

Qiang Sun

List of Publications by Citations

Source: <https://exaly.com/author-pdf/9035160/qiang-sun-publications-by-citations.pdf>

Version: 2024-04-20

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

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

298
papers

13,280
citations

56
h-index

106
g-index

308
ext. papers

14,912
ext. citations

6.3
avg, IF

6.91
L-index

#	Paper	IF	Citations
298	Ferromagnetism in semihydrogenated graphene sheet. <i>Nano Letters</i> , 2009 , 9, 3867-70	11.5	686
297	Clustering of Ti on a C60 surface and its effect on hydrogen storage. <i>Journal of the American Chemical Society</i> , 2005 , 127, 14582-3	16.4	606
296	First-principles study of hydrogen storage on Li12C60. <i>Journal of the American Chemical Society</i> , 2006 , 128, 9741-5	16.4	474
295	Epitaxial monolayer MoS2 on mica with novel photoluminescence. <i>Nano Letters</i> , 2013 , 13, 3870-7	11.5	456
294	Vacancy-induced magnetism in ZnO thin films and nanowires. <i>Physical Review B</i> , 2008 , 77,	3.3	381
293	Structures and Phase Transition of a MoS2 Monolayer. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 1515-1522	3.3	356
292	Magnetism of phthalocyanine-based organometallic single porous sheet. <i>Journal of the American Chemical Society</i> , 2011 , 133, 15113-9	16.4	289
291	Super Atomic Clusters: Design Rules and Potential for Building Blocks of Materials. <i>Chemical Reviews</i> , 2018 , 118, 5755-5870	68.1	265
290	Freestanding film made by necklace-like N-doped hollow carbon with hierarchical pores for high-performance potassium-ion storage. <i>Energy and Environmental Science</i> , 2019 , 12, 1605-1612	35.4	253
289	Electronic and magnetic properties of a BN sheet decorated with hydrogen and fluorine. <i>Physical Review B</i> , 2010 , 81,	3.3	247
288	Heterogeneous catalytic conversion of CO2: a comprehensive theoretical review. <i>Nanoscale</i> , 2015 , 7, 8663-83	7.7	241
287	Recent Advances in Breaking Scaling Relations for Effective Electrochemical Conversion of CO2. <i>Advanced Energy Materials</i> , 2016 , 6, 1600463	21.8	234
286	Amino acid modified copper electrodes for the enhanced selective electroreduction of carbon dioxide towards hydrocarbons. <i>Energy and Environmental Science</i> , 2016 , 9, 1687-1695	35.4	204
285	Exfoliating biocompatible ferromagnetic Cr-trihalide monolayers. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 8777-84	3.6	198
284	Direct observation of key reaction intermediates on gold clusters. <i>Journal of the American Chemical Society</i> , 2003 , 125, 2848-9	16.4	196
283	Electric field enhanced hydrogen storage on polarizable materials substrates. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010 , 107, 2801-6	11.5	194
282	Tuning electronic and magnetic properties of graphene by surface modification. <i>Applied Physics Letters</i> , 2009 , 95, 103108	3.4	185

281	Potential of AlN nanostructures as hydrogen storage materials. <i>ACS Nano</i> , 2009 , 3, 621-6	16.7	183
280	Electronic structures and bonding of graphyne sheet and its BN analog. <i>Journal of Chemical Physics</i> , 2011 , 134, 174701	3.9	163
279	CO ₂ Electroreduction Performance of Transition Metal Dimers Supported on Graphene: A Theoretical Study. <i>ACS Catalysis</i> , 2015 , 5, 6658-6664	13.1	162
278	Lithium Chlorides and Bromides as Promising Solid-State Chemistries for Fast Ion Conductors with Good Electrochemical Stability. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 8039-8043	16.4	151
277	Ferromagnetism in MnX ₂ (X = S, Se) monolayers. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 4990-4	3.6	145
276	The Intrinsic Ferromagnetism in a MnO ₂ Monolayer. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 3382-6.4	6.4	142
275	On-surface formation of one-dimensional polyphenylene through Bergman cyclization. <i>Journal of the American Chemical Society</i> , 2013 , 135, 8448-51	16.4	142
274	Functionalized Graphitic Carbon Nitride for Efficient Energy Storage. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 6055-6059	3.8	131
273	Dehalogenative Homocoupling of Terminal Alkynyl Bromides on Au(111): Incorporation of Acetylenic Scaffolding into Surface Nanostructures. <i>ACS Nano</i> , 2016 , 10, 7023-30	16.7	130
272	Theoretical Study of Hydrogen Storage in Ca-Coated Fullerenes. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 374-9	6.4	115
271	Unravelling orientation distribution and merging behavior of monolayer MoS ₂ domains on sapphire. <i>Nano Letters</i> , 2015 , 15, 198-205	11.5	110
270	Carrier-mediated ferromagnetism in N codoped (Zn,Mn)O (101 $\bar{1}$ 0) thin films. <i>Physical Review B</i> , 2004 , 70,	3.3	109
269	Appearance of bulk properties in small tungsten oxide clusters. <i>Journal of Chemical Physics</i> , 2004 , 121, 9417-22	3.9	105
268	Interactions of Au cluster anions with oxygen. <i>Journal of Chemical Physics</i> , 2004 , 120, 6510-5	3.9	101
267	A Three-Dimensional Carbon Framework Constructed by N/S Co-doped Graphene Nanosheets with Expanded Interlayer Spacing Facilitates Potassium Ion Storage. <i>ACS Energy Letters</i> , 2020 , 5, 1653-1661	20.1	99
266	Storage of molecular hydrogen in B-N cage: energetics and thermal stability. <i>Nano Letters</i> , 2005 , 5, 1273-17.5	17.5	96
265	On-surface aryl-aryl coupling via selective C-H activation. <i>Chemical Communications</i> , 2014 , 50, 11825-8	5.8	95
264	A density functional theory study of the tunable structure, magnetism and metal-insulator phase transition in VS ₂ monolayers induced by in-plane biaxial strain. <i>Nano Research</i> , 2015 , 8, 1348-1356	10	89

