

# Rui-Qin Zhang

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

372  
papers

9,494  
citations

48  
h-index

80  
g-index

385  
ext. papers

10,359  
ext. citations

4.4  
avg, IF

6.32  
L-index

#	Paper	IF	Citations
372	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
371	Volcano Plots of Reaction Yields in Cross-Coupling Catalysis.. <i>Journal of Physical Chemistry Letters</i> , <b>2022</b> , 520-526	6.4	1
370	The thermal and elastic properties of U3Si5 and their variations induced by incorporated aluminum. <i>Journal of Nuclear Materials</i> , <b>2022</b> , 558, 153331	3.3	0
369	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
368	1/f Noise responses of Ultra-Thin Body and Buried oxide FD-SOI PMOSFETs under total ionizing dose irradiation. <i>Radiation Effects and Defects in Solids</i> , <b>2021</b> , 176, 1202-1214	0.9	
367	Crowding-induced polymer trapping in a channel.. <i>Physical Review E</i> , <b>2021</b> , 104, 054502	2.4	0
366	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
365	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
364	Strong Interaction between Cyclo[18]Carbon and Graphene. <i>Advanced Theory and Simulations</i> , <b>2021</b> , 4, 2100022	3.5	2
363	Biochemical analyses of a novel thermostable GH5 endo $\alpha$ ,4-mannanase with minor $\alpha$ ,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>2021</b> , 166, 778-788	7.9	3
362	An efficient Z-scheme (Cr, B) codoped g-C3N4/BiVO4 photocatalyst for water splitting: A hybrid DFT study. <i>International Journal of Hydrogen Energy</i> , <b>2021</b> , 46, 247-261	6.7	18
361	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
360	Adenine ultrafast photorelaxation electron-driven proton transfer. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 23090-23095	3.6	0
359	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
358	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
357	A pseudo-metal-free strategy for constructing high performance photoelectrodes. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 12767-12773	13	3
356	Atomic Sulfur Passivation Improves the Photoelectrochemical Performance of ZnSe Nanorods. <i>Nanomaterials</i> , <b>2020</b> , 10,	5.4	4

355	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
354	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
353	Colorful carbon nitride based composite films. <i>Applied Surface Science</i> , <b>2020</b> , 511, 145535	6.7	8
352	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
351	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
350	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
349	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
348	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
347	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
346	Charge Transfer Boosting Moisture Resistance of Sem nude Perovskite Nanocrystals via Hierarchical Alumina Modulation. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 3159-3165	6.4	8
345	A novel glycoside hydrolase family 42 enzyme with bifunctional $\alpha$ -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
344	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	
343	Thermal vacuum de-oxygenation and post oxidation of TiO <sub>2</sub> nanorod arrays for enhanced photoelectrochemical properties. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 5434-5441	13	11
342	Revealing the trap emission in graphene-based nanostructures. <i>Carbon</i> , <b>2019</b> , 150, 439-445	10.4	5
341	Mechanism of the charge separation improvement in carbon-nanodot sensitized g-C <sub>3</sub> N <sub>4</sub> . <i>Applied Surface Science</i> , <b>2019</b> , 487, 151-158	6.7	12
340	Hydrogen-Location-Sensitive Modulation of the Redox Reactivity for Oxygen-Deficient TiO. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 8407-8411	16.4	43
339	n $\rightarrow$ $\pi$ 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
338	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

