

Mingwen Zhao

List of Publications by Year in descending order

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363
papers

13,985
citations

23500

58
h-index

33814

99
g-index

365
all docs

365
docs citations

365
times ranked

13627
citing authors

#	ARTICLE	IF	CITATIONS
1	Broadband Few-Layer MoS ₂ Saturable Absorbers. <i>Advanced Materials</i> , 2014, 26, 3538-3544.	11.1	645
2	From UV to Near-Infrared, WS ₂ Nanosheet: A Novel Photocatalyst for Full Solar Light Spectrum Photodegradation. <i>Advanced Materials</i> , 2015, 27, 363-369.	11.1	494
3	Phagraphene: A Low-Energy Graphene Allotrope Composed of 5-6-7 Carbon Rings with Distorted Dirac Cones. <i>Nano Letters</i> , 2015, 15, 6182-6186.	4.5	482
4	Exfoliation of Hexagonal Boron Nitride by Molten Hydroxides. <i>Advanced Materials</i> , 2013, 25, 2200-2204.	11.1	275
5	Ultrabroadband MoS ₂ Photodetector with Spectral Response from 445 to 2717 nm. <i>Advanced Materials</i> , 2017, 29, 1605972.	11.1	256
6	A Photoresponsive Rutile TiO ₂ Heterojunction with Enhanced Electron-Hole Separation for High-Performance Hydrogen Evolution. <i>Advanced Materials</i> , 2019, 31, e1806596.	11.1	240
7	Strain energy and electronic structures of silicon carbide nanotubes: Density functional calculations. <i>Physical Review B</i> , 2005, 71, .	1.1	239
8	High Mobility and High Storage Capacity of Lithium in sp ² Hybridized Carbon Network: The Case of Graphyne. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8845-8850.	1.5	228
9	Tunable electronic structures of graphene/boron nitride heterobilayers. <i>Applied Physics Letters</i> , 2011, 98, .	1.5	211
10	Strain-driven band inversion and topological aspects in Antimonene. <i>Scientific Reports</i> , 2015, 5, 16108.	1.6	203
11	Germanium sulfide nanosheet: a universal anode material for alkali metal ion batteries. <i>Journal of Materials Chemistry A</i> , 2016, 4, 8905-8912.	5.2	188
12	A niobium and tantalum co-doped perovskite cathode for solid oxide fuel cells operating below 500 °C. <i>Nature Communications</i> , 2017, 8, 13990.	5.8	180
13	Sulfur and nitrogen self-doped carbon nanosheets derived from peanut root nodules as high-efficiency non-metal electrocatalyst for hydrogen evolution reaction. <i>Nano Energy</i> , 2015, 16, 357-366.	8.2	162
14	Spontaneous full photocatalytic water splitting on 2D MoSe ₂ /SnSe ₂ and WSe ₂ /SnSe ₂ vdW heterostructures. <i>Nanoscale</i> , 2019, 11, 14836-14843.	2.8	156
15	Stability and electronic structure of AlN nanotubes. <i>Physical Review B</i> , 2003, 68, .	1.1	148
16	An ab initio study on gas sensing properties of graphene and Si-doped graphene. <i>European Physical Journal B</i> , 2011, 81, 475-479.	0.6	143
17	Isoelectronic Doping of Graphdiyne with Boron and Nitrogen: Stable Configurations and Band Gap Modification. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3934-3939.	1.1	142
18	Two-dimensional carbon topological insulators superior to graphene. <i>Scientific Reports</i> , 2013, 3, 3532.	1.6	140

