Qiang Sun

List of Publications by Year in descending order

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353 17,282 65 117
papers citations h-index g-index

365 365 365 17110 all docs docs citations times ranked citing authors

#	Article	IF	CITATIONS
1	Clustering of Ti on a C60Surface and Its Effect on Hydrogen Storage. Journal of the American Chemical Society, 2005, 127, 14582-14583.	13.7	675
2	First-Principles Study of Hydrogen Storage on Li12C60. Journal of the American Chemical Society, 2006, 128, 9741-9745.	13.7	533
3	Epitaxial Monolayer MoS ₂ on Mica with Novel Photoluminescence. Nano Letters, 2013, 13, 3870-3877.	9.1	512
4	Super Atomic Clusters: Design Rules and Potential for Building Blocks of Materials. Chemical Reviews, 2018, 118, 5755-5870.	47.7	426
5	Vacancy-induced magnetism in ZnO thin films and nanowires. Physical Review B, 2008, 77, .	3.2	409
6	Magnetism of Phthalocyanine-Based Organometallic Single Porous Sheet. Journal of the American Chemical Society, 2011, 133, 15113-15119.	13.7	350
7	Freestanding film made by necklace-like N-doped hollow carbon with hierarchical pores for high-performance potassium-ion storage. Energy and Environmental Science, 2019, 12, 1605-1612.	30 . 8	349
8	Lithium Chlorides and Bromides as Promising Solidâ€State Chemistries for Fast Ion Conductors with Good Electrochemical Stability. Angewandte Chemie - International Edition, 2019, 58, 8039-8043.	13.8	322
9	Recent Advances in Breaking Scaling Relations for Effective Electrochemical Conversion of CO ₂ . Advanced Energy Materials, 2016, 6, 1600463.	19.5	308
10	Heterogeneous catalytic conversion of CO ₂ : a comprehensive theoretical review. Nanoscale, 2015, 7, 8663-8683.	5.6	306
11	Amino acid modified copper electrodes for the enhanced selective electroreduction of carbon dioxide towards hydrocarbons. Energy and Environmental Science, 2016, 9, 1687-1695.	30.8	290
12	Electronic and magnetic properties of a BN sheet decorated with hydrogen and fluorine. Physical Review B, 2010, 81, .	3.2	278
13	Exfoliating biocompatible ferromagnetic Cr-trihalide monolayers. Physical Chemistry Chemical Physics, 2016, 18, 8777-8784.	2.8	273
14	Solid Oxide Fuel Cell Anode Materials for Direct Hydrocarbon Utilization. Advanced Energy Materials, 2012, 2, 1156-1181.	19.5	253
15	Inoculation treatment of an additively manufactured 2024 aluminium alloy with titanium nanoparticles. Acta Materialia, 2020, 196, 1-16.	7.9	247
16	CO ₂ Electroreduction Performance of Transition Metal Dimers Supported on Graphene: A Theoretical Study. ACS Catalysis, 2015, 5, 6658-6664.	11.2	227
17	Direct Observation of Key Reaction Intermediates on Gold Clusters. Journal of the American Chemical Society, 2003, 125, 2848-2849.	13.7	206
18	A Three-Dimensional Carbon Framework Constructed by N/S Co-doped Graphene Nanosheets with Expanded Interlayer Spacing Facilitates Potassium Ion Storage. ACS Energy Letters, 2020, 5, 1653-1661.	17.4	202

