 2009, 105, .	2.5	212
244	Photo and pH Stable, Highly-Luminescent Silicon Nanospheres and Their Bioconjugates for Immunofluorescent Cell Imaging. Journal of the American Chemical Society, 2009, 131, 4434-4438.	13.7	193
245	Covalent-adsorption induced magnetism in graphene. Journal of Materials Chemistry, 2009, 19, 9274.	6.7	58
246	Atomistic Simulations of Self-Trapped Exciton Formation in Silicon Nanostructures: The Transition from Quantum Dots to Nanowires. Journal of Physical Chemistry C, 2009, 113, 12935-12938.	3.1	25
247	Computation of large systems with an economic basis set: systems in excited states. Theoretical Chemistry Accounts, 2008, 119, 437-443.	1.4	4
248	Structural and electronic properties of single-walled carbon nanotubes adsorbed with 1-pyrenebutanoic acid, succinimidyl ester. Science in China Series B: Chemistry, 2008, 51, 1203-1210.	0.8	20
249	Motility of Metal Nanoparticles in Silicon and Induced Anisotropic Silicon Etching. Advanced Functional Materials, 2008, 18, 3026-3035.	14.9	427
250	A surface-enhanced Raman spectroscopy substrate for highly sensitive label-free immunoassay. Applied Physics Letters, 2008, 92, .	3.3	67
251	Preparation of Large-Area Uniform Silicon Nanowires Arrays through Metal-Assisted Chemical Etching. Journal of Physical Chemistry C, 2008, 112, 4444-4450.	3.1	504
252	Optimal surface functionalization of silicon quantum dots. Journal of Chemical Physics, 2008, 128, 244714.	3.0	57

#	Article	IF	Citations
253	Anomalous size dependence of the luminescence in reconstructed silicon nanoparticles. Applied Physics Letters, 2008, 93, .	3.3	23
254	Effect of B-complexes on lattice structure and electronic properties in heavily boron-doped diamond. Diamond and Related Materials, 2008, 17, 234-239.	3.9	18
255	First-Principles Study of the Structural Stability and Electronic Properties of ZnS Nanowires. Journal of Physical Chemistry C, 2008, 112, 20291-20294.	3.1	11
256	Theoretical Models of Silica Nanorings: First-Principles Calculations. Journal of Physical Chemistry C, 2008, 112, 17071-17075.	3.1	3
257	Single-Crystal 9,10-Diphenylanthracene Nanoribbons and Nanorods. Chemistry of Materials, 2008, 20, 6945-6950.	6.7	71
258	INTRAMOLECULAR CHARGE TRANSFER AND PHOTOISOMERIZATION OF THE DCM STYRENE DYE: A THEORETICAL STUDY. Journal of Theoretical and Computational Chemistry, 2008, 07, 719-736.	1.8	12
259	First principles studies for formation mechanism and properties of ethylene molecule adsorbing on diamond (100) surface. Journal of Chemical Physics, 2008, 128, 114710.	3.0	2
260	Energy alignment induced negative differential resistance: The role of hybrid states in aromatic molecular devices. Journal of Chemical Physics, 2008, 129, 074710.	3.0	16
261	Unique electronic band structures of hydrogen-terminated langle 112angle silicon nanowires. Nanotechnology, 2008, 19, 035708.	2.6	10
262	Mechanical properties of solid C₆₀studied with density functional tight binding method augmented by an empirical dispersion term. Journal of Physics Condensed Matter, 2008, 20, 275240.	1.8	5
263	Negative differential resistance and tunable peak-to-valley ratios in a silicon nanochain. Journal of Applied Physics, 2008, 103, 103719.	2.5	5
264	Amine-capped silicon quantum dots. Applied Physics Letters, 2008, 92, 053107.	3.3	35
265	Facet dependent reactivity and selective deposition of nanometer sized Î²-SiC on diamond surfaces. Applied Physics Letters, 2008, 92, .	3.3	15
266	Indirect-to-direct band gap transitions in phosphorus adsorbed âŸ¨112âŸ© silicon nanowires. Applied Physics Letters, 2008, 93, .	3.3	20
267	Tunable electronic band structures of hydrogen-terminated âŸ¨112âŸ© silicon nanowires. Applied Physics Letters, 2008, 92, 203109.	3.3	22
268	Valence band offset of InN/4H-SiC heterojunction measured by x-ray photoelectron spectroscopy. Applied Physics Letters, 2008, 93, .	3.3	14
269	AN ITERATION SCHEME FOR CALCULATING TRANSPORT PROPERTIES OF MOLECULAR SYSTEMS. Journal of Theoretical and Computational Chemistry, 2007, 06, 975-984.	1.8	0