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19	A Highly Active Perovskite Electrode for the Oxygen Reduction Reaction Below 600°C. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 14036-14040.	7.2	138
20	Tunable Hydrogen Separation in sp^2 Hybridized Carbon Membranes: A First-Principles Prediction. <i>Journal of Physical Chemistry C</i> , 2012, 116, 16634-16638.	1.5	135
21	Anchoring effects of S-terminated Ti ₂ C MXene for lithium-sulfur batteries: A first-principles study. <i>Applied Surface Science</i> , 2018, 455, 522-526.	3.1	134
22	Graphdiyne: A promising anode material for lithium ion batteries with high capacity and rate capability. <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	131
23	High activity and durability of novel perovskite electrocatalysts for water oxidation. <i>Materials Horizons</i> , 2015, 2, 495-501.	6.4	128
24	One-Step Exfoliation and Fluorination of Boron Nitride Nanosheets and a Study of Their Magnetic Properties. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 3645-3649.	7.2	127
25	Promotion of Overall Water Splitting Activity Over a Wide pH Range by Interfacial Electrical Effects of Metallic NiCo-nitrides Nanoparticle/NiCo ₂ O ₄ Nanoflake/graphite Fibers. <i>Advanced Science</i> , 2019, 6, 1801829.	5.6	122
26	Efficient helium separation of graphitic carbon nitride membrane. <i>Carbon</i> , 2015, 95, 51-57.	5.4	115
27	Novel Conductive Metal-Organic Framework for a High-Performance Lithium-Sulfur Battery Host: 2D Cu-Benzenehexathial (BHT). <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 15012-15020.	4.0	105
28	Tunable Magnetism in Carbon-Implanted Highly Oriented Pyrolytic Graphite. <i>Advanced Materials</i> , 2008, 20, 4679-4683.	11.1	103
29	Effective hydrogen storage in single-wall carbon nanotubes. <i>Physical Review B</i> , 2001, 63, .	1.1	101
30	Conductive and Polar Titanium Boride as a Sulfur Host for Advanced Lithium-Sulfur Batteries. <i>Chemistry of Materials</i> , 2018, 30, 6969-6977.	3.2	101
31	Correlation between the vacancy defects and ferromagnetism in graphite. <i>Carbon</i> , 2009, 47, 1399-1406.	5.4	94
32	First-principles calculations for nitrogen-containing single-walled carbon nanotubes. <i>Journal of Applied Physics</i> , 2003, 94, 2398-2402.	1.1	93
33	Giant Topological Nontrivial Band Gaps in Chloridized Gallium Bismuthide. <i>Nano Letters</i> , 2015, 15, 1296-1301.	4.5	92
34	An unprecedented high-temperature-tolerance 2D laminar MXene membrane for ultrafast hydrogen sieving. <i>Journal of Membrane Science</i> , 2019, 569, 117-123.	4.1	87
35	Theoretical Discovery of a Superconducting Two-Dimensional Metal-Organic Framework. <i>Nano Letters</i> , 2017, 17, 6166-6170.	4.5	86
36	Half-metallicity of a kagome spin lattice: the case of a manganese bis-dithiolene monolayer. <i>Nanoscale</i> , 2013, 5, 10404.	2.8	84

