Qian Wang

List of Publications by Citations

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	Carbon materials for high volumetric performance supercapacitors: design, progress, challenges and opportunities. *Energy and Environmental Science*, **2016**, 9, 729-762	35.4	876
257	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
256	Ferromagnetism in semihydrogenated graphene sheet. *Nano Letters*, **2009**, 9, 3867-70	11.5	686
255	Clustering of Ti on a C60 surface and its effect on hydrogen storage. *Journal of the American Chemical Society*, **2005**, 127, 14582-3	16.4	606
254	First-principles study of hydrogen storage on Li12C60. *Journal of the American Chemical Society*, **2006**, 128, 9741-5	16.4	474
253	Vacancy-induced magnetism in ZnO thin films and nanowires. *Physical Review B*, **2008**, 77,	3.3	381
252	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
251	Sulfur/Oxygen Codoped Porous Hard Carbon Microspheres for High-Performance Potassium-Ion Batteries. *Advanced Energy Materials*, **2018**, 8, 1800171	21.8	272
250	3D⁄2D⁄0D Interface Profiling for Record Efficiency All-Inorganic CsPbBrI2 Perovskite Solar Cells with Superior Stability. *Advanced Energy Materials*, **2018**, 8, 1703246	21.8	256
249	Electronic and magnetic properties of a BN sheet decorated with hydrogen and fluorine. *Physical Review B*, **2010**, 81,	3.3	247
248	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
247	Potential of AlN nanostructures as hydrogen storage materials. *ACS Nano*, **2009**, 3, 621-6	16.7	183
246	Thermoelectric properties of single-layered SnSe sheet. *Nanoscale*, **2015**, 7, 15962-70	7.7	181
245	Electronic structures and bonding of graphyne sheet and its BN analog. *Journal of Chemical Physics*, **2011**, 134, 174701	3.9	163
244	Functionalized Graphitic Carbon Nitride for Efficient Energy Storage. *Journal of Physical Chemistry C* , **2013**, 117, 6055-6059	3.8	131
243	Beyond Graphitic Carbon Nitride: Nitrogen-Rich Penta-CN2 Sheet. *Journal of Physical Chemistry C*, **2016**, 120, 3993-3998	3.8	125
242	Theoretical Study of Hydrogen Storage in Ca-Coated Fullerenes. *Journal of Chemical Theory and Computation*, **2009**, 5, 374-9	6.4	115

241	Three-dimensional metallic boron nitride. *Journal of the American Chemical Society*, **2013**, 135, 18216-21	16.4	113
240	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
239	Carrier-mediated ferromagnetism in N codoped (Zn,Mn)O (101 0) thin films. *Physical Review B*, **2004**, 70,	3.3	109
238	TiC2: a new two-dimensional sheet beyond MXenes. *Nanoscale*, **2016**, 8, 233-42	7.7	107
237	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
236	Storage of molecular hydrogen in B-N cage: energetics and thermal stability. *Nano Letters*, **2005**, 5, 1273-7	11.5	96
235	Ferromagnetism in Mn-doped GaN nanowires. *Physical Review Letters*, **2005**, 95, 167202	7.4	89
234	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
233	Stabilization of Si60 cage structure. *Physical Review Letters*, **2003**, 90, 135503	7.4	83
232	Tuning the electronic and mechanical properties of penta-graphene via hydrogenation and fluorination. *Physical Chemistry Chemical Physics*, **2016**, 18, 14191-7	3.6	83
231	Functionalized heterofullerenes for hydrogen storage. *Applied Physics Letters*, **2009**, 94, 013111	3.4	82
230	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
229	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
228	Synergistic Effect of Co-Ni Hybrid Phosphide Nanocages for Ultrahigh Capacity Fast Energy Storage. *Advanced Science*, **2019**, 6, 1802005	13.6	80
227	Magnetic properties of transition-metal-doped Zn1 TxO (T=Cr, Mn, Fe, Co, and Ni) thin films with and without intrinsic defects: A density functional study. *Physical Review B*, **2009**, 79,	3.3	79
226	Tuning the band gap and magnetic properties of BN sheets impregnated with graphene flakes. *Physical Review B*, **2011**, 84,	3.3	77
225	Lattice thermal conductivity of penta-graphene. *Carbon*, **2016**, 105, 424-429	10.4	77
224	Iodine-Optimized Interface for Inorganic CsPbIBr Perovskite Solar Cell to Attain High Stabilized Efficiency Exceeding 14. *Advanced Science*, **2018**, 5, 1801123	13.6	76