270	Surface structures and electronic states of silicon nanotubes stabilized by oxygen atoms. Journal of Applied Physics, 2007, 102, .	2.5	7

#	Article	IF	Citations
271	Theoretical study of the chemical gap tuning in silicon nanowires. Physical Review B, 2007, 76, .	3.2	65
272	Unusual size dependence of the optical emission gap in small hydrogenated silicon nanoparticles. Applied Physics Letters, 2007, 90, 123116.	3.3	61
273	Stabilizing excited-state silicon nanoparticle by surface oxidation. Applied Physics Letters, 2007, 91, .	3.3	27
274	Effect of thickness on the electronic structure of poly(vinylidene fluoride) molecular films from first-principles calculations. Physical Review B, 2007, 75, .	3.2	14
275	Theoretical Studies on Optical and Electronic Properties of Propionic-Acid-Terminated Silicon Quantum Dots. Journal of Chemical Theory and Computation, 2007, 3, 1518-1526.	5.3	36
276	First-principles calculations of reconstructed [0001] ZnO nanowires. Physical Review B, 2007, 76, .	3.2	58
277	Ordered silicon nanowire arrays via nanosphere lithography and metal-induced etching. Applied Physics Letters, 2007, 90, 163123.	3.3	286
278	Stress-induced band gap tuning in âŸ¨112âŸ© silicon nanowires. Applied Physics Letters, 2007, 91, .	3.3	71
279	Density-functional theory calculations of bare and passivated triangular-shaped ZnO nanowires. Applied Physics Letters, 2007, 91, 031914.	3.3	41
280	Faceted Silicon Nanotubes:â€‰ Structure, Energetic, and Passivation Effects. Journal of Physical Chemistry C, 2007, 111, 1234-1238.	3.1	32
281	Signatures in Vibrational Spectra of Ice Nanotubes Revealed by a Density Functional Tight Binding Method. Journal of Physical Chemistry C, 2007, 111, 14131-14138.	3.1	14
282	Hydrogenated Silicon Nanoparticles Relaxed in Excited States. Journal of Physical Chemistry C, 2007, 111, 12588-12593.	3.1	32
283	Effect of Câ‹¯HÂ·Â·Â·F and Oâ‹¯HÂ·Â·Â·O Hydrogen Bonding in Forming Self-Assembled Monolayers of BF2-Substituted Î²-Dicarbonyl Derivatives on HOPG:â€‰ STM Investigation. Journal of Physical Chemistry C, 2007, 111, 13851-13854.	3.1	18
284	Possible Gas-Phase Reactions of H2/CH4/Tetramethylsilane in Diamond/Î²-SiC Nanocomposite Film Deposition:Â An Ab-Initio Study. Journal of Physical Chemistry A, 2007, 111, 3554-3559.	2.5	16
285	Structural and electronic properties of ZnO nanotubes from density functional calculations. Nanotechnology, 2007, 18, 485713.	2.6	72
286	Geometric and Electronic Structures of Carbon Nanotubes Adsorbed with Flavin Adenine Dinucleotide:â€‰ A Theoretical Study. Journal of Physical Chemistry C, 2007, 111, 4069-4073.	3.1	74
287	Computation of large systems with an economic basis set: Structures and reactivity indices of nucleic acid base pairs from density functional theory. Journal of Computational Chemistry, 2007, 28, 967-974.	3.3	15
288	Effective simulation of biological systems: Choice of density functional and basis set for heme-containing complexes. Chemical Physics Letters, 2007, 434, 149-154.	2.6	39

#	Article	IF	Citations
289	Diameter-dependent spin polarization of injected carriers in carbon-doped zigzag boron nitride nanotubes. Applied Physics Letters, 2006, 89, 123103.	3.3	20
290	Structural characterization of fully coordinated ultrathin silica nanotubes by first-principles calculations. Physical Review B, 2006, 73, .	3.2	21
291	Silica Nanoarchitectures with Tailored Pores Based on the Hybrid Three- and Four-Membered Rings. Journal of Physical Chemistry B, 2006, 110, 15269-15274.	2.6	12
292	A Synthetic Route toward Well-Defined Stoichiometric Silica Fullerene and Nanotubes Based on Metastable Four-Membered Rings. Journal of Physical Chemistry B, 2006, 110, 8992-8997.	2.6	6
293	Dimensionality Dependence of Optical Properties and Quantum Confinement Effects of Hydrogenated Silicon Nanostructures. Journal of Physical Chemistry B, 2006, 110, 21528-21535.	2.6	12