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37	Two-dimensional topological insulators with binary honeycomb lattices: Si_3C siligraphene and its analogs. <i>Physical Review B</i> , 2014, 89, .	1.1	83
38	Spin-polarization and ferromagnetism of graphitic carbon nitride materials. <i>Journal of Materials Chemistry C</i> , 2013, 1, 6265.	2.7	82
39	First-principles LDA+U calculations of the Co-doped ZnO magnetic semiconductor. <i>Physical Review B</i> , 2006, 73, .	1.1	81
40	Topological insulator states in a honeycomb lattice of s-triazines. <i>Nanoscale</i> , 2014, 6, 11157-11162.	2.8	79
41	Structures, Energetics, and Electronic Properties of Multifarious Stacking Patterns for High-Buckled and Low-Buckled Silicene on the MoS_2 Substrate. <i>Journal of Physical Chemistry C</i> , 2014, 118, 19129-19138.	1.5	76
42	Tuning of Interlayer Coupling in Large-Area Graphene/ WSe_2 van der Waals Heterostructure via Ion Irradiation: Optical Evidences and Photonic Applications. <i>ACS Photonics</i> , 2017, 4, 1531-1538.	3.2	75
43	Manipulating the electronic structures of silicon carbide nanotubes by selected hydrogenation. <i>Journal of Chemical Physics</i> , 2005, 122, 214707.	1.2	72
44	First-Principles Calculations of AlN Nanowires and Nanotubes: Atomic Structures, Energetics, and Surface States. <i>Journal of Physical Chemistry B</i> , 2006, 110, 8764-8768.	1.2	72
45	Spin-gapless semiconducting graphitic carbon nitrides: A theoretical design from first principles. <i>Carbon</i> , 2015, 84, 1-8.	5.4	72
46	Electron stopping power and mean free path in organic compounds over the energy range of 20 eV–10,000 eV. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2004, 222, 27-43.	0.6	71
47	First-principles study of hydrogenated graphyne and its family: Stable configurations and electronic structures. <i>Diamond and Related Materials</i> , 2012, 29, 42-47.	1.8	71
48	Diffusion and condensation of lithium atoms in single-walled carbon nanotubes. <i>Physical Review B</i> , 2005, 71, .	1.1	70
49	Prediction of a flexible anode material for Li/Na ion batteries: Phosphorous carbide monolayer ($\hat{\pm}$ -PC). <i>Carbon</i> , 2019, 141, 444-450.	5.4	70
50	Chemical Weathering-Exfoliation of Atom-Thick Transition Metal Dichalcogenides and Their Ultrafast Saturable Absorption Properties. <i>Advanced Functional Materials</i> , 2015, 25, 5292-5299.	7.8	69
51	Tunable C ₂ N Membrane for High Efficient Water Desalination. <i>Scientific Reports</i> , 2016, 6, 29218.	1.6	67
52	Bifunctional HER/OER or OER/ORR Catalytic Activity of Two-Dimensional TM ₃ (HITP) ₂ with TM = Fe–Zn. <i>Journal of Physical Chemistry C</i> , 2020, 124, 9350-9359.	1.5	67
53	Diffusion and coalescence of vacancies and interstitials in graphite: A first-principles study. <i>Diamond and Related Materials</i> , 2010, 19, 1240-1244.	1.8	66
54	Ultra-high hydrogen storage capacity of Li-decorated graphyne: A first-principles prediction. <i>Journal of Applied Physics</i> , 2012, 112, .	1.1	64

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55	Strain energy and thermal stability of single-walled aluminum nitride nanotubes from first-principles calculations. <i>Chemical Physics Letters</i> , 2004, 389, 160-164.	1.2	63
56	Prediction of an ultrasoft graphene allotrope with Dirac cones. <i>Carbon</i> , 2016, 105, 323-329.	5.4	62
57	Intrinsic multiferroicity in two-dimensional VOCl ₂ monolayers. <i>Nanoscale</i> , 2019, 11, 1103-1110.	2.8	62
58	Tight-binding model for the electronic structures of SiC and BN nanoribbons. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2010, 43, 440-445.	1.3	59
59	Covalent-adsorption induced magnetism in graphene. <i>Journal of Materials Chemistry</i> , 2009, 19, 9274.	6.7	58
60	Two-dimensional transition metal borides as highly efficient N ₂ fixation catalysts. <i>Applied Surface Science</i> , 2021, 536, 147742.	3.1	58
61	Metal-free highly efficient photocatalysts for overall water splitting: C ₃ N ₅ multilayers. <i>Nanoscale</i> , 2020, 12, 306-315.	2.8	57
62	Theoretical study of hydrogen atom adsorbed on carbon-doped BN nanotubes. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2006, 357, 369-373.	0.9	56
63	First-principles identifications of superstructures of germanene on Ag(111) surface and h-BN substrate. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 16853.	1.3	56
64	Nanophysical Antimicrobial Strategies: A Rational Deployment of Nanomaterials and Physical Stimulations in Combating Bacterial Infections. <i>Advanced Science</i> , 2022, 9, e2105252.	5.6	56
65	Silicon Monoxide Clusters: The Favorable Precursors for Forming Silicon Nanostructures. <i>Physical Review Letters</i> , 2004, 93, 095503.	2.9	55
66	Driving a GaAs film to a large-gap topological insulator by tensile strain. <i>Scientific Reports</i> , 2015, 5, 8441.	1.6	55
67	Theoretical Design of an InSe/GaTe vdW Heterobilayer: A Potential Visible-Light Photocatalyst for Water Splitting. <i>Journal of Physical Chemistry C</i> , 2018, 122, 27803-27810.	1.5	55
68	Design and energetic characterization of ZnO clusters from first-principles calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2007, 372, 39-43.	0.9	54
69	Highly-efficient overall water splitting in 2D Janus group-III chalcogenide multilayers: the roles of intrinsic electric field and vacancy defects. <i>Science Bulletin</i> , 2020, 65, 27-34.	4.3	54
70	In-situ Nano-Crystallization and Solvation Modulation to Promote Highly Stable Anode Involving Alloy/Dealloy for Potassium Ion Batteries. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 15381-15389.	7.2	54
71	SiC coating: An alternative for the protection of nuclear graphite from liquid fluoride salt. <i>Journal of Nuclear Materials</i> , 2014, 448, 1-3.	1.3	53
72	Fluorination-induced magnetism in boron nitride nanotubes from ab initio calculations. <i>Applied Physics Letters</i> , 2008, 92, 102515.	1.5	52

