Mingwen Zhao

List of Publications by Year
in descending order

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363 papers	13,985 citations	23567 58 h-index	33894 99 g-index
365 all docs	365 docs citations	365 times ranked	13627 citing authors

#	Article	IF	Citations
1	Broadband Fewâ€Layer MoS₂ Saturable Absorbers. Advanced Materials, 2014, 26, 3538-3544.	21.0	645
2	From UV to Nearâ€Infrared, WS₂ Nanosheet: A Novel Photocatalyst for Full Solar Light Spectrum Photodegradation. Advanced Materials, 2015, 27, 363-369.	21.0	494
3	Phagraphene: A Low-Energy Graphene Allotrope Composed of 5â€“6â€“7 Carbon Rings with Distorted Dirac Cones. Nano Letters, 2015, 15, 6182-6186.	9.1	482
4	Exfoliation of Hexagonal Boron Nitride by Molten Hydroxides. Advanced Materials, 2013, 25, 2200-2204.	21.0	275
5	Ultrabroadband MoS₂ Photodetector with Spectral Response from 445 to 2717 nm. Advanced Materials, 2017, 29, 1605972.	21.0	256
6	A Photoresponsive Rutile TiO₂ Heterojunction with Enhanced Electronâ€“Hole Separation for Highâ€Performance Hydrogen Evolution. Advanced Materials, 2019, 31, e1806596.	21.0	240
7	Strain energy and electronic structures of silicon carbide nanotubes: Density functional calculations. Physical Review B, 2005, 71, .	3.2	239
8	High Mobility and High Storage Capacity of Lithium in spâ€“sp² Hybridized Carbon Network: The Case of Graphyne. Journal of Physical Chemistry C, 2011, 115, 8845-8850.	3.1	228
9	Tunable electronic structures of graphene/boron nitride heterobilayers. Applied Physics Letters, 2011, 98, .	3.3	211
10	Strain-driven band inversion and topological aspects in Antimonene. Scientific Reports, 2015, 5, 16108.	3.3	203
11	Germanium sulfide nanosheet: a universal anode material for alkali metal ion batteries. Journal of Materials Chemistry A, 2016, 4, 8905-8912.	10.3	188
12	A niobium and tantalum co-doped perovskite cathode for solid oxide fuel cells operating below 500â€‰Â°C. Nature Communications, 2017, 8, 13990.	12.8	180
13	Sulfur and nitrogen self-doped carbon nanosheets derived from peanut root nodules as high-efficiency non-metal electrocatalyst for hydrogen evolution reaction. Nano Energy, 2015, 16, 357-366.	16.0	162
14	Spontaneous full photocatalytic water splitting on 2D MoSe₂/SnSe₂ and WSe₂/SnSe₂ vdW heterostructures. Nanoscale, 2019, 11, 14836-14843.	5.6	156
15	Stability and electronic structure of AlN nanotubes. Physical Review B, 2003, 68, .	3.2	148
16	An ab initio study on gas sensing properties of graphene and Si-doped graphene. European Physical Journal B, 2011, 81, 475-479.	1.5	143
17	Isoelectronic Doping of Graphdiyne with Boron and Nitrogen: Stable Configurations and Band Gap Modification. Journal of Physical Chemistry A, 2012, 116, 3934-3939.	2.5	142
18	Two-dimensional carbon topological insulators superior to graphene. Scientific Reports, 2013, 3, 3532.	3.3	140

