Qian Wang

List of Publications by Year in Descending Order

258 papers	11,658 citations	51 h-index	101 g-index
273 ext. papers	13,457 ext. citations	6.8 avg, IF	6.82 L-index

#	Paper	IF	Citations
258	Toward stable zinc aqueous rechargeable batteries by anode morphology modulation via polyaspartic acid additive. *Energy Storage Materials*, **2022**, 45, 777-785	19.4	5
257	Design of 3D topological nodal-net porous carbon for sodium-ion battery anodes. *Journal of Materials Chemistry A*, **2022**, 10, 7754-7763	13	1
256	MXene-Supported, Atomic-Layered Iridium Catalysts Created by Nanoparticle Re-Dispersion for Efficient Alkaline Hydrogen Evolution.. *Small*, **2022**, 18, e2105226	11	2
255	Screening transition metal-based polar pentagonal monolayers with large piezoelectricity and shift current. *Npj Computational Materials*, **2022**, 8,	10.9	4
254	A novel construction of Ti3C2@complete edge-nitrogen doped carbon spheres with excellent K-ion storage performance. *Nano Energy*, **2022**, 97, 107161	17.1	1
253	Pentagon-based 2D materials: Classification, properties and applications. *Physics Reports*, **2022**, 964, 1-42	27.7	3
252	Research progress on penta-graphene and its related materials: Properties and applications. *Nano Today*, **2022**, 44, 101501	17.9	5
251	Two Birds with One Stone: Interfacial Engineering of Multifunctional Janus Separator for Lithium-Sulfur Batteries. *Advanced Materials*, **2021**, e2107638	24	11
250	Origins of low lattice thermal conductivity in 2D carbon allotropes. *Journal of Materials Research and Technology*, **2021**, 11, 1982-1990	5.5	4
249	Identifying key parameters for predicting materials with low defect generation efficiency by machine learning. *Computational Materials Science*, **2021**, 191, 110306	3.2	1
248	Pentagonal BN-based 3D metallic boron nitride with high energy density. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	1
247	SnS Nanosheets Anchored on Nitrogen and Sulfur Co-Doped MXene Sheets for High-Performance Potassium-Ion Batteries. *ACS Applied Materials & Interfaces*, **2021**, 13, 17668-17676	9.5	13
246	A New Porous Metallic Carbon Allotrope with Interlocking Pentagons for Sodium-Ion Battery Anode Material. *Advanced Theory and Simulations*, **2021**, 4, 2100025	3.5	2
245	Marrying Ester Group with Lithium Salt: Cellulose-Acetate-Enabled LiF-Enriched Interface for Stable Lithium Metal Anodes. *Advanced Functional Materials*, **2021**, 31, 2102228	15.6	22
244	Low lattice thermal conductivity of pentadiamond. *Journal of Applied Physics*, **2021**, 129, 215107	2.5	5
243	Advanced electrolyte design for stable lithium metal anode: From liquid to solid. *Nano Energy*, **2021**, 80, 105516	17.1	34
242	Imidazole-graphyne: a new 2D carbon nitride with a direct bandgap and strong IR refraction. *Physical Chemistry Chemical Physics*, **2021**, 23, 10274-10280	3.6	1

241	1,2,4-Azadiphosphole-based piezoelectric penta-CNP sheet with high spontaneous polarization. *Applied Surface Science*, **2021**, 554, 149499	6.7	6
240	Hex-C558: A new porous metallic carbon allotrope for lithium-ion battery anode. *Carbon*, **2021**, 183, 652-659	10.4	3
239	Low lattice thermal conductivity of a 5-8-peanut-shaped carbon nanotube. *Physical Chemistry Chemical Physics*, **2021**, 23, 5460-5466	3.6	3