223	Manganese-based magnetic superhalogens. *Angewandte Chemie - International Edition*, **2011**, 50, 2568-72	16.4	74
222	Zero-strain K0.6Mn1F2.7 hollow nanocubes for ultrastable potassium ion storage. *Energy and Environmental Science*, **2018**, 11, 3033-3042	35.4	67
221	Fabrication of Hollow CoP/TiO Heterostructures for Enhanced Oxygen Evolution Reaction. *Small*, **2020**, 16, e1905075	11	67
220	Dendrite-Free Lithium Deposition via a Superfilling Mechanism for High-Performance Li-Metal Batteries. *Advanced Materials*, **2019**, 31, e1903248	24	66
219	A New Silicon Phase with Direct Band Gap and Novel Optoelectronic Properties. *Scientific Reports*, **2015**, 5, 14342	4.9	62
218	First-principles calculations of metal stabilized Si20 cages. *Physical Review B*, **2002**, 65,	3.3	62
217	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
216	Tuning magnetic properties of graphene nanoribbons with topological line defects: From antiferromagnetic to ferromagnetic. *Physical Review B*, **2012**, 85,	3.3	59
215	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
214	Stability and physical properties of a tri-ring based porous g-C4N3 sheet. *Physical Chemistry Chemical Physics*, **2013**, 15, 7142-6	3.6	58
213	Magnetic coupling between Cr atoms doped at bulk and surface sites of ZnO. *Applied Physics Letters*, **2005**, 87, 162509	3.4	56
212	Stable Li metal anode with protected interface for high-performance Li metal batteries. *Energy Storage Materials*, **2018**, 15, 249-256	19.4	55
211	Octa-coordinated alkaline earth metal-dinitrogen complexes M(N) (M=Ca, Sr, Ba). *Nature Communications*, **2019**, 10, 3375	17.4	55
210	Magnetism and energetics of Mn-Doped ZnO (101□0) thin films. *Physical Review B*, **2004**, 69,	3.3	55
209	Antiferromagnetic coupling driven by bond length contraction near the Ga1-xMnxN film surface. *Physical Review Letters*, **2004**, 93, 155501	7.4	54
208	Patterning Graphitic C-N Sheets into a Kagome Lattice for Magnetic Materials. *Journal of Physical Chemistry Letters*, **2013**, 4, 259-63	6.4	52
207	Robust ferromagnetism in monolayer chromium nitride. *Scientific Reports*, **2014**, 4, 5241	4.9	50
206	Body-Centered Tetragonal C : A Novel Topological Node-Line Semimetallic Carbon Composed of Tetrarings. *Small*, **2017**, 13, 1602894	11	49

205	A New Anisotropic Dirac Cone Material: A BS Honeycomb Monolayer. *Journal of Physical Chemistry Letters*, **2018**, 9, 1815-1820	6.4	49
204	Superhalogen properties of CuF(n) clusters. *Journal of Chemical Physics*, **2009**, 131, 124301	3.9	49
203	Structure of SiAu16: can a silicon atom be stabilized in a gold cage?. *Journal of Chemical Physics*, **2007**, 127, 214706	3.9	49
202	Rational design of super-alkalis and their role in CO activation. *Nanoscale*, **2017**, 9, 4891-4897	7.7	47
201	Exceptional Thermoelectric Properties of Layered GeAs2. *Chemistry of Materials*, **2017**, 29, 9300-9307	9.6	47
200	Ferromagnetic GaN--Cr Nanowires. *Nano Letters*, **2005**, 5, 1587-90	11.5	47
199	CsPbCl-Driven Low-Trap-Density Perovskite Grain Growth for >20% Solar Cell Efficiency. *Advanced Science*, **2018**, 5, 1800474	13.6	47
198	Strain-Induced Spin Crossover in Phthalocyanine-Based Organometallic Sheets. *Journal of Physical Chemistry Letters*, **2012**, 3, 3109-14	6.4	46
197	Density Functional Theory Study of the Interaction of Hydrogen with Li6C60. *Journal of Physical Chemistry Letters*, **2012**, 3, 1084-8	6.4	46
196	Geometry and electronic structure of magic iron oxide clusters. *Physical Review B*, **1999**, 59, 12672-12677	3.3	46
195	Ferromagnetic and Half-Metallic FeC Monolayer Containing C Dimers. *ACS Applied Materials & Interfaces*, **2016**, 8, 26207-26212	9.5	44
194	Effect of Au coating on the magnetic and structural properties of Fe nanoclusters for use in biomedical applications: A density-functional theory study. *Physical Review B*, **2006**, 73,	3.3	44
193	Electronic structure and bonding of Au on a SiO2 cluster: a nanobullet for tumors. *Physical Review Letters*, **2004**, 93, 186803	7.4	42
192	Structure and properties of Mn4Cl9: an antiferromagnetic binary hyperhalogen. *Journal of Chemical Physics*, **2013**, 138, 054309	3.9	41
191	Geometry and electronic structures of magic transition-metal oxide clusters M9O6 (M=Fe, Co, and Ni). *Physical Review B*, **2000**, 62, 8500-8507	3.3	39
190	Intrinsic ferromagnetism in two-dimensional carbon structures: Triangular graphene nanoflakes linked by carbon chains. *Physical Review B*, **2011**, 84,	3.3	38
189	First-principles studies of the geometry and energetics of the Si36 cluster. *Physical Review A*, **2003**, 67,	2.6	38
188	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

