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	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
2	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
3	Motility of Metal Nanoparticles in Silicon and Induced Anisotropic Silicon Etching. Advanced Functional Materials, 2008, 18, 3026-3035.	14.9	427
4	Ordered silicon nanowire arrays via nanosphere lithography and metal-induced etching. Applied Physics Letters, 2007, 90, 163123.	3.3	286
5	Strain energy and electronic structures of silicon carbide nanotubes: Density functional calculations. Physical Review B, 2005, 71, .	3.2	239
6	Al doped graphene: A promising material for hydrogen storage at room temperature. Journal of Applied Physics, 2009, 105, .	2.5	212
7	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
8	The Mechanism of Diamond Nucleation from Energetic Species. Science, 2002, 297, 1531-1533.	12.6	202
9	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
10	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
11	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
12	Efficiency Enhancement of Carbon Nitride Photoelectrochemical Cells via Tailored Monomers Design. Advanced Energy Materials, 2016, 6, 1600263.	19.5	116
13	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
14	Structures and energetics of hydrogen-terminated silicon nanowire surfaces. Journal of Chemical Physics, 2005, 123, 144703.	3.0	109
15	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
16	Vacancy-defectâ€“induced diminution of thermal conductivity in silicene. Europhysics Letters, 2012, 99, 36001.	2.0	101
17	Geometric and Electronic Structures of Silicon Oxide Clusters. Journal of Physical Chemistry B, 2001, 105, 1705-1709.	2.6	100
18	Graphitic Carbon Nitride Film: An Emerging Star for Catalytic and Optoelectronic Applications. ChemSusChem, 2016, 9, 2723-2735.	6.8	96

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19	Simulation of Water Cluster Assembly on a Graphite Surface. Journal of Physical Chemistry B, 2005, 109, 14183-14188.	2.6	95
20	First-principles calculations for nitrogen-containing single-walled carbon nanotubes. Journal of Applied Physics, 2003, 94, 2398-2402.	2.5	93
21	Electronic and geometric structure of thin stable short silicon nanowires. Physical Review B, 2002, 65, .	3.2	88
22	Low-dimensional Mo:BiVO₄ photoanodes for enhanced photoelectrochemical activity. Journal of Materials Chemistry A, 2018, 6, 3602-3609.	10.3	86
23	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
24	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
25	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
26	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
27	Stable calcium adsorbates on carbon nanostructures: Applications for high-capacity hydrogen storage. Physical Review B, 2009, 79, .	3.2	74
28	Moleculeâ€“substrate interaction channels of metal-phthalocyanines on graphene on Ni(111) surface. Journal of Chemical Physics, 2011, 134, 094705.	3.0	74
29	Spin-orbit torque in a completely compensated synthetic antiferromagnet. Physical Review B, 2018, 97, .	3.2	73
30	Chemical reaction dynamics of barium atom with alkyl bromides. Chemical Physics Letters, 1991, 181, 474-478.	2.6	72
31	Manipulating the electronic structures of silicon carbide nanotubes by selected hydrogenation. Journal of Chemical Physics, 2005, 122, 214707.	3.0	72
32	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
33	Structural and electronic properties of ZnO nanotubes from density functional calculations. Nanotechnology, 2007, 18, 485713.	2.6	72
34	Tunable Electrical Properties of Silicon Nanowires via Surface-Ambient Chemistry. ACS Nano, 2010, 4, 3045-3052.	14.6	72
35	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
36	Stress-induced band gap tuning in âŸ¨112âŸ© silicon nanowires. Applied Physics Letters, 2007, 91, .	3.3	71