263	Ferromagnetism in Mn-doped GaN nanowires. <i>Physical Review Letters</i> , 2005 , 95, 167202	7.4	89
262	All-carbon-based porous topological semimetal for Li-ion battery anode material. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 651-656	11.5	86
261	On-Surface Synthesis of Carbon Nanostructures. <i>Advanced Materials</i> , 2018 , 30, e1705630	24	86
260	Curvature-Dependent Selectivity of CO ₂ Electrocatalytic Reduction on Cobalt Porphyrin Nanotubes. <i>ACS Catalysis</i> , 2016 , 6, 6294-6301	13.1	83
259	Stabilization of Si ₆₀ cage structure. <i>Physical Review Letters</i> , 2003 , 90, 135503	7.4	83
258	Functionalized heterofullerenes for hydrogen storage. <i>Applied Physics Letters</i> , 2009 , 94, 013111	3.4	82
257	Bottom-Up Synthesis of Metalated Carbyne. <i>Journal of the American Chemical Society</i> , 2016 , 138, 1106-916.4	16.4	79
256	Magnetic properties of transition-metal-doped Zn _{1-x} T _x O (T=Cr, Mn, Fe, Co, and Ni) thin films with and without intrinsic defects: A density functional study. <i>Physical Review B</i> , 2009 , 79,	3.3	79
255	Magic behavior and bonding nature in hydrogenated aluminum clusters. <i>Physical Review B</i> , 2001 , 65,	3.3	79
254	Tuning the band gap and magnetic properties of BN sheets impregnated with graphene flakes. <i>Physical Review B</i> , 2011 , 84,	3.3	77
253	Manganese-based magnetic superhalogens. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 2568-726.4	26.4	74
252	A Honeycomb BeN ₂ Sheet with a Desirable Direct Band Gap and High Carrier Mobility. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 2664-70	6.4	72
251	C3B monolayer as an anchoring material for lithium-sulfur batteries. <i>Carbon</i> , 2018 , 129, 38-44	10.4	72
250	Phase stability and Raman vibration of the molybdenum ditelluride (MoTe ₂) monolayer. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 14866-71	3.6	70
249	Energetics and local spin magnetic moment of single 3,4d impurities encapsulated in an icosahedral Au ₁₂ cage. <i>Physical Review B</i> , 2004 , 70,	3.3	68
248	CO ₂ Electroreduction Performance of Phthalocyanine Sheet with Mn Dimer: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 3963-3969	3.8	66
247	On-surface construction of a metal-organic Sierpiński triangle. <i>Chemical Communications</i> , 2015 , 51, 14164-568	568	63
246	First-principles calculations of metal stabilized Si ₂₀ cages. <i>Physical Review B</i> , 2002 , 65,	3.3	62

245	Tuning magnetic properties of graphene nanoribbons with topological line defects: From antiferromagnetic to ferromagnetic. <i>Physical Review B</i> , 2012 , 85,	3.3	59
244	Dehydrogenative homocoupling of terminal alkenes on copper surfaces: a route to dienes. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 4549-52	16.4	58
243	Magnetic coupling between Cr atoms doped at bulk and surface sites of ZnO. <i>Applied Physics Letters</i> , 2005 , 87, 162509	3.4	56
242	Magnetism and energetics of Mn-Doped ZnO (1010) thin films. <i>Physical Review B</i> , 2004 , 69,	3.3	55
241	Antiferromagnetic coupling driven by bond length contraction near the Ga _{1-x} Mn _x N film surface. <i>Physical Review Letters</i> , 2004 , 93, 155501	7.4	54
240	Metal adatoms-decorated silicene as hydrogen storage media. <i>International Journal of Hydrogen Energy</i> , 2014 , 39, 14027-14032	6.7	53
239	Lithium-doped triazine-based graphitic C ₃ N ₄ sheet for hydrogen storage at ambient temperature. <i>Computational Materials Science</i> , 2014 , 81, 275-279	3.2	53
238	Calcium-decorated graphyne nanotubes as promising hydrogen storage media: A first-principles study. <i>Journal of Solid State Chemistry</i> , 2013 , 197, 323-328	3.3	52
237	Local magnetic properties and electronic structures of 3d and 4d impurities in Cu clusters. <i>Physical Review B</i> , 1996 , 54, 10896-10904	3.3	52
236	Production of sustainable methane from renewable energy and captured carbon dioxide with the use of Solid Oxide Electrolyzer: A thermodynamic assessment. <i>Energy</i> , 2015 , 82, 714-721	7.9	49
235	Superhalogen properties of CuF _n clusters. <i>Journal of Chemical Physics</i> , 2009 , 131, 124301	3.9	49
234	Structure of SiAu ₁₆ : can a silicon atom be stabilized in a gold cage?. <i>Journal of Chemical Physics</i> , 2007 , 127, 214706	3.9	49
233	Thermodynamic analysis of combined Solid Oxide Electrolyzer and Fischer-Tropsch processes. <i>Energy</i> , 2015 , 81, 682-690	7.9	48
232	Ferromagnetic GaN-Cr Nanowires. <i>Nano Letters</i> , 2005 , 5, 1587-90	11.5	47
231	Competition between Hydrogen Bonds and Coordination Bonds Steered by the Surface Molecular Coverage. <i>ACS Nano</i> , 2017 , 11, 3727-3732	16.7	46
230	Strain-Induced Spin Crossover in Phthalocyanine-Based Organometallic Sheets. <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 3109-14	6.4	46
229	Influence of dislocations on photoluminescence of InGa _{1-x} GaN multiple quantum wells. <i>Applied Physics Letters</i> , 2005 , 87, 071908	3.4	46
228	Experimental and theoretical studies on inorganic magic clusters: M ₄ X ₆ (M=W, Mo, X=O, S). <i>Chemical Physics Letters</i> , 2004 , 396, 341-345	2.5	46