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73	First-principles prediction of the transition from graphdiyne to a superlattice of carbon nanotubes and graphene nanoribbons. Carbon, 2013, 65, 341-348.	5.4	52
74	A comparative study of SrCo _{0.8} Nb _{0.2} O ₃ and SrCo _{0.8} Ta _{0.2} O ₃ as low-temperature solid oxide fuel cell cathodes: effect of non-geometry factors on the oxygen reduction reaction. Journal of Materials Chemistry A, 2015, 3, 24064-24070.	5.2	52
75	Tungsten boride: a 2D multiple Dirac semimetal for the hydrogen evolution reaction. Journal of Materials Chemistry C, 2019, 7, 8868-8873.	2.7	52
76	Moiré superstructures of silicene on hexagonal boron nitride: A first-principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 2628-2632.	0.9	51
77	Negative Poisson's ratio and high-mobility transport anisotropy in SiC ₆ siligraphene. Nanoscale, 2018, 10, 2108-2114.	2.8	51
78	Direct Z-scheme photocatalytic overall water splitting on 2D CdS/InSe heterostructures. Journal Physics D: Applied Physics, 2018, 51, 395501.	1.3	51
79	pH-switchable nanozyme cascade catalysis: a strategy for spatial-temporal modulation of pathological wound microenvironment to rescue stalled healing in diabetic ulcer. Journal of Nanobiotechnology, 2022, 20, 12.	4.2	50
80	Spin-polarized Dirac cones and topological nontriviality in a metal-organic framework Ni ₂ C ₂₄ S ₆ H ₁₂ . Physical Chemistry Chemical Physics, 2016, 18, 8059-8064.	1.3	48
81	Manipulating Electrocatalytic Polysulfide Redox Kinetics by 1D Core-Shell Like Composite for Lithium-Sulfur Batteries. Advanced Energy Materials, 2022, 12, .	10.2	47
82	Distribution patterns and controllable transport of water inside and outside charged single-walled carbon nanotubes. Journal of Chemical Physics, 2005, 122, 084708.	1.2	46
83	Hybrid density functional study of band alignment in ZnO-GaN and ZnO-(Ga _{1-x} Zn _x)N _{1-x} O _x -GaN heterostructures. Physical Chemistry Chemical Physics, 2012, 14, 15693.	1.3	46
84	Dirac node lines in two-dimensional Lieb lattices. Nanoscale, 2017, 9, 8740-8746.	2.8	46
85	Stable Multifunctional Single-Atom Catalysts Resulting from the Synergistic Effect of Anchored Transition-Metal Atoms and Host Covalent-Organic Frameworks. Journal of Physical Chemistry C, 2020, 124, 17675-17683.	1.5	46
86	Exohedral and endohedral adsorption of nitrogen on the sidewall of single-walled carbon nanotubes. Physical Review B, 2002, 66, .	1.1	45
87	Tensile strength of single-walled carbon nanotubes with defects under hydrostatic pressure. Physical Review B, 2002, 65, .	1.1	45
88	Tensile strain induced half-metallicity in graphene-like carbon nitride. Physical Chemistry Chemical Physics, 2015, 17, 6028-6035.	1.3	45
89	Highly Efficient Quantum Sieving in Porous Graphene-like Carbon Nitride for Light Isotopes Separation. Scientific Reports, 2016, 6, 19952.	1.6	45
90	Monolayer Fe ₃ GeX ₂ (X = S, Se, and Te) as Highly Efficient Electrocatalysts for Lithium-Sulfur Batteries. ACS Applied Materials & Interfaces, 2021, 13, 11845-11851.	4.0	45