- 337 Substrate-mediated and temperature-modulated long-range interactions between bromine adatom stripes on Cu(1 1 1). *Applied Surface Science*, **2019**, 463, 253-260 6.7 2
- 336 Photoinduced Water-Heptazine Electron-Driven Proton Transfer: Perspective for Water Splitting with g-CN. *Journal of Physical Chemistry Letters*, **2019**, 10, 4310-4316 6.4 23
- 335 The nature of small molecules adsorbed on defective carbon nanotubes. *Royal Society Open Science*, **2019**, 6, 190727 3.3 3
- 334 Nonradiative Excited-State Decay via Conical Intersection in Graphene Nanostructures. *ChemPhysChem*, **2019**, 20, 2754-2758 3.2 4
- 333 Unusual self-assembly of chloroaluminium phthalocyanine on graphite. *Surface Science*, **2019**, 681, 104-118 2
- 332 Formation Mechanism of Atmospheric Ammonium Bisulfate: Hydrogen-Bond-Promoted Nearly Barrierless Reactions of SO with NH and H O. *ChemPhysChem*, **2018**, 19, 967-972 3.2 8
- 331 Interlocking Mechanism between Molecular Gears Attached to Surfaces. *ACS Nano*, **2018**, 12, 3020-3029 16.7 18
- 330 Engineering the Band Gap States of the Rutile TiO (110) Surface by Modulating the Active Heteroatom. *Angewandte Chemie - International Edition*, **2018**, 57, 8550-8554 16.4 14
- 329 2p-insulator heterointerfaces: Creation of half-metallicity and anionogenic ferromagnetism via double exchange. *Physical Review B*, **2018**, 97, 3.3 2
- 328 Selective interface transparency in graphene nanoribbon based molecular junctions. *Nanoscale*, **2018**, 10, 4861-4864 7.7 7
- 327 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. *Solar Energy*, **2018**, 162, 306-316 6.8 17
- 326 Low-dimensional Mo:BiVO<sub>4</sub> photoanodes for enhanced photoelectrochemical activity. *Journal of Materials Chemistry A*, **2018**, 6, 3602-3609 13 56
- 325 Interlocking Molecular Gear Chains Built on Surfaces. *Journal of Physical Chemistry Letters*, **2018**, 9, 2611-2619 16.1 15
- 324 Engineering the Band Gap States of the Rutile TiO<sub>2</sub>(110) Surface by Modulating the Active Heteroatom. *Angewandte Chemie*, **2018**, 130, 8686-8690 3.6 8
- 323 Surface effects on the thermal conductivity of silicon nanowires. *Chinese Physics B*, **2018**, 27, 036801 1.2 5
- 322 Design of conjugated microporous polymer nanotubes for efficient benzene molecular adsorptions. *International Journal of Quantum Chemistry*, **2018**, 118, e25492 2.1 5
- 321 Collaborative enhancement of photon harvesting and charge carrier dynamics in carbon nitride photoelectrode. *Applied Catalysis B: Environmental*, **2018**, 237, 783-790 21.8 27
- 320 Exciton Self-Trapping in sp Carbon Nanostructures Induced by Edge Ether Groups. *Journal of Physical Chemistry Letters*, **2018**, 9, 4857-4864 6.4 37

3 <sup>19</sup>	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
3 <sup>18</sup>	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
3 <sup>17</sup>	Spin-orbit torque in a completely compensated synthetic antiferromagnet. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	48
3 <sup>16</sup>	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
3 <sup>15</sup>	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
3 <sup>14</sup>	Intermolecular orbital interaction in $\beta$ systems. <i>Molecular Physics</i> , <b>2018</b> , 116, 978-986	1.7	1
3 <sup>13</sup>	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
3 <sup>12</sup>	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
3 <sup>11</sup>	How Does the Flexibility of Molecules Affect the Performance of Molecular Rotors?. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 25067-25074	3.8	12
3 <sup>10</sup>	Theoretical and Experimental Methods for Determining the Thermal Conductivity of Nanostructures. <i>SpringerBriefs in Physics</i> , <b>2018</b> , 11-40	0.6	
3 <sup>09</sup>	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
3 <sup>08</sup>	Phonon Thermal Transport in Silicene and Its Defect Effects. <i>SpringerBriefs in Physics</i> , <b>2018</b> , 67-80	0.6	
3 <sup>07</sup>	Thermal Stability and Phonon Thermal Transport in Spherical Silicon Nanoclusters. <i>SpringerBriefs in Physics</i> , <b>2018</b> , 41-51	0.6	
3 <sup>06</sup>	Phonon Thermal Transport in Silicon Nanowires and Its Surface Effects. <i>SpringerBriefs in Physics</i> , <b>2018</b> , 53-66	0.6	
3 <sup>05</sup>	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
3 <sup>04</sup>	Crystal-Face Tailored Graphitic Carbon Nitride Films for High-Performance Photoelectrochemical Cells. <i>ChemSusChem</i> , <b>2018</b> , 11, 2497-2501	8.3	23
3 <sup>03</sup>	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
3 <sup>02</sup>	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