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19	Potential of AlN Nanostructures as Hydrogen Storage Materials. ACS Nano, 2009, 3, 621-626.	14.6	201
20	Tuning electronic and magnetic properties of graphene by surface modification. Applied Physics Letters, 2009, 95, .	3.3	199
21	Ferromagnetism in MnX2 (X = S, Se) monolayers. Physical Chemistry Chemical Physics, 2014, 16, 4990.	2.8	199
22	Strong Phonon–Phonon Interactions Securing Extraordinary Thermoelectric Ge _{1–<i>x</i>} Sb _{<i>x</i>} Te with Zn-Alloying-Induced Band Alignment. Journal of the American Chemical Society, 2019, 141, 1742-1748.	13.7	199
23	Electronic structures and bonding of graphyne sheet and its BN analog. Journal of Chemical Physics, 2011, 134, 174701.	3.0	182
24	Functionalized Graphitic Carbon Nitride for Efficient Energy Storage. Journal of Physical Chemistry C, 2013, 117, 6055-6059.	3.1	171
25	On-Surface Formation of One-Dimensional Polyphenylene through Bergman Cyclization. Journal of the American Chemical Society, 2013, 135, 8448-8451.	13.7	154
26	Dehalogenative Homocoupling of Terminal Alkynyl Bromides on Au(111): Incorporation of Acetylenic Scaffolding into Surface Nanostructures. ACS Nano, 2016, 10, 7023-7030.	14.6	150
27	High Thermoelectric Performance in pâ€type Polycrystalline Cdâ€doped SnSe Achieved by a Combination of Cation Vacancies and Localized Lattice Engineering. Advanced Energy Materials, 2019, 9, 1803242.	19.5	150
28	Rashba Effect Maximizes Thermoelectric Performance of GeTe Derivatives. Joule, 2020, 4, 2030-2043.	24.0	138
29	Ternary MOF-on-MOF heterostructures with controllable architectural and compositional complexity via multiple selective assembly. Nature Communications, 2020, 11, 4971.	12.8	138
30	Unravelling Orientation Distribution and Merging Behavior of Monolayer MoS ₂ Domains on Sapphire. Nano Letters, 2015, 15, 198-205.	9.1	136
31	Free convection in a triangle cavity filled with a porous medium saturated with nanofluids with flush mounted heater on the wall. International Journal of Thermal Sciences, 2011, 50, 2141-2153.	4.9	134
32	Symmetry-breaking induced large piezoelectricity in Janus tellurene materials. Physical Chemistry Chemical Physics, 2019, 21, 1207-1216.	2.8	134
33	Theoretical Study of Hydrogen Storage in Ca-Coated Fullerenes. Journal of Chemical Theory and Computation, 2009, 5, 374-379.	5 . 3	130
34	All-carbon-based porous topological semimetal for Li-ion battery anode material. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 651-656.	7.1	125
35	Onâ€Surface Synthesis of Carbon Nanostructures. Advanced Materials, 2018, 30, e1705630.	21.0	121
36	Exfoliated graphene-supported Pt and Pt-based alloys as electrocatalysts for direct methanol fuel cells. Carbon, 2013, 52, 595-604.	10.3	117

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37	A density functional theory study of the tunable structure, magnetism and metal-insulator phase transition in VS2 monolayers induced by in-plane biaxial strain. Nano Research, 2015, 8, 1348-1356.	10.4	116
38	Curvature-Dependent Selectivity of CO ₂ Electrocatalytic Reduction on Cobalt Porphyrin Nanotubes. ACS Catalysis, 2016, 6, 6294-6301.	11.2	113
39	Interactions of Au cluster anions with oxygen. Journal of Chemical Physics, 2004, 120, 6510-6515.	3.0	107
40	N-Doped Carbon Nanosheet Networks with Favorable Active Sites Triggered by Metal Nanoparticles as Bifunctional Oxygen Electrocatalysts. ACS Energy Letters, 2018, 3, 2914-2920.	17.4	107
41	High-performance in n-type PbTe-based thermoelectric materials achieved by synergistically dynamic doping and energy filtering. Nano Energy, 2022, 91, 106706.	16.0	107
42	Storage of Molecular Hydrogen in Bâ^'N Cage:  Energetics and Thermal Stability. Nano Letters, 2005, 5, 1273-1277.	9.1	106
43	On-surface aryl–aryl coupling via selective C–H activation. Chemical Communications, 2014, 50, 11825-11828.	4.1	106
44	C3B monolayer as an anchoring material for lithium-sulfur batteries. Carbon, 2018, 129, 38-44.	10.3	105
45	Phase stability and Raman vibration of the molybdenum ditelluride (MoTe ₂) monolayer. Physical Chemistry Chemical Physics, 2015, 17, 14866-14871.	2.8	104
46	Bottom-Up Synthesis of Metalated Carbyne. Journal of the American Chemical Society, 2016, 138, 1106-1109.	13.7	104
47	Bi0.5Sb1.5Te3/PEDOT:PSS-based flexible thermoelectric film and device. Chemical Engineering Journal, 2020, 397, 125360.	12.7	104
48	Computer-aided design of high-efficiency GeTe-based thermoelectric devices. Energy and Environmental Science, 2020, 13, 1856-1864.	30.8	103
49	A Honeycomb BeN ₂ Sheet with a Desirable Direct Band Gap and High Carrier Mobility. Journal of Physical Chemistry Letters, 2016, 7, 2664-2670.	4.6	100
50	CO ₂ Electroreduction Performance of Phthalocyanine Sheet with Mn Dimer: A Theoretical Study. Journal of Physical Chemistry C, 2017, 121, 3963-3969.	3.1	95
51	Biomimetic Sn ₄ P ₃ Anchored on Carbon Nanotubes as an Anode for High-Performance Sodium-Ion Batteries. ACS Nano, 2020, 14, 8826-8837.	14.6	95
52	Bi2O2Se nanosheet: An excellent high-temperature n-type thermoelectric material. Applied Physics Letters, 2018, 112, .	3.3	94
53	Functionalized heterofullerenes for hydrogen storage. Applied Physics Letters, 2009, 94, .	3.3	89
54	Site-specific growth of MOF-on-MOF heterostructures with controllable nano-architectures: beyond the combination of MOF analogues. Chemical Science, 2020, 11, 3680-3686.	7.4	89