227	Geometry and electronic structure of magic iron oxide clusters. <i>Physical Review B</i> , 1999 , 59, 12672-12673,	3.3	46
226	Effect of Au coating on the magnetic and structural properties of Fe nanoclusters for use in biomedical applications: A density-functional theory study. <i>Physical Review B</i> , 2006 , 73,	3.3	44
225	Photoelectron spectroscopy and density functional calculations of CuSi(n)- (n = 4-18) clusters. <i>Journal of Chemical Physics</i> , 2012 , 136, 104308	3.9	42
224	Electronic structure and bonding of Au on a SiO ₂ cluster: a nanobullet for tumors. <i>Physical Review Letters</i> , 2004 , 93, 186803	7.4	42
223	The superior catalytic CO oxidation capacity of a Cr-phthalocyanine porous sheet. <i>Scientific Reports</i> , 2014 , 4, 4098	4.9	41
222	On-Surface Formation of Cumulene by Dehalogenative Homocoupling of Alkenyl gem-Dibromides. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 12165-12169	16.4	41
221	Superhalogen-based lithium superionic conductors. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 13373-13381	3.1	40
220	Tetragonal C24: a topological nodal-surface semimetal with potential as an anode material for sodium ion batteries. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 5733-5739	13	40
219	On-surface synthesis and characterization of individual polyacetylene chains. <i>Nature Chemistry</i> , 2019 , 11, 924-930	17.6	39
218	Direct Formation of C-C Triple-Bonded Structural Motifs by On-Surface Dehalogenative Homocouplings of Tribromomethyl-Substituted Arenes. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 4035-4038	16.4	39
217	Carrier induced magnetic coupling transitions in phthalocyanine-based organometallic sheet. <i>Nanoscale</i> , 2014 , 6, 328-33	7.7	39
216	Geometry and electronic structures of magic transition-metal oxide clusters M ₉ O ₆ (M=Fe, Co, and Ni). <i>Physical Review B</i> , 2000 , 62, 8500-8507	3.3	39
215	On-surface formation of two-dimensional polymer via direct C-H activation of metal phthalocyanine. <i>Chemical Communications</i> , 2015 , 51, 2836-9	5.8	38
214	Physical principles for the calculation of equilibrium potential for co-electrolysis of steam and carbon dioxide in a Solid Oxide Electrolyzer Cell (SOEC). <i>Electrochimica Acta</i> , 2014 , 147, 490-497	6.7	38
213	Intrinsic ferromagnetism in two-dimensional carbon structures: Triangular graphene nanoflakes linked by carbon chains. <i>Physical Review B</i> , 2011 , 84,	3.3	38
212	First-principles studies of the geometry and energetics of the Si ₃₆ cluster. <i>Physical Review A</i> , 2003 , 67,	2.6	38
211	Chain growth mechanism on bimetallic surfaces for higher alcohol synthesis from syngas. <i>Catalysis Communications</i> , 2015 , 61, 57-61	3.2	36
210	Performance of power generation extension system based on solid-oxide electrolyzer cells under various design conditions. <i>Energy</i> , 2013 , 55, 647-657	7.9	36

209	Tailoring Li adsorption on graphene. <i>Physical Review B</i> , 2014 , 90,	3.3	36
208	Enhanced Hydrogen Storage on Li Functionalized BC ₃ Nanotube. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 6136-6140	3.8	36
207	Cu atomic chains supported on Borophene sheets for effective CO electroreduction. <i>Nanoscale</i> , 2018 , 10, 11064-11071	7.7	36
206	First-principles study of magnetic properties in V-doped ZnO. <i>Applied Physics Letters</i> , 2007 , 91, 063116	3.4	35
205	Enhanced ferromagnetism in a Mn(3)C(12)N(12)H(12) sheet. <i>ChemPhysChem</i> , 2015 , 16, 614-20	3.2	34
204	Identifying the Ground State Geometry of a MoN ₂ Sheet through a Global Structure Search and Its Tunable p-Electron Half-Metallicity. <i>Chemistry of Materials</i> , 2017 , 29, 8588-8593	9.6	33
203	High-temperature superconductivity in heavily N- or B-doped graphene. <i>Physical Review B</i> , 2015 , 92,	3.3	33
202	Energy and exergy analysis of Solid Oxide Electrolyser Cell (SOEC) working as a CO ₂ mitigation device. <i>International Journal of Hydrogen Energy</i> , 2012 , 37, 14518-14527	6.7	33
201	Ligand induced ferromagnetism in ZnO nanostructures. <i>Journal of Chemical Physics</i> , 2008 , 129, 164714	3.9	33
200	Design of Janus nanoparticles with atomic precision: tungsten-doped gold nanostructures. <i>ACS Nano</i> , 2008 , 2, 341-7	16.7	33
199	Nitrogen-induced magnetic transition in small chromium clusters. <i>Journal of Chemical Physics</i> , 2003 , 119, 7124-7130	3.9	33
198	Ground state of spin-1 Bose-Einstein condensates with spin-orbit coupling in a Zeeman field. <i>Physical Review A</i> , 2012 , 86,	2.6	31
197	How to fabricate a semihydrogenated graphene sheet? A promising strategy explored. <i>Applied Physics Letters</i> , 2012 , 101, 073114	3.4	31
196	Structures of neutral and anionic Au(16) clusters revisited. <i>Journal of Chemical Physics</i> , 2010 , 132, 194306.9	3.9	31
195	Cyclic and linear polymeric structures of Al _n H _{3n} (n=3-7) molecules. <i>Physical Review A</i> , 2003 , 67,	2.6	31
194	Recent advances in hybrid graphene-BN planar structures. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016 , 6, 65-82	7.9	31
193	Clustering of Cr in GaN nanotubes and the onset of ferrimagnetic order. <i>Physical Review B</i> , 2006 , 73,	3.3	29
192	Effect of sequential oxidation on the electronic structure of tungsten clusters. <i>Chemical Physics Letters</i> , 2004 , 387, 29-34	2.5	29