#	Article	IF	Citations
37	Single-Crystal 9,10-Diphenylanthracene Nanoribbons and Nanorods. Chemistry of Materials, 2008, 20, 6945-6950.	6.7	71
38	Smallest diameter carbon nanotubes. Applied Physics Letters, 2000, 77, 2831-2833.	3.3	68
39	Recent developments in carbon nitride based films for photoelectrochemical water splitting. Sustainable Energy and Fuels, 2020, 4, 485-503.	4.9	68
40	A surface-enhanced Raman spectroscopy substrate for highly sensitive label-free immunoassay. Applied Physics Letters, 2008, 92, .	3.3	67
41	Theoretical study of the chemical gap tuning in silicon nanowires. Physical Review B, 2007, 76, .	3.2	65
42	Unusual size dependence of the optical emission gap in small hydrogenated silicon nanoparticles. Applied Physics Letters, 2007, 90, 123116.	3.3	61
43	DFT calculations on structural and electronic properties of Bi2MO6 (M = Cr, Mo, W). Rare Metals, 2011, 30, 166-172.	7.1	60
44	Energetics of segregation in Î²-C2BN. Applied Physics Letters, 1999, 75, 2259-2261.	3.3	59
45	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
46	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
47	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
48	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
49	First-principles calculations of reconstructed [0001] ZnO nanowires. Physical Review B, 2007, 76, .	3.2	58
50	Covalent-adsorption induced magnetism in graphene. Journal of Materials Chemistry, 2009, 19, 9274.	6.7	58
51	Optimal surface functionalization of silicon quantum dots. Journal of Chemical Physics, 2008, 128, 244714.	3.0	57
52	Surface Passivation and Transfer Doping of Silicon Nanowires. Angewandte Chemie - International Edition, 2009, 48, 9896-9900.	13.8	57
53	Structural transition in nanosized silicon clusters. Physical Review B, 2002, 65, .	3.2	56
54	Silicon Monoxide Clusters: The Favorable Precursors for Forming Silicon Nanostructures. Physical Review Letters, 2004, 93, 095503.	7.8	55

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55	Structural, Electronic, Dynamical, and Superconducting Properties in Dense GeH₄(H₂)₂. Journal of Physical Chemistry C, 2012, 116, 5225-5234.	3.1	55
56	Exciton Self-Trapping in sp² Carbon Nanostructures Induced by Edge Ether Groups. Journal of Physical Chemistry Letters, 2018, 9, 4857-4864.	4.6	55
57	High reactivity of silicon suboxide clusters. Physical Review B, 2001, 64, .	3.2	54
58	Strain Induced Band Dispersion Engineering in Si Nanosheets. Journal of Physical Chemistry C, 2011, 115, 23682-23687.	3.1	54
59	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
60	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
61	Hydrogen and oxygen adsorption on ZnO nanowires: A first-principles study. Physical Review B, 2009, 79, .	3.2	51
62	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
63	Dynamic crystallography reveals early signalling events in ultraviolet photoreceptor UVR8. Nature Plants, 2015, 1, .	9.3	48
64	A new insight into Ï€â€“Ï€ stacking involving remarkable orbital interactions. Physical Chemistry Chemical Physics, 2016, 18, 25452-25457.	2.8	48
65	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
66	Adsorption and properties of aromatic amino acids on single-walled carbon nanotubes. Nanoscale, 2012, 4, 1146-1153.	5.6	45
67	Molecular orbital analysis of the hydrogen bonded water dimer. Scientific Reports, 2016, 6, 22099.	3.3	45
68	Density-functional theory calculations of bare and passivated triangular-shaped ZnO nanowires. Applied Physics Letters, 2007, 91, 031914.	3.3	41
69	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
70	Survey of structural and electronic properties of C60 on close-packed metal surfaces. Journal of Materials Science, 2012, 47, 7341-7355.	3.7	41
71	Role of structural saturation and geometry in the luminescence of silicon-based nanostructured materials. Physical Review B, 1996, 53, 7847-7850.	3.2	40
72	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

