

# Rui-Qin Zhang

## List of Publications by Citations

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372  
papers

9,494  
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48  
h-index

80  
g-index

385  
ext. papers

10,359  
ext. citations

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L-index

#	Paper	IF	Citations
372	A Strategy of Enhancing the Photoactivity of g-C <sub>3</sub> N <sub>4</sub> via Doping of Nonmetal Elements: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 23485-23493	3.8	471
371	Preparation of Large-Area Uniform Silicon Nanowires Arrays through Metal-Assisted Chemical Etching. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 4444-4450	3.8	448
370	Motility of Metal Nanoparticles in Silicon and Induced Anisotropic Silicon Etching. <i>Advanced Functional Materials</i> , <b>2008</b> , 18, 3026-3035	15.6	387
369	Ordered silicon nanowire arrays via nanosphere lithography and metal-induced etching. <i>Applied Physics Letters</i> , <b>2007</b> , 90, 163123	3.4	251
368	Strain energy and electronic structures of silicon carbide nanotubes: Density functional calculations. <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	224
367	Al doped graphene: A promising material for hydrogen storage at room temperature. <i>Journal of Applied Physics</i> , <b>2009</b> , 105, 074307	2.5	183
366	The mechanism of diamond nucleation from energetic species. <i>Science</i> , <b>2002</b> , 297, 1531-3	33.3	179
365	Photo and pH stable, highly-luminescent silicon nanospheres and their bioconjugates for immunofluorescent cell imaging. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 4434-8	16.4	176
364	Thermal vapor condensation of uniform graphitic carbon nitride films with remarkable photocurrent density for photoelectrochemical applications. <i>Nano Energy</i> , <b>2015</b> , 15, 353-361	17.1	158
363	Carbon dot loading and TiO <sub>2</sub> nanorod length dependence of photoelectrochemical properties in carbon dot/TiO <sub>2</sub> nanorod array nanocomposites. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2014</b> , 6, 4883-90	9.5	151
362	Tris(trimethylsilyl)borate as an electrolyte additive for improving interfacial stability of high voltage layered lithium-rich oxide cathode/carbonate-based electrolyte. <i>Journal of Power Sources</i> , <b>2015</b> , 285, 360-366	8.9	107
361	Contact formation of LiF/Al cathodes in Alq <sub>3</sub> -based organic light-emitting diodes. <i>Journal Physics D: Applied Physics</i> , <b>2002</b> , 35, 103-107	3	102
360	Structures and energetics of hydrogen-terminated silicon nanowire surfaces. <i>Journal of Chemical Physics</i> , <b>2005</b> , 123, 144703	3.9	98
359	Efficiency Enhancement of Carbon Nitride Photoelectrochemical Cells via Tailored Monomers Design. <i>Advanced Energy Materials</i> , <b>2016</b> , 6, 1600263	21.8	96
358	Geometric and Electronic Structures of Silicon Oxide Clusters. <i>Journal of Physical Chemistry B</i> , <b>2001</b> , 105, 1705-1709	3.4	90
357	Simulation of water cluster assembly on a graphite surface. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 14183-8	3.4	89
356	First-principles calculations for nitrogen-containing single-walled carbon nanotubes. <i>Journal of Applied Physics</i> , <b>2003</b> , 94, 2398-2402	2.5	88

355	Vacancy-defect-induced diminution of thermal conductivity in silicene. <i>Europhysics Letters</i> , <b>2012</b> , 99, 36001	1.6	85
354	Electronic and geometric structure of thin stable short silicon nanowires. <i>Physical Review B</i> , <b>2002</b> , 65,	3.3	85
353	A novel electrolyte additive for improving the interfacial stability of high voltage lithium nickel manganese oxide cathode. <i>Journal of Power Sources</i> , <b>2015</b> , 293, 71-77	8.9	75
352	Molecule-substrate interaction channels of metal-phthalocyanines on graphene on Ni(111) surface. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 094705	3.9	71
351	Stable calcium adsorbates on carbon nanostructures: Applications for high-capacity hydrogen storage. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	71
350	Geometric and Electronic Structures of Carbon Nanotubes Adsorbed with Flavin Adenine Dinucleotide: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 4069-4073	3.8	69
349	Structural and electronic properties of ZnO nanotubes from density functional calculations. <i>Nanotechnology</i> , <b>2007</b> , 18, 485713	3.4	68
348	Manipulating the electronic structures of silicon carbide nanotubes by selected hydrogenation. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 214707	3.9	68
347	Chemical reaction dynamics of barium atom with alkyl bromides. <i>Chemical Physics Letters</i> , <b>1991</b> , 181, 474-478	2.5	67
346	Two-dimensional topological insulators with binary honeycomb lattices: SiC <sub>3</sub> siligraphene and its analogs. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	65
345	Tunable electrical properties of silicon nanowires via surface-ambient chemistry. <i>ACS Nano</i> , <b>2010</b> , 4, 3045-3052	5.7	65
344	Graphitic Carbon Nitride Film: An Emerging Star for Catalytic and Optoelectronic Applications. <i>ChemSusChem</i> , <b>2016</b> , 9, 2723-2735	8.3	62
343	Single-Crystal 9,10-Diphenylanthracene Nanoribbons and Nanorods. <i>Chemistry of Materials</i> , <b>2008</b> , 20, 6945-6950	9.6	62
342	Stress-induced band gap tuning in <112> silicon nanowires. <i>Applied Physics Letters</i> , <b>2007</b> , 91, 263107	3.4	62
341	Efficient emission facilitated by multiple energy level transitions in uniform graphitic carbon nitride films deposited by thermal vapor condensation. <i>ChemPhysChem</i> , <b>2015</b> , 16, 954-9	3.2	61
340	A surface-enhanced Raman spectroscopy substrate for highly sensitive label-free immunoassay. <i>Applied Physics Letters</i> , <b>2008</b> , 92, 043116	3.4	61
339	Investigation of possible structures of silicon nanotubes via density-functional tight-binding molecular dynamics simulations and ab initio calculations. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 8605-12	3.4	60
338	Unusual size dependence of the optical emission gap in small hydrogenated silicon nanoparticles. <i>Applied Physics Letters</i> , <b>2007</b> , 90, 123116	3.4	59

- 337 Theoretical study of the chemical gap tuning in silicon nanowires. *Physical Review B*, **2007**, 76, 3-3 58
- 336 Smallest diameter carbon nanotubes. *Applied Physics Letters*, **2000**, 77, 2831-2833 3-4 58
- 335 Low-dimensional Mo:BiVO<sub>4</sub> photoanodes for enhanced photoelectrochemical activity. *Journal of Materials Chemistry A*, **2018**, 6, 3602-3609 13 56
- 334 Covalent-adsorption induced magnetism in graphene. *Journal of Materials Chemistry*, **2009**, 19, 9274 56
- 333 First-principles calculations of reconstructed [0001] ZnO nanowires. *Physical Review B*, **2007**, 76, 3-3 56
- 332 Improved performance and stability of organic light-emitting devices with silicon oxy-nitride buffer layer. *Applied Physics Letters*, **2003**, 83, 1038-1040 3-4 56
- 331 Energetics of segregation in  $\text{SiC}_2\text{BN}$ . *Applied Physics Letters*, **1999**, 75, 2259-2261 3-4 56
- 330 Surface passivation and transfer doping of silicon nanowires. *Angewandte Chemie - International Edition*, **2009**, 48, 9896-9900 16.4 55
- 329 Optimal surface functionalization of silicon quantum dots. *Journal of Chemical Physics*, **2008**, 128, 244714.9 53
- 328 Structural transition in nanosized silicon clusters. *Physical Review B*, **2002**, 65, 3-3 51
- 327 Silicon monoxide clusters: the favorable precursors for forming silicon nanostructures. *Physical Review Letters*, **2004**, 93, 095503 7-4 51
- 326 Spin-orbit torque in a completely compensated synthetic antiferromagnet. *Physical Review B*, **2018**, 97, 3-3 48
- 325 Structural, Electronic, Dynamical, and Superconducting Properties in Dense GeH<sub>4</sub>(H<sub>2</sub>)<sub>2</sub>. *Journal of Physical Chemistry C*, **2012**, 116, 5225-5234 3.8 48
- 324 Ab Initio Calculations of Hydrogen-Bonded Carboxylic Acid Cluster Systems: Dimer Evaporations. *The Journal of Physical Chemistry*, **1996**, 100, 960-966 48
- 323 High reactivity of silicon suboxide clusters. *Physical Review B*, **2001**, 64, 3-3 48
- 322 Time-dependent quantum wave packet studies of the F+HCl and F+DCI reactions. *Journal of Chemical Physics*, **2000**, 113, 10105-10113 3-9 48
- 321 DFT calculations on structural and electronic properties of Bi<sub>2</sub>MO<sub>6</sub> (M = Cr, Mo, W). *Rare Metals*, **2011**, 30, 166-172 5-5 46
- 320 Hydrogen and oxygen adsorption on ZnO nanowires: A first-principles study. *Physical Review B*, **2009**, 79, 3-3 46