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19	A Highly Active Perovskite Electrode for the Oxygen Reduction Reaction Below 600â€‰Â°C. Angewandte Chemie - International Edition, 2013, 52, 14036-14040.	13.8	138
20	Tunable Hydrogen Separation in spâ€“sp² Hybridized Carbon Membranes: A First-Principles Prediction. Journal of Physical Chemistry C, 2012, 116, 16634-16638.	3.1	135
21	Anchoring effects of S-terminated Ti2C MXene for lithium-sulfur batteries: A first-principles study. Applied Surface Science, 2018, 455, 522-526.	6.1	134
22	Graphdiyne: A promising anode material for lithium ion batteries with high capacity and rate capability. Journal of Applied Physics, 2013, 113, .	2.5	131
23	High activity and durability of novel perovskite electrocatalysts for water oxidation. Materials Horizons, 2015, 2, 495-501.	12.2	128
24	Oneâ€Step Exfoliation and Fluorination of Boron Nitride Nanosheets and a Study of Their Magnetic Properties. Angewandte Chemie - International Edition, 2014, 53, 3645-3649.	13.8	127
25	Promotion of Overall Water Splitting Activity Over a Wide pH Range by Interfacial Electrical Effects of Metallic NiCoâ€nitrides Nanoparticle/NiCo₂O₄ Nanoflake/graphite Fibers. Advanced Science, 2019, 6, 1801829.	11.2	122
26	Efficient helium separation of graphitic carbon nitride membrane. Carbon, 2015, 95, 51-57.	10.3	115
27	Novel Conductive Metalâ€“Organic Framework for a High-Performance Lithiumâ€“Sulfur Battery Host: 2D Cu-Benzenehexathial (BHT). ACS Applied Materials & Interfaces, 2018, 10, 15012-15020.	8.0	105
28	Tunable Magnetism in Carbonâ€Ionâ€Implanted Highly Oriented Pyrolytic Graphite. Advanced Materials, 2008, 20, 4679-4683.	21.0	103
29	Effective hydrogen storage in single-wall carbon nanotubes. Physical Review B, 2001, 63, .	3.2	101
30	Conductive and Polar Titanium Boride as a Sulfur Host for Advanced Lithiumâ€“Sulfur Batteries. Chemistry of Materials, 2018, 30, 6969-6977.	6.7	101
31	Correlation between the vacancy defects and ferromagnetism in graphite. Carbon, 2009, 47, 1399-1406.	10.3	94
32	First-principles calculations for nitrogen-containing single-walled carbon nanotubes. Journal of Applied Physics, 2003, 94, 2398-2402.	2.5	93
33	Giant Topological Nontrivial Band Gaps in Chloridized Gallium Bismuthide. Nano Letters, 2015, 15, 1296-1301.	9.1	92
34	An unprecedented high-temperature-tolerance 2D laminar MXene membrane for ultrafast hydrogen sieving. Journal of Membrane Science, 2019, 569, 117-123.	8.2	87
35	Theoretical Discovery of a Superconducting Two-Dimensional Metalâ€“Organic Framework. Nano Letters, 2017, 17, 6166-6170.	9.1	86
36	Half-metallicity of a kagome spin lattice: the case of a manganese bis-dithiolene monolayer. Nanoscale, 2013, 5, 10404.	5.6	84

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37	Two-dimensional topological insulators with binary honeycomb lattices:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Si</mml:mi><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>siligraphene and its analogs. Physical Review B, 2014, 89, .	3.2	83
38	Spin-polarization and ferromagnetism of graphitic carbon nitride materials. Journal of Materials Chemistry C, 2013, 1, 6265.	5.5	82
39	First-principlesLDA+Ucalculations of the Co-dopedZnOmagnetic semiconductor. Physical Review B, 2006, 73, .	3.2	81
40	Topological insulator states in a honeycomb lattice of s-triazines. Nanoscale, 2014, 6, 11157-11162.	5.6	79
41	Structures, Energetics, and Electronic Properties of Multifarious Stacking Patterns for High-Buckled and Low-Buckled Silicene on the MoS₂ Substrate. Journal of Physical Chemistry C, 2014, 118, 19129-19138.	3.1	76
42	Tuning of Interlayer Coupling in Large-Area Graphene/WSe₂ van der Waals Heterostructure via Ion Irradiation: Optical Evidences and Photonic Applications. ACS Photonics, 2017, 4, 1531-1538.	6.6	75
43	Manipulating the electronic structures of silicon carbide nanotubes by selected hydrogenation. Journal of Chemical Physics, 2005, 122, 214707.	3.0	72
44	First-Principles Calculations of AlN Nanowires and Nanotubes:Â Atomic Structures, Energetics, and Surface States. Journal of Physical Chemistry B, 2006, 110, 8764-8768.	2.6	72
45	Spin-gapless semiconducting graphitic carbon nitrides: A theoretical design from first principles. Carbon, 2015, 84, 1-8.	10.3	72
46	Electron stopping power and mean free path in organic compounds over the energy range of 20â€“10,000 eV. Nuclear Instruments & Methods in Physics Research B, 2004, 222, 27-43.	1.4	71
47	First-principles study of hydrogenated graphyne and its family: Stable configurations and electronic structures. Diamond and Related Materials, 2012, 29, 42-47.	3.9	71
48	Diffusion and condensation of lithium atoms in single-walled carbon nanotubes. Physical Review B, 2005, 71, .	3.2	70
49	Prediction of a flexible anode material for Li/Na ion batteries: Phosphorous carbide monolayer (Î±-PC). Carbon, 2019, 141, 444-450.	10.3	70
50	â€œChemical Weatheringâ€•Exfoliation of Atomâ€Thick Transition Metal Dichalcogenides and Their Ultrafast Saturable Absorption Properties. Advanced Functional Materials, 2015, 25, 5292-5299.	14.9	69
51	Tunable C2N Membrane for High Efficient Water Desalination. Scientific Reports, 2016, 6, 29218.	3.3	67
52	Bifunctional HER/OER or OER/ORR Catalytic Activity of Two-Dimensional TM₃(HITP)₂ with TM = Feâ€“Zn. Journal of Physical Chemistry C, 2020, 124, 9350-9359.	3.1	67
53	Diffusion and coalescence of vacancies and interstitials in graphite: A first-principles study. Diamond and Related Materials, 2010, 19, 1240-1244.	3.9	66
54	Ultra-high hydrogen storage capacity of Li-decorated graphyne: A first-principles prediction. Journal of Applied Physics, 2012, 112, .	2.5	64