187	Tailoring Li adsorption on graphene. *Physical Review B*, **2014**, 90,	3.3	36
186	Enhanced Hydrogen Storage on Li Functionalized BC3 Nanotube. *Journal of Physical Chemistry C*, **2011**, 115, 6136-6140	3.8	36
185	First-principles study of magnetic properties in V-doped ZnO. *Applied Physics Letters*, **2007**, 91, 063116	3.4	35
184	Magnetism in ZnO nanowire with Fe/Co codoping: First-principles density functional calculations. *Physical Review B*, **2010**, 81,	3.3	34
183	Advanced electrolyte design for stable lithium metal anode: From liquid to solid. *Nano Energy*, **2021**, 80, 105516	17.1	34
182	Broadband Reflection in Polymer-Stabilized Cholesteric Liquid Crystals via Thiol-Acrylate Chemistry. *Angewandte Chemie - International Edition*, **2019**, 58, 6698-6702	16.4	33
181	High-temperature superconductivity in heavily N- or B-doped graphene. *Physical Review B*, **2015**, 92,	3.3	33
180	Ligand induced ferromagnetism in ZnO nanostructures. *Journal of Chemical Physics*, **2008**, 129, 164714	3.9	33
179	Design of Janus nanoparticles with atomic precision: tungsten-doped gold nanostructures. *ACS Nano*, **2008**, 2, 341-7	16.7	33
178	Nitrogen-induced magnetic transition in small chromium clusters. *Journal of Chemical Physics*, **2003**, 119, 7124-7130	3.9	33
177	New Phosphorene Allotropes Containing Ridges with 2- and 4-Coordination. *Journal of Physical Chemistry C*, **2015**, 119, 24674-24680	3.8	32
176	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
175	Structures of neutral and anionic Au(16) clusters revisited. *Journal of Chemical Physics*, **2010**, 132, 194306	3.9	31
174	Penta-BCN: A New Ternary Pentagonal Monolayer with Intrinsic Piezoelectricity. *Journal of Physical Chemistry Letters*, **2020**, 11, 3501-3506	6.4	31
173	Tuning electronic and magnetic properties of silicene with magnetic superhalogens. *Physical Chemistry Chemical Physics*, **2014**, 16, 22979-86	3.6	30
172	Clustering of Cr in GaN nanotubes and the onset of ferrimagnetic order. *Physical Review B*, **2006**, 73,	3.3	29
171	A new C=C embedded porphyrin sheet with superior oxygen reduction performance. *Nano Research*, **2015**, 8, 2901-2912	10	28
170	Sc-phthalocyanine sheet: Promising material for hydrogen storage. *Applied Physics Letters*, **2011**, 99, 163104	3.4	28