319	Engineering of Facets, Band Structure, and Gas-Sensing Properties of Hierarchical Sn <sup>2+</sup> -Doped SnO <sub>2</sub> Nanostructures. <i>Advanced Functional Materials</i> , <b>2013</b> , 23, n/a-n/a	15.6	45
318	Strain Induced Band Dispersion Engineering in Si Nanosheets. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 23682-23687	3.8	45
317	Recent developments in carbon nitride based films for photoelectrochemical water splitting. <i>Sustainable Energy and Fuels</i> , <b>2020</b> , 4, 485-503	5.8	44
316	Hydrogen-Location-Sensitive Modulation of the Redox Reactivity for Oxygen-Deficient TiO <sub>2</sub> . <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 8407-8411	16.4	43
315	Tuning the optical properties of graphene quantum dots by selective oxidation: a theoretical perspective. <i>Journal of Materials Chemistry C</i> , <b>2018</b> , 6, 6875-6883	7.1	43
314	Dynamic Crystallography Reveals Early Signalling Events in Ultraviolet Photoreceptor UVR8. <i>Nature Plants</i> , <b>2015</b> , 1,	11.5	42
313	Stacking of polycyclic aromatic hydrocarbons as prototype for graphene multilayers, studied using density functional theory augmented with a dispersion term. <i>Journal of Chemical Physics</i> , <b>2009</b> , 131, 1947-1952	3.0	41
312	Adsorption and properties of aromatic amino acids on single-walled carbon nanotubes. <i>Nanoscale</i> , <b>2012</b> , 4, 1146-53	7.7	40
311	Density-functional theory calculations of bare and passivated triangular-shaped ZnO nanowires. <i>Applied Physics Letters</i> , <b>2007</b> , 91, 031914	3.4	40
310	Survey of structural and electronic properties of C <sub>60</sub> on close-packed metal surfaces. <i>Journal of Materials Science</i> , <b>2012</b> , 47, 7341-7355	4.3	39
309	Two-dimensional metal-organic coordination networks of Mn-7,7,8,8-tetracyanoquinodimethane assembled on Cu(100): Structural, electronic, and magnetic properties. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	39
308	Enhanced optical absorption and photocatalytic H <sub>2</sub> production activity of g-C <sub>3</sub> N <sub>4</sub> /TiO <sub>2</sub> heterostructure by interfacial coupling: A DFT+U study. <i>International Journal of Hydrogen Energy</i> , <b>2017</b> , 42, 9903-9913	6.7	38
307	Evaluating frontier orbital energy and HOMO/LUMO gap with descriptors from density functional reactivity theory. <i>Journal of Molecular Modeling</i> , <b>2017</b> , 23, 3	2	38
306	Role of structural saturation and geometry in the luminescence of silicon-based nanostructured materials. <i>Physical Review B</i> , <b>1996</b> , 53, 7847-7850	3.3	38
305	Exciton Self-Trapping in sp Carbon Nanostructures Induced by Edge Ether Groups. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 4857-4864	6.4	37
304	The electronic structures and properties of Alq <sub>3</sub> and NPB molecules in organic light emitting devices: Decompositions of density of states. <i>Journal of Chemical Physics</i> , <b>2000</b> , 112, 8614-8620	3.9	37
303	Molecular orbital analysis of the hydrogen bonded water dimer. <i>Scientific Reports</i> , <b>2016</b> , 6, 22099	4.9	36
302	Optical spectra of single-walled boron nitride nanotubes. <i>Physical Review B</i> , <b>2004</b> , 69,	3.3	36

301	Structural properties of hydrogenated silicon nanocrystals and nanoclusters. <i>Journal of Applied Physics</i> , <b>2002</b> , 92, 7453-7458	2.5	36
300	Quantum Mechanical Quantification of Weakly Interacting Complexes of Peptides with Single-Walled Carbon Nanotubes. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 2879-85	6.4	35
299	Effective simulation of biological systems: Choice of density functional and basis set for heme-containing complexes. <i>Chemical Physics Letters</i> , <b>2007</b> , 434, 149-154	2.5	35
298	Theoretical Exploration of the Structural, Electronic, and Magnetic Properties of ZnO Nanotubes with Vacancies, Antisites, and Nitrogen Substitutional Defects. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 5760-5766	3.8	33
297	Amine-capped silicon quantum dots. <i>Applied Physics Letters</i> , <b>2008</b> , 92, 053107	3.4	33
296	Theoretical Studies on Optical and Electronic Properties of Propionic-Acid-Terminated Silicon Quantum Dots. <i>Journal of Chemical Theory and Computation</i> , <b>2007</b> , 3, 1518-26	6.4	33
295	A new insight into $\pi$ -stacking involving remarkable orbital interactions. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 25452-25457	3.6	32
294	$\pi$ - $\rightarrow$ Imma- $\rightarrow$ sh phase transitions of germanium. <i>Physical Review Letters</i> , <b>2011</b> , 106, 135502	7.4	32
293	Tuning Electronic Structures of ZnO Nanowires by Surface Functionalization: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 8861-8866	3.8	32
292	Exact solutions of the Schrödinger equation for some quantum-mechanical many-body systems. <i>Physical Review A</i> , <b>1993</b> , 47, 71-77	2.6	32
291	Facet-Controlling Agents Free Synthesis of Hematite Crystals with High-Index Planes: Excellent Photodegradation Performance and Mechanism Insight. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2016</b> , 8, 142-51	9.5	31
290	Faceted Silicon Nanotubes: Structure, Energetic, and Passivation Effects. <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 1234-1238	3.8	31
289	Metal/Alq <sub>3</sub> interactions in organic light emitting devices: The different roles of Mg, Al, and Li atoms. <i>Journal of Chemical Physics</i> , <b>2002</b> , 116, 8827-8837	3.9	31
288	Theory of magnesium/Alq <sub>3</sub> interaction in organic light emitting devices. <i>Applied Physics Letters</i> , <b>1999</b> , 74, 1612-1614	3.4	31
287	Defect induced electronic structure of uranofullerene. <i>Scientific Reports</i> , <b>2013</b> , 3, 1341	4.9	30
286	Signature of nanodiamond in Raman spectra: a density functional theoretical study. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 9006-13	3.4	30
285	Gold nanowires from silicon nanowire templates. <i>Applied Physics Letters</i> , <b>2004</b> , 84, 407-409	3.4	30
284	Hydrogenated Silicon Nanoparticles Relaxed in Excited States. <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 12588-12593	3.8	29