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73	Optical spectra of single-walled boron nitride nanotubes. Physical Review B, 2004, 69, .	3.2	40
74	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
75	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
76	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
77	Structural properties of hydrogenated silicon nanocrystals and nanoclusters. Journal of Applied Physics, 2002, 92, 7453-7458.	2.5	38
78	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
79	<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
80	Collaborative enhancement of photon harvesting and charge carrier dynamics in carbon nitride photoelectrode. Applied Catalysis B: Environmental, 2018, 237, 783-790.	20.2	38
81	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
82	Na₂C monolayer: a novel 2p Dirac half-metal with multiple symmetry-protected Dirac cones. Nanoscale, 2018, 10, 13645-13651.	5.6	38
83	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
84	Exact solutions of the SchrÃ¶dinger equation for some quantum-mechanical many-body systems. Physical Review A, 1993, 47, 71-77.	2.5	36
85	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
86	Amine-capped silicon quantum dots. Applied Physics Letters, 2008, 92, 053107.	3.3	35
87	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
88	Gold nanowires from silicon nanowire templates. Applied Physics Letters, 2004, 84, 407-409.	3.3	34
89	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
90	Crystalâ€Face Tailored Graphitic Carbon Nitride Films for Highâ€Performance Photoelectrochemical Cells. ChemSusChem, 2018, 11, 2497-2501.	6.8	34

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91	Theory of magnesium/Alq3 interaction in organic light emitting devices. Applied Physics Letters, 1999, 74, 1612-1614.	3.3	33
92	A scheme for the economical use of numerical basis sets in calculations with SIESTA. Theoretical Chemistry Accounts, 2004, 112, 158.	1.4	33
93	Diamond nucleation by energetic pure carbon bombardment. Physical Review B, 2005, 72, .	3.2	33
94	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
95	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
96	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
97	Faceted Silicon Nanotubes:â€‰ Structure, Energetic, and Passivation Effects. Journal of Physical Chemistry C, 2007, 111, 1234-1238.	3.1	32
98	Hydrogenated Silicon Nanoparticles Relaxed in Excited States. Journal of Physical Chemistry C, 2007, 111, 12588-12593.	3.1	32
99	Signature of Nanodiamond in Raman Spectra:Â A Density Functional Theoretical Study. Journal of Physical Chemistry B, 2005, 109, 9006-9013.	2.6	31
100	Cooperative Modulation of Electronic Structures of Aromatic Molecules Coupled to Multiple Metal Contacts. Physical Review Letters, 2013, 110, 046802.	7.8	31
101	Defect Induced Electronic Structure of Uranofullerene. Scientific Reports, 2013, 3, 1341.	3.3	30
102	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
103	Nonresonant chemical mechanism in surface-enhanced Raman scattering of pyridine on M@Au₁₂clusters. Nanoscale, 2016, 8, 4086-4093.	5.6	30
104	External Electric Field Modulated Electronic and Structural Properties of â€˜111â€‰ Si Nanowires. Journal of Physical Chemistry C, 2009, 113, 10384-10389.	3.1	29
105	Oxygen vacancy diffusion in bare ZnO nanowires. Nanoscale, 2014, 6, 11882-11886.	5.6	29
106	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
107	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
108	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

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109	Stable and extendable cage containing nanosize silica clusters based on three-membered rings. Physical Review B, 2004, 69, .	3.2	28
110	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
111	Stabilizing excited-state silicon nanoparticle by surface oxidation. Applied Physics Letters, 2007, 91, .	3.3	27
112	Band gap engineering of GaN nanowires by surface functionalization. Applied Physics Letters, 2009, 94, .	3.3	27
113	Detailed low-energy electron diffraction analysis of the (<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 602 Td (xmlns:mml= 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
114	Mechanism of the charge separation improvement in carbon-nanodot sensitized g-C3N4. Applied Surface Science, 2019, 487, 151-158.	6.1	27
115	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
116	Solution of atomic and molecular SchrÃ¶dinger equation described by hyperspherical coordinates. International Journal of Quantum Chemistry, 1993, 45, 385-390.	2.0	24
117	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
118	Excited state properties of Si quantum dots. Physica Status Solidi (B): Basic Research, 2012, 249, 401-412.	1.5	24
119	Boundary and Symmetry Determined Exciton Distribution in Two Dimensional Silicon Nanosheets. Journal of Physical Chemistry C, 2014, 118, 20070-20076.	3.1	24
120	Two- and Three-Membered-Ring Hybrid Structures of Silica Nanoclusters. Journal of Physical Chemistry B, 2004, 108, 18451-18454.	2.6	23
121	Anomalous size dependence of the luminescence in reconstructed silicon nanoparticles. Applied Physics Letters, 2008, 93, .	3.3	23
122	Prediction of energetically optimal single-walled carbon nanotubes for hydrogen physisorption. Applied Physics Letters, 2009, 95, 013116.	3.3	23
123	Rectifying Properties of Oligo(Phenylene Ethynylene) Heterometallic Molecular Junctions: Molecular Length and Side Group Effects. Scientific Reports, 2014, 4, 6357.	3.3	23
124	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
125	An effective scheme for selecting basis sets forab initio calculations. Science in China Series B: Chemistry, 2000, 43, 375-388.	0.8	22
126	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