169	Real-space representation of electron localization and shell structure in jelliumlike clusters. *Physical Review B*, **2001**, 63,	3.3	28
168	Monoclinic C16: sp-sp hybridized nodal-line semimetal protected by PT-symmetry. *Carbon*, **2018**, 127, 527-532	10.4	28
167	First-principles study of magnetism in (112 0) Zn1−xMnxO thin film. *Applied Physics Letters*, **2004**, 84, 4170-4172	3.4	27
166	Piezoelectric Effects in Surface-Engineered Two-Dimensional Group III Nitrides. *ACS Applied Materials & Interfaces*, **2019**, 11, 1033-1039	9.5	27
165	Controlled Air-Etching Synthesis of Porous-Carbon Nanotube Aerogels with Ultrafast Charging at 1000 A g. *Small*, **2018**, 14, e1802394	11	27
164	Ground-State Structure of YN2 Monolayer Identified by Global Search. *Journal of Physical Chemistry C*, **2017**, 121, 10258-10264	3.8	26
163	Theoretical Study on Gold-Coated Iron Oxide Nanostructure: Magnetism and Bioselectivity for Amino Acids. *Journal of Physical Chemistry C*, **2007**, 111, 4159-4163	3.8	26
162	Ferromagnetism in Al1−xCrxN thin films by density functional calculations. *Physical Review B*, **2006**, 73,	3.3	25
161	2D SnSe-based vdW heterojunctions: tuning the Schottky barrier by reducing Fermi level pinning. *Nanoscale*, **2018**, 10, 13767-13772	7.7	24
160	N-doped ZnO thin films and nanowires: energetics, impurity distribution and magnetism. *New Journal of Physics*, **2009**, 11, 063035	2.9	24
159	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
158	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
157	First-principles study of hydrogen adsorption in metal-doped COF-10. *Journal of Chemical Physics*, **2010**, 133, 154706	3.9	23
156	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
155	Like Charges Attract?. *Journal of Physical Chemistry Letters*, **2016**, 7, 2689-95	6.4	23
154	Tunable ferromagnetism in assembled two dimensional triangular graphene nanoflakes. *Physical Chemistry Chemical Physics*, **2012**, 14, 2065-9	3.6	22
153	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
152	Topological insulating states in 2D transition metal dichalcogenides induced by defects and strain. *Nanoscale*, **2017**, 9, 562-569	7.7	21

151	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
150	2D planar penta-MN (M = Pd, Pt) sheets identified through structure search. *Physical Chemistry Chemical Physics*, **2018**, 21, 246-251	3.6	21
149	Structure, Stability, and Property Modulations of Stoichiometric Graphene Oxide. *Journal of Physical Chemistry C*, **2013**, 117, 1064-1070	3.8	21
148	Hydrogen Storage in Organometallic Structures Grafted on Silsesquioxanes. *Chemistry of Materials*, **2007**, 19, 3074-3078	9.6	21
147	First-principles studies on the intrinsic stability of the magic Fe13O8 cluster. *Physical Review B*, **2000**, 61, 5781-5785	3.3	21
146	Self-consistent determination of Hubbard U for explaining the anomalous magnetism of the Gd13 cluster. *Physical Review B*, **2014**, 89,	3.3	20
145	Cluster-Inspired Design of High-Capacity Anode for Li-Ion Batteries. *ACS Energy Letters*, **2016**, 1, 202-208	20.1	19
144	Surface-Based Li+ Complex Enables Uniform Lithium Deposition for Stable Lithium Metal Anodes. *ACS Applied Energy Materials*, **2019**, 2, 4602-4608	6.1	19
143	Ab initio study of ferromagnetism in Ga1−xCrxN thin films. *Physical Review B*, **2005**, 72,	3.3	19
142	Pressure-induced magnetic crossover driven by hydrogen bonding in CuF(HFO)(3-chloropyridine). *Scientific Reports*, **2014**, 4, 6054	4.9	18
141	2D halide perovskite-based van der Waals heterostructures: contact evaluation and performance modulation. *2D Materials*, **2017**, 4, 035009	5.9	18
140	Ab initio study of electronic and magnetic properties of the C-codoped Ga1−xMnxN (10−10) surface. *Physical Review B*, **2007**, 75,	3.3	18
139	Comment on "Fully coordinated silica nanoclusters: (SiO2)N molecular rings". *Physical Review Letters*, **2004**, 92, 039601; author reply 039602	7.4	18
138	TiS sheet based van der Waals heterostructures with a tunable Schottky barrier. *Nanoscale*, **2018**, 10, 807-815	7.7	18
137	N-doped peanut-shaped carbon nanotubes for efficient CO2 electrocatalytic reduction. *Carbon*, **2019**, 152, 241-246	10.4	17
136	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
135	Strain Effect on Thermoelectric Performance of InSe Monolayer. *Nanoscale Research Letters*, **2019**, 14, 287	5	17
134	Magnetism of two-dimensional triangular nanoflake-based kagome lattices. *New Journal of Physics*, **2012**, 14, 033043	2.9	17