283	Diamond nucleation by energetic pure carbon bombardment. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	29
282	NaC monolayer: a novel 2p Dirac half-metal with multiple symmetry-protected Dirac cones. <i>Nanoscale</i> , <b>2018</b> , 10, 13645-13651	7.7	29
281	External Electric Field Modulated Electronic and Structural Properties of <111> Si Nanowires. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 10384-10389	3.8	28
280	Stable and extendable cage containing nanosize silica clusters based on three-membered rings. <i>Physical Review B</i> , <b>2004</b> , 69,	3.3	28
279	Collaborative enhancement of photon harvesting and charge carrier dynamics in carbon nitride photoelectrode. <i>Applied Catalysis B: Environmental</i> , <b>2018</b> , 237, 783-790	21.8	27
278	Interactions between free radicals and a graphene fragment: physical versus chemical bonding, charge transfer, and deformation. <i>Journal of Computational Chemistry</i> , <b>2011</b> , 32, 3264-8	3.5	27
277	Stabilizing excited-state silicon nanoparticle by surface oxidation. <i>Applied Physics Letters</i> , <b>2007</b> , 91, 043104	10.6	27
276	Photocatalytic water splitting of (F, Ti) codoped heptazine/triazine based g-C <sub>3</sub> N <sub>4</sub> heterostructure: A hybrid DFT study. <i>Applied Surface Science</i> , <b>2019</b> , 463, 809-819	6.7	26
275	Cooperative modulation of electronic structures of aromatic molecules coupled to multiple metal contacts. <i>Physical Review Letters</i> , <b>2013</b> , 110, 046802	7.4	26
274	Structural Analysis and Electronic Properties of Negatively Charged TCNQ: 2D Networks of (TCNQ) <sub>2</sub> Mn Assembled on Cu(100)□ <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 17197-17204	3.8	26
273	Computation of large systems with an economic basis set: Ab initio calculations of silicon oxide clusters. <i>Journal of Chemical Physics</i> , <b>2001</b> , 114, 5531-5536	3.9	26
272	C=C Bond Modified Graphitic Carbon Nitride Films for Enhanced Photoelectrochemical Cell Performance. <i>Chemistry - an Asian Journal</i> , <b>2017</b> , 12, 1005-1012	4.5	25
271	Nonresonant chemical mechanism in surface-enhanced Raman scattering of pyridine on M@Au <sub>12</sub> clusters. <i>Nanoscale</i> , <b>2016</b> , 8, 4086-93	7.7	24
270	Oxygen vacancy diffusion in bare ZnO nanowires. <i>Nanoscale</i> , <b>2014</b> , 6, 11882-6	7.7	24
269	Excited state properties of Si quantum dots. <i>Physica Status Solidi (B): Basic Research</i> , <b>2012</b> , 249, 401-412	1.3	24
268	Atomistic Simulations of Self-Trapped Exciton Formation in Silicon Nanostructures: The Transition from Quantum Dots to Nanowires. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 12935-12938	3.8	24
267	Physisorption of benzene derivatives on graphene: critical roles of steric and stereoelectronic effects of the substituent. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 12185-93	3.6	23
266	Photoinduced Water-Heptazine Electron-Driven Proton Transfer: Perspective for Water Splitting with g-CN. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 4310-4316	6.4	23

265	Boundary and Symmetry Determined Exciton Distribution in Two Dimensional Silicon Nanosheets. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 20070-20076	3.8	23
264	Reproducible and recyclable SERS substrates: Flower-like Ag structures with concave surfaces formed by electrodeposition. <i>Applied Surface Science</i> , <b>2015</b> , 333, 126-133	6.7	23
263	Detailed low-energy electron diffraction analysis of the (4 $\times$ 4) surface structure of C60 on Cu(111): Seven-atom-vacancy reconstruction. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	23
262	Band gap engineering of GaN nanowires by surface functionalization. <i>Applied Physics Letters</i> , <b>2009</b> , 94, 073116	3.4	23
261	Anomalous size dependence of the luminescence in reconstructed silicon nanoparticles. <i>Applied Physics Letters</i> , <b>2008</b> , 93, 243120	3.4	23
260	Crystal-Face Tailored Graphitic Carbon Nitride Films for High-Performance Photoelectrochemical Cells. <i>ChemSusChem</i> , <b>2018</b> , 11, 2497-2501	8.3	23
259	Rectifying properties of oligo(phenylene ethynylene) heterometallic molecular junctions: molecular length and side group effects. <i>Scientific Reports</i> , <b>2014</b> , 4, 6357	4.9	22
258	Structural transitions of solid germane under pressure. <i>Europhysics Letters</i> , <b>2010</b> , 90, 66006	1.6	22
257	C60 on the Pt(111) surface: Structural tuning of electronic properties. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	22
256	Superconductivity in Hydrogen-rich Material: GeH <sub>4</sub> . <i>Journal of Superconductivity and Novel Magnetism</i> , <b>2010</b> , 23, 717-719	1.5	22
255	N-doped ZnO nanowires: Surface segregation, the effect of hydrogen passivation and applications in spintronics. <i>Physica Status Solidi (B): Basic Research</i> , <b>2010</b> , 247, 2195-2201	1.3	22
254	An effective scheme for selecting basis sets for ab initio calculations. <i>Science in China Series B: Chemistry</i> , <b>2000</b> , 43, 375-388		22
253	Prediction of energetically optimal single-walled carbon nanotubes for hydrogen physisorption. <i>Applied Physics Letters</i> , <b>2009</b> , 95, 013116	3.4	21
252	Tunable electronic band structures of hydrogen-terminated <112> silicon nanowires. <i>Applied Physics Letters</i> , <b>2008</b> , 92, 203109	3.4	21
251	Geometrical structures and electronic properties of AlN fullerenes: A comparative theoretical study of AlN fullerenes with BN and C fullerenes. <i>Journal of Materials Chemistry</i> , <b>2005</b> , 15, 3034		21
250	A scheme for the economical use of numerical basis sets in calculations with SIESTA. <i>Theoretical Chemistry Accounts</i> , <b>2004</b> , 112, 158	1.9	21
249	Kinetics and Mechanism of O (3P) Reaction with CH <sub>3</sub> CHF <sub>2</sub> : A Theoretical Study. <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 1064-1068	2.8	21
248	Two- and Three-Membered-Ring Hybrid Structures of Silica Nanoclusters. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 18451-18454	3.4	21



247	Solution of atomic and molecular Schrödinger equation described by hyperspherical coordinates. <i>International Journal of Quantum Chemistry</i> , <b>1993</b> , 45, 385-390	2.1	21
246	Energetics of hexagonal boron nitride nanostructures: edge dependence and truncation effects. <i>Nanoscale</i> , <b>2017</b> , 9, 6734-6740	7.7	20
245	Prospects for resolving chemical structure by atomic force microscopy: a first-principles study. <i>Langmuir</i> , <b>2010</b> , 26, 16271-7	4	20
244	Interaction of O <sub>2</sub> , H <sub>2</sub> O, N <sub>2</sub> , and O <sub>3</sub> with stoichiometric and reduced ZnO(101̄0) surface. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	20
243	Adsorbate-induced reconstruction by C <sub>60</sub> on close-packed metal surfaces: Mechanism for different types of reconstruction. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	20
242	Diameter-dependent spin polarization of injected carriers in carbon-doped zigzag boron nitride nanotubes. <i>Applied Physics Letters</i> , <b>2006</b> , 89, 123103	3.4	20
241	Structural characterization of fully coordinated ultrathin silica nanotubes by first-principles calculations. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	20
240	Fluorination-induced back-bond weakening and hydrogen passivation on HF-etched Si surfaces. <i>Physical Review B</i> , <b>2004</b> , 69,	3.3	20
239	The mechanism of N-Ag bonding determined tunability of surface-enhanced Raman scattering of pyridine on MAg (M = Cu, Ag, Au) diatomic clusters. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 20665-71	3.6	19
238	Roles of the active species involved in the photocatalytic oxidation of benzyl alcohol into benzaldehyde on TiO <sub>2</sub> under UV light: Experimental and DFT studies. <i>Journal of Molecular Catalysis A</i> , <b>2016</b> , 420, 82-87		19
237	Interlocking Mechanism between Molecular Gears Attached to Surfaces. <i>ACS Nano</i> , <b>2018</b> , 12, 3020-3029	16.7	18
236	The structure, electronic, and optical properties of (Sm,N)-codoped anatase TiO <sub>2</sub> photocatalyst: A density functional study. <i>Journal of Catalysis</i> , <b>2014</b> , 309, 115-120	7.3	18
235	Surface Passivation and Transfer Doping of Silicon Nanowires. <i>Angewandte Chemie</i> , <b>2009</b> , 121, 10080-10084	9.4	18
234	Indirect-to-direct band gap transitions in phosphorus adsorbed <112> silicon nanowires. <i>Applied Physics Letters</i> , <b>2008</b> , 93, 173108	3.4	18
233	Effect of C≡N and O≡N Hydrogen Bonding in Forming Self-Assembled Monolayers of BF <sub>2</sub> -Substituted Dicarboxyl Derivatives on HOPG: STM Investigation. <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 13851-13854	3.8	18
232	Structural and electronic properties of single-walled carbon nanotubes adsorbed with 1-pyrenebutanoic acid, succinimidyl ester. <i>Science in China Series B: Chemistry</i> , <b>2008</b> , 51, 1203-1210		18
231	An efficient Z-scheme (Cr, B) codoped g-C <sub>3</sub> N <sub>4</sub> /BiVO <sub>4</sub> photocatalyst for water splitting: A hybrid DFT study. <i>International Journal of Hydrogen Energy</i> , <b>2021</b> , 46, 247-261	6.7	18
230	Electronic and optical performances of (Cu, N) codoped TiO <sub>2</sub> /g-C <sub>3</sub> N <sub>4</sub> heterostructure photocatalyst: A spin-polarized DFT + U study. <i>Solar Energy</i> , <b>2018</b> , 162, 306-316	6.8	17