301	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
300	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
299	Energetics of hexagonal boron nitride nanostructures: edge dependence and truncation effects. <i>Nanoscale</i> , <b>2017</b> , 9, 6734-6740	7.7	20
298	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
297	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
296	Beyond the electrostatic model: the significant roles of orbital interaction and the dispersion effect in aqueous- $\beta$ systems. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 1298-1302	3.6	7
295	Donor/Acceptor Properties of Aromatic Molecules in Complex Metal-Molecule Interfaces. <i>Langmuir</i> , <b>2017</b> , 33, 451-458	4	12
294	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
293	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
292	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	
291	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
290	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
289	Role of Cl Ion Desorption in Photocurrent Enhancement of the Annealed Rutile Single-Crystalline TiO <sub>2</sub> Nanorod Arrays. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 18892-18899	3.8	12
288	A Thermodynamic Model of Diameter- and Temperature-dependent Semiconductor Nanowire Growth. <i>Scientific Reports</i> , <b>2017</b> , 7, 15029	4.9	3
287	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
286	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
285	Hydrogen-terminated silicon quantum dots <b>2017</b> , 413-432		
284	Hydrogen-terminated silicon quantum dots. <i>Series in Materials Science and Engineering</i> , <b>2017</b> , 413-432		

283	A new insight into $\pi$ - $\pi$ stacking involving remarkable orbital interactions. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 25452-25457	3.6	32
282	Graphitic Carbon Nitride Film: An Emerging Star for Catalytic and Optoelectronic Applications. <i>ChemSusChem</i> , <b>2016</b> , 9, 2723-2735	8.3	62
281	Molecular orbital analysis of the hydrogen bonded water dimer. <i>Scientific Reports</i> , <b>2016</b> , 6, 22099	4.9	36
280	Strong orbital interaction in a weak CH- $\pi$ hydrogen bonding system. <i>Scientific Reports</i> , <b>2016</b> , 6, 22304	4.9	13
279	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
278	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
277	Composition dependent reactivity of titanium oxide clusters. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 10594-9	3.6	6
276	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
275	Chirality dependent spin polarization of carbon nanotubes. <i>New Journal of Physics</i> , <b>2016</b> , 18, 023029	2.9	7
274	Efficiency Enhancement of Carbon Nitride Photoelectrochemical Cells via Tailored Monomers Design. <i>Advanced Energy Materials</i> , <b>2016</b> , 6, 1600263	21.8	96
273	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
272	Dual response of graphene-based ultra-small molecular junctions to defect engineering. <i>Nano Research</i> , <b>2016</b> , 9, 1480-1488	10	9
271	Intramolecular torque, an indicator of the internal rotation direction of rotor molecules and similar systems. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 29665-29672	3.6	12
270	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
269	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
268	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
267	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
266	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



265	Strong [email protected] Dependence in Surface-Enhanced Raman Scattering of Pyridine on Stable 13-Atom Silver-Caged Bimetallic Clusters. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 17429-17437	3.8	15
264	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
263	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
262	Dynamic Crystallography Reveals Early Signalling Events in Ultraviolet Photoreceptor UVR8. <i>Nature Plants</i> , <b>2015</b> , 1,	11.5	42
261	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
260	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
259	Water Clusters on Graphitic Carbon Surfaces. <i>Journal of Cluster Science</i> , <b>2015</b> , 26, 361-373	3	2
258	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
257	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
256	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
255	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
254	Strong orbital deformation due to CH $\cdots$ interaction in the benzene-methane complex. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 29489-91	3.6	11
253	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
252	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
251	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, 30744-50	3.6	5
250	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
249	Self-doping and magnetic ordering induced by extended line defects in graphene. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	14
248	Electronic delocalization in small water rings. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 2987-90	3.6	17



247	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
246	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
245	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
244	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
243	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
242	Point defect weakened thermal contraction in monolayer graphene. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 064705	3.9	11
241	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
240	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
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	Anomalous effect of hydrogenation on phonon thermal conductivity in thin silicon nanowires. <i>Europhysics Letters</i> , <b>2014</b> , 105, 56003	1.6	15
237	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
236	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
235	Oxygen vacancy diffusion in bare ZnO nanowires. <i>Nanoscale</i> , <b>2014</b> , 6, 11882-6	7.7	24
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