238	Boron-Functionalized Organic Framework as a High-Performance Metal-Free Catalyst for N Fixation.. *Journal of Physical Chemistry Letters*, **2021**, 12, 12142-12149	6.4	0
237	Porous-Carbon Aerogels with Tailored Sub-Nanopores for High Cycling Stability and Rate Capability Potassium-Ion Battery Anodes. *ACS Applied Materials & Interfaces*, **2020**, 12, 27045-27054	9.5	11
236	Binder-Free TiO2-Coated Polypropylene Separators for Advanced Lithium-Ion Batteries. *Energy Technology*, **2020**, 8, 2000228	3.5	6
235	Ground state structure and physical properties of silicon monoxide sheet. *Applied Surface Science*, **2020**, 527, 146759	6.7	0
234	An asymmetric quasi-solid electrolyte for high-performance Li metal batteries. *Chemical Communications*, **2020**, 56, 7195-7198	5.8	8
233	A 3D porous honeycomb carbon as Na-ion battery anode material with high capacity, excellent rate performance, and robust stability. *Carbon*, **2020**, 168, 163-168	10.4	11
232	Large Second Harmonic Generation in Elemental □Sb and □Bi Monolayers. *Journal of Physical Chemistry C*, **2020**, 124, 5506-5513	3.8	9
231	Large Out-of-Plane Second Harmonic Generation Susceptibility in Penta-ZnS2 Sheet. *Advanced Theory and Simulations*, **2020**, 3, 2000027	3.5	6
230	Fabrication of Hollow CoP/TiO Heterostructures for Enhanced Oxygen Evolution Reaction. *Small*, **2020**, 16, e1905075	11	67
229	High Curie temperature ferromagnetism in penta-MnN2 monolayer. *Applied Surface Science*, **2020**, 505, 144620	6.7	9
228	Low thermal conductivity of peanut-shaped carbon nanotube and its insensitive response to uniaxial strain. *Nanotechnology*, **2020**, 31, 115701	3.4	2
227	□CsCu5Se3: A Promising Thermoelectric Material going beyond Photovoltaic Application. *Advanced Theory and Simulations*, **2020**, 3, 2000169	3.5	1
226	Potential of porous nodal-line semi-metallic carbon for sodium-ion battery anode. *Journal of Power Sources*, **2020**, 478, 228746	8.9	7
225	The geometry, electronic and magnetic properties of VLin (n = 2□13) clusters using the first-principles and PSO method. *Molecular Physics*, **2020**, 118, e1791990	1.7	1
224	Enhancing power factor of SnSe sheet with grain boundary by doping germanium or silicon. *Npj Computational Materials*, **2020**, 6,	10.9	4

223	Performance of the Pentagonal PdSe2 Sheet as a Channel Material in Contact with Metal Surfaces and Graphene. *ACS Applied Electronic Materials*, **2020**, 2, 2535-2542	4	4
222	Strain-engineering of bandgaps in pristine and fully hydrogenated hexagonal boron phosphide. *Journal of Applied Physics*, **2020**, 128, 094302	2.5	2
221	Integrating conductivity and active sites: Fe/Fe3C@GNC as an trapping-catalyst interlayer and dendrite-free lithium host for the lithium–sulfur cell with outstanding rate performance. *Journal of Materials Chemistry A*, **2020**, 8, 18987-19000	13	23
220	Na-functionalized IrTe2 monolayer: Suppressed charge ordering and electric field tuned topological phase transition. *Physical Review B*, **2020**, 102,	3.3	3
219	Ultralow thermal conductivity and negative thermal expansion of CuSCN. *Nano Energy*, **2020**, 73, 104822	17.1	9
218	Penta-BCN: A New Ternary Pentagonal Monolayer with Intrinsic Piezoelectricity. *Journal of Physical Chemistry Letters*, **2020**, 11, 3501-3506	6.4	31