- 229 Electronic delocalization in small water rings. *Physical Chemistry Chemical Physics*, **2015**, 17, 2987-90 3.6 17
- 228 Strong interactions and charge transfers between a charged benzene molecule and multilayer graphenes. *Journal of Materials Chemistry*, **2012**, 22, 23380 17
- 227 Chemical Trend of Pressure-Induced Metallization in Alkaline Earth Hydrides. *Journal of Physical Chemistry C*, **2010**, 114, 14614-14617 3.8 17
- 226 Effect of B-complexes on lattice structure and electronic properties in heavily boron-doped diamond. *Diamond and Related Materials*, **2008**, 17, 234-239 3.5 17
- 225 Structures and Properties of Silicon Oxide Clusters by Theoretical Investigations. *Journal of Cluster Science*, **2006**, 17, 541-563 3 17
- 224 Local strain in interface: Origin of grain tilting in diamond (001)/silicon (001) heteroepitaxy. *Physical Review B*, **1998**, 58, 15351-15354 3.3 17
- 223 Hyperspherical approach for charged excitons in quantum wells. *Physical Review B*, **1999**, 60, 5714-5720 3.3 17
- 222 Interactions between Organics and Metal Surfaces in the Intermediate Regime between Physisorption and Chemisorption. *Journal of Physical Chemistry C*, **2012**, 116, 23603-23607 3.8 16
- 221 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 16
- 220 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 2.9 16
- 219 Strong [email protected] 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 3.8 15
- 218 Interlocking Molecular Gear Chains Built on Surfaces. *Journal of Physical Chemistry Letters*, **2018**, 9, 26116-26119 4.19 15
- 217 Anomalous effect of hydrogenation on phonon thermal conductivity in thin silicon nanowires. *Europhysics Letters*, **2014**, 105, 56003 1.6 15
- 216 Signatures in vibrational and UV-visible absorption spectra for identifying cyclic hydrocarbons by graphene fragments. *Nanoscale*, **2013**, 5, 12178-84 7.7 15
- 215 Energetics and dynamics of a new type of extended line defects in graphene. *Nanoscale*, **2012**, 4, 2580-37.7 15
- 214 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 3.8 15
- 213 Resonance and antiresonance effects in electronic transport through several-quantum-dot combinations. *Journal of Applied Physics*, **2009**, 105, 043706 2.5 15
- 212 Energy alignment induced negative differential resistance: the role of hybrid states in aromatic molecular devices. *Journal of Chemical Physics*, **2008**, 129, 074710 3.9 15

211	Structural modeling of the possible growth of oriented textured single-crystal diamond film on a silicon (111) surface. <i>Applied Physics Letters</i> , <b>1996</b> , 69, 1086-1088	3.4	15
210	The electronic structure, optical absorption and photocatalytic water splitting of (Fe <sup>3+</sup> /Ni)-codoped TiO <sub>2</sub> : A DFT +U study. <i>International Journal of Hydrogen Energy</i> , <b>2017</b> , 42, 4966-4976	6.7	14
209	Revealing highly unbalanced energy barriers in the extension and contraction of the muscle-like motion of a [c2]daisy chain. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 18318-26	3.6	14
208	The role of tryptophans in the UV-B absorption of a UVR8 photoreceptor--a computational study. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 10786-94	3.6	14
207	Engineering the Band Gap States of the Rutile TiO (110) Surface by Modulating the Active Heteroatom. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 8550-8554	16.4	14
206	Synthesis of Carbon Materials-TiO Hybrid Nanostructures and Their Visible-Light Photo-catalytic Activity. <i>ChemPlusChem</i> , <b>2014</b> , 79, 454-461	2.8	14
205	Strong Adsorption Between Uranium Dicarbide and Graphene Surface Induced by f Electrons. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 26849-26857	3.8	14
204	Self-doping and magnetic ordering induced by extended line defects in graphene. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	14
203	Characteristic Vibrational Modes and Electronic Structures of Carbon Nanotubes Containing Defects. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 292-297	3.8	14
202	An energetic stability predictor of hydrogen-terminated Si nanostructures. <i>Applied Physics Letters</i> , <b>2009</b> , 95, 253106	3.4	14
201	Valence band offset of InN/4H-SiC heterojunction measured by x-ray photoelectron spectroscopy. <i>Applied Physics Letters</i> , <b>2008</b> , 93, 242107	3.4	14
200	Possible gas-phase reactions of H <sub>2</sub> /CH <sub>4</sub> /tetramethylsilane in diamond/beta-SiC nanocomposite film deposition: an ab-initio study. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 3554-9	2.8	14
199	Computation of large systems with an economic basis set: structures and reactivity indices of nucleic acid base pairs from density functional theory. <i>Journal of Computational Chemistry</i> , <b>2007</b> , 28, 967-74	3.5	14
198	Structural model of silica nanowire assembled from a highly stable (SiO <sub>2</sub> ) <sub>8</sub> unit. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 1338-43	3.4	14
197	Stable tetrahedral structure of the silica cluster (SiO <sub>2</sub> ) <sub>10</sub> . <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	14
196	Strong orbital interaction in a weak CH- $\pi$ hydrogen bonding system. <i>Scientific Reports</i> , <b>2016</b> , 6, 22304	4.9	13
195	New superhard carbon allotropes based on C <sub>20</sub> fullerene. <i>Carbon</i> , <b>2013</b> , 63, 571-573	10.4	13
194	Ab Initio Study on Thermal and Chemical Stabilities of Silicon Monoxide Clusters. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 12736-12741	3.8	13