191	Enhanced CO ₂ electroreduction on armchair graphene nanoribbons edge-decorated with copper. <i>Nano Research</i> , 2017 , 10, 1641-1650	10	28
190	A new C=C embedded porphyrin sheet with superior oxygen reduction performance. <i>Nano Research</i> , 2015 , 8, 2901-2912	10	28
189	Sc-phthalocyanine sheet: Promising material for hydrogen storage. <i>Applied Physics Letters</i> , 2011 , 99, 163104	3.4	28
188	Structural and bonding properties of ScSi _n (n = 2 ~ 6) clusters: photoelectron spectroscopy and density functional calculations. <i>Chinese Physics B</i> , 2011 , 20, 043102	1.2	28
187	Real-space representation of electron localization and shell structure in jelliumlike clusters. <i>Physical Review B</i> , 2001 , 63,	3.3	28
186	High-pressure-assisted design of porous topological semimetal carbon for Li-ion battery anode with high-rate performance. <i>Physical Review Materials</i> , 2018 , 2,	3.2	28
185	Recent advances in computational studies of organometallic sheets: Magnetism, adsorption and catalysis. <i>Computational Materials Science</i> , 2016 , 112, 492-502	3.2	27
184	High-temperature electrolysis of synthetic seawater using solid oxide electrolyzer cells. <i>Journal of Power Sources</i> , 2017 , 342, 79-87	8.9	27
183	Pre-combustion CO ₂ capture by transition metal ions embedded in phthalocyanine sheets. <i>Journal of Chemical Physics</i> , 2012 , 136, 234703	3.9	27
182	First-principles investigation of mechanical and electronic properties of MNi ₃ (M=Zn, Mg, or Cd). <i>Journal of Applied Physics</i> , 2009 , 105, 123921	2.5	26
181	Theoretical Study on Gold-Coated Iron Oxide Nanostructure: Magnetism and Bioselectivity for Amino Acids. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 4159-4163	3.8	26
180	Boron-graphdiyne as an anode material for Li, Na, and K ion batteries with high capacities and low diffusion barriers. <i>Journal of Renewable and Sustainable Energy</i> , 2019 , 11, 014106	2.5	25
179	Stability and properties of 2D porous nanosheets based on tetraoxa[8]circulene analogues. <i>Nanoscale</i> , 2014 , 6, 14962-70	7.7	25
178	First-principles study of the magnetic and the electronic properties of Fem/Aun multilayers. <i>Journal of Magnetism and Magnetic Materials</i> , 1998 , 183, 42-48	2.8	25
177	Ferromagnetism in Al _{1-x} Cr _x N thin films by density functional calculations. <i>Physical Review B</i> , 2006 , 73,	3.3	25
176	Topological semimetal porous carbon as a high-performance anode for Li-ion batteries. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 14253-14259	13	24
175	Controllable Scission and Seamless Stitching of Metal-Organic Clusters by STM Manipulation. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 6526-30	16.4	24
174	Li and Ca Co-decorated carbon nitride nanostructures as high-capacity hydrogen storage media. <i>Journal of Applied Physics</i> , 2011 , 110, 094311	2.5	24

173	N-doped ZnO thin films and nanowires: energetics, impurity distribution and magnetism. <i>New Journal of Physics</i> , 2009 , 11, 063035	2.9	24
172	Single-molecule insight into Wurtz reactions on metal surfaces. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 2730-5	3.6	23
171	Solventless Formation of G-Quartet Complexes Based on Alkali and Alkaline Earth Salts on Au(111). <i>ChemPhysChem</i> , 2015 , 16, 2099-105	3.2	23
170	First-principles study of hydrogen adsorption in metal-doped COF-10. <i>Journal of Chemical Physics</i> , 2010 , 133, 154706	3.9	23
169	The stereoselective synthesis of dienes through dehalogenative homocoupling of terminal alkenyl bromides on Cu(110). <i>Chemical Communications</i> , 2016 , 52, 6009-12	5.8	23
168	The acceleration of methanol synthesis and C2 oxygenates formation on copper grain boundary from syngas. <i>Applied Catalysis A: General</i> , 2016 , 509, 97-104	5.1	22
167	Valley-Polarized Quantum Anomalous Hall Effect in Ferrimagnetic Honeycomb Lattices. <i>Physical Review Letters</i> , 2017 , 119, 046403	7.4	22
166	C 20 - T carbon: a novel superhard sp ³ carbon allotrope with large cavities. <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 475402	1.8	22
165	Electric field improved hydrogen storage of Ca-decorated monolayer MoS ₂ . <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2015 , 379, 815-819	2.3	21
164	Hydrogen Storage in Organometallic Structures Grafted on Silsesquioxanes. <i>Chemistry of Materials</i> , 2007 , 19, 3074-3078	9.6	21
163	First-principles studies on the intrinsic stability of the magic Fe ₁₃ O ₈ cluster. <i>Physical Review B</i> , 2000 , 61, 5781-5785	3.3	21
162	Self-consistent determination of Hubbard U for explaining the anomalous magnetism of the Gd ₁₃ cluster. <i>Physical Review B</i> , 2014 , 89,	3.3	20
161	Chemisorption of atomic and molecular oxygen on Au and Ag cluster anions: discrimination of different isomers. <i>Chemical Physics Letters</i> , 2004 , 396, 69-74	2.5	20
160	Theoretical prediction of hydrogen storage on Li decorated planar boron sheets. <i>Applied Surface Science</i> , 2012 , 258, 8874-8879	6.7	19
159	Ab initio study of ferromagnetism in Ga _{1-x} Cr _x N thin films. <i>Physical Review B</i> , 2005 , 72,	3.3	19
158	Real-Space Evidence of Rare Guanine Tautomer Induced by Water. <i>ACS Nano</i> , 2016 , 10, 3776-82	16.7	18
157	Li and Na Co-decorated carbon nitride nanotubes as promising new hydrogen storage media. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012 , 376, 631-636	2.3	18
156	Metal decorated monolayer BC ₂ N for hydrogen storage. <i>Computational Materials Science</i> , 2012 , 60, 181-185	3.85	18