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55	Strain energy and thermal stability of single-walled aluminum nitride nanotubes from first-principles calculations. Chemical Physics Letters, 2004, 389, 160-164.	2.6	63
56	Prediction of an ultrasoft graphene allotrope with Dirac cones. Carbon, 2016, 105, 323-329.	10.3	62
57	Intrinsic multiferroicity in two-dimensional VOCl₂ monolayers. Nanoscale, 2019, 11, 1103-1110.	5.6	62
58	Tight-binding model for the electronic structures of SiC and BN nanoribbons. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 43, 440-445.	2.7	59
59	Covalent-adsorption induced magnetism in graphene. Journal of Materials Chemistry, 2009, 19, 9274.	6.7	58
60	Two-dimensional transition metal borides as highly efficient N2 fixation catalysts. Applied Surface Science, 2021, 536, 147742.	6.1	58
61	Metal-free highly efficient photocatalysts for overall water splitting: C₃N₅ multilayers. Nanoscale, 2020, 12, 306-315.	5.6	57
62	Theoretical study of hydrogen atom adsorbed on carbon-doped BN nanotubes. Physics Letters, Section A: General, Atomic and Solid State Physics, 2006, 357, 369-373.	2.1	56
63	First-principles identifications of superstructures of germanene on Ag(111) surface and h-BN substrate. Physical Chemistry Chemical Physics, 2013, 15, 16853.	2.8	56
64	Nanophysical Antimicrobial Strategies: A Rational Deployment of Nanomaterials and Physical Stimulations in Combating Bacterial Infections. Advanced Science, 2022, 9, e2105252.	11.2	56
65	Silicon Monoxide Clusters: The Favorable Precursors for Forming Silicon Nanostructures. Physical Review Letters, 2004, 93, 095503.	7.8	55
66	Driving a GaAs film to a large-gap topological insulator by tensile strain. Scientific Reports, 2015, 5, 8441.	3.3	55
67	Theoretical Design of an InSe/GaTe vdW Heterobilayer: A Potential Visible-Light Photocatalyst for Water Splitting. Journal of Physical Chemistry C, 2018, 122, 27803-27810.	3.1	55
68	Design and energetic characterization of ZnO clusters from first-principles calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2007, 372, 39-43.	2.1	54
69	Highly-efficient overall water splitting in 2D Janus group-III chalcogenide multilayers: the roles of intrinsic electric filed and vacancy defects. Science Bulletin, 2020, 65, 27-34.	9.0	54
70	Inâ€šitu Nanoâ€Crystallization and Solvation Modulation to Promote Highly Stable Anode Involving Alloy/Deâ€šalloy for Potassium Ion Batteries. Angewandte Chemie - International Edition, 2021, 60, 15381-15389.	13.8	54
71	SiC coating: An alternative for the protection of nuclear graphite from liquid fluoride salt. Journal of Nuclear Materials, 2014, 448, 1-3.	2.7	53
72	Fluorination-induced magnetism in boron nitride nanotubes from ab initio calculations. Applied Physics Letters, 2008, 92, 102515.	3.3	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.	10.3	52
74	A comparative study of SrCo_{0.8}Nb_{0.2}O_{3â^'Î´}and SrCo_{0.8}Ta_{0.2}O_{3â^'Î´}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.	10.3	52
75	Tungsten boride: a 2D multiple Dirac semimetal for the hydrogen evolution reaction. Journal of Materials Chemistry C, 2019, 7, 8868-8873.	5.5	52
76	MoirÃ© 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.	2.1	51
77	Negative Poisson's ratio and high-mobility transport anisotropy in SiC₆siligraphene. Nanoscale, 2018, 10, 2108-2114.	5.6	51
78	Direct Z-scheme photocatalytic overall water splitting on 2D CdS/InSe heterostructures. Journal Physics D: Applied Physics, 2018, 51, 395501.	2.8	51
79	pH-switchable nanozyme cascade catalysis: a strategy for spatialâ€“temporal modulation of pathological wound microenvironment to rescue stalled healing in diabetic ulcer. Journal of Nanobiotechnology, 2022, 20, 12.	9.1	50
80	Spin-polarized Dirac cones and topological nontriviality in a metalâ€“organic framework Ni₂C₂₄S₆H₁₂. Physical Chemistry Chemical Physics, 2016, 18, 8059-8064.	2.8	48
81	Manipulating Electrocatalytic Polysulfide Redox Kinetics by 1D Coreâ€“Shell Like Composite for Lithiumâ€“Sulfur Batteries. Advanced Energy Materials, 2022, 12, .	19.5	47
82	Distribution patterns and controllable transport of water inside and outside charged single-walled carbon nanotubes. Journal of Chemical Physics, 2005, 122, 084708.	3.0	46
83	Hybrid density functional study of band alignment in ZnOâ€“GaN and ZnOâ€“(Ga1â^'xZnx)(N1â^'xOx)â€“GaN heterostructures. Physical Chemistry Chemical Physics, 2012, 14, 15693.	2.8	46
84	Dirac node lines in two-dimensional Lieb lattices. Nanoscale, 2017, 9, 8740-8746.	5.6	46
85	Stable Multifunctional Single-Atom Catalysts Resulting from the Synergistic Effect of Anchored Transition-Metal Atoms and Host Covalentâ€“Organic Frameworks. Journal of Physical Chemistry C, 2020, 124, 17675-17683.	3.1	46
86	Exohedral and endohedral adsorption of nitrogen on the sidewall of single-walled carbon nanotubes. Physical Review B, 2002, 66, .	3.2	45
87	Tensile strength of single-walled carbon nanotubes with defects under hydrostatic pressure. Physical Review B, 2002, 65, .	3.2	45
88	Tensile strain induced half-metallicity in graphene-like carbon nitride. Physical Chemistry Chemical Physics, 2015, 17, 6028-6035.	2.8	45
89	Highly Efficient Quantum Sieving in Porous Graphene-like Carbon Nitride for Light Isotopes Separation. Scientific Reports, 2016, 6, 19952.	3.3	45
90	Monolayer Fe₃GeX₂ (X = S, Se, and Te) as Highly Efficient Electrocatalysts for Lithiumâ€“Sulfur Batteries. ACS Applied Materials & Interfaces, 2021, 13, 11845-11851.	8.0	45