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55	Electrocatalytic Interlayer with Fast Lithium–Polysulfides Diffusion for Lithium–Sulfur Batteries to Enhance Electrochemical Kinetics under Lean Electrolyte Conditions. Advanced Functional Materials, 2020, 30, 2000742. Magnetic properties of transition-metal-doped <mml:math <="" td="" xmlns:mml="http://www.w3.org/1998/Math/MathML"><td>14.9</td><td>87</td></mml:math>	14.9	87
56	xmins:mml="http://www.w3.org/1998/Math/MathML"		

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73	Formation of polyphenyl chains through hierarchical reactions: Ullmann coupling followed by cross-dehydrogenative coupling. Chemical Communications, 2015, 51, 495-498.	4.1	58
74	Production of sustainable methane from renewable energy and captured carbon dioxide with the use of Solid Oxide Electrolyzer: AÂthermodynamic assessment. Energy, 2015, 82, 714-721.	8.8	58
75	Computation-guided design of high-performance flexible thermoelectric modules for sunlight-to-electricity conversion. Energy and Environmental Science, 2020, 13, 3480-3488.	30.8	57
76	Superhalogen-based lithium superionic conductors. Journal of Materials Chemistry A, 2017, 5, 13373-13381.	10.3	55
77	Strain-Induced Spin Crossover in Phthalocyanine-Based Organometallic Sheets. Journal of Physical Chemistry Letters, 2012, 3, 3109-3114.	4.6	54
78	SiTe monolayers: Si-based analogues of phosphorene. Journal of Materials Chemistry C, 2016, 4, 6353-6361.	5.5	54
79	Structure of SiAu16: Can a silicon atom be stabilized in a gold cage?. Journal of Chemical Physics, 2007, 127, 214706.	3.0	52
80	Photoelectron spectroscopy and density functional calculations of CuSinâ^' (n = 4â€"18) clusters. Journal of Chemical Physics, 2012, 136, 104308.	3.0	52
81	Mixed convection in gravity-driven nano-liquid film containing both nanoparticles and gyrotactic microorganisms. Applied Mathematics and Mechanics (English Edition), 2015, 36, 163-178.	3.6	52
82	Onâ€Surface Formation of Cumulene by Dehalogenative Homocoupling of Alkenyl <i>gem</i> å€Dibromides. Angewandte Chemie - International Edition, 2017, 56, 12165-12169.	13.8	52
83	High Carrier Mobility and High Figure of Merit in the CuBiSe ₂ Alloyed GeTe. Advanced Energy Materials, 2021, 11, 2102913.	19.5	52
84	Hierarchical Structures Advance Thermoelectric Properties of Porous n-type β-Ag ₂ Se. ACS Applied Materials & Distribution (12, 51523-51529).	8.0	51
85	Direct Formation of Câ^C Tripleâ€Bonded Structural Motifs by Onâ€Surface Dehalogenative Homocouplings of Tribromomethylâ€Substituted Arenes. Angewandte Chemie - International Edition, 2018, 57, 4035-4038.	13.8	50
86	Cu atomic chains supported on \hat{l}^2 -borophene sheets for effective CO $<$ sub $>$ 2 $<$ /sub $>$ electroreduction. Nanoscale, 2018, 10, 11064-11071.	5.6	50
87	Physical principles for the calculation of equilibrium potential for co-electrolysis of steam and carbon dioxide in a Solid Oxide Electrolyzer Cell (SOEC). Electrochimica Acta, 2014, 147, 490-497.	5.2	49
88	The superior catalytic CO oxidation capacity of a Cr-phthalocyanine porous sheet. Scientific Reports, 2014, 4, 4098.	3.3	49
89	Rational Electronic and Structural Designs Advance BiCuSeO Thermoelectrics. Advanced Functional Materials, 2021, 31, 2101289.	14.9	48
90	On-surface formation of two-dimensional polymer via direct C–H activation of metal phthalocyanine. Chemical Communications, 2015, 51, 2836-2839.	4.1	46