217	Rational Design of Porous Nodal-Line Semimetallic Carbon for K-Ion Battery Anode Materials. *Journal of Physical Chemistry Letters*, **2019**, 10, 6360-6367	6.4	21
216	Two-Dimensional T-NiSe as a Promising Anode Material for Potassium-Ion Batteries with Low Average Voltage, High Ionic Conductivity, and Superior Carrier Mobility. *ACS Applied Materials & Interfaces*, **2019**, 11, 35661-35666	9.5	23
215	PCF-Graphene: A 2D sp2-Hybridized Carbon Allotrope with a Direct Band Gap. *Journal of Physical Chemistry C*, **2019**, 123, 4567-4573	3.8	13
214	Thermoelectric Properties of Two-Dimensional Gallium Telluride. *Journal of Electronic Materials*, **2019**, 48, 5988-5994	1.9	12
213	N-doped peanut-shaped carbon nanotubes for efficient CO2 electrocatalytic reduction. *Carbon*, **2019**, 152, 241-246	10.4	17
212	Rational Design of Stable Dianions and the Concept of Super-Chalcogens. *Journal of Physical Chemistry A*, **2019**, 123, 5753-5761	2.8	5
211	Broadband Reflection in Polymer-Stabilized Cholesteric Liquid Crystals via Thiol-Acrylate Chemistry. *Angewandte Chemie - International Edition*, **2019**, 58, 6698-6702	16.4	33
210	Broadband Reflection in Polymer-Stabilized Cholesteric Liquid Crystals via Thiol–Acrylate Chemistry. *Angewandte Chemie*, **2019**, 131, 6770-6774	3.6	7
209	Classifying superheavy elements by machine learning. *Physical Review A*, **2019**, 99,	2.6	8
208	Unidirectional Spin-Orbit Interaction Induced by the Line Defect in Monolayer Transition Metal Dichalcogenides for High-Performance Devices. *Nano Letters*, **2019**, 19, 6005-6012	11.5	8
207	Lattice Dynamic and Instability in Pentasilicene: A Light Single-Element Ferroelectric Material With High Curie Temperature. *Physical Review Applied*, **2019**, 11,	4.3	14
206	Octa-coordinated alkaline earth metal-dinitrogen complexes M(N) (M=Ca, Sr, Ba). *Nature Communications*, **2019**, 10, 3375	17.4	55

205	Surface-Based Li+ Complex Enables Uniform Lithium Deposition for Stable Lithium Metal Anodes. *ACS Applied Energy Materials*, **2019**, 2, 4602-4608	6.1	19
204	Dendrite-Free Lithium Deposition via a Superfilling Mechanism for High-Performance Li-Metal Batteries. *Advanced Materials*, **2019**, 31, e1903248	24	66
203	Strain Effect on Thermoelectric Performance of InSe Monolayer. *Nanoscale Research Letters*, **2019**, 14, 287	5	17
202	Synergistic Effect of Co-Ni Hybrid Phosphide Nanocages for Ultrahigh Capacity Fast Energy Storage. *Advanced Science*, **2019**, 6, 1802005	13.6	80
201	Ultrahigh thermal conductivity of carbon allotropes with correlations with the scaled Pugh ratio. *Journal of Materials Chemistry A*, **2019**, 7, 6259-6266	13	14
200	Interfacial properties of penta-graphene-metal contacts. *Journal of Applied Physics*, **2019**, 125, 065308	2.5	6
199	Co-doped 1T-MoS2 nanosheets embedded in N, S-doped carbon nanobowls for high-rate and ultra-stable sodium-ion batteries. *Nano Research*, **2019**, 12, 2218-2223	10	59
198	Piezoelectric Effects in Surface-Engineered Two-Dimensional Group III Nitrides. *ACS Applied Materials & Interfaces*, **2019**, 11, 1033-1039	9.5	27
197	Thermal transport properties of penta-graphene with grain boundaries. *Carbon*, **2019**, 145, 445-451	10.4	10
196	A C-based 3D carbon allotrope with high thermal conductivity. *Physical Chemistry Chemical Physics*, **2019**, 22, 306-312	3.6	7