155	Ab initio study of electronic and magnetic properties of the C-codoped Ga _{1-x} MnxN (101 $\bar{0}$) surface. <i>Physical Review B</i> , 2007 , 75,	3.3	18
154	Comment on "Fully coordinated silica nanoclusters: (SiO ₂) _n molecular rings". <i>Physical Review Letters</i> , 2004 , 92, 039601; author reply 039602	7.4	18
153	Porphyrin-based porous sheet: Optoelectronic properties and hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2015 , 40, 3689-3696	6.7	17
152	Photoelectron spectroscopy and theoretical study of M(IO ₃) ₂ (-) (M = H, Li, Na, K): structural evolution, optical isomers, and hyperhalogen behavior. <i>Journal of Chemical Physics</i> , 2013 , 139, 044312	3.9	17
151	Hydrogen storage in AlN cage based nanostructures. <i>Applied Physics Letters</i> , 2009 , 94, 103105	3.4	17
150	Electronic structures of perovskite-type ScRh ₃ Bx (0 $\bar{0}$ 1): X-ray photoelectron and nuclear magnetic resonance spectroscopies and ab initio band calculation. <i>Journal of Alloys and Compounds</i> , 2002 , 339, 317-326	5.7	17
149	First-principles studies on magnetism of Ni clusters coated and alloyed with Pd. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2000 , 267, 394-402	2.3	17
148	Design of tetracene-based metallic 2D carbon materials for Na- and K-Ion batteries. <i>Applied Surface Science</i> , 2020 , 521, 146456	6.7	16
147	Structure and Properties of Egyptian Blue Monolayer Family: XCuSi ₄ O ₁₀ (X = Ca, Sr, and Ba). <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 399-405	6.4	16
146	Direct Formation of C-C Double-Bonded Structural Motifs by On-Surface Dehalogenative Homocoupling of gem-Dibromomethyl Molecules. <i>ACS Nano</i> , 2018 , 12, 7959-7966	16.7	16
145	Using carbon chains to mediate magnetic coupling in zigzag graphene nanoribbons. <i>Applied Physics Letters</i> , 2012 , 100, 173106	3.4	16
144	Local Magnetism of 3d and 4d Impurities in Ag and Pd Clusters. <i>Journal De Physique, I</i> , 1997 , 7, 1233-1244		16
143	Yttrium-Sodium Halides as Promising Solid-State Electrolytes with High Ionic Conductivity and Stability for Na-Ion Batteries. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 3376-3383	6.4	16
142	Giant magnetocrystalline anisotropy of 5d transition metal-based phthalocyanine sheet. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 17182-9	3.6	15
141	Absorption induced modulation of magnetism in two-dimensional metal-phthalocyanine porous sheets. <i>Journal of Chemical Physics</i> , 2013 , 138, 204706	3.9	15
140	Mg-doped GaN nanostructures: Energetics, magnetism, and H ₂ adsorption. <i>Applied Physics Letters</i> , 2009 , 94, 013108	3.4	15
139	First-principles study of ferromagnetic coupling in Zn _{1-x} Cr _x Te thin film. <i>Journal of Applied Physics</i> , 2005 , 97, 043904	2.5	15
138	Structures of magic Ba clusters and magic Ba suboxide clusters. <i>Physical Review A</i> , 2000 , 62,	2.6	15

137	Surface thermal stability of nickel clusters. <i>Physica Status Solidi (B): Basic Research</i> , 1996 , 193, 355-361	1.3	15
136	A new porous metallic silicon dicarbide for highly efficient Li-ion battery anode identified by targeted structure search. <i>Carbon</i> , 2018 , 140, 680-687	10.4	15
135	The selectivity and activity of catalyst for CO hydrogenation to methanol and hydrocarbon: A comparative study on Cu, Co and Ni surfaces. <i>Surface Science</i> , 2016 , 645, 30-40	1.8	14
134	New allotropes of Li ₂ MnO ₃ as cathode materials with better cycling performance predicted in high pressure synthesis. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 16936-16943	13	14
133	On-Surface Formation of Cumulene by Dehalogenative Homocoupling of Alkenyl gem-Dibromides. <i>Angewandte Chemie</i> , 2017 , 129, 12333-12337	3.6	14
132	Metastability of a gold nanoring: Density-functional calculations. <i>Physical Review B</i> , 2004 , 70,	3.3	14
131	Dehydrogenative Homocoupling of Alkyl Chains on Cu(110). <i>Chemistry - A European Journal</i> , 2016 , 22, 1918-1921	4.8	14
130	Gaussian approximation potential for studying the thermal conductivity of silicene. <i>Journal of Applied Physics</i> , 2019 , 126, 105103	2.5	13
129	Graphdiyne-Based Monolayers as Promising Anchoring Materials for Lithium-Sulfur Batteries: A Theoretical Study. <i>Advanced Theory and Simulations</i> , 2020 , 3, 1900236	3.5	13
128	Theoretical prediction of hydrogen storage on Li-decorated boron nitride atomic chains. <i>Journal of Applied Physics</i> , 2013 , 113, 064309	2.5	13
127	Stability and electronic structure of bilayer graphone. <i>Applied Physics Letters</i> , 2011 , 98, 063108	3.4	13
126	Soft breakdown of an insulating nanowire in an electric field. <i>Nanotechnology</i> , 2004 , 15, 260-263	3.4	13
125	Interaction of magic gold cluster with Si ₆₀ cage. <i>European Physical Journal D</i> , 2004 , 29, 231-234	3.4	13
124	Changes in the interface capacitance for fatigued lead-zirconate-titanate capacitors. <i>Applied Physics Letters</i> , 2001 , 78, 2548-2550	3.4	13
123	Design of a heterostructure peapod using magic silicon clusters. <i>Physical Review B</i> , 2002 , 66,	3.3	13
122	Interpenetrating silicene networks: A topological nodal-line semimetal with potential as an anode material for sodium ion batteries. <i>Physical Review Materials</i> , 2018 , 2,	3.2	13
121	The ultralow thermal conductivity and ultrahigh thermoelectric performance of fluorinated Sn ₂ Bi sheet in room temperature. <i>Nano Energy</i> , 2020 , 67, 104283	17.1	13
120	Three-dimensional porous phosphorus-graphdiyne as a universal anode material for both K- and Ca-ion batteries with high performance. <i>Journal of Power Sources</i> , 2020 , 480, 228876	8.9	13