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91	Optimization of sodium hydroxide for securing high thermoelectric performance in polycrystalline Sn _{1 â^' <i>x</i>} Se via anisotropy and vacancy synergy. InformaÄnÃ-Materiály, 2020, 2, 1201-1215.	17.3	46
92	High-temperature superconductivity in heavily N- or B-doped graphene. Physical Review B, 2015, 92, .	3.2	45
93	High-temperature electrolysis of synthetic seawater using solid oxide electrolyzer cells. Journal of Power Sources, 2017, 342, 79-87.	7.8	45
94	Energy and exergy analysis of Solid Oxide Electrolyser Cell (SOEC) working as a CO2 mitigation device. International Journal of Hydrogen Energy, 2012, 37, 14518-14527.	7.1	44
95	Carrier induced magnetic coupling transitions in phthalocyanine-based organometallic sheet. Nanoscale, 2014, 6, 328-333.	5.6	44
96	Identifying the Ground State Geometry of a MoN ₂ Sheet through a Global Structure Search and Its Tunable p-Electron Half-Metallicity. Chemistry of Materials, 2017, 29, 8588-8593.	6.7	44
97	Performance of power generation extension system based on solid-oxide electrolyzer cells under various design conditions. Energy, 2013, 55, 647-657.	8.8	43
98	Ultralow lattice thermal conductivity induced high thermoelectric performance in the Î'-Cu ₂ S monolayer. Nanoscale, 2019, 11, 10306-10313.	5.6	43
99	Yttrium–Sodium Halides as Promising Solid-State Electrolytes with High Ionic Conductivity and Stability for Na-Ion Batteries. Journal of Physical Chemistry Letters, 2020, 11, 3376-3383.	4.6	43
100	Versatile Vanadium Doping Induces High Thermoelectric Performance in GeTe via Band Alignment and Structural Modulation. Advanced Energy Materials, 2021, 11, 2100544.	19.5	43
101	Non-singular boundary integral methods for fluid mechanics applications. Journal of Fluid Mechanics, 2012, 696, 468-478.	3.4	42
102	Tailoring Li adsorption on graphene. Physical Review B, 2014, 90, .	3.2	42
103	Boron-graphdiyne as an anode material for Li, Na, and K ion batteries with high capacities and low diffusion barriers. Journal of Renewable and Sustainable Energy, $2019,11,1$	2.0	42
104	Optimizing Electronic Quality Factor toward Highâ€Performance Ge _{1â^¹} <i>_××</i> > Ta <i>_×</i> Sb <i>_{> Thermoelectrics: The Role of Transition Metal Doping. Advanced Materials, 2021, 33, e2102575.}</i>	y 2/1500 b> </td <td>i⋊ī́e</td>	i⋊ī́e
105	Intrinsic ferromagnetism in two-dimensional carbon structures: Triangular graphene nanoflakes linked by carbon chains. Physical Review B, 2011, 84, .	3.2	40
106	Ni-induced supramolecular structural transformation of cytosine on Au(111): from one-dimensional chains to zero-dimensional clusters. Chemical Communications, 2014, 50, 3242.	4.1	39
107	Enhanced Ferromagnetism in a Mn ₃ C ₁₂ N ₁₂ H ₁₂ Sheet. ChemPhysChem, 2015, 16, 614-620.	2.1	39
108	First-principles study of magnetic properties in V-doped ZnO. Applied Physics Letters, 2007, 91, 063116.	3.3	38