133	First-principles studies on magnetism of Ni clusters coated and alloyed with Pd. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2000**, 267, 394-402	2.3	17
132	Local Magnetism of 3d and 4d Impurities in Ag and Pd Clusters. *Journal De Physique, I*, **1997**, 7, 1233-1244		16
131	Colossal Stability of Gas-Phase Trianions: Super-Pnictogens. *Angewandte Chemie - International Edition*, **2017**, 56, 13421-13425	16.4	15
130	Weak interlayer dependence of lattice thermal conductivity on stacking thickness of penta-graphene. *Applied Physics Letters*, **2017**, 111, 192102	3.4	15
129	Giant magnetocrystalline anisotropy of 5d transition metal-based phthalocyanine sheet. *Physical Chemistry Chemical Physics*, **2015**, 17, 17182-9	3.6	15
128	Anisotropy and Transport Properties of Tubular C-BN Janus Nanostructures. *Journal of Physical Chemistry C*, **2011**, 115, 23978-23983	3.8	15
127	Mg-doped GaN nanostructures: Energetics, magnetism, and H2 adsorption. *Applied Physics Letters*, **2009**, 94, 013108	3.4	15
126	First-principles study of LaB36N36 cage. *Physica B: Condensed Matter*, **2003**, 339, 105-109	2.8	15
125	First-principles study of ferromagnetic coupling in Zn1−xCrxTe thin film. *Journal of Applied Physics*, **2005**, 97, 043904	2.5	15
124	Structures of magic Ba clusters and magic Ba suboxide clusters. *Physical Review A*, **2000**, 62,	2.6	15
123	Lattice Dynamic and Instability in Pentasilicene: A Light Single-Element Ferroelectric Material With High Curie Temperature. *Physical Review Applied*, **2019**, 11,	4.3	14
122	Metastability of a gold nanoring: Density-functional calculations. *Physical Review B*, **2004**, 70,	3.3	14
121	Ultrahigh thermal conductivity of carbon allotropes with correlations with the scaled Pugh ratio. *Journal of Materials Chemistry A*, **2019**, 7, 6259-6266	13	14
120	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
119	Bonding-restricted structure search for novel 2D materials with dispersed C2 dimers. *Scientific Reports*, **2016**, 6, 29531	4.9	13
118	Stability and electronic structure of bilayer graphone. *Applied Physics Letters*, **2011**, 98, 063108	3.4	13
117	Soft breakdown of an insulating nanowire in an electric field. *Nanotechnology*, **2004**, 15, 260-263	3.4	13
116	Interaction of magic gold cluster with Si(_mathsf{60}) cage. *European Physical Journal D*, **2004**, 29, 231-234	1.3	13

115	Design of a heterostructure peapod using magic silicon clusters. *Physical Review B*, **2002**, 66,	3.3	13
114	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
113	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
112	Thermoelectric Properties of Two-Dimensional Gallium Telluride. *Journal of Electronic Materials*, **2019**, 48, 5988-5994	1.9	12
111	Electronic and optical properties of silicon based porous sheets. *Physical Chemistry Chemical Physics* , **2014**, 16, 16832-6	3.6	12
110	First-principles studies on pure and doped C32clusters. *Journal of Physics Condensed Matter*, **2001**, 13, 1931-1938	1.8	12
109	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
108	Transformation of monolayer MoS2 into multiphasic MoTe2: Chalcogen atom-exchange synthesis route. *Nano Research*, **2017**, 10, 2761-2771	10	11
107	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
106	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
105	A simple method for understanding the triangular growth patterns of transition metal dichalcogenide sheets. *AIP Advances*, **2015**, 5, 107105	1.5	11
104	Reaction-induced magnetic transition in Mn2 dimers. *Journal of Physical Chemistry A*, **2011**, 115, 549-55	2.8	11
103	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
102	Two Birds with One Stone: Interfacial Engineering of Multifunctional Janus Separator for Lithium-Sulfur Batteries. *Advanced Materials*, **2021**, e2107638	24	11
101	Experimental observation of TiN cluster and theoretical investigation of its stable and metastable isomers. *Chemical Science*, **2015**, 6, 4723-4729	9.4	10
100	Self-assembly of metal atoms (Na, K, Ca) on graphene. *Nanoscale*, **2015**, 7, 2352-9	7.7	10
99	Structure and interaction mechanism in the magic Al13+H2O cluster. *Physical Review A*, **2001**, 64,	2.6	10
98	Thermal transport properties of penta-graphene with grain boundaries. *Carbon*, **2019**, 145, 445-451	10.4	10