- 193 Facet dependent reactivity and selective deposition of nanometer sized  $\beta$ -SiC on diamond surfaces. *Applied Physics Letters*, **2008**, 92, 243107 3.4 13
- 192 Signatures in Vibrational Spectra of Ice Nanotubes Revealed by a Density Functional Tight Binding Method. *Journal of Physical Chemistry C*, **2007**, 111, 14131-14138 3.8 13
- 191 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 13
- 190 Size-dependent oxidation of hydrogenated silicon clusters. *Applied Physics Letters*, **2002**, 80, 4223-4225 3.4 13
- 189 Donor/Acceptor Properties of Aromatic Molecules in Complex Metal-Molecule Interfaces. *Langmuir*, **2017**, 33, 451-458 4 12
- 188 Mechanism of the charge separation improvement in carbon-nanodot sensitized g-C<sub>3</sub>N<sub>4</sub>. *Applied Surface Science*, **2019**, 487, 151-158 6.7 12
- 187 Anomalous stability of graphene containing defects covered by a water layer. *Nanoscale*, **2013**, 5, 6767-727 12
- 186 Role of Cl Ion Desorption in Photocurrent Enhancement of the Annealed Rutile Single-Crystalline TiO<sub>2</sub> Nanorod Arrays. *Journal of Physical Chemistry C*, **2017**, 121, 18892-18899 3.8 12
- 185 Atomic nitrogen chemisorption on graphene with extended line defects. *Journal of Materials Chemistry*, **2012**, 22, 21167 12
- 184 Spin-polarized transport through ZnMnSe/ZnSe/ZnBeSe heterostructures. *Journal of Applied Physics*, **2011**, 110, 093717 2.5 12
- 183 Surface-nitrogenation-induced thermal conductivity attenuation in silicon nanowires. *Europhysics Letters*, **2011**, 96, 56007 1.6 12
- 182 Intramolecular torque, an indicator of the internal rotation direction of rotor molecules and similar systems. *Physical Chemistry Chemical Physics*, **2016**, 18, 29665-29672 3.6 12
- 181 How Does the Flexibility of Molecules Affect the Performance of Molecular Rotors?. *Journal of Physical Chemistry C*, **2018**, 122, 25067-25074 3.8 12
- 180 Thermal vacuum de-oxygenation and post oxidation of TiO<sub>2</sub> nanorod arrays for enhanced photoelectrochemical properties. *Journal of Materials Chemistry A*, **2019**, 7, 5434-5441 13 11
- 179 Strong orbital deformation due to CH $\cdots$ H interaction in the benzene-methane complex. *Physical Chemistry Chemical Physics*, **2015**, 17, 29489-91 3.6 11
- 178 Point defect weakened thermal contraction in monolayer graphene. *Journal of Chemical Physics*, **2014**, 141, 064705 3.9 11
- 177 Stable electronic structures of a defective uranofullerene. *Carbon*, **2014**, 78, 19-25 10.4 11
- 176 Effect of thickness on the electronic structure of poly(vinylidene fluoride) molecular films from first-principles calculations. *Physical Review B*, **2007**, 75, 3.3 11

175	Ab initio and variational transition state approach to beta-C3N4 formation: kinetics for the reaction of CH3NH2 with H. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 9112-7	2.8	11
174	Silica nanoarchitectures with tailored pores based on the hybrid three- and four-membered rings. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 15269-74	3.4	11
173	Dimensionality dependence of optical properties and quantum confinement effects of hydrogenated silicon nanostructures. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 21528-35	3.4	11
172	On the Stability of Hydride Configurations on Silicon Cluster Surfaces: A First-Principle Theoretical Study. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 1967-1973	3.4	11
171	A Theoretical Study on the Interactions of Hydrogen Species with Various Carbon and Boron Nitride Phases. <i>Journal of Physical Chemistry B</i> , <b>2000</b> , 104, 6761-6766	3.4	11
170	Theory of the charge-transport properties of naphthyl diamine used in organic light-emitting devices. <i>Applied Physics Letters</i> , <b>1999</b> , 75, 2418-2420	3.4	11
169	Mo2B, an MBene member with high electrical and thermal conductivities, and satisfactory performances in lithium ion batteries. <i>Nanoscale Advances</i> , <b>2020</b> , 2, 347-355	5.1	11
168	Tailoring the transmission lineshape spectrum of zigzag graphene nanoribbon based heterojunctions via controlling their width and edge protrusions. <i>Nanoscale</i> , <b>2015</b> , 7, 20003-8	7.7	10
167	Growth Mechanisms and Novel Properties of Silicon Nanostructures from Quantum-Mechanical Calculations. <i>Springer Briefs in Molecular Science</i> , <b>2014</b> ,	0.6	10
166	Prediction of surface passivation doping of silicon nanowires with phosphorus. <i>Applied Physics Letters</i> , <b>2009</b> , 95, 193105	3.4	10
165	First-Principles Study of the Structural Stability and Electronic Properties of ZnS Nanowires. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 20291-20294	3.8	10
164	INTRAMOLECULAR CHARGE TRANSFER AND PHOTOISOMERIZATION OF THE DCM STYRENE DYE: A THEORETICAL STUDY. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2008</b> , 07, 719-736	1.8	10
163	Unique electronic band structures of hydrogen-terminated [Formula: see text] silicon nanowires. <i>Nanotechnology</i> , <b>2008</b> , 19, 035708	3.4	10
162	Density functional theory study of geometrical structures and electronic properties of silica nanowires. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 23633-6	3.4	10
161	Computation of Large Systems with Economic Basis Set: Simulation of Diamond Metallization Using Titanium. <i>Journal of Physical Chemistry B</i> , <b>2002</b> , 106, 625-631	3.4	10
160	Aggregation of metal-free organic sensitizers on TiO <sub>2</sub> (1 0 1) surface for use in dye-sensitized solar cells: A computational investigation. <i>Computational and Theoretical Chemistry</i> , <b>2016</b> , 1093, 1-8	2	10
159	Efficient degradation of industrial pollutants with sulfur (IV) mediated by LiCoO cathode powders of spent lithium ion batteries: A "treating waste with waste" strategy. <i>Journal of Hazardous Materials</i> , <b>2020</b> , 399, 123090	12.8	9
158	Excited State Relaxation and Stabilization of Hydrogen Terminated Silicon Quantum Dots. <i>Journal of Cluster Science</i> , <b>2013</b> , 24, 381-397	3	9

157	Zwitterions are the most stable form for neutral arginylglycine in gas phase: Clear theoretical evidence. <i>Computational and Theoretical Chemistry</i> , <b>2013</b> , 1008, 96-102	2	9
156	Possible cage-like nanostructures formed by amino acids. <i>Organic and Biomolecular Chemistry</i> , <b>2012</b> , 10, 5049-54	3.9	9
155	Calcium/poly(9,9-dioctylfluorene) interaction: a theoretical study. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 12868-73	3.4	9
154	Theoretical study on the substituent effect of a Wittig reaction. <i>Theoretical Chemistry Accounts</i> , <b>2002</b> , 107, 206-210	1.9	9
153	Theoretical Prediction on Efficient Formation of Imino Acid via an Aza-Wittig Reaction. <i>Journal of Physical Chemistry B</i> , <b>2003</b> , 107, 2061-2067	3.4	9
152	Interactions of Li, Ca, and Al with aromatic carbon materials: an ab initio study. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 194322	3.9	9
151	Dual response of graphene-based ultra-small molecular junctions to defect engineering. <i>Nano Research</i> , <b>2016</b> , 9, 1480-1488	10	9
150	The electronic structure and optical absorption of rutile TiO <sub>2</sub> with La and N dopants from first-principles calculation. <i>Computational Materials Science</i> , <b>2017</b> , 131, 178-186	3.2	8
149	New insight into the spin-conserving excitation of the negatively charged nitrogen-vacancy center in diamond. <i>Scientific Reports</i> , <b>2014</b> , 4, 5144	4.9	8
148	Colorful carbon nitride based composite films. <i>Applied Surface Science</i> , <b>2020</b> , 511, 145535	6.7	8
147	Formation Mechanism of Atmospheric Ammonium Bisulfate: Hydrogen-Bond-Promoted Nearly Barrierless Reactions of SO with NH and H <sub>2</sub> O. <i>ChemPhysChem</i> , <b>2018</b> , 19, 967-972	3.2	8
146	Engineering the Band Gap States of the Rutile TiO <sub>2</sub> (110) Surface by Modulating the Active Heteroatom. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 8686-8690	3.6	8
145	Electronic and vibrational properties of stable isomers of (SiO) <sub>n</sub> ((0,⊕)) (n = 2-7) clusters. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 8893-900	2.8	8
144	Intramolecular triplet energy transfer in donor-acceptor molecules linked by a crown ether bridge. <i>Chemistry - A European Journal</i> , <b>2006</b> , 12, 5238-45	4.8	8
143	A family of stable silica fullerenes with fully coordinated structures. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 17757-62	3.4	8
142	Fluorination Induced Etching Selectivity of Boron Nitride Phases. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 7597-7602	3.4	8
141	Charge Transfer Boosting Moisture Resistance of Semimetal Perovskite Nanocrystals via Hierarchical Alumina Modulation. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 3159-3165	6.4	8
140	Actinide embedded nearly planar gold superatoms: structural properties and applications in surface-enhanced Raman scattering (SERS). <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 27523-27527	3.6	8