195	2D planar penta-MN (M = Pd, Pt) sheets identified through structure search. *Physical Chemistry Chemical Physics*, **2018**, 21, 246-251	3.6	21
194	A C fullerene-based sheet with ultrahigh thermal conductivity. *Nanoscale*, **2018**, 10, 6099-6104	7.7	6
193	A metallic peanut-shaped carbon nanotube and its potential for CO2 capture. *Carbon*, **2018**, 132, 249-256	10.4	7
192	Prediction of a BeP2 monolayer with a compression-induced Dirac semimetal state. *Physical Review B*, **2018**, 97,	3.3	8
191	3D□D□D Interface Profiling for Record Efficiency All-Inorganic CsPbBrI2 Perovskite Solar Cells with Superior Stability. *Advanced Energy Materials*, **2018**, 8, 1703246	21.8	256
190	Stable Li metal anode with protected interface for high-performance Li metal batteries. *Energy Storage Materials*, **2018**, 15, 249-256	19.4	55
189	Interstitial Mn2+-Driven High-Aspect-Ratio Grain Growth for Low-Trap-Density Microcrystalline Films for Record Efficiency CsPbI2Br Solar Cells. *ACS Energy Letters*, **2018**, 3, 970-978	20.1	285
188	A New Anisotropic Dirac Cone Material: A BS Honeycomb Monolayer. *Journal of Physical Chemistry Letters*, **2018**, 9, 1815-1820	6.4	49

187	Thermoelectric properties of two-dimensional hexagonal indium-VA. *Chinese Physics B*, **2018**, 27, 026802	1.2	9
186	Sulfur/Oxygen Codoped Porous Hard Carbon Microspheres for High-Performance Potassium-Ion Batteries. *Advanced Energy Materials*, **2018**, 8, 1800171	21.8	272
185	2D SnSe-based vdW heterojunctions: tuning the Schottky barrier by reducing Fermi level pinning. *Nanoscale*, **2018**, 10, 13767-13772	7.7	24
184	High n-type and p-type thermoelectric performance of two-dimensional SiTe at high temperature.. *RSC Advances*, **2018**, 8, 21280-21287	3.7	7
183	Zero-strain K0.6Mn1F2.7 hollow nanocubes for ultrastable potassium ion storage. *Energy and Environmental Science*, **2018**, 11, 3033-3042	35.4	67
182	Graphdiyne as an ideal monolayer coating material for lithium-ion battery cathodes with ultralow areal density and ultrafast Li penetration. *Journal of Materials Chemistry A*, **2018**, 6, 12630-12636	13	17
181	A new 3D Dirac nodal-line semi-metallic graphene monolith for lithium ion battery anode materials. *Journal of Materials Chemistry A*, **2018**, 6, 13816-13824	13	31
180	Monoclinic C16: sp-sp hybridized nodal-line semimetal protected by PT-symmetry. *Carbon*, **2018**, 127, 527-532	10.4	28
179	TiS sheet based van der Waals heterostructures with a tunable Schottky barrier. *Nanoscale*, **2018**, 10, 807-815	7.7	18
178	Stabilizing benzene-like planar N rings to form a single atomic honeycomb BeN sheet with high carrier mobility. *Nanoscale*, **2018**, 10, 949-957	7.7	13
177	Physical Properties and Photovoltaic Application of Semiconducting $PdSe_2$ Monolayer. *Nanomaterials*, **2018**, 8,	5.4	10
176	Iodine-Optimized Interface for Inorganic CsPbIBr Perovskite Solar Cell to Attain High Stabilized Efficiency Exceeding 14. *Advanced Science*, **2018**, 5, 1801123	13.6	76
175	Contact properties of a vdW heterostructure composed of penta-graphene and penta-BN2 sheets. *Journal of Applied Physics*, **2018**, 124, 165103	2.5	10
174	Hydrogenated NaTiO Epitaxially Grown on Flexible N-Doped Carbon Sponge for Potassium-Ion Batteries. *ACS Applied Materials & Interfaces*, **2018**, 10, 37974-37980	9.5	37