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91	Ferromagnetic ordering of silicon vacancies in N-doped silicon carbide. Applied Physics Letters, 2010, 96, .	1.5	44
92	Silicene and germanene on InSe substrates: structures and tunable electronic properties. Physical Chemistry Chemical Physics, 2018, 20, 11369-11377.	1.3	44
93	Stable ferromagnetism and half-metallicity in two-dimensional polyporphyrin frameworks. RSC Advances, 2013, 3, 7016.	1.7	43
94	Curvature-induced condensation of lithium confined inside single-walled carbon nanotubes: First-principles calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2005, 340, 434-439.	0.9	42
95	Layered Titanium Oxide Nanosheet and Ultrathin Nanotubes: A First-Principles Prediction. Journal of Physical Chemistry C, 2009, 113, 13610-13615.	1.5	41
96	Metal-free Ternary BCN Nanosheets with Synergetic Effect of Band Gap Engineering and Magnetic Properties. Scientific Reports, 2017, 7, 6617.	1.6	41
97	Magnetic and optical properties of Cu-doped ZnO nanosheet: First-principles calculations. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 53, 101-105.	1.3	40
98	A metallic carbon allotrope with superhardness: a first-principles prediction. Journal of Materials Chemistry C, 2014, 2, 2751-2757.	2.7	40
99	Predicting a graphene-like WB4 nanosheet with a double Dirac cone, an ultra-high Fermi velocity and significant gap opening by spin-orbit coupling. Physical Chemistry Chemical Physics, 2017, 19, 5449-5453.	1.3	40
100	A promising alkali-metal ion battery anode material: 2D metallic phosphorus carbide (β -2O-PC). Electrochimica Acta, 2017, 258, 582-590.	2.6	40
101	Li-III-VI bilayers for efficient photocatalytic overall water splitting: the role of intrinsic electric field. Journal of Materials Chemistry A, 2019, 7, 26123-26130.	5.2	40
102	Strain-Modulated Electronic Structure and Infrared Light Adsorption in Palladium Diselenide Monolayer. Scientific Reports, 2017, 7, 39995.	1.6	39
103	Porous-hollow nanorods constructed from alternate intercalation of carbon and MoS2 monolayers for lithium and sodium storage. Nano Research, 2019, 12, 1912-1920.	5.8	39
104	Highly Efficient Photocatalytic CO ₂ Reduction in Two-Dimensional Ferroelectric CuInP ₂ S ₆ Bilayers. ACS Applied Materials & Interfaces, 2021, 13, 34486-34494.	4.0	39
105	Reversible out-of-plane spin texture in a two-dimensional ferroelectric material for persistent spin helix. Physical Review Materials, 2019, 3, .	0.9	39
106	OnionNet-2: A Convolutional Neural Network Model for Predicting Protein-Ligand Binding Affinity Based on Residue-Atom Contacting Shells. Frontiers in Chemistry, 2021, 9, 753002.	1.8	39
107	Tunable topological states in electron-doped HTT-Pt. Physical Review B, 2016, 93, .	1.1	38
108	Two-dimensional graphyne-like carbon nitrides: Moderate band gaps, high carrier mobility, high flexibility and type-II band alignment. Carbon, 2019, 149, 234-241.	5.4	38