97	Physical Properties and Photovoltaic Application of Semiconducting $PdSe_2$ Monolayer. *Nanomaterials*, **2018**, 8,	5.4	10
96	Contact properties of a vdW heterostructure composed of penta-graphene and penta-BN2 sheets. *Journal of Applied Physics*, **2018**, 124, 165103	2.5	10
95	Large Second Harmonic Generation in Elemental Sb and Bi Monolayers. *Journal of Physical Chemistry C*, **2020**, 124, 5506-5513	3.8	9
94	Thermoelectric properties of two-dimensional hexagonal indium-VA. *Chinese Physics B*, **2018**, 27, 026802	1.2	9
93	Phosphorus K Crystal: A New Stable Allotrope. *Scientific Reports*, **2016**, 6, 37528	4.9	9
92	Ferromagnetic to ferrimagnetic crossover in Cr-doped GaN nanohole arrays. *Physical Review B*, **2007**, 75,	3.3	9
91	Dimer interactions of magic W@Si12 clusters. *Journal of Physics Condensed Matter*, **2002**, 14, 4503-4508	1.8	9
90	High Curie temperature ferromagnetism in penta-MnN2 monolayer. *Applied Surface Science*, **2020**, 505, 144620	6.7	9
89	Ultralow thermal conductivity and negative thermal expansion of CuSCN. *Nano Energy*, **2020**, 73, 104822	17.1	9
88	Classifying superheavy elements by machine learning. *Physical Review A*, **2019**, 99,	2.6	8
87	An asymmetric quasi-solid electrolyte for high-performance Li metal batteries. *Chemical Communications*, **2020**, 56, 7195-7198	5.8	8
86	Prediction of a BeP2 monolayer with a compression-induced Dirac semimetal state. *Physical Review B*, **2018**, 97,	3.3	8
85	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
84	All-metal clusters that mimic the chemistry of halogens. *ChemPhysChem*, **2013**, 14, 3227-32	3.2	8
83	Communication: In search of four-atom chiral metal clusters. *Journal of Chemical Physics*, **2013**, 139, 111101	3.9	8
82	Broadband Reflection in Polymer-Stabilized Cholesteric Liquid Crystals via Thiol–Acrylate Chemistry. *Angewandte Chemie*, **2019**, 131, 6770-6774	3.6	7
81	A metallic peanut-shaped carbon nanotube and its potential for CO2 capture. *Carbon*, **2018**, 132, 249-256	10.4	7
80	Thermal exfoliation of stoichiometric single-layer silica from the stishovite phase: insight from first-principles calculations. *Nanoscale*, **2016**, 8, 10598-606	7.7	7

79	High n-type and p-type thermoelectric performance of two-dimensional SiTe at high temperature.. *RSC Advances*, **2018**, 8, 21280-21287	3.7	7
78	Quasi-freestanding, striped WS2 monolayer with an invariable band gap on Au(001). *Nano Research*, **2017**, 10, 3875-3884	10	7
77	Geometry and energetics of Si60 isomers. *Science and Technology of Advanced Materials*, **2003**, 4, 361-365	7.1	7
76	Potential of porous nodal-line semi-metallic carbon for sodium-ion battery anode. *Journal of Power Sources*, **2020**, 478, 228746	8.9	7
75	A C-based 3D carbon allotrope with high thermal conductivity. *Physical Chemistry Chemical Physics*, **2019**, 22, 306-312	3.6	7
74	Binder-Free TiO2-Coated Polypropylene Separators for Advanced Lithium-Ion Batteries. *Energy Technology*, **2020**, 8, 2000228	3.5	6
73	Large Out-of-Plane Second Harmonic Generation Susceptibility in Penta-ZnS2 Sheet. *Advanced Theory and Simulations*, **2020**, 3, 2000027	3.5	6
72	A C fullerene-based sheet with ultrahigh thermal conductivity. *Nanoscale*, **2018**, 10, 6099-6104	7.7	6
71	Colossal Stability of Gas-Phase Trianions: Super-Pnictogens. *Angewandte Chemie*, **2017**, 129, 13606-13610	3.6	6
70	Magnetism of triangular nanoflakes with different compositions and edge terminations. *Journal of Nanoparticle Research*, **2012**, 14, 1	2.3	6
69	Geometry, Electronic Properties, and Hydrogen Adsorption Properties of Li3N-Based Nanostructures. *Journal of Physical Chemistry C*, **2010**, 114, 19202-19205	3.8	6
68	Can 5d transition-metal monolayers BE magnetic on ferromagnetic substrate?. *Solid State Communications*, **1998**, 106, 665-667	1.6	6
67	Effect of Hydrogen on the Magnetism and Its Solubility in Ferromagnetic Nickel. *Materials Transactions, JIM*, **1999**, 40, 1244-1248		6
66	Interfacial properties of penta-graphene-metal contacts. *Journal of Applied Physics*, **2019**, 125, 065308	2.5	6
65	1,2,4-Azadiphosphole-based piezoelectric penta-CNP sheet with high spontaneous polarization. *Applied Surface Science*, **2021**, 554, 149499	6.7	6
64	Rational Design of Stable Dianions and the Concept of Super-Chalcogens. *Journal of Physical Chemistry A*, **2019**, 123, 5753-5761	2.8	5
63	Magnetic properties of two dimensional silicon carbide triangular nanoflakes-based kagome lattices. *Journal of Nanoparticle Research*, **2012**, 14, 1	2.3	5
62	Adsorption of oxygen-containing functional groups on free and supported graphene using point contact. *Physical Review B*, **2012**, 85,	3.3	5