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109	Enhanced Hydrogen Storage on Li Functionalized BC ₃ Nanotube. Journal of Physical Chemistry C, 2011, 115, 6136-6140.	3.1	38
110	Atomic-Scale Investigation on the Facilitation and Inhibition of Guanine Tautomerization at $Au(111)$ Surface. ACS Nano, 2014, 8, 1804-1808.	14.6	38
111	Design of Janus Nanoparticles with Atomic Precision: Tungsten-Doped Gold Nanostructures. ACS Nano, 2008, 2, 341-347.	14.6	37
112	Chain growth mechanism on bimetallic surfaces for higher alcohol synthesis from syngas. Catalysis Communications, 2015, 61, 57-61.	3.3	37
113	Cyclic and linear polymeric structures ofAlnH3n(n=3–7) molecules. Physical Review A, 2003, 67, .	2.5	36
114	A Universal Length-Dependent Vibrational Mode in Graphene Nanoribbons. ACS Nano, 2019, 13, 13083-13091.	14.6	36
115	Topological semimetal porous carbon as a high-performance anode for Li-ion batteries. Journal of Materials Chemistry A, 2019, 7, 14253-14259.	10.3	36
116	Ligand induced ferromagnetism in ZnO nanostructures. Journal of Chemical Physics, 2008, 129, 164714.	3.0	35
117	Formation of a G-Quartet-Fe Complex and Modulation of Electronic and Magnetic Properties of the Fe Center. ACS Nano, 2014, 8, 11799-11805.	14.6	35
118	A new C=C embedded porphyrin sheet with superior oxygen reduction performance. Nano Research, 2015, 8, 2901-2912.	10.4	35
119	Enhanced CO2 electroreduction on armchair graphene nanoribbons edge-decorated with copper. Nano Research, 2017, 10, 1641-1650.	10.4	35
120	Simultaneously achieving high ZT and mechanical hardness in highly alloyed GeTe with symmetric nanodomains. Chemical Engineering Journal, 2022, 441, 136131.	12.7	35
121	Structural and bonding properties of ScSi $\langle \sup \hat{a}^* \langle \sup \rangle \langle \sup \rangle \langle i \rangle n \langle i \rangle \langle \sup \rangle = 2 \hat{a}^4 6$ clusters: photoelectron spectroscopy and density functional calculations. Chinese Physics B, 2011, 20, 043102.	1.4	34
122	How to fabricate a semihydrogenated graphene sheet? A promising strategy explored. Applied Physics Letters, 2012, 101, 073114.	3.3	34
123	Three-dimensional stagnation flow of a nanofluid containing both nanoparticles and microorganisms on a moving surface with anisotropic slip. Applied Mathematical Modelling, 2016, 40, 4136-4150.	4.2	34
124	A highly efficient porous rod-like Ce-doped ZnO photocatalyst for the degradation of dye contaminants in water. Beilstein Journal of Nanotechnology, 2019, 10, 1157-1165.	2.8	34
125	Structures of neutral and anionic Au16 clusters revisited. Journal of Chemical Physics, 2010, 132, 194306.	3.0	33
126	Reactive molten salt synthesis of natural graphite flakes decorated with SnO2 nanorods as high performance, low cost anode material for lithium ion batteries. Journal of Alloys and Compounds, 2019, 792, 1213-1222.	5.5	33