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109	Theoretical Insight into Faceted ZnS Nanowires and Nanotubes from Interatomic Potential and First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3509-3514.	1.5	37
110	Valley-selective circular dichroism and high carrier mobility of graphene-like BC ₆ N. <i>Nanoscale</i> , 2018, 10, 13179-13186.	2.8	37
111	First-principles study of ZnS nanostructures: nanotubes, nanowires and nanosheets. <i>Nanotechnology</i> , 2008, 19, 305708.	1.3	36
112	Chemical Reactivity of Single-Walled Carbon Nanotubes to Amidogen from Density Functional Calculations. <i>Journal of Physical Chemistry B</i> , 2004, 108, 9599-9603.	1.2	35
113	Density-functional theory calculations of XH ₃ -decorated SiC nanotubes (X={C,Si}): Structures, energetics, and electronic structures. <i>Journal of Applied Physics</i> , 2005, 97, 104311.	1.1	35
114	First-principles prediction of a new Dirac-fermion material: silicon germanide monolayer. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 395501.	0.7	35
115	Low-energy transmission electron diffraction and imaging of large-area graphene. <i>Science Advances</i> , 2017, 3, e1603231.	4.7	35
116	Electronic properties of BN/C nanotube heterostructures. <i>Journal of Applied Physics</i> , 2010, 107, .	1.1	34
117	Dirac cones and highly anisotropic electronic structure of super-graphyne. <i>Carbon</i> , 2017, 113, 40-45.	5.4	34
118	Synergistic trifunctional electrocatalysis of pyridinic nitrogen and single transition-metal atoms anchored on pyrazine-modified graphdiyne. <i>Science Bulletin</i> , 2020, 65, 995-1002.	4.3	34
119	Regulating polysulfide intermediates by ultrathin Co-Bi nanosheet electrocatalyst in lithium-sulfur batteries. <i>Nano Today</i> , 2021, 40, 101246.	6.2	34
120	Ultrafine zirconium boride nanoparticles constructed bidirectional catalyst for ultrafast and long-lived lithium-sulfur batteries. <i>Energy Storage Materials</i> , 2022, 45, 130-141.	9.5	34
121	Plasma properties of a laser-ablated aluminum target in air. <i>Laser and Particle Beams</i> , 2003, 21, 97-101.	0.4	33
122	A scheme for the economical use of numerical basis sets in calculations with SIESTA. <i>Theoretical Chemistry Accounts</i> , 2004, 112, 158.	0.5	33
123	Faceted Silicon Nanotubes: Structure, Energetic, and Passivation Effects. <i>Journal of Physical Chemistry C</i> , 2007, 111, 1234-1238.	1.5	32
124	Graphyne-based carbon allotropes with tunable properties: From Dirac fermion to semiconductor. <i>Diamond and Related Materials</i> , 2014, 41, 65-72.	1.8	32
125	High-efficiency helium separation through an inorganic graphenylene membrane: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9789-9795.	1.3	32
126	Stable multifunctional single-atom catalysts adsorbed on pyrazine-modified graphyne. <i>Applied Surface Science</i> , 2021, 553, 149464.	3.1	32