61	Dependence of Magnetism on Doping Concentration in V-Doped Bulk ZnO. *Materials Transactions*, **2008**, 49, 2469-2473	1.3	5
60	Theoretical Study of Hydrogen Solubility in Fe, Co and Ni. *Materials Transactions, JIM*, **1999**, 40, 855-858		5
59	Toward stable zinc aqueous rechargeable batteries by anode morphology modulation via polyaspartic acid additive. *Energy Storage Materials*, **2022**, 45, 777-785	19.4	5
58	Low lattice thermal conductivity of pentadiamond. *Journal of Applied Physics*, **2021**, 129, 215107	2.5	5
57	Strain and carrier-induced coexistence of topologically insulating and superconducting phase in iodized Si(111) films. *Nano Research*, **2016**, 9, 1578-1589	10	5
56	Research progress on penta-graphene and its related materials: Properties and applications. *Nano Today*, **2022**, 44, 101501	17.9	5
55	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
54	Tuning magnetic properties of Mn(4) cluster with gold coating. *Physical Chemistry Chemical Physics*, **2010**, 12, 1493-6	3.6	4
53	First-principles study on the local magnetism of Fe/Nb multilayers. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1998**, 239, 406-410	2.3	4
52	Interactions of uranium atom with tetraketone complexes. *Chemical Physics Letters*, **2005**, 415, 243-245	2.5	4
51	First-Principles Calculation on Dissociation of Hydrogen Molecule in Nickel. *Materials Transactions, JIM*, **2000**, 41, 1114-1117		4
50	Enhancing power factor of SnSe sheet with grain boundary by doping germanium or silicon. *Npj Computational Materials*, **2020**, 6,	10.9	4
49	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
48	Origins of low lattice thermal conductivity in 2D carbon allotropes. *Journal of Materials Research and Technology*, **2021**, 11, 1982-1990	5.5	4
47	Integrating superconducting phase and topological crystalline quantum spin Hall effect in hafnium intercalated gallium film. *Applied Physics Letters*, **2016**, 108, 253102	3.4	4
46	Screening transition metal-based polar pentagonal monolayers with large piezoelectricity and shift current. *Npj Computational Materials*, **2022**, 8,	10.9	4
45	Structural, electronic and magnetic properties of neutral and anionic Fe2(BO2)n (n=1□) clusters. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 2959-2964	2.3	3
44	Effects of charging and doping on orbital hybridizations and distributions in TiO2 clusters. *Physica B: Condensed Matter*, **2011**, 406, 4322-4326	2.8	3