173	Controlled Air-Etching Synthesis of Porous-Carbon Nanotube Aerogels with Ultrafast Charging at 1000 A g. *Small*, **2018**, 14, e1802394	11	27
172	CsPbCl-Driven Low-Trap-Density Perovskite Grain Growth for >20% Solar Cell Efficiency. *Advanced Science*, **2018**, 5, 1800474	13.6	47
171	Body-Centered Tetragonal C : A Novel Topological Node-Line Semimetallic Carbon Composed of Tetrarings. *Small*, **2017**, 13, 1602894	11	49
170	Rational design of super-alkalis and their role in CO activation. *Nanoscale*, **2017**, 9, 4891-4897	7.7	47

169	Transformation of monolayer MoS2 into multiphasic MoTe2: Chalcogen atom-exchange synthesis route. *Nano Research*, **2017**, 10, 2761-2771	10	11
168	A new metallic carbon allotrope with high stability and potential for lithium ion battery anode material. *Nano Energy*, **2017**, 38, 263-270	17.1	60
167	Ground-State Structure of YN2 Monolayer Identified by Global Search. *Journal of Physical Chemistry C*, **2017**, 121, 10258-10264	3.8	26
166	Topological insulating states in 2D transition metal dichalcogenides induced by defects and strain. *Nanoscale*, **2017**, 9, 562-569	7.7	21
165	Structural Stabilities and Electronic Properties of High-Angle Grain Boundaries in Perovskite Cesium Lead Halides. *Journal of Physical Chemistry C*, **2017**, 121, 1715-1722	3.8	80
164	Exceptional Thermoelectric Properties of Layered GeAs2. *Chemistry of Materials*, **2017**, 29, 9300-9307	9.6	47
163	Boron-Doped Graphene as a Promising Anode Material for Potassium-Ion Batteries with a Large Capacity, High Rate Performance, and Good Cycling Stability. *Journal of Physical Chemistry C*, **2017**, 121, 24418-24424	3.8	86
162	An all-carbon vdW heterojunction composed of penta-graphene and graphene: Tuning the Schottky barrier by electrostatic gating or nitrogen doping. *Applied Physics Letters*, **2017**, 111, 073503	3.4	23
161	Titelbild: Colossal Stability of Gas-Phase Trianions: Super-Pnictogens (Angew. Chem. 43/2017). *Angewandte Chemie*, **2017**, 129, 13333-13333	3.6	
160	Colossal Stability of Gas-Phase Trianions: Super-Pnictogens. *Angewandte Chemie*, **2017**, 129, 13606-13610	3.6	6
159	Colossal Stability of Gas-Phase Trianions: Super-Pnictogens. *Angewandte Chemie - International Edition*, **2017**, 56, 13421-13425	16.4	15
158	Weak interlayer dependence of lattice thermal conductivity on stacking thickness of penta-graphene. *Applied Physics Letters*, **2017**, 111, 192102	3.4	15
157	Quasi-freestanding, striped WS2 monolayer with an invariable band gap on Au(001). *Nano Research*, **2017**, 10, 3875-3884	10	7
156	2D halide perovskite-based van der Waals heterostructures: contact evaluation and performance modulation. *2D Materials*, **2017**, 4, 035009	5.9	18
155	Graphene: A New Metallic Allotrope of Planar Carbon with Potential Applications as Anode Materials for Lithium-Ion Batteries. *Journal of Physical Chemistry Letters*, **2017**, 8, 3234-3241	6.4	109
154	Modulating the phases of iron carbide nanoparticles: from a perspective of interfering with the carbon penetration of Fe@FeO by selectively adsorbed halide ions. *Chemical Science*, **2017**, 8, 473-481	9.4	80
153	TiC2: a new two-dimensional sheet beyond MXenes. *Nanoscale*, **2016**, 8, 233-42	7.7	107