139	Beyond the electrostatic model: the significant roles of orbital interaction and the dispersion effect in aqueous-systems. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 1298-1302	3.6	7
138	Selective interface transparency in graphene nanoribbon based molecular junctions. <i>Nanoscale</i> , <b>2018</b> , 10, 4861-4864	7.7	7
137	Chirality dependent spin polarization of carbon nanotubes. <i>New Journal of Physics</i> , <b>2016</b> , 18, 023029	2.9	7
136	Mechanism of Charge Separation and Frontier Orbital Structure in Graphitic Carbon Nitride and Graphene Quantum Dots. <i>ChemPhysChem</i> , <b>2018</b> , 19, 2534-2539	3.2	7
135	Selective adsorption of L-serine functional groups on the anatase TiO <sub>2</sub> (101) surface in benthic microbial fuel cells. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 20806-17	3.6	7
134	Tuning thermal expansions of zinc oxide sheets by varying the layer thickness. <i>Europhysics Letters</i> , <b>2014</b> , 107, 26007	1.6	7
133	Symmetry-dependent band gap opening in graphene induced by g-C <sub>3</sub> N <sub>4</sub> substrates. <i>RSC Advances</i> , <b>2014</b> , 4, 64577-64582	3.7	7
132	Inducing extended line defects in graphene by linear adsorption of C and N atoms. <i>Applied Physics Letters</i> , <b>2012</b> , 101, 253105	3.4	7
131	First-principles calculations of atomic and electronic properties of ZnO nanostructures. <i>Physica Status Solidi (B): Basic Research</i> , <b>2010</b> , 247, 2581-2593	1.3	7
130	Stabilizing and activating dopants in <112> silicon nanowires by alkene adsorptions: A first-principles study. <i>Applied Physics Letters</i> , <b>2011</b> , 98, 073115	3.4	7
129	A COMPARATIVE STUDY ON INTERMOLECULAR HYDROGEN BOND INTERACTIONS IN MOLECULAR DIMERS USING DIFFERENT LEVELS OF COMPUTATIONAL METHODS. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2012</b> , 11, 1237-1259	1.8	7
128	Surface passivation-induced strong ferromagnetism of zinc oxide nanowires. <i>Chemistry - A European Journal</i> , <b>2010</b> , 16, 13072-6	4.8	7
127	Simulation of gate-controlled Coulomb blockades in carbon nanotubes. <i>Journal of Applied Physics</i> , <b>2004</b> , 95, 5729-5735	2.5	7
126	Theoretical study of structure-dependent Coulomb blockade in carbon nanotubes. <i>Physical Review B</i> , <b>2002</b> , 66,	3.3	7
125	Oxygen adsorption on small Si clusters: a full-potential linear-muffin-tin-orbital molecular-dynamics study. <i>Journal of Physics Condensed Matter</i> , <b>2002</b> , 14, 1723-1733	1.8	7
124	Bonding reactivity descriptor from conceptual density functional theory and its applications to elucidate bonding formation. <i>Journal of Chemical Physics</i> , <b>2017</b> , 147, 134303	3.9	6
123	Composition dependent reactivity of titanium oxide clusters. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 10594-9	3.6	6
122	A durable surface-enhanced Raman scattering substrate: ultrathin carbon layer encapsulated Ag nanoparticle arrays on indium-tin-oxide glass. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 14849-55	3.6	6

121	Size dependent catalytic effect of TiO <sub>2</sub> clusters in water dissociation. <i>Journal of Molecular Catalysis A</i> , <b>2013</b> , 366, 163-170		6
120	Intramolecular Torsion Based Molecular Switch Functionality Enhanced in $\pi$ -Conjugated Oligomolecules by a $\pi$ -Conjugated Pendant Group. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 13911-13918	3.8	6
119	Significant negative differential resistance predicted in scanning tunneling spectroscopy for a C60 monolayer on a metal surface. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	6
118	SENSITIVITY OF HYDROGENATED SILICON NANODOT ON SMALL POLAR MOLECULES. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2009</b> , 08, 299-316	1.8	6
117	Tunable optical and electronic properties of Si nanowires by electric bias. <i>Journal of Applied Physics</i> , <b>2011</b> , 109, 083106	2.5	6
116	A synthetic route toward well-defined stoichiometric silica fullerene and nanotubes based on metastable four-membered rings. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 8992-7	3.4	6
115	Geometric and excited-state properties of 1,4-bis(benzothiazolylvinyl)benzene interacting with 2,2',2''-(1,3,5-phenylene)tris[1-phenyl-1H-benzimidazole] studied by a density-functional tight-binding method. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 20847-51	3.4	6
114	Electrical Transport and Electronic Delocalization of Small Fullerenes. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 16636-16641	3.4	6
113	A thermodynamic and kinetic study of the formation of C <sub>20</sub> compounds encapsulating H, He and Ne atoms. <i>Theoretical Chemistry Accounts</i> , <b>2003</b> , 109, 278-283	1.9	6
112	In situ textured carbon nitride photoanodes with enhanced photoelectrochemical activity by band-gap state modulation. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 24005-24012	13	6
111	Intramolecular Torque Study of a Molecular Rotation Stimulated by Electron Injection and Extraction. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 7614-7619	2.8	6
110	Revealing the trap emission in graphene-based nanostructures. <i>Carbon</i> , <b>2019</b> , 150, 439-445	10.4	5
109	Economical basis sets and their uses in ab initio calculations. <i>International Journal of Quantum Chemistry</i> , <b>2015</b> , 115, 570-577	2.1	5
108	Charging-induced asymmetric spin distribution in an asymmetric (9,0) carbon nanotube. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 28860-5	3.6	5
107	Surface effects on the thermal conductivity of silicon nanowires. <i>Chinese Physics B</i> , <b>2018</b> , 27, 036801	1.2	5
106	Design of conjugated microporous polymer nanotubes for efficient benzene molecular adsorptions. <i>International Journal of Quantum Chemistry</i> , <b>2018</b> , 118, e25492	2.1	5
105	Structural Evolution of Cu/ZnO Active Sites: From Reactive Environment to Ultrahigh Vacuum. <i>ChemCatChem</i> , <b>2014</b> , 6, 2322-2326	5.2	5
104	Enhancement of spin polarization induced by Coulomb on-site repulsion between localized pz electrons in graphene embedded with line defects. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 30744-30750	3.6	5



103	A unique feature of chiral transition of a difluorobenzo[c]phenanthrene molecule confined in a boron-nitride nanotube based on molecular dynamics simulations. <i>Chemical Physics Letters</i> , <b>2014</b> , 591, 265-267	2.5	5
102	Size-dependent structural characteristics and phonon thermal transport in silicon nanoclusters. <i>AIP Advances</i> , <b>2013</b> , 3, 082114	1.5	5
101	Inducing novel electronic properties in Ge nanowires by means of variations in their size, shape and strain: a first-principles computational study. <i>Journal of Physics Condensed Matter</i> , <b>2012</b> , 24, 015301	1.8	5
100	Size dependence of nanoscale confinement on chiral transformation. <i>Chemistry - A European Journal</i> , <b>2010</b> , 16, 6482-7	4.8	5
99	Mechanical properties of solid C(60) studied with density functional tight binding method augmented by an empirical dispersion term. <i>Journal of Physics Condensed Matter</i> , <b>2008</b> , 20, 275240	1.8	5
98	Negative differential resistance and tunable peak-to-valley ratios in a silicon nanochain. <i>Journal of Applied Physics</i> , <b>2008</b> , 103, 103719	2.5	5
97	Surface structures and electronic states of silicon nanotubes stabilized by oxygen atoms. <i>Journal of Applied Physics</i> , <b>2007</b> , 102, 024313	2.5	5
96	Interactions of hydride species and their roles in carbon nitride growth. <i>Physical Review B</i> , <b>2001</b> , 63,	3.3	5
95	Origin and nature of gap states in a-Si:H alloys. <i>Solid State Communications</i> , <b>1989</b> , 69, 681-684	1.6	5
94	Solvents Hinder the Interlocking Rotation between Molecular Gears, as Revealed by Torque Calculations. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 17612-17621	3.8	5
93	Correlation between electron delocalization and structural planarization in small water rings. <i>International Journal of Quantum Chemistry</i> , <b>2015</b> , 115, 817-819	2.1	4
92	Atomic Sulfur Passivation Improves the Photoelectrochemical Performance of ZnSe Nanorods. <i>Nanomaterials</i> , <b>2020</b> , 10,	5.4	4
91	Computational prediction of optimal metal ions to induce coordinated polymerization of muscle-like [c2]daisy chains. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 7419-26	3.6	4
90	Fragment motion in motor molecules: basic concepts and application to intra-molecular rotations. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 21487-21497	3.6	4
89	Nonradiative Excited-State Decay via Conical Intersection in Graphene Nanostructures. <i>ChemPhysChem</i> , <b>2019</b> , 20, 2754-2758	3.2	4
88	Remarkable Thermal Contraction in Small Size Single-Walled Boron Nanotubes. <i>Communications in Computational Physics</i> , <b>2014</b> , 16, 201-212	2.4	4
87	Basis set effect on defect induced spin polarization of a carbon nanotube in density functional theory calculations. <i>Chemical Physics Letters</i> , <b>2013</b> , 585, 107-111	2.5	4
86	INTERACTION IN BENZENE DIMER STUDIED USING DENSITY FUNCTIONAL THEORY AUGMENTED WITH AN EMPIRICAL DISPERSION TERM. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2010</b> , 09, 109-123	1.8	4

