

Qiang Sun

List of Publications by Year in Descending Order

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

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	Three-dimensional tetrahexcarbon: Stability and properties. <i>Materials Today Physics</i> , 2022 , 23, 100628	8	0
297	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
296	Screening Topological Quantum Materials for Na-Ion Battery Cathode 2022 , 4, 175-180		1
295	Recent advances in topological quantum anode materials for metal-ion batteries. <i>Journal of Power Sources</i> , 2022 , 540, 231655	8.9	1
294	Atomically Precise Synthesis of Chemically Modified Superatoms 2021 , 141-181		
293	Rational Design of Superatoms Using Electron-Counting Rules 2021 , 15-51		
292	Atomically Precise Noble Metals in the Nanoscale, Stabilized by Ligands 2021 , 183-208		
291	Cluster-based Materials for Energy Harvesting and Storage 2021 , 277-316		
290	Superhalogens [Enormously Strong Electron Acceptors 2021 , 53-84		1
289	Superatoms as Building Blocks of 2D Materials 2021 , 209-255		
288	Endohedrally Doped Superatoms and Assemblies 2021 , 85-127		
287	Clusters for CO ₂ Activation and Conversion 2021 , 349-374		
286	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
285	3D Porous Metallic Boron Carbide Crystal Structure with Excellent Ductility. <i>Advanced Theory and Simulations</i> , 2021 , 4, 2100325	3.5	1
284	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
283	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
282	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

281	Theory-Guided Discovery of Novel Materials. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 6499-6513	6.4	6
280	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
279	A topological semimetal LiCrN sheet as a promising hydrogen storage material. <i>Nanoscale</i> , 2020 , 12, 12106-12113	7.7	2
278	2D CrCl(pyrazine) monolayer: high-temperature ferromagnetism and half-metallicity. <i>Journal of Physics Condensed Matter</i> , 2020 , 32, 135801	1.8	2
277	Metal-free Catalyst B S Sheet for Effective CO Electrochemical Reduction to CH OH. <i>ChemPhysChem</i> , 2020 , 21, 779-784	3.2	2
276	Electronic band structure phase diagram of 3D carbon allotropes from machine learning. <i>Diamond and Related Materials</i> , 2020 , 108, 107990	3.5	2
275	Cu Atomic Chain Supported on Graphene Nanoribbon for Effective Conversion of CO to Ethanol. <i>ChemPhysChem</i> , 2020 , 21, 1768-1774	3.2	7
274	Triphenylene and tetracene based porous sheet: Stability and electronic properties. <i>Computational Materials Science</i> , 2020 , 176, 109529	3.2	2
273	Graphdiyne-Based Monolayers as Promising Anchoring Materials for LithiumSulfur Batteries: A Theoretical Study. <i>Advanced Theory and Simulations</i> , 2020 , 3, 1900236	3.5	13
272	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
271	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
270	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
269	The ultralow thermal conductivity and ultrahigh thermoelectric performance of fluorinated Sn2Bi sheet in room temperature. <i>Nano Energy</i> , 2020 , 67, 104283	17.1	13
268	Three-dimensional porous borocarbonitride BC2N with negative Poissons ratio. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 15771-15777	7.1	3
267	A stable metallic 3D porous BPC2 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
266	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
265	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
264	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