294	Structural Model of Silica Nanowire Assembled from a Highly Stable (SiO2)8 Unit. Journal of Physical Chemistry B, 2006, 110, 1338-1343.	2.6	16
295	A Family of Stable Silica Fullerenes with Fully Coordinated Structures. Journal of Physical Chemistry B, 2006, 110, 17757-17762.	2.6	8
296	Density Functional Theory Study of Geometrical Structures and Electronic Properties of Silica Nanowires. Journal of Physical Chemistry B, 2006, 110, 23633-23636.	2.6	11
297	Geometric and Excited-State Properties of 1,4-Bis(benzothiazolylvinyl)benzene Interacting with 2,2â€˜,2â€˜Ââ€˜-(1,3,5-phenylene)tris[1-phenyl-1H-benzimidazole] Studied by a Density-Functional Tight-Binding Method. Journal of Physical Chemistry B, 2006, 110, 20847-20851.	2.6	6
298	Photoluminescence and electroluminescence of 3-methyl-8-dimethylaminophenazine. Synthetic Metals, 2006, 156, 185-189.	3.9	3
299	Structures and Properties of Silicon Oxide Clusters by Theoretical Investigations. Journal of Cluster Science, 2006, 17, 541-563.	3.3	20
300	Intramolecular Triplet Energy Transfer in Donorâ€“Acceptor Molecules Linked by a Crown Ether Bridge. Chemistry - A European Journal, 2006, 12, 5238-5245.	3.3	13
301	COMPUTATION OF LARGE SYSTEMS WITH AN ECONOMIC BASIS SET: AB INITIO CALCULATIONS OF BIOLOGICAL NUCLEIC ACID BASE PAIRS. Journal of Theoretical and Computational Chemistry, 2006, 05, 411-420.	1.8	2
302	Oxide-Assisted Growth of Silicon and Related Nanowires: Growth Mechanism, Structure and Properties. , 2005, , 308-370.		3
303	Interactions of Li, Ca, and Al with aromatic carbon materials: Anab initiostudy. Journal of Chemical Physics, 2005, 122, 194322.	3.0	10
304	A comparative study of optical properties of poly(9,9-dioctylfluorene) and poly(p-phenylenevinylene) oligomers. Journal of Applied Physics, 2005, 97, 103513.	2.5	15
305	Manipulating the electronic structures of silicon carbide nanotubes by selected hydrogenation. Journal of Chemical Physics, 2005, 122, 214707.	3.0	72
306	Diamond nucleation by energetic pure carbon bombardment. Physical Review B, 2005, 72, .	3.2	33

#	Article	IF	Citations
307	Potential visible light absorption in 3-Ã…-diam carbon nanotubes. Physical Review B, 2005, 72, .	3.2	4
308	Simulation of Water Cluster Assembly on a Graphite Surface. Journal of Physical Chemistry B, 2005, 109, 14183-14188.	2.6	95
309	Ab Initio and Variational Transition State Approach to Î²-C3N4Formation:Â Kinetics for the Reaction of CH3NH2with H. Journal of Physical Chemistry A, 2005, 109, 9112-9117.	2.5	13
310	Investigation of Possible Structures of Silicon Nanotubes via Density-Functional Tight-Binding Molecular Dynamics Simulations and ab Initio Calculations. Journal of Physical Chemistry B, 2005, 109, 8605-8612.	2.6	72
311	Geometrical structures and electronic properties of AlN fullerenes: A comparative theoretical study of AlN fullerenes with BN and C fullerenes. Journal of Materials Chemistry, 2005, 15, 3034.	6.7	22
312	Structures and energetics of hydrogen-terminated silicon nanowire surfaces. Journal of Chemical Physics, 2005, 123, 144703.	3.0	109
313	Signature of Nanodiamond in Raman Spectra:Â A Density Functional Theoretical Study. Journal of Physical Chemistry B, 2005, 109, 9006-9013.	2.6	31
314	Calcium/Poly(9,9-dioctylfluorene) Interaction:â€‰ A Theoretical Study. Journal of Physical Chemistry B, 2005, 109, 12868-12873.	2.6	9
315	Strain energy and electronic structures of silicon carbide nanotubes: Density functional calculations. Physical Review B, 2005, 71, .	3.2	239
316	Fluorination-induced back-bond weakening and hydrogen passivation on HF-etched Si surfaces. Physical Review B, 2004, 69, .	3.2	21
317	Gold nanowires from silicon nanowire templates. Applied Physics Letters, 2004, 84, 407-409.	3.3	34
318	Simulation of gate-controlled Coulomb blockades in carbon nanotubes. Journal of Applied Physics, 2004, 95, 5729-5735.	2.5	7