85	Metallization induced by nitrogen atom adsorption on silicon nanofilms and nanowires. <i>Applied Physics Letters</i> , <b>2009</b> , 94, 113101	3.4	4
84	Silicon nanowires for high-specificity and high-selectivity sensors under low-frequency scanning. <i>Applied Physics Letters</i> , <b>2011</b> , 98, 043108	3.4	4
83	Computation of large systems with an economic basis set: systems in excited states. <i>Theoretical Chemistry Accounts</i> , <b>2008</b> , 119, 437-443	1.9	4
82	Engineering the excited state of graphitic carbon nitride nanostructures by covalently bonding with graphene quantum dots. <i>Theoretical Chemistry Accounts</i> , <b>2020</b> , 139, 1	1.9	4
81	An ultra-sensitive gas sensor based on a two-dimensional manganese porphyrin monolayer. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 11852-11862	3.6	4
80	Enhanced optical absorption and photocatalytic activity of anatase TiO <sub>2</sub> through C Nd-codoped: A DFT+ U calculations. <i>Journal of Physics and Chemistry of Solids</i> , <b>2017</b> , 109, 70-77	3.9	3
79	n → π* Interaction Promoted Charge Carrier Transfer between Helical SWNTs and a 4-(1-Pyrenyl)phenyl Group. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 13976-13982	3.8	3
78	Tunable dipole induced hydrogen bonds between a hydrogen molecule and alkali halides. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 20361-7	3.6	3
77	A pseudo-metal-free strategy for constructing high performance photoelectrodes. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 12767-12773	1.3	3
76	High-Angular-Momentum Orbitals and Superatomic Characteristics of Boron-Nitrogen Cages. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 3881-3885	3.8	3
75	The nature of small molecules adsorbed on defective carbon nanotubes. <i>Royal Society Open Science</i> , <b>2019</b> , 6, 190727	3.3	3
74	Strong slip-induced anomalous enhancement and red-shifts in wide-range optical absorption of graphite under uniaxial pressure. <i>Nanoscale</i> , <b>2014</b> , 6, 8943-8	7.7	3
73	DFT study of benzyl alcohol/TiO <sub>2</sub> interfacial surface complex: reaction pathway and mechanism of visible light absorption. <i>Journal of Molecular Modeling</i> , <b>2017</b> , 23, 285	2	3
72	A Thermodynamic Model of Diameter- and Temperature-dependent Semiconductor Nanowire Growth. <i>Scientific Reports</i> , <b>2017</b> , 7, 15029	4.9	3
71	STABLE STRUCTURES AND CHARACTERISTIC VIBRATIONAL SPECTRA OF TinOm (n = 2m; m = 1/2n) CLUSTERS. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2013</b> , 12, 1250094	1.8	3
70	Possible Reaction Paths of Small Silicon Clusters with Oxygen Explored with Density Functional Theory. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 13196-13203	3.8	3
69	Electron Transport Suppression from Tip-Induced State Interaction on Si(100)-2 × 1 Surfaces. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 707-12	6.4	3
68	Adsorptions of Tetrafluorotetracyanoquinodimethane on Entirely and Partially Hydrogenated C(100)-2 × 1 Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 8829-8835	3.8	3

67	Theoretical Models of Silica Nanorings: First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 17071-17075	3.8	3
66	Photoluminescence and electroluminescence of 3-methyl-8-dimethylaminophenazine. <i>Synthetic Metals</i> , <b>2006</b> , 156, 185-189	3.6	3
65	Potential visible light absorption in 3- $\mu$ m diam carbon nanotubes. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	3
64	The Effects of Hydrogen Etching on Different Carbon and Boron Nitride Phases. <i>Chemical Vapor Deposition</i> , <b>2000</b> , 6, 227-230		3
63	Role of hydrogen in doping mechanism for a-Si:H alloys. <i>Solid State Communications</i> , <b>1988</b> , 65, 1625-1627	7.6	3
62	Biochemical analyses of a novel thermostable GH5 endo $\beta$ -1,4-mannanase with minor $\beta$ -1,4-glucosidic cleavage activity from <i>Bacillus</i> sp. KW1 and its synergism with a commercial $\beta$ -galactosidase on galactomannan hydrolysis. <i>International Journal of Biological Macromolecules</i> , <b>2004</b> , 35, 773-780	7.9	3
61	A novel glycoside hydrolase family 42 enzyme with bifunctional $\beta$ -galactosidase and $\beta$ -L-arabinopyranosidase activities and its synergistic effects with cognate glycoside hydrolases in plant polysaccharides degradation. <i>International Journal of Biological Macromolecules</i> , <b>2019</b> , 140, 129-139	7.9	2
60	Theoretical study on catalyzed selective photoreduction mechanism for 4-bromobenzaldehyde in two different solvents. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 19997-20005	3.6	2
59	Water Clusters on Graphitic Carbon Surfaces. <i>Journal of Cluster Science</i> , <b>2015</b> , 26, 361-373	3	2
58	2p-insulator heterointerfaces: Creation of half-metallicity and anionogenic ferromagnetism via double exchange. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	2
57	Substrate-mediated and temperature-modulated long-range interactions between bromine adatom stripes on Cu(1 1 1). <i>Applied Surface Science</i> , <b>2019</b> , 463, 253-260	6.7	2
56	Structural Asymmetry-Facilitated Tunability of Spin Distribution in the (10, 0) Carbon Nanotube Induced by Charging. <i>Journal of Electronic Materials</i> , <b>2017</b> , 46, 3857-3861	1.9	2
55	Chemical Coupling SERS Properties of Pyridine on Silver-Caged Metal Clusters M@Ag <sub>12</sub> (M = V, Nb, Ta, Cr, Mo, W, Mn <sup>+</sup> , Tc <sup>+</sup> , Re <sup>+</sup> ). <i>Journal of Electronic Materials</i> , <b>2017</b> , 46, 3904-3909	1.9	2
54	Intermolecular $\pi$ - $\pi$ and H/ $\pi$ Interactions in dimers researched by different computational methods. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2014</b> , 13, 1450057	1.8	2
53	Stabilizing reconstruction induced by O protrusions of the ZnO (0001) polar surface. <i>RSC Advances</i> , <b>2014</b> , 4, 54249-54255	3.7	2
52	A random rotor molecule: Vibrational analysis and molecular dynamics simulations. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 234302	3.9	2
51	Barrier dependent electron tunneling lifetime in one-dimensional device structures. <i>Journal of Applied Physics</i> , <b>2010</b> , 108, 104514	2.5	2
50	APPLICATIONS OF DISCRETE SINGULAR CONVOLUTION ALGORITHM IN ONE-ELECTRON SYSTEMS: HYDROGEN ATOM. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2009</b> , 08, 813-826	1.8	2