152	Ferromagnetic and Half-Metallic FeC Monolayer Containing C Dimers. *ACS Applied Materials & Interfaces*, **2016**, 8, 26207-26212	9.5	44

151	Phosphorus K Crystal: A New Stable Allotrope. *Scientific Reports*, **2016**, 6, 37528	4.9	9
150	Bonding-restricted structure search for novel 2D materials with dispersed C2 dimers. *Scientific Reports*, **2016**, 6, 29531	4.9	13
149	Cluster-Inspired Design of High-Capacity Anode for Li-Ion Batteries. *ACS Energy Letters*, **2016**, 1, 202-208	20.1	19
148	Carbon materials for high volumetric performance supercapacitors: design, progress, challenges and opportunities. *Energy and Environmental Science*, **2016**, 9, 729-762	35.4	876
147	Beyond Graphitic Carbon Nitride: Nitrogen-Rich Penta-CN2 Sheet. *Journal of Physical Chemistry C*, **2016**, 120, 3993-3998	3.8	125
146	Thermal exfoliation of stoichiometric single-layer silica from the stishovite phase: insight from first-principles calculations. *Nanoscale*, **2016**, 8, 10598-606	7.7	7
145	Like Charges Attract?. *Journal of Physical Chemistry Letters*, **2016**, 7, 2689-95	6.4	23
144	Integrating superconducting phase and topological crystalline quantum spin Hall effect in hafnium intercalated gallium film. *Applied Physics Letters*, **2016**, 108, 253102	3.4	4
143	Many faces of carbon **2016**,		1
142	Tuning the electronic and mechanical properties of penta-graphene via hydrogenation and fluorination. *Physical Chemistry Chemical Physics*, **2016**, 18, 14191-7	3.6	83
141	Lattice thermal conductivity of penta-graphene. *Carbon*, **2016**, 105, 424-429	10.4	77
140	Strain and carrier-induced coexistence of topologically insulating and superconducting phase in iodized Si(111) films. *Nano Research*, **2016**, 9, 1578-1589	10	5
139	Intrinsic quantum spin Hall and anomalous Hall effects in h-Sb/Bi epitaxial growth on a ferromagnetic MnO2 thin film. *Nanoscale*, **2016**, 8, 11202-9	7.7	12
138	Experimental observation of TiN cluster and theoretical investigation of its stable and metastable isomers. *Chemical Science*, **2015**, 6, 4723-4729	9.4	10
137	A new C=C embedded porphyrin sheet with superior oxygen reduction performance. *Nano Research* , **2015**, 8, 2901-2912	10	28
136	New Phosphorene Allotropes Containing Ridges with 2- and 4-Coordination. *Journal of Physical Chemistry C*, **2015**, 119, 24674-24680	3.8	32
135	Thermoelectric properties of single-layered SnSe sheet. *Nanoscale*, **2015**, 7, 15962-70	7.7	181
134	Self-assembly of metal atoms (Na, K, Ca) on graphene. *Nanoscale*, **2015**, 7, 2352-9	7.7	10

133	High-temperature superconductivity in heavily N- or B-doped graphene. *Physical Review B*, **2015**, 92,	3.3	33
132	A New Silicon Phase with Direct Band Gap and Novel Optoelectronic Properties. *Scientific Reports*, **2015**, 5, 14342	4.9	62
131	A simple method for understanding the triangular growth patterns of transition metal dichalcogenide sheets. *AIP Advances*, **2015**, 5, 107105	1.5	11
130	Giant magnetocrystalline anisotropy of 5d transition metal-based phthalocyanine sheet. *Physical Chemistry Chemical Physics*, **2015**, 17, 17182-9	3.6	15
129	Penta-graphene: A new carbon allotrope. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 2372-7	11.5	763
128	Pressure-induced magnetic crossover driven by hydrogen bonding in CuF(HF)(3-chloropyridine). *Scientific Reports*, **2014**, 4, 6054	4.9	18