263	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
262	Tuning the Properties of Tetracene-Based Nanoribbons by Fluorination and N-Doping. <i>ChemPhysChem</i> , 2019 , 20, 2799-2805	3.2	8
261	On-surface synthesis and characterization of individual polyacetylene chains. <i>Nature Chemistry</i> , 2019 , 11, 924-930	17.6	39
260	Gaussian approximation potential for studying the thermal conductivity of silicene. <i>Journal of Applied Physics</i> , 2019 , 126, 105103	2.5	13
259	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
258	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
257	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
256	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
255	A BN analog of two-dimensional triphenylene-graphdiyne: stability and properties. <i>Nanoscale</i> , 2019 , 11, 9000-9007	7.7	8
254	Classifying superheavy elements by machine learning. <i>Physical Review A</i> , 2019 , 99,	2.6	8
253	Tetragonal C ₂₄ : 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
252	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
251	Three dimensional metallic porous SiC ₄ allotropes: Stability and battery applications. <i>Nano Energy</i> , 2019 , 63, 103862	17.1	7
250	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
249	Two-Dimensional Fe-Hexaaminobenzene Metal-Organic Frameworks as Promising CO ₂ Catalysts with High Activity and Selectivity. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 26460-26466	3.8	11
248	Tuning CO ₂ Electroreduction of Cu Atoms on Triphenylene-Cored Graphdiyne. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 29776-29782	3.8	10
247	Edge-State-Enhanced CO ₂ Electroreduction on Topological Nodal-Line Semimetal Cu ₂ Si Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 2837-2842	3.8	12
246	On-surface stereoconvergent synthesis, dimerization and hybridization of organocopper complexes. <i>Science China Chemistry</i> , 2019 , 62, 126-132	7.9	

245	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
244	On-Surface Synthesis of Carbon Nanostructures. <i>Advanced Materials</i> , 2018 , 30, e1705630	24	86
243	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
242	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	7
241	Bipolar Magnetic Materials Based on 2D Ni[TCNE] Metal-Organic Coordination Networks. <i>Advanced Electronic Materials</i> , 2018 , 4, 1700323	6.4	10
240	Cluster correlation and fragment emission in C12+C12 at 95 MeV/nucleon. <i>Physical Review C</i> , 2018 , 97,	2.7	6
239	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
238	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
237	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
236	Nickel Adatoms Induced Tautomeric Dehydrogenation of Thymine Molecules on Au(111). <i>ACS Nano</i> , 2018 , 12, 9033-9039	16.7	8
235	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
234	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
233	Applying machine learning to accelerate new materials development. <i>Scientia Sinica: Physica, Mechanica Et Astronomica</i> , 2018 , 48, 107001	1.5	5
232	C3B monolayer as an anchoring material for lithium-sulfur batteries. <i>Carbon</i> , 2018 , 129, 38-44	10.4	72
231	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
230	Three-dimensional pentagonal silicon: Stability and properties. <i>Computational Materials Science</i> , 2018 , 155, 373-377	3.2	5
229	Super Atomic Clusters: Design Rules and Potential for Building Blocks of Materials. <i>Chemical Reviews</i> , 2018 , 118, 5755-5870	68.1	265
228	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

227	Cu atomic chains supported on Eborophene sheets for effective CO electroreduction. <i>Nanoscale</i> , 2018 , 10, 11064-11071	7.7	36
226	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
225	BeO Nano-cage as a Promising Catalyst for CO Hydrogenation. <i>Scientific Reports</i> , 2017 , 7, 40562	4.9	4
224	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
223	Self-assembled nanostructures of a di-carbonitrile molecule on copper single-crystal surfaces. <i>RSC Advances</i> , 2017 , 7, 1771-1775	3.7	
222	Enhanced CO ₂ electroreduction on armchair graphene nanoribbons edge-decorated with copper. <i>Nano Research</i> , 2017 , 10, 1641-1650	10	28
221	Superhalogen-based lithium superionic conductors. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 13373-13381	3.1	40
220	Competition between Hydrogen Bonds and Coordination Bonds Steered by the Surface Molecular Coverage. <i>ACS Nano</i> , 2017 , 11, 3727-3732	16.7	46
219	High-temperature electrolysis of synthetic seawater using solid oxide electrolyzer cells. <i>Journal of Power Sources</i> , 2017 , 342, 79-87	8.9	27
218	Magnetic two-dimensional organic topological insulator: Au-1,3,5-triethynylbenzene framework. <i>Journal of Chemical Physics</i> , 2017 , 147, 104704	3.9	6
217	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
216	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
215	Valley-Polarized Quantum Anomalous Hall Effect in Ferrimagnetic Honeycomb Lattices. <i>Physical Review Letters</i> , 2017 , 119, 046403	7.4	22
214	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
213	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
212	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
211	On-Surface Formation of Cumulene by Dehalogenative Homocoupling of Alkenyl gem-Dibromides. <i>Angewandte Chemie</i> , 2017 , 129, 12333-12337	3.6	14
210	Exfoliating biocompatible ferromagnetic Cr-trihalide monolayers. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 8777-84	3.6	198