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127	Sc-phthalocyanine sheet: Promising material for hydrogen storage. Applied Physics Letters, 2011, 99, .	3.3	32
128	Recent advances in hybrid grapheneâ€BN planar structures. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 65-82.	14.6	32
129	High-pressure-assisted design of porous topological semimetal carbon for Li-ion battery anode with high-rate performance. Physical Review Materials, 2018, 2, .	2.4	32
130	Single-molecule insight into Wurtz reactions on metal surfaces. Physical Chemistry Chemical Physics, 2016, 18, 2730-2735.	2.8	31
131	High Thermoelectric Figure of Merit Achieved in Cu ₂ S _{1–<i>x</i>} Te _{<i>x</i>} Alloys Synthesized by Mechanical Alloying and Spark Plasma Sintering. ACS Applied Materials & Interfaces, 2018, 10, 32201-32211.	8.0	31
132	Superstructured Macroporous Carbon Rods Composed of Defective Graphitic Nanosheets for Efficient Oxygen Reduction Reaction. Advanced Science, 2021, 8, e2100120.	11.2	31
133	Pre-combustion CO2 capture by transition metal ions embedded in phthalocyanine sheets. Journal of Chemical Physics, 2012, 136, 234703.	3.0	30
134	Recent advances in computational studies of organometallic sheets: Magnetism, adsorption and catalysis. Computational Materials Science, 2016, 112, 492-502.	3.0	29
135	Two-dimensional flexible thermoelectric devices: Using modeling to deliver optimal capability. Applied Physics Reviews, 2021, 8, .	11.3	29
136	Boundary regularized integral equation formulation of the Helmholtz equation in acoustics. Royal Society Open Science, 2015, 2, 140520.	2.4	28
137	Solventless Formation of Gâ€Quartet Complexes Based on Alkali and Alkaline Earth Salts on Au(111). ChemPhysChem, 2015, 16, 2099-2105.	2.1	28
138	Controllable Scission and Seamless Stitching of Metal–Organic Clusters by STM Manipulation. Angewandte Chemie - International Edition, 2015, 54, 6526-6530.	13.8	28
139	Nonsingular Field-Only Surface Integral Equations for Electromagnetic Scattering. IEEE Transactions on Antennas and Propagation, 2017, 65, 972-977.	5.1	28
140	A cost-effective Fe-rich compositionally complicated alloy with superior high-temperature oxidation resistance. Corrosion Science, 2021, 180, 109190.	6.6	28
141	Mechanical alloying boosted SnTe thermoelectrics. Materials Today Physics, 2021, 17, 100340.	6.0	28
142	Graphite Nanosheets as Multifunctional Nanoinclusions to Boost the Thermoelectric Performance of the Shearâ€Exfoliated Bi ₂ O ₂ Se. Advanced Functional Materials, 2022, 32, .	14.9	28
143	Stability and properties of 2D porous nanosheets based on tetraoxa[8]circulene analogues. Nanoscale, 2014, 6, 14962-14970.	5.6	27
144	Lithium Chlorides and Bromides as Promising Solidâ€State Chemistries for Fast Ion Conductors with Good Electrochemical Stability. Angewandte Chemie, 2019, 131, 8123-8127.	2.0	27

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145	Engineering of three-dimensional nanohybrids: Co9S8 nanocrystal coated hollow carbon nanosphere for advanced lithium storage. Applied Surface Science, 2020, 514, 146092.	6.1	27
146	Simultaneously enhanced strength and plasticity of Ag2Se-based thermoelectric materials endowed by nano-twinned CuAgSe secondary phase. Acta Materialia, 2021, 220, 117335.	7.9	27
147	Atomic-scale structures and interactions between the guanine quartet and potassium. Chemical Communications, 2013, 49, 7210.	4.1	26
148	Self-consistent determination of Hubbard <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math> for explaining the anomalous magnetism of the Gd <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow< td=""><td>3.2</td><td>26</td></mml:mrow<></mml:msub></mml:math>	3.2	26
149	/> <mml:mn>13</mml:mn> cluster. Physical Review B, 2014, 89, . The stereoselective synthesis of dienes through dehalogenative homocoupling of terminal alkenyl bromides on Cu(110). Chemical Communications, 2016, 52, 6009-6012.	4.1	26
150	Edge-State-Enhanced CO ₂ Electroreduction on Topological Nodal-Line Semimetal Cu ₂ Si Nanoribbons. Journal of Physical Chemistry C, 2019, 123, 2837-2842.	3.1	26
151	A novel lapping process for single-crystal sapphire using hybrid nanoparticle suspensions. International Journal of Mechanical Sciences, 2021, 191, 106099.	6.7	26
152	A simple d-band model for the magnetic property of ferromagnetic transition-metal clusters. Physics Letters, Section A: General, Atomic and Solid State Physics, 1995, 205, 308-312.	2.1	25
153	First-principles study of the magnetic and the electronic properties of Fem/Aun multilayers. Journal of Magnetism and Magnetic Materials, 1998, 183, 42-48.	2.3	25
154	N-doped ZnO thin films and nanowires: energetics, impurity distribution and magnetism. New Journal of Physics, 2009, 11, 063035.	2.9	25
155	First-principles study of hydrogen adsorption in metal-doped COF-10. Journal of Chemical Physics, 2010, 133, 154706.	3.0	25
156	A robust and non-singular formulation of the boundary integral method for the potential problem. Engineering Analysis With Boundary Elements, 2014, 43, 117-123.	3.7	25
157	A new porous metallic silicon dicarbide for highly efficient Li-ion battery anode identified by targeted structure search. Carbon, 2018, 140, 680-687.	10.3	25
158	Outstanding thermoelectric properties of solvothermal-synthesized Sn _{1a^3x} In _x Ag _{2x} Te micro-crystals through defect engineering and band tuning. Journal of Materials Chemistry A, 2020, 8, 3978-3987.	10.3	25
159	Assembling Si ₂ BN nanoribbons into a 3D porous structure as a universal anode material for both Li- and Na-ion batteries with high performance. Nanoscale, 2020, 12, 19367-19374.	5.6	25
160	Structure and Properties of Egyptian Blue Monolayer Family: XCuSi ₄ O ₁₀ (X =) Tj ETQ	q0 <u>Q</u> Q rgB	T /9yerlock 10
161	A box model for representing estuarine physical processes in Earth system models. Ocean Modelling, 2017, 112, 139-153.	2.4	24
162	Direct Formation of C–C Double-Bonded Structural Motifs by On-Surface Dehalogenative Homocoupling of <i>gem</i> -Dibromomethyl Molecules. ACS Nano, 2018, 12, 7959-7966.	14.6	24