319	Response to â€œComment on â€˜Gold nanowires from silicon nanowire templatesâ€™â€‰â€•[Appl. Phys. Lett. 85, 692 (2004)]. Applied Physics Letters, 2004, 85, 693-693.	3.3	1
320	A scheme for the economical use of numerical basis sets in calculations with SIESTA. Theoretical Chemistry Accounts, 2004, 112, 158.	1.4	33
321	On the Stability of Hydride Configurations on Silicon Cluster Surfaces:Â A First-Principle Theoretical Study. Journal of Physical Chemistry B, 2004, 108, 1967-1973.	2.6	11
322	Stable and extendable cage containing nanosize silica clusters based on three-membered rings. Physical Review B, 2004, 69, .	3.2	28
323	Kinetics and Mechanism of O (3P) Reaction with CH3CHF2:Â A Theoretical Study. Journal of Physical Chemistry A, 2004, 108, 1064-1068.	2.5	21
324	Electrical Transport and Electronic Delocalization of Small Fullerenes. Journal of Physical Chemistry B, 2004, 108, 16636-16641.	2.6	10

#	Article	IF	Citations
325	Fluorination Induced Etching Selectivity of Boron Nitride Phases. Journal of Physical Chemistry B, 2004, 108, 7597-7602.	2.6	8
326	Stable tetrahedral structure of the silica cluster(SiO2)10. Physical Review B, 2004, 70, .	3.2	15
327	Two- and Three-Membered-Ring Hybrid Structures of Silica Nanoclusters. Journal of Physical Chemistry B, 2004, 108, 18451-18454.	2.6	23
328	Optical spectra of single-walled boron nitride nanotubes. Physical Review B, 2004, 69, .	3.2	40
329	Silicon Monoxide Clusters: The Favorable Precursors for Forming Silicon Nanostructures. Physical Review Letters, 2004, 93, 095503.	7.8	55
330	Theoretical Prediction on Efficient Formation of Imino Acid via an Aza-Wittig Reaction. Journal of Physical Chemistry B, 2003, 107, 2061-2067.	2.6	10
331	A thermodynamic and kinetic study of the formation of C20 compounds encapsulating H, He and Ne atoms. Theoretical Chemistry Accounts, 2003, 109, 278-283.	1.4	6
332	Improved performance and stability of organic light-emitting devices with silicon oxy-nitride buffer layer. Applied Physics Letters, 2003, 83, 1038-1040.	3.3	59
333	First-principles calculations for nitrogen-containing single-walled carbon nanotubes. Journal of Applied Physics, 2003, 94, 2398-2402.	2.5	93
334	Silicon-Based Nanowires. , 2003, , 413-462.		0
335	Metal/Alq3 interactions in organic light emitting devices: The different roles of Mg, Al, and Li atoms. Journal of Chemical Physics, 2002, 116, 8827-8837.	3.0	32
336	Electronic and geometric structure of thin stable short silicon nanowires. Physical Review B, 2002, 65, .	3.2	88
337	Theoretical study of structure-dependent Coulomb blockade in carbon nanotubes. Physical Review B, 2002, 66, .	3.2	7
338	Oxygen adsorption on small Si clusters: a full-potential linear-muffin-tin-orbital molecular-dynamics study. Journal of Physics Condensed Matter, 2002, 14, 1723-1733.	1.8	8
339	Computation of Large Systems with Economic Basis Set:Â Simulation of Diamond Metallization Using Titanium. Journal of Physical Chemistry B, 2002, 106, 625-631.	2.6	10
340	Structural properties of hydrogenated silicon nanocrystals and nanoclusters. Journal of Applied Physics, 2002, 92, 7453-7458.	2.5	38
341	Contact formation of LiF/Al cathodes in Alq-based organic light-emitting diodes. Journal Physics D: Applied Physics, 2002, 35, 103-107.	2.8	115
342	The Mechanism of Diamond Nucleation from Energetic Species. Science, 2002, 297, 1531-1533.	12.6	202

#	Article	IF	Citations
343	Size-dependent oxidation of hydrogenated silicon clusters. Applied Physics Letters, 2002, 80, 4223-4225.	3.3	13
344	Theoretical study on the substituent effect of a Wittig reaction. Theoretical Chemistry Accounts, 2002, 107, 206-210.	1.4	9
345	Structural transition in nanosized silicon clusters. Physical Review B, 2002, 65, .	3.2	56
346	Geometric and Electronic Structures of Silicon Oxide Clusters. Journal of Physical Chemistry B, 2001, 105, 1705-1709.	2.6	100
347	Computation of large systems with an economic basis set: Ab initio calculations of silicon oxide clusters. Journal of Chemical Physics, 2001, 114, 5531-5536.	3.0	28