127	Robust ferromagnetism in monolayer chromium nitride. *Scientific Reports*, **2014**, 4, 5241	4.9	50
126	Tuning electronic and magnetic properties of silicene with magnetic superhalogens. *Physical Chemistry Chemical Physics*, **2014**, 16, 22979-86	3.6	30
125	Structural, electronic and magnetic properties of neutral and anionic Fe2(BO2)n (n=1-3) clusters. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 2959-2964	2.3	3
124	Electronic and optical properties of silicon based porous sheets. *Physical Chemistry Chemical Physics* , **2014**, 16, 16832-6	3.6	12
123	Tailoring Li adsorption on graphene. *Physical Review B*, **2014**, 90,	3.3	36
122	Self-consistent determination of Hubbard U for explaining the anomalous magnetism of the Gd13 cluster. *Physical Review B*, **2014**, 89,	3.3	20
121	Stable three-dimensional metallic carbon with interlocking hexagons. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 18809-13	11.5	100
120	Structure and properties of Mn4Cl9: an antiferromagnetic binary hyperhalogen. *Journal of Chemical Physics*, **2013**, 138, 054309	3.9	41
119	Three-dimensional metallic boron nitride. *Journal of the American Chemical Society*, **2013**, 135, 18216-21	16.4	113
118	All-metal clusters that mimic the chemistry of halogens. *ChemPhysChem*, **2013**, 14, 3227-32	3.2	8
117	Functionalized Graphitic Carbon Nitride for Efficient Energy Storage. *Journal of Physical Chemistry C* , **2013**, 117, 6055-6059	3.8	131
116	Stability and physical properties of a tri-ring based porous g-C4N3 sheet. *Physical Chemistry Chemical Physics*, **2013**, 15, 7142-6	3.6	58

115	Structure, Stability, and Property Modulations of Stoichiometric Graphene Oxide. *Journal of Physical Chemistry C*, **2013**, 117, 1064-1070	3.8	21
114	Patterning Graphitic C-N Sheets into a Kagome Lattice for Magnetic Materials. *Journal of Physical Chemistry Letters*, **2013**, 4, 259-63	6.4	52
113	Communication: In search of four-atom chiral metal clusters. *Journal of Chemical Physics*, **2013**, 139, 111101	3.1	8
112	Magnetic properties of two dimensional silicon carbide triangular nanoflakes-based kagome lattices. *Journal of Nanoparticle Research*, **2012**, 14, 1	2.3	5
111	Magnetism of triangular nanoflakes with different compositions and edge terminations. *Journal of Nanoparticle Research*, **2012**, 14, 1	2.3	6
110	Strain-Induced Spin Crossover in Phthalocyanine-Based Organometallic Sheets. *Journal of Physical Chemistry Letters*, **2012**, 3, 3109-14	6.4	46
109	Tunable ferromagnetism in assembled two dimensional triangular graphene nanoflakes. *Physical Chemistry Chemical Physics*, **2012**, 14, 2065-9	3.6	22
108	Density Functional Theory Study of the Interaction of Hydrogen with Li6C60. *Journal of Physical Chemistry Letters*, **2012**, 3, 1084-8	6.4	46
107	Tuning magnetic properties of graphene nanoribbons with topological line defects: From antiferromagnetic to ferromagnetic. *Physical Review B*, **2012**, 85,	3.3	59
106	Magnetism of two-dimensional triangular nanoflake-based kagome lattices. *New Journal of Physics*, **2012**, 14, 033043	2.9	17
105	Adsorption of oxygen-containing functional groups on free and supported graphene using point contact. *Physical Review B*, **2012**, 85,	3.3	5