- 119 Dehydrogenative Homocoupling of Terminal Alkenes on Copper Surfaces: A Route to Dienes. *Angewandte Chemie*, **2015**, 127, 4632-4635 3.6 12
- 118 Theoretical consideration of Solid Oxide Electrolyzer Cell with zirconia-based electrolyte operated under extreme polarization or with low supply of feedstock chemicals. *Electrochimica Acta*, **2014**, 130, 718-727 6.7 12
- 117 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
- 116 Edge-State-Enhanced CO₂ Electroreduction on Topological Nodal-Line Semimetal Cu₂Si Nanoribbons. *Journal of Physical Chemistry C*, **2019**, 123, 2837-2842 3.8 12
- 115 Two-Dimensional Fe-Hexaaminobenzene Metal-Organic Frameworks as Promising CO₂ Catalysts with High Activity and Selectivity. *Journal of Physical Chemistry C*, **2019**, 123, 26460-26466 3.8 11
- 114 Surface-assisted cis-trans isomerization of an alkene molecule on Cu(110). *Chemical Communications*, **2014**, 50, 1728-30 5.8 11
- 113 Controllable Scission and Seamless Stitching of Metal-Organic Clusters by STM Manipulation. *Angewandte Chemie*, **2015**, 127, 6626-6630 3.6 11
- 112 Reaction-induced magnetic transition in Mn₂ dimers. *Journal of Physical Chemistry A*, **2011**, 115, 549-55 2.8 11
- 111 The structures and magnetic properties of small clusters. *Journal of Physics Condensed Matter*, **1996**, 8, 1805-1810 1.8 11
- 110 Bipolar Magnetic Materials Based on 2D Ni[TCNE] Metal-Organic Coordination Networks. *Advanced Electronic Materials*, **2018**, 4, 1700323 6.4 10
- 109 High-energy proton emission and Fermi motion in intermediate-energy heavy-ion collisions. *Physical Review C*, **2016**, 94, 2.7 10
- 108 Tuning CO₂ Electroreduction of Cu Atoms on Triphenylene-Cored Graphdiyne. *Journal of Physical Chemistry C*, **2019**, 123, 29776-29782 3.8 10
- 107 Structure and interaction mechanism in the magic Al₁₃+H₂O cluster. *Physical Review A*, **2001**, 64, 2.6 10
- 106 Preferential Formation of Fe₁₃O₈ Clusters in a Reactive Laser Vaporization Cluster Source. *Journal of the Physical Society of Japan*, **1999**, 68, 3497-3499 1.5 10
- 105 New template for Li and Ca decoration and hydrogen adsorption on graphene-like SiC: A first-principles study. *Computational Materials Science*, **2015**, 99, 150-155 3.2 9
- 104 Phthalocyanine-based organometallic nanocages: properties and gas storage. *ChemPhysChem*, **2014**, 15, 126-31 3.2 9
- 103 Ferromagnetic to ferrimagnetic crossover in Cr-doped GaN nanohole arrays. *Physical Review B*, **2007**, 75, 3.3 9
- 102 Dimer interactions of magic W@Si₁₂ clusters. *Journal of Physics Condensed Matter*, **2002**, 14, 4503-4508 1.8 9

101	Tuning the Properties of Tetracene-Based Nanoribbons by Fluorination and N-Doping. <i>ChemPhysChem</i> , 2019 , 20, 2799-2805	3.2	8
100	A BN analog of two-dimensional triphenylene-graphdiyne: stability and properties. <i>Nanoscale</i> , 2019 , 11, 9000-9007	7.7	8
99	Classifying superheavy elements by machine learning. <i>Physical Review A</i> , 2019 , 99,	2.6	8
98	Nickel Adatoms Induced Tautomeric Dehydrogenation of Thymine Molecules on Au(111). <i>ACS Nano</i> , 2018 , 12, 9033-9039	16.7	8
97	Sulfur Tolerant LSCM-based Composite Cathode for High Temperature Electrolysis/Co-electrolysis of H ₂ O and CO ₂ . <i>Fuel Cells</i> , 2017 , 17, 464-472	2.9	8
96	Intrinsic spin dependent and ferromagnetic stability on edge saturated zigzag graphene-like carbon-nitride nanoribbons. <i>Applied Physics Letters</i> , 2014 , 104, 172111	3.4	8
95	Li ₂ O clusters for high-capacity hydrogen storage: A first principles study. <i>Chemical Physics</i> , 2013 , 415, 26-30	2.3	8
94	Controlling on-surface molecular diffusion behaviors by functionalizing the organic molecules with tert-butyl groups. <i>Applied Physics Letters</i> , 2013 , 103, 013103	3.4	8
93	Phase behavior of coherent tunneling through a quantum dot: A consideration of the off-diagonal elastic coupling. <i>European Physical Journal B</i> , 1998 , 5, 913-917	1.2	8
92	A stable metallic 3D porous BPC ₂ as a universal anode material for Li, Na, and K ion batteries with high performance. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 25824-25830	13	8
91	Assembling SiBN nanoribbons into a 3D porous structure as a universal anode material for both Li- and Na-ion batteries with high performance. <i>Nanoscale</i> , 2020 , 12, 19367-19374	7.7	8
90	Cu Atomic Chain Supported on Graphene Nanoribbon for Effective Conversion of CO to Ethanol. <i>ChemPhysChem</i> , 2020 , 21, 1768-1774	3.2	7
89	Direct Formation of C≡C Triple-Bonded Structural Motifs by On-Surface Dehalogenative Homocouplings of Tribromomethyl-Substituted Arenes. <i>Angewandte Chemie</i> , 2018 , 130, 4099-4102	3.6	7
88	Three dimensional metallic porous SiC ₄ allotropes: Stability and battery applications. <i>Nano Energy</i> , 2019 , 63, 103862	17.1	7
87	Anisotropic Mo ₂ -phthalocyanine sheet: a new member of the organometallic family. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 304-7	2.8	7
86	Oxygen-induced self-assembly of quaterphenyl molecules on metal surfaces. <i>Chemical Communications</i> , 2014 , 50, 12112-5	5.8	7
85	Nuclear stopping and light charged particle emission in C ¹² +C ¹² at 95 MeV/nucleon. <i>Physical Review C</i> , 2017 , 95,	2.7	7
84	Manganese-Based Magnetic Superhalogens. <i>Angewandte Chemie</i> , 2011 , 123, 2616-2620	3.6	7