43	Stabilizing a 22 karat nanogolden cage. *Journal of Chemical Physics*, **2009**, 131, 204501	3.9	3
42	Geometry and Energetics of Nano Gears. *Journal of Computational and Theoretical Nanoscience*, **2010**, 7, 1457-1461	0.3	3
41	The local magnetic properties of sp impurities in alkali metal clusters. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1997**, 228, 297-300	2.3	3
40	The local magnetism of Fe impurity in Nbn and NbnMom clusters. *Journal of Magnetism and Magnetic Materials*, **1998**, 184, 106-110	2.8	3
39	Structures and stability of Al 7 C and Al 7 N clusters. *European Physical Journal D*, **2002**, 18, 77-81	1.3	3
38	First-Principles Study of the Magic Ar6Fe+ Cluster. *Materials Transactions*, **2001**, 42, 2172-2174	1.3	3
37	Quantum size effect and temperature effect on spin-polarized transport in ZnSe/Zn1−xMnxSe multilayers. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2001**, 284, 205-215	2.3	3
36	Capacitance of magic Ba n clusters. *Scripta Materialia*, **2001**, 44, 1959-1962	5.6	3
35	First-principles studies on the adsorptive properties of hydrogenated Si cluster. *Physica B: Condensed Matter*, **1999**, 269, 239-243	2.8	3
34	Atomic Structure of Pd-Intercalated Graphite by High-Resolution Electron Microscopy and First Principles Calculations. *Materials Transactions, JIM*, **1999**, 40, 1213-1218		3
33	Na-functionalized IrTe2 monolayer: Suppressed charge ordering and electric field tuned topological phase transition. *Physical Review B*, **2020**, 102,	3.3	3
32	Hex-C558: A new porous metallic carbon allotrope for lithium-ion battery anode. *Carbon*, **2021**, 183, 652-659	10.4	3
31	Low lattice thermal conductivity of a 5-8-peanut-shaped carbon nanotube. *Physical Chemistry Chemical Physics*, **2021**, 23, 5460-5466	3.6	3
30	Pentagon-based 2D materials: Classification, properties and applications. *Physics Reports*, **2022**, 964, 1-42	27.7	3
29	Doping induced anisotropic growth in C60. *Journal of Chemical Physics*, **2009**, 130, 184714	3.9	2
28	Effect of Magnetic Transition on Hydrogen Solubility in Ni. *Materials Transactions, JIM*, **2000**, 41, 621-623		2
27	Low thermal conductivity of peanut-shaped carbon nanotube and its insensitive response to uniaxial strain. *Nanotechnology*, **2020**, 31, 115701	3.4	2
26	Strain-engineering of bandgaps in pristine and fully hydrogenated hexagonal boron phosphide. *Journal of Applied Physics*, **2020**, 128, 094302	2.5	2

25	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
24	A new 3D metallic carbon allotrope composed of penta-graphene nanoribbons as a high-performance anode material for sodium-ion batteries. *Journal of Materials Chemistry A*,	13	2
23	MXene-Supported, Atomic-Layered Iridium Catalysts Created by Nanoparticle Re-Dispersion for Efficient Alkaline Hydrogen Evolution.. *Small*, **2022**, 18, e2105226	11	2
22	Probing the existence of energetically degenerate cluster isomers by chemical tagging. *Applied Physics Letters*, **2010**, 97, 223104	3.4	1
21	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
20	Nonmetal□metal transition in Ban clusters. *Solid State Communications*, **2001**, 117, 635-639	1.6	1
19	First-Principles Studies on Pd Intercalated Graphite. *Molecular Crystals and Liquid Crystals*, **2000**, 340, 283-288		1
18	Capacitance of Microclusters. *Materials Transactions, JIM*, **1999**, 40, 1224-1227		1
17	Porous Carbon Tubes Constructing Freestanding Flexible Electrodes for Symmetric Potassium-Ion Hybrid Capacitors. *ACS Applied Energy Materials*,	6.1	1
16	□CsCu5Se3: A Promising Thermoelectric Material going beyond Photovoltaic Application. *Advanced Theory and Simulations*, **2020**, 3, 2000169	3.5	1
15	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
14	Identifying key parameters for predicting materials with low defect generation efficiency by machine learning. *Computational Materials Science*, **2021**, 191, 110306	3.2	1
13	Pentagonal BN-based 3D metallic boron nitride with high energy density. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	1
12	Many faces of carbon **2016**,		1
11	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
10	Design of 3D topological nodal-net porous carbon for sodium-ion battery anodes. *Journal of Materials Chemistry A*, **2022**, 10, 7754-7763	13	1
9	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
8	Ground state structure and physical properties of silicon monoxide sheet. *Applied Surface Science*, **2020**, 527, 146759	6.7	0

7	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
6	In-Situ Construction of Ceramic□Polymer All-Solid-State Electrolytes for High-Performance Room-Temperature Lithium Metal Batteries1297-1305		0
5	Titelbild: Colossal Stability of Gas-Phase Trianions: Super-Pnictogens (Angew. Chem. 43/2017). *Angewandte Chemie*, **2017**, 129, 13333-13333	3.6	
4	Effects of cluster□cluster interactions on the structure and magnetic properties in (Fe6)2. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **1998**, 241, 137-140	5.3	
3	Magnetic phase transition and hydrogen solubility in Fe, Co, and Ni. *Journal of Phase Equilibria and Diffusion*, **2001**, 22, 504-507		
2	Deep Traps in LiF: Mg, Ti. *Physica Status Solidi A*, **1994**, 145, K1-K4		
1	On the Metastable States of Low Dimensional Magnetic Systems. *Journal of the Magnetics Society of Japan*, **1999**, 23, 590-592		