209	Recent advances in computational studies of organometallic sheets: Magnetism, adsorption and catalysis. <i>Computational Materials Science</i> , 2016 , 112, 492-502	3.2	27
208	Curvature-Dependent Selectivity of CO ₂ Electrocatalytic Reduction on Cobalt Porphyrin Nanotubes. <i>ACS Catalysis</i> , 2016 , 6, 6294-6301	13.1	83
207	High-energy proton emission and Fermi motion in intermediate-energy heavy-ion collisions. <i>Physical Review C</i> , 2016 , 94,	2.7	10
206	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	
205	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
204	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
203	Recent Advances in Breaking Scaling Relations for Effective Electrochemical Conversion of CO ₂ . <i>Advanced Energy Materials</i> , 2016 , 6, 1600463	21.8	234
202	Bottom-Up Synthesis of Metalated Carbyne. <i>Journal of the American Chemical Society</i> , 2016 , 138, 1106-9	16.4	79
201	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
200	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
199	Single-molecule insight into Wurtz reactions on metal surfaces. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 2730-5	3.6	23
198	Real-Space Evidence of Rare Guanine Tautomer Induced by Water. <i>ACS Nano</i> , 2016 , 10, 3776-82	16.7	18
197	The acceleration of methanol synthesis and C ₂ oxygenates formation on copper grain boundary from syngas. <i>Applied Catalysis A: General</i> , 2016 , 509, 97-104	5.1	22
196	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
195	Dehydrogenative Homocoupling of Alkyl Chains on Cu(110). <i>Chemistry - A European Journal</i> , 2016 , 22, 1918-1921	4.8	14
194	Recent advances in 2D thermoelectric materials 2016 ,		4
193	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
192	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

191	Intrinsic quantum spin Hall and anomalous Hall effects in h-Sb/Bi epitaxial growth on a ferromagnetic MnO ₂ thin film. <i>Nanoscale</i> , 2016 , 8, 11202-9	7.7	12
190	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
189	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
188	Recent advances in hybrid graphene-BN planar structures. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016 , 6, 65-82	7.9	31
187	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
186	On-surface construction of a metal-organic Sierpiński triangle. <i>Chemical Communications</i> , 2015 , 51, 14164-68	5.8	63
185	Heterogeneous catalytic conversion of CO ₂ : a comprehensive theoretical review. <i>Nanoscale</i> , 2015 , 7, 8663-83	7.7	241
184	Thermodynamic analysis of combined Solid Oxide Electrolyzer and Fischer-Tropsch processes. <i>Energy</i> , 2015 , 81, 682-690	7.9	48
183	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
182	A new C=C embedded porphyrin sheet with superior oxygen reduction performance. <i>Nano Research</i> , 2015 , 8, 2901-2912	10	28
181	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
180	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
179	Chain growth mechanism on bimetallic surfaces for higher alcohol synthesis from syngas. <i>Catalysis Communications</i> , 2015 , 61, 57-61	3.2	36
178	Unravelling orientation distribution and merging behavior of monolayer MoS ₂ domains on sapphire. <i>Nano Letters</i> , 2015 , 15, 198-205	11.5	110
177	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
176	High-temperature superconductivity in heavily N- or B-doped graphene. <i>Physical Review B</i> , 2015 , 92,	3.3	33
175	Controllable Scission and Seamless Stitching of Metal-Organic Clusters by STM Manipulation. <i>Angewandte Chemie</i> , 2015 , 127, 6626-6630	3.6	11
174	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