348	The properties and possible transformation path for C12B24N24. International Journal of Quantum Chemistry, 2001, 84, 363-368.	2.0	2
349	Interactions of hydride species and their roles in carbon nitride growth. Physical Review B, 2001, 63, .	3.2	5
350	High reactivity of silicon suboxide clusters. Physical Review B, 2001, 64, .	3.2	54
351	The Effects of Hydrogen Etching on Different Carbon and Boron Nitride Phases. Chemical Vapor Deposition, 2000, 6, 227-230.	1.3	3
352	An effective scheme for selecting basis sets forab initio calculations. Science in China Series B: Chemistry, 2000, 43, 375-388.	0.8	22
353	Smallest diameter carbon nanotubes. Applied Physics Letters, 2000, 77, 2831-2833.	3.3	68
354	Time-dependent quantum wave packet studies of the F+HCl and F+DCl reactions. Journal of Chemical Physics, 2000, 113, 10105-10113.	3.0	52
355	A Theoretical Study on the Interactions of Hydrogen Species with Various Carbon and Boron Nitride Phases. Journal of Physical Chemistry B, 2000, 104, 6761-6766.	2.6	12
356	The electronic structures and properties of Alq3 and NPB molecules in organic light emitting devices: Decompositions of density of states. Journal of Chemical Physics, 2000, 112, 8614-8620.	3.0	40
357	Theory of the charge-transport properties of naphthyl diamine used in organic light-emitting devices. Applied Physics Letters, 1999, 75, 2418-2420.	3.3	14
358	Hyperspherical approach for charged excitons in quantum wells. Physical Review B, 1999, 60, 5714-5720.	3.2	19
359	Energetics of segregation in Î²-C2BN. Applied Physics Letters, 1999, 75, 2259-2261.	3.3	59
360	Theory of magnesium/Alq3 interaction in organic light emitting devices. Applied Physics Letters, 1999, 74, 1612-1614.	3.3	33

#	Article	IF	Citations
361	Local strain in interface: Origin of grain tilting in diamond (001)/silicon (001) heteroepitaxy. Physical Review B, 1998, 58, 15351-15354.	3.2	19
362	Bonding Regeneration: The Driving Force of Hetero-Epitaxial Diamond Grain Coalescence on (001) Silicon. Materials Research Society Symposia Proceedings, 1998, 529, 133.	0.1	2
363	The Origin of Mis-Oriented Diamond Grains Nucleated Directly on (001) Silicon Surface. Materials Research Society Symposia Proceedings, 1998, 529, 139.	0.1	1
364	Improved scheme to solve the atomic Schrï¿½dinger equation in hyperspherical coordinates. International Journal of Quantum Chemistry, 1996, 59, 203-207.	2.0	5
365	Production of nanometric particles in radio frequency glow discharges in mixtures of silane and methane. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1996, 14, 567-571.	2.1	17
366	Role of structural saturation and geometry in the luminescence of silicon-based nanostructured materials. Physical Review B, 1996, 53, 7847-7850.	3.2	40
367	Structural modeling of the possible growth of oriented textured singleâ€crystal diamond film on a silicon (111) surface. Applied Physics Letters, 1996, 69, 1086-1088.	3.3	15
368	Ab Initio Calculations of Hydrogen-Bonded Carboxylic Acid Cluster Systems:Â Dimer Evaporations. The Journal of Physical Chemistry, 1996, 100, 960-966.	2.9	52
369	Solution of atomic and molecular SchrÃ¶dinger equation described by hyperspherical coordinates. International Journal of Quantum Chemistry, 1993, 45, 385-390.	2.0	24
370	Exact solutions of the SchrÃ¶dinger equation for some quantum-mechanical many-body systems. Physical Review A, 1993, 47, 71-77.	2.5	36
371	Chemical reaction dynamics of barium atom with alkyl bromides. Chemical Physics Letters, 1991, 181, 474-478.	2.6	72
372	Origin and nature of gap states in a-Si:H alloys. Solid State Communications, 1989, 69, 681-684.	1.9	6
373	Role of hydrogen in doping mechanism for a-Si:H alloys. Solid State Communications, 1988, 65, 1625-1627.	1.9	3
374	A revised mechanism of band gap evolution of TMDC nanotubes and its application to Janus TMDC nanotubes: negative electron and hole compressibility. Journal of Materials Chemistry C, 0, , .	5.5	7