83	First-principles study of quantum size effects in ultrathin Pb-Bi metal alloy films. <i>Physical Review B</i> , 2010 , 81,	3.3	7
82	Geometry and energetics of Si ₆₀ isomers. <i>Science and Technology of Advanced Materials</i> , 2003 , 4, 361-365.	1	7
81	Comparison of electronic structures of ScAl ₃ and ScRh ₃ : X-ray photoelectron spectroscopy and ab initio band calculation. <i>Journal of Alloys and Compounds</i> , 2003 , 358, 264-267	5.7	7
80	Adsorption of O adatoms on hydrogenated Si cluster. <i>Europhysics Letters</i> , 1998 , 43, 47-52	1.6	7
79	Borophene-Based Three-Dimensional Porous Structures as Anode Materials for Alkali Metal-Ion Batteries with Ultrahigh Capacity. <i>Chemistry of Materials</i> , 2021 , 33, 2976-2983	9.6	7
78	Measurement of leakage neutron spectra from graphite cylinders irradiated with D-T neutrons for validation of evaluated nuclear data. <i>Applied Radiation and Isotopes</i> , 2016 , 116, 185-9	1.7	7
77	Highly sensitive tuning of lattice thermal conductivity of graphene-like borophene by fluorination and chlorination. <i>Nano Research</i> , 2020 , 13, 1171-1177	10	7
76	B Cluster-Based 3D Porous Topological Metal as an Anode Material for Both Li- and Na-Ion Batteries with a Superhigh Capacity. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 1548-1553	6.4	7
75	CO oxidation on Ni doped and Ni-M (M = Ca, Sc, V, Cu) bimetal-doped graphene: A first-principles study. <i>Computational Materials Science</i> , 2018 , 151, 189-195	3.2	7
74	Cluster correlation and fragment emission in C ₁₂ +C ₁₂ at 95 MeV/nucleon. <i>Physical Review C</i> , 2018 , 97,	2.7	6
73	A Low Cost Large-Area Solid Oxide Cells Fabrication Technology based on Aqueous Co-Tape Casting and Co-Sintering. <i>Fuel Cells</i> , 2014 , 14, 667-670	2.9	6
72	Magnetic two-dimensional organic topological insulator: Au-1,3,5-triethynylbenzene framework. <i>Journal of Chemical Physics</i> , 2017 , 147, 104704	3.9	6
71	Geometry, Electronic Properties, and Hydrogen Adsorption Properties of Li ₃ N-Based Nanostructures. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 19202-19205	3.8	6
70	Effect of boron non-stoichiometry on B-site in perovskite type structure ScB _x Rh ₃ and CeB _x Rh ₃ on charges of atoms on A-site: study by X-ray photoelectron and nuclear magnetic resonance spectroscopies. <i>Journal of Solid State Chemistry</i> , 2004 , 177, 457-460	3.3	6
69	Effect of Hydrogen on the Magnetism and Its Solubility in Ferromagnetic Nickel. <i>Materials Transactions, JIM</i> , 1999 , 40, 1244-1248		6
68	Structural, Electronic, and Vibrational Properties of a Two-Dimensional Graphdiyne-like Carbon Nanonetwork Synthesized on Au(111): Implications for the Engineering of sp-sp Carbon Nanostructures. <i>ACS Applied Nano Materials</i> , 2020 , 3, 12178-12187	5.6	6
67	Theory-Guided Discovery of Novel Materials. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 6499-6513	6.4	6
66	A high-pressure induced stable phase of Li ₂ MnSiO ₄ as an effective poly-anion cathode material from simulations. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 16406-16413	13	5

65	High inertness of W@Si ₁₂ cluster toward O ₂ molecule. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012 , 376, 1454-1459	2.3	5
64	Theoretical Study of Hydrogen Solubility in Fe, Co and Ni. <i>Materials Transactions, JIM</i> , 1999 , 40, 855-858		5
63	Applying machine learning to accelerate new materials development. <i>Scientia Sinica: Physica, Mechanica Et Astronomica</i> , 2018 , 48, 107001	1.5	5
62	Assembling biphenylene into 3D porous metallic carbon allotrope for promising anode of lithium-ion batteries. <i>Carbon</i> , 2022 , 188, 95-103	10.4	5
61	Strain and carrier-induced coexistence of topologically insulating and superconducting phase in iodized Si(111) films. <i>Nano Research</i> , 2016 , 9, 1578-1589	10	5
60	Three-dimensional pentagonal silicon: Stability and properties. <i>Computational Materials Science</i> , 2018 , 155, 373-377	3.2	5
59	Identifying lithium fluorides for promising solid-state electrolyte and coating material of high-voltage cathode. <i>Materials Today Energy</i> , 2021 , 21, 100719	7	5
58	BeO Nano-cage as a Promising Catalyst for CO Hydrogenation. <i>Scientific Reports</i> , 2017 , 7, 40562	4.9	4
57	Discovery of a high-pressure phase of rutile-like CoO ₂ and its potential as a cathode material. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 18449-18457	13	4
56	Identification of Molecular-Adsorption Geometries and Intermolecular Hydrogen-Bonding Configurations by In Situ STM Manipulation. <i>Angewandte Chemie</i> , 2013 , 125, 7590-7593	3.6	4
55	First-principles study of the effect of vacancies on magnetic properties of Zn _{1-x} Co _x O thin films. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 076002	1.8	4
54	Tuning magnetic properties of Mn(4) cluster with gold coating. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 1493-6	3.6	4
53	First-principles study on the local magnetism of Fe/Nb multilayers. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 1998 , 239, 406-410	2.3	4
52	Interactions of uranium atom with tetraketone complexes. <i>Chemical Physics Letters</i> , 2005 , 415, 243-245	2.5	4
51	First-Principles Calculation on Dissociation of Hydrogen Molecule in Nickel. <i>Materials Transactions, JIM</i> , 2000 , 41, 1114-1117		4
50	Recent advances in 2D thermoelectric materials 2016 ,		4
49	2D carbon sheets with negative Gaussian curvature assembled from pentagonal carbon nanoflakes. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 9123-9129	3.6	3
48	Tripyrrylmethane based 2D porous structure for hydrogen storage. <i>Frontiers of Physics</i> , 2011 , 6, 220-223	3.7	3