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127	Screening of Transition-Metal Single-Atom Catalysts Anchored on Covalent Organic Frameworks for Efficient Nitrogen Fixation. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 1024-1033.	4.0	32
128	Hydrogen storage capacity in single-walled carbon nanotubes. <i>Physical Review B</i> , 2002, 65, .	1.1	31
129	Proton stopping power in a group of bioorganic compounds over the energy range of 0.05–10 MeV. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2006, 248, 1-6.	0.6	31
130	Hydrogen saturation stabilizes vacancy-induced ferromagnetic ordering in graphene. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13699.	1.3	31
131	Gas Adsorption Effects on the Electronic Properties of Two-Dimensional Nickel Bis(dithiolene) Complex. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3846-3852.	1.5	31
132	Collision of hydrogen atom with single-walled carbon nanotube: Adsorption, insertion, and healing. <i>Journal of Chemical Physics</i> , 2001, 115, 8152-8156.	1.2	30
133	Theoretical study of the OH reaction with cytosine. <i>Computational and Theoretical Chemistry</i> , 2005, 723, 123-129.	1.5	30
134	Tuning the electronic structures of semiconducting SiC nanotubes by N and NH _x (x=1,2) groups. <i>Journal of Chemical Physics</i> , 2006, 125, 194710.	1.2	30
135	Manifold electronic structure transition of BNC biribbons. <i>Journal of Applied Physics</i> , 2011, 110, .	1.1	30
136	Characterization of the effects of 3-MeV proton irradiation on fine-grained isotropic nuclear graphite. <i>Carbon</i> , 2014, 77, 311-318.	5.4	30
137	Large-Scale Synthesis of Few-Layer F-BN Nanocages with Zigzag-Edge Triangular Antidot Defects and Investigation of the Advanced Ferromagnetism. <i>Nano Letters</i> , 2015, 15, 8122-8128.	4.5	30
138	Chern Insulator and Chern Half-Metal States in the Two-Dimensional Spin-Gapless Semiconductor Mn ₂ C ₆ S ₁₂ . <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3770-3775.	2.1	30
139	Robust half-metallicity and topological aspects in two-dimensional Cu-TPyB. <i>Scientific Reports</i> , 2015, 5, 14098.	1.6	29
140	Cu ₃ N and its analogs: a new class of electrodes for lithium ion batteries. <i>Journal of Materials Chemistry A</i> , 2017, 5, 8762-8768.	5.2	29
141	Orientational DNA binding and directed transport on nanomaterial heterojunctions. <i>Nanoscale</i> , 2020, 12, 5217-5226.	2.8	29
142	Cross sections of electron inelastic interactions in DNA. <i>Radiation and Environmental Biophysics</i> , 2004, 43, 173-182.	0.6	28
143	Stable and extendable cage containing nanosize silica clusters based on three-membered rings. <i>Physical Review B</i> , 2004, 69, .	1.1	28
144	Electron stopping power and inelastic mean free path in amino acids and protein over the energy range of 20–20,000 eV. <i>Radiation and Environmental Biophysics</i> , 2006, 45, 135-143.	0.6	28

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145	Energetic Minimum Structures of Imogolite Nanotubes: A First-Principles Prediction. <i>Journal of Physical Chemistry C</i> , 2009, 113, 14834-14837.	1.5	28
146	Can cation vacancy defects induce room temperature ferromagnetism in GaN?. <i>Applied Physics Letters</i> , 2013, 102, 062411.	1.5	28
147	Study of the plasma produced from laser ablation of a KTP crystal. <i>Applied Surface Science</i> , 2003, 207, 227-235.	3.1	27
148	Orientation-Dependent Stability and Quantum-Confinement Effects of Silicon Carbide Nanowires. <i>Journal of Physical Chemistry C</i> , 2009, 113, 12731-12735.	1.5	27
149	A comparative first-principles study of the electronic, mechanical, defect and acoustic properties of Ti ₂ AlC and Ti ₃ AlC. <i>Journal Physics D: Applied Physics</i> , 2014, 47, 215301.	1.3	27
150	Photo-assisted high performance single atom electrocatalysis of the N ₂ reduction reaction by a Mo-embedded covalent organic framework. <i>Journal of Materials Chemistry A</i> , 2021, 9, 19949-19957.	5.2	27
151	Reactions of •OH with thymine studied using density functional theory. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 211-218.	1.0	26
152	Neutral vacancy-defect-induced magnetism in SiC monolayer. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2010, 42, 2451-2454.	1.3	26
153	Protection of nuclear graphite toward liquid fluoride salt by isotropic pyrolytic carbon coating. <i>Journal of Nuclear Materials</i> , 2013, 442, 306-308.	1.3	26
154	Prediction of quantum anomalous Hall effect on graphene nanomesh. <i>RSC Advances</i> , 2015, 5, 9875-9880.	1.7	26
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