173	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
172	Dehydrogenative Homocoupling of Terminal Alkenes on Copper Surfaces: A Route to Dienes. <i>Angewandte Chemie</i> , 2015 , 127, 4632-4635	3.6	12
171	Giant magnetocrystalline anisotropy of 5d transition metal-based phthalocyanine sheet. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 17182-9	3.6	15
170	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
169	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
168	Porphyrin-based porous sheet: Optoelectronic properties and hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2015 , 40, 3689-3696	6.7	17
167	Enhanced ferromagnetism in a Mn(3)C(12)N(12)H(12) sheet. <i>ChemPhysChem</i> , 2015 , 16, 614-20	3.2	34
166	New template for Li and Ca decoration and hydrogen adsorption on graphene-like SiC: A first-principles study. <i>Computational Materials Science</i> , 2015 , 99, 150-155	3.2	9
165	The superior catalytic CO oxidation capacity of a Cr-phthalocyanine porous sheet. <i>Scientific Reports</i> , 2014 , 4, 4098	4.9	41
164	Carrier induced magnetic coupling transitions in phthalocyanine-based organometallic sheet. <i>Nanoscale</i> , 2014 , 6, 328-33	7.7	39
163	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
162	Surface-assisted cis-trans isomerization of an alkene molecule on Cu(110). <i>Chemical Communications</i> , 2014 , 50, 1728-30	5.8	11
161	Ferromagnetism in MnX ₂ (X = S, Se) monolayers. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 4990-4	3.6	145
160	Structures and Phase Transition of a MoS ₂ Monolayer. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 1515-1522	5.8	356
159	On-surface aryl-aryl coupling via selective C-H activation. <i>Chemical Communications</i> , 2014 , 50, 11825-8	5.8	95
158	Oxygen-induced self-assembly of quaterphenyl molecules on metal surfaces. <i>Chemical Communications</i> , 2014 , 50, 12112-5	5.8	7
157	Metal adatoms-decorated silicene as hydrogen storage media. <i>International Journal of Hydrogen Energy</i> , 2014 , 39, 14027-14032	6.7	53
156	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

155	Stability and properties of 2D porous nanosheets based on tetraoxa[8]circulene analogues. <i>Nanoscale</i> , 2014 , 6, 14962-70	7.7	25
154	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
153	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
152	Tailoring Li adsorption on graphene. <i>Physical Review B</i> , 2014 , 90,	3.3	36
151	Self-consistent determination of Hubbard U for explaining the anomalous magnetism of the Gd13 cluster. <i>Physical Review B</i> , 2014 , 89,	3.3	20
150	Phthalocyanine-based organometallic nanocages: properties and gas storage. <i>ChemPhysChem</i> , 2014 , 15, 126-31	3.2	9
149	Ultrathin Carbon Nanotubes for Efficient Energy Storage: A First-Principles Study. <i>Chinese Physics Letters</i> , 2014 , 31, 026801	1.8	
148	Lithium-doped triazine-based graphitic C3N4 sheet for hydrogen storage at ambient temperature. <i>Computational Materials Science</i> , 2014 , 81, 275-279	3.2	53
147	Theoretical consideration of Solid Oxide Electrolyzer Cell with zirconia-based electrolyte operated under extreme polarization or with low supply of feedstock chemicals. <i>Electrochimica Acta</i> , 2014 , 130, 718-727	6.7	12
146	Epitaxial monolayer MoS2 on mica with novel photoluminescence. <i>Nano Letters</i> , 2013 , 13, 3870-7	11.5	456
145	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
144	The Intrinsic Ferromagnetism in a MnO2 Monolayer. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 3382-6.4	6.4	142
143	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
142	Functionalized Graphitic Carbon Nitride for Efficient Energy Storage. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 6055-6059	3.8	131
141	Li2O clusters for high-capacity hydrogen storage: A first principles study. <i>Chemical Physics</i> , 2013 , 415, 26-30	2.3	8
140	Theoretical prediction of hydrogen storage on Li-decorated boron nitride atomic chains. <i>Journal of Applied Physics</i> , 2013 , 113, 064309	2.5	13
139	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
138	Absorption induced modulation of magnetism in two-dimensional metal-phthalocyanine porous sheets. <i>Journal of Chemical Physics</i> , 2013 , 138, 204706	3.9	15

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