104	Electronic structures and bonding of graphyne sheet and its BN analog. *Journal of Chemical Physics*, **2011**, 134, 174701	3.9	163
103	Enhanced Hydrogen Storage on Li Functionalized BC3 Nanotube. *Journal of Physical Chemistry C*, **2011**, 115, 6136-6140	3.8	36
102	Effects of charging and doping on orbital hybridizations and distributions in TiO2 clusters. *Physica B: Condensed Matter*, **2011**, 406, 4322-4326	2.8	3
101	Manganese-based magnetic superhalogens. *Angewandte Chemie - International Edition*, **2011**, 50, 2568-72	6.4	74
100	Reaction-induced magnetic transition in Mn2 dimers. *Journal of Physical Chemistry A*, **2011**, 115, 549-55	2.8	11
99	Anisotropy and Transport Properties of Tubular C-BN Janus Nanostructures. *Journal of Physical Chemistry C*, **2011**, 115, 23978-23983	3.8	15
98	Sc-phthalocyanine sheet: Promising material for hydrogen storage. *Applied Physics Letters*, **2011**, 99, 163104	3.4	28

97	Ferromagnetism in Two-Dimensional Carbon Chains Linked by 1,3,5-Benzenetriyl Units. *Journal of Physical Chemistry C*, **2011**, 115, 19621-19625	3.8	11
96	Intrinsic ferromagnetism in two-dimensional carbon structures: Triangular graphene nanoflakes linked by carbon chains. *Physical Review B*, **2011**, 84,	3.3	38
95	Tuning the band gap and magnetic properties of BN sheets impregnated with graphene flakes. *Physical Review B*, **2011**, 84,	3.3	77
94	Stability and electronic structure of bilayer graphone. *Applied Physics Letters*, **2011**, 98, 063108	3.4	13
93	Electric field enhanced hydrogen storage on polarizable materials substrates. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 2801-6	11.5	194
92	Structures of neutral and anionic Au(16) clusters revisited. *Journal of Chemical Physics*, **2010**, 132, 194306	3.9	31
91	Probing the existence of energetically degenerate cluster isomers by chemical tagging. *Applied Physics Letters*, **2010**, 97, 223104	3.4	1
90	Magnetism in ZnO nanowire with Fe/Co codoping: First-principles density functional calculations. *Physical Review B*, **2010**, 81,	3.3	34
89	Electronic and magnetic properties of a BN sheet decorated with hydrogen and fluorine. *Physical Review B*, **2010**, 81,	3.3	247
88	Interaction of C(59)Si with Si based clusters: a study of Janus nanostructures. *Journal of Physics Condensed Matter*, **2010**, 22, 275303	1.8	1
87	Geometry, Electronic Properties, and Hydrogen Adsorption Properties of Li3N-Based Nanostructures. *Journal of Physical Chemistry C*, **2010**, 114, 19202-19205	3.8	6
86	First-principles study of hydrogen adsorption in metal-doped COF-10. *Journal of Chemical Physics*, **2010**, 133, 154706	3.9	23
85	First-principles study of the effect of vacancies on magnetic properties of Zn1 - xCoxO thin films. *Journal of Physics Condensed Matter*, **2010**, 22, 076002	1.8	4
84	Tuning magnetic properties of Mn(4) cluster with gold coating. *Physical Chemistry Chemical Physics*, **2010**, 12, 1493-6	3.6	4
83	Geometry and Energetics of Nano Gears. *Journal of Computational and Theoretical Nanoscience*, **2010**, 7, 1457-1461	0.3	3
82	Mg-doped GaN nanostructures: Energetics, magnetism, and H2 adsorption. *Applied Physics Letters*, **2009**, 94, 013108	3.4	15
81	Stabilizing a 22 karat nanogolden cage. *Journal of Chemical Physics*, **2009**, 131, 204501	3.9	3
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