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127	Tunable electronic band structures of hydrogen-terminated âŸ¨112âŸ© silicon nanowires. Applied Physics Letters, 2008, 92, 203109.	3.3	22
128	Superconductivity in Hydrogen-rich Material: GeH4. Journal of Superconductivity and Novel Magnetism, 2010, 23, 717-719.	1.8	22
129	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
130	Structural transitions of solid germane under pressure. Europhysics Letters, 2010, 90, 66006.	2.0	22
131	Prospects for Resolving Chemical Structure by Atomic Force Microscopy: A First-Principles Study. Langmuir, 2010, 26, 16271-16277.	3.5	22
132	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 different types of reconstruction. Physical Review B, 2012, 85, .	3.2	22
133	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
134	Energetics of hexagonal boron nitride nanostructures: edge dependence and truncation effects. Nanoscale, 2017, 9, 6734-6740.	5.6	22
135	Fluorination-induced back-bond weakening and hydrogen passivation on HF-etched Si surfaces. Physical Review B, 2004, 69, .	3.2	21
136	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
137	Structural characterization of fully coordinated ultrathin silica nanotubes by first-principles calculations. Physical Review B, 2006, 73,	3.2	21
138	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:mrow></mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>N</mml:mtext><mml:mn>2</mml:mn></mml:m. Physical Revi	3.2	21
139	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
140	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
141	Anomalous effect of hydrogenation on phonon thermal conductivity in thin silicon nanowires. Europhysics Letters, 2014, 105, 56003.	2.0	21
142	Interlocking Mechanism between Molecular Gears Attached to Surfaces. ACS Nano, 2018, 12, 3020-3029.	14.6	21
143	Diameter-dependent spin polarization of injected carriers in carbon-doped zigzag boron nitride nanotubes. Applied Physics Letters, 2006, 89, 123103.	3.3	20
144	Structures and Properties of Silicon Oxide Clusters by Theoretical Investigations. Journal of Cluster Science, 2006, 17, 541-563.	3.3	20

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145	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
146	Indirect-to-direct band gap transitions in phosphorus adsorbed âŸ¨112âŸ© silicon nanowires. Applied Physics Letters, 2008, 93, .	3.3	20
147	Chemical Trend of Pressure-Induced Metallization in Alkaline Earth Hydrides. Journal of Physical Chemistry C, 2010, 114, 14614-14617.	3.1	20
148	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
149	Local strain in interface: Origin of grain tilting in diamond (001)/silicon (001) heteroepitaxy. Physical Review B, 1998, 58, 15351-15354.	3.2	19
150	Hyperspherical approach for charged excitons in quantum wells. Physical Review B, 1999, 60, 5714-5720.	3.2	19
151	Strong interactions and charge transfers between a charged benzene molecule and multilayer graphenes. Journal of Materials Chemistry, 2012, 22, 23380.	6.7	19
152	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
153	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
154	Strong orbital interaction in a weak CH·Ï€ hydrogen bonding system. Scientific Reports, 2016, 6, 22304.	3.3	19
155	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
156	Effect of Câˆ'HÂ·Â·Â·F and Oâˆ'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
157	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
158	Electronic delocalization in small water rings. Physical Chemistry Chemical Physics, 2015, 17, 2987-2990.	2.8	18
159	Formation Mechanism of Atmospheric Ammonium Bisulfate: Hydrogenâ€Bondâ€Promoted Nearly Barrierless Reactions of SO₃ with NH₃ and H₂O. ChemPhysChem, 2018, 19, 967-972.	2.1	18
160	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
161	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
162	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

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