47	The local magnetic properties of sp impurities in alkali metal clusters. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 1997 , 228, 297-300	2.3	3
46	The local magnetism of Fe impurity in Nbn and NbnMom clusters. <i>Journal of Magnetism and Magnetic Materials</i> , 1998 , 184, 106-110	2.8	3
45	Capacitance of magic Ba n clusters. <i>Scripta Materialia</i> , 2001 , 44, 1959-1962	5.6	3
44	Three-dimensional porous borocarbonitride BC2N with negative Poissons ratio. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 15771-15777	7.1	3
43	Two-dimensional metallic pentadiamond as anode material for Li-/Na-/K-ion batteries with high performance. <i>Materials Today Energy</i> , 2021 , 20, 100664	7	3
42	A topological semimetal LiCrN sheet as a promising hydrogen storage material. <i>Nanoscale</i> , 2020 , 12, 12106-12113	7.7	2
41	2D CrCl(pyrazine) monolayer: high-temperature ferromagnetism and half-metallicity. <i>Journal of Physics Condensed Matter</i> , 2020 , 32, 135801	1.8	2
40	Metal-free Catalyst B S Sheet for Effective CO Electrochemical Reduction to CH OH. <i>ChemPhysChem</i> , 2020 , 21, 779-784	3.2	2
39	Electronic band structure phase diagram of 3D carbon allotropes from machine learning. <i>Diamond and Related Materials</i> , 2020 , 108, 107990	3.5	2
38	Triphenylene and tetracene based porous sheet: Stability and electronic properties. <i>Computational Materials Science</i> , 2020 , 176, 109529	3.2	2
37	Hydrogen Storage Materials Based on Single-Layer Aluminum Nitride Nanostructures. <i>Chinese Physics Letters</i> , 2011 , 28, 116801	1.8	2
36	Doping induced anisotropic growth in C60. <i>Journal of Chemical Physics</i> , 2009 , 130, 184714	3.9	2
35	Electronic structure of perovskite-type YBRh3: X-ray photoelectron spectroscopy and ab initio band calculations. <i>Journal of Alloys and Compounds</i> , 2003 , 349, 206-210	5.7	2
34	Effect of Magnetic Transition on Hydrogen Solubility in Ni. <i>Materials Transactions, JIM</i> , 2000 , 41, 621-623		2
33	The Stereoselective Formation of trans-Cumulene through Dehalogenative Homocoupling of Alkenyl gem-Dibromides on Cu(110). <i>ChemCatChem</i> , 2019 , 11, 5417-5420	5.2	1
32	Probing the existence of energetically degenerate cluster isomers by chemical tagging. <i>Applied Physics Letters</i> , 2010 , 97, 223104	3.4	1
31	FIRST-PRINCIPLES INVESTIGATION OF STRUCTURAL AND ELECTRONIC PROPERTIES OF THE RECONSTRUCTED ZnO\$(000\bar{1})\$ and \$(0001) (\sqrt{3}\times\sqrt{3})\text{-R}30^{\text{circ}}\$ SURFACES. <i>Modern Physics Letters B</i> , 2010 , 24, 2803-2814	1.6	1
30	Interaction of C(59)Si with Si based clusters: a study of Janus nanostructures. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 275303	1.8	1

29	Nonmetal-metal transition in Boron clusters. <i>Solid State Communications</i> , 2001 , 117, 635-639	1.6	1
28	Capacitance of Microclusters. <i>Materials Transactions, JIM</i> , 1999 , 40, 1224-1227		1
27	Superhalogens [Enormously Strong Electron Acceptors 2021 , 53-84		1
26	Topological Quantum Cathode Materials for Fast Charging Li-Ion Battery Identified by Machine Learning and First Principles Calculation. <i>Advanced Theory and Simulations</i> , 2021 , 4, 2100325	3.5	1
25	3D Porous Metallic Boron Carbide Crystal Structure with Excellent Ductility. <i>Advanced Theory and Simulations</i> , 2021 , 4, 2100325	3.5	1
24	Screening Topological Quantum Materials for Na-Ion Battery Cathode 2022 , 4, 175-180		1
23	Recent advances in topological quantum anode materials for metal-ion batteries. <i>Journal of Power Sources</i> , 2022 , 540, 231655	8.9	1
22	Three-dimensional tetrahexcarbon: Stability and properties. <i>Materials Today Physics</i> , 2022 , 23, 100628	8	0
21	Stronger three-phonon interactions revealed by molecular dynamics in materials with restricted phase space. <i>Journal of Applied Physics</i> , 2021 , 130, 205101	2.5	0
20	Mechanisms of Ionic Diffusion and Stability of the Na ₄ MnCr(PO ₄) ₃ Cathode 2021 , 860-867		0
19	Self-assembled nanostructures of a di-carbonitrile molecule on copper single-crystal surfaces. <i>RSC Advances</i> , 2017 , 7, 1771-1775	3.7	
18	Measurements and analysis of leakage neutron spectra from multiple-slab sample assemblies comprising W,U,C, and CH with D-T neutron irradiation. <i>Applied Radiation and Isotopes</i> , 2018 , 137, 123-128	1.7	
17	Assembling a bi-coordinated Cr complex for ferromagnetic nanorings: insight from first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 17868-74	3.6	
16	Structures and hydrogen adsorption of (MgCN ₂) _n (n=1-4) clusters. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012 , 376, 864-868	2.3	
15	Quantum phase transitions and coherent tunneling in a bilayer of ultracold atoms with dipole interactions. <i>European Physical Journal B</i> , 2012 , 85, 1	1.2	
14	Ultrathin Carbon Nanotubes for Efficient Energy Storage: A First-Principles Study. <i>Chinese Physics Letters</i> , 2014 , 31, 026801	1.8	
13	Atomic-Scale Probing the Priority of Oxidation Sites of an Organic Molecule Adsorbed at the Cu ₂ O/Cu(1 1 0) Interface. <i>ChemCatChem</i> , 2013 , 5, 2662-2666	5.2	
12	ATOMISTIC VIEWS OF DYNAMICAL FRACTURE INSTABILITIES IN SILICON: MOLECULAR DYNAMICS STUDIES. <i>Modern Physics Letters B</i> , 2013 , 27, 1350171	1.6	

- 11 Effects of cluster-cluster interactions on the structure and magnetic properties in $(\text{Fe}_6)_2$. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **1998**, 241, 137-140 5.3
- 10 Magnetic phase transition and hydrogen solubility in Fe, Co, and Ni. *Journal of Phase Equilibria and Diffusion*, **2001**, 22, 504-507
- 9 Atomically Precise Synthesis of Chemically Modified Superatoms **2021**, 141-181
- 8 Rational Design of Superatoms Using Electron-Counting Rules **2021**, 15-51
- 7 Atomically Precise Noble Metals in the Nanoscale, Stabilized by Ligands **2021**, 183-208
- 6 Cluster-based Materials for Energy Harvesting and Storage **2021**, 277-316
- 5 Superatoms as Building Blocks of 2D Materials **2021**, 209-255
- 4 Endohedrally Doped Superatoms and Assemblies **2021**, 85-127
- 3 Clusters for CO₂ Activation and Conversion **2021**, 349-374
- 2 On the Metastable States of Low Dimensional Magnetic Systems. *Journal of the Magnetism Society of Japan*, **1999**, 23, 590-592
- 1 On-surface stereoconvergent synthesis, dimerization and hybridization of organocopper complexes. *Science China Chemistry*, **2019**, 62, 126-132 7.9