49	Single-electron tunneling and Coulomb blockade in carbon-based quantum dots. <i>Frontiers of Physics in China</i> , <b>2009</b> , 4, 315-326		2
48	First principles studies for formation mechanism and properties of ethylene molecule adsorbing on diamond (100) surface. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 114710	3.9	2
47	COMPUTATION OF LARGE SYSTEMS WITH AN ECONOMIC BASIS SET: AB INITIO CALCULATIONS OF BIOLOGICAL NUCLEIC ACID BASE PAIRS. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2006</b> , 05, 411-420	1.8	2
46	Oxide-Assisted Growth of Silicon and Related Nanowires: Growth Mechanism, Structure and Properties <b>2005</b> , 308-370		2
45	The properties and possible transformation path for C12B24N24. <i>International Journal of Quantum Chemistry</i> , <b>2001</b> , 84, 363-368	2.1	2
44	Bonding Regeneration: The Driving Force of Hetero-Epitaxial Diamond Grain Coalescence on (001) Silicon. <i>Materials Research Society Symposia Proceedings</i> , <b>1998</b> , 529, 133		2
43	Improved scheme to solve the atomic Schrödinger equation in hyperspherical coordinates. <i>International Journal of Quantum Chemistry</i> , <b>1996</b> , 59, 203-207	2.1	2
42	Machine learning-driven discovery of double hybrid organic/inorganic perovskites. <i>Journal of Materials Chemistry A</i> , <b>2022</b> , 10, 1402-1413	13	2
41	The Stability and Mechanical Properties of Boron Nanotubes Explored through Density Functional Calculations. <i>International Journal for Multiscale Computational Engineering</i> , <b>2010</b> , 8, 245-250	2.4	2
40	Novel Two-Step Surface Boron Decoration of Graphitic Carbon Nitride Photoelectrodes for Efficient Charge Transport and Separation. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 25207-25216	3.8	2
39	Numerical variational solution of hydrogen molecule and ions using one-dimensional hydrogen as basis functions. <i>New Journal of Physics</i> , <b>2020</b> , 22, 093059	2.9	2
38	Photoelectrochemical Performance Enhancement of ZnSe Nanorods versus Dots: Combined Experimental and Computational Insights. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 10414-10420	6.4	2
37	Strong Interaction between Cyclo[18]Carbon and Graphene. <i>Advanced Theory and Simulations</i> , <b>2021</b> , 4, 2100022	3.5	2
36	Unusual self-assembly of chloroaluminium phthalocyanine on graphite. <i>Surface Science</i> , <b>2019</b> , 681, 104-110		2
35	Excited state dynamics study of the self-trapped exciton formation in silicon nanosheets. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 29299-29305	3.6	2
34	A scheme of numerical solution for three-dimensional isoelectronic series of hydrogen atom using one-dimensional basis functions. <i>International Journal of Quantum Chemistry</i> , <b>2018</b> , 118, e25694	2.1	2
33	A Green's function approach to the nonrelativistic radial wave equation of hydrogen atom. <i>International Journal of Quantum Chemistry</i> , <b>2017</b> , 117, e25360	2.1	1
32	Tunneling lifetimes of electrons escaping from atoms under a static electric field. <i>Journal of Chemical Physics</i> , <b>2017</b> , 147, 064109	3.9	1

31	Surface modification of TiO <sub>2</sub> and ZnO nanosurfaces and applications <b>2010</b> ,		1
30	First-principles study of silicon bulk and nanowire (111) surfaces terminated with trihydrides: Symmetric, rotated, and tilted. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	1
29	CHARACTERISTIC VIBRATIONAL MODES OF H <sub>2</sub> O ADSORBED MOLECULARLY AND DISSOCIATIVELY ON TITANIUM OXIDE CLUSTERS. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2012</b> , 11, 1289-1295 <sup>1,8</sup>	1.8	1
28	The Origin of Mis-Oriented Diamond Grains Nucleated Directly on (001) Silicon Surface. <i>Materials Research Society Symposia Proceedings</i> , <b>1998</b> , 529, 139		1
27	Volcano Plots of Reaction Yields in Cross-Coupling Catalysis.. <i>Journal of Physical Chemistry Letters</i> , <b>2022</b> , 520-526	6.4	1
26	Revealing the tunability of electronic structures and optical properties of novel SWCNT derivatives, phenine nanotubes. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 24239-24248	3.6	1
25	A revised mechanism of band gap evolution of TMDC nanotubes and its application to Janus TMDC nanotubes: negative electron and hole compressibility. <i>Journal of Materials Chemistry C</i> ,	7.1	1
24	Intermolecular orbital interaction in $\pi$ systems. <i>Molecular Physics</i> , <b>2018</b> , 116, 978-986	1.7	1
23	Crowding-induced polymer trapping in a channel.. <i>Physical Review E</i> , <b>2021</b> , 104, 054502	2.4	0
22	The thermal and elastic properties of U <sub>3</sub> Si <sub>5</sub> and their variations induced by incorporated aluminum. <i>Journal of Nuclear Materials</i> , <b>2022</b> , 558, 153331	3.3	0
21	Adenine ultrafast photorelaxation electron-driven proton transfer. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 23090-23095	3.6	0
20	Solution of two-electron Schrödinger equations using a residual minimization method and one-dimensional basis functions. <i>AIP Advances</i> , <b>2021</b> , 11, 025228	1.5	0
19	Crystal growth engineering and origin of the weak ferromagnetism in antiferromagnetic matrix of orthochromates from - orbital hybridization.. <i>IScience</i> , <b>2022</b> , 25, 104111	6.1	0
18	Periodicity-dependent long range coulomb on-site repulsion in hydrogen adsorbed graphene: A DFT+U study. <i>Progress in Natural Science: Materials International</i> , <b>2019</b> , 29, 362-366	3.6	
17	Electronic structure and properties of highly ordered C <sub>60</sub> nano arrays on Au (111): STM & DFT study. <i>Journal of Physics: Conference Series</i> , <b>2017</b> , 864, 012076	0.3	
16	Environmental-confinement-induced stability enhancement of chiral molecules. <i>ChemPhysChem</i> , <b>2014</b> , 15, 2672-5	3.2	
15	A NONSELF-CONSISTENT METHOD FOR THE NONEQUILIBRIUM GREEN'S FUNCTION TECHNIQUE. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2009</b> , 08, 423-431	1.8	
14	AN ITERATION SCHEME FOR CALCULATING TRANSPORT PROPERTIES OF MOLECULAR SYSTEMS. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2007</b> , 06, 975-984	1.8	

- 13 Response to Comment on Gold nanowires from silicon nanowire templates [Appl. Phys. Lett. 85, 692 (2004)]. *Applied Physics Letters*, **2004**, 85, 693-693 3.4
- 12 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 0.9
- 11 Silicon-Based Nanowires **2003**, 413-462
- 10 Hydrogen-terminated silicon quantum dots **2017**, 413-432
- 9 Hydrogen-terminated silicon quantum dots. *Series in Materials Science and Engineering*, **2017**, 413-432
- 8 Modeling Silicon Nanostructure Surface Functionalization for Biological Detections **2012**, 33-51
- 7 Novel Electronic Properties of Silicon Nanostructures. *Springer Briefs in Molecular Science*, **2014**, 31-63 0.6
- 6 Growth Mechanism of Silicon Nanowires. *Springer Briefs in Molecular Science*, **2014**, 7-12 0.6
- 5 Stability of Silicon Nanostructures. *Springer Briefs in Molecular Science*, **2014**, 13-30 0.6
- 4 Theoretical and Experimental Methods for Determining the Thermal Conductivity of Nanostructures. *Springer Briefs in Physics*, **2018**, 11-40 0.6
- 3 Phonon Thermal Transport in Silicene and Its Defect Effects. *Springer Briefs in Physics*, **2018**, 67-80 0.6
- 2 Thermal Stability and Phonon Thermal Transport in Spherical Silicon Nanoclusters. *Springer Briefs in Physics*, **2018**, 41-51 0.6
- 1 Phonon Thermal Transport in Silicon Nanowires and Its Surface Effects. *Springer Briefs in Physics*, **2018**, 53-66 0.6