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163	Scanning tunneling microscopy and Raman spectroscopy of polymeric sp–sp ² carbon atomic wires synthesized on the Au(111) surface. Nanoscale, 2019, 11, 18191-18200.	5.6	24
164	Real-Space Evidence of Rare Guanine Tautomer Induced by Water. ACS Nano, 2016, 10, 3776-3782.	14.6	23
165	The acceleration of methanol synthesis and C2 oxygenates formation on copper grain boundary from syngas. Applied Catalysis A: General, 2016, 509, 97-104.	4.3	23
166	Robust multiscale field-only formulation of electromagnetic scattering. Physical Review B, 2017, 95, .	3.2	23
167	On-surface synthesis of polyazulene with 2,6-connectivity. Chemical Communications, 2019, 55, 13466-13469.	4.1	23
168	Morphology and Texture Engineering Enhancing Thermoelectric Performance of Solvothermal Synthesized Ultralarge SnS Microcrystal. ACS Applied Energy Materials, 2020, 3, 2192-2199.	5.1	23
169	Achieving high-performance n-type PbTe via synergistically optimizing effective mass and carrier concentration and suppressing lattice thermal conductivity. Chemical Engineering Journal, 2022, 428, 132601.	12.7	23
170	Tight-binding study of the structural and magnetic properties of vanadium clusters. Physica B: Condensed Matter, 1995, 215, 377-382.	2.7	22
171	Hydrogen Storage in Organometallic Structures Grafted on Silsesquioxanes. Chemistry of Materials, 2007, 19, 3074-3078.	6.7	22
172	Porphyrin-based porous sheet: Optoelectronic properties and hydrogen storage. International Journal of Hydrogen Energy, 2015, 40, 3689-3696.	7.1	22
173	Single-layer BiOBr: An effective <i>p</i> -type 2D thermoelectric material. Journal of Applied Physics, 2019, 125, .	2.5	22
174	Gaussian approximation potential for studying the thermal conductivity of silicene. Journal of Applied Physics, 2019, 126, .	2.5	21
175	Structural Evolution of Highâ€Performance Mnâ€Alloyed Thermoelectric Materials: A Case Study of SnTe. Small, 2021, 17, e2100525.	10.0	21
176	Thermoelectric performance of p-type (Bi,Sb)2Te3 incorporating amorphous Sb2S3 nanospheres. Chemical Engineering Journal, 2022, 430, 132738.	12.7	21
177	Interpenetrating silicene networks: A topological nodal-line semimetal with potential as an anode material for sodium ion batteries. Physical Review Materials, 2018, 2, .	2.4	21
178	Field-only surface integral equations: scattering from a dielectric body. Journal of the Optical Society of America A: Optics and Image Science, and Vision, 2020, 37, 284.	1.5	21
179	Field-only surface integral equations: scattering from a perfect electric conductor. Journal of the Optical Society of America A: Optics and Image Science, and Vision, 2020, 37, 276.	1.5	21
180	Hydrogen storage in Al–N cage based nanostructures. Applied Physics Letters, 2009, 94, .	3.3	20

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181	Ricocheting Droplets Moving on Superâ€Repellent Surfaces. Advanced Science, 2019, 6, 1901846.	11.2	20
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