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91	Ferromagnetic ordering of silicon vacancies in N-doped silicon carbide. Applied Physics Letters, 2010, 96, .	3.3	44
92	Silicene and germanene on InSe substrates: structures and tunable electronic properties. Physical Chemistry Chemical Physics, 2018, 20, 11369-11377.	2.8	44
93	Stable ferromagnetism and half-metallicity in two-dimensional polyporphyrin frameworks. RSC Advances, 2013, 3, 7016.	3.6	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.	2.1	42
95	Layered Titanium Oxide Nanosheet and Ultrathin Nanotubes: A First-Principles Prediction. Journal of Physical Chemistry C, 2009, 113, 13610-13615.	3.1	41
96	Metal-free Ternary BCN Nanosheets with Synergetic Effect of Band Gap Engineering and Magnetic Properties. Scientific Reports, 2017, 7, 6617.	3.3	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.	2.7	40
98	A metallic carbon allotrope with superhardness: a first-principles prediction. Journal of Materials Chemistry C, 2014, 2, 2751-2757.	5.5	40
99	Predicting a graphene-like WB4 nanosheet with a double Dirac cone, an ultra-high Fermi velocity and significant gap opening by spinâ€“orbit coupling. Physical Chemistry Chemical Physics, 2017, 19, 5449-5453.	2.8	40
100	A promising alkali-metal ion battery anode material: 2D metallic phosphorus carbide (Î²0-PC). Electrochimica Acta, 2017, 258, 582-590.	5.2	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.	10.3	40
102	Strain-Modulated Electronic Structure and Infrared Light Adsorption in Palladium Diselenide Monolayer. Scientific Reports, 2017, 7, 39995.	3.3	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.	10.4	39
104	Highly Efficient Photocatalytic CO₂ Reduction in Two-Dimensional Ferroelectric CuInP₂S₆ Bilayers. ACS Applied Materials & Interfaces, 2021, 13, 34486-34494.	8.0	39
105	Reversible out-of-plane spin texture in a two-dimensional ferroelectric material for persistent spin helix. Physical Review Materials, 2019, 3, .	2.4	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.	3.6	39
107	Tunable topological states in electron-doped HTT-Pt. Physical Review B, 2016, 93, .	3.2	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.	10.3	38

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109	Theoretical Insight into Faceted ZnS Nanowires and Nanotubes from Interatomic Potential and First-Principles Calculations. Journal of Physical Chemistry C, 2008, 112, 3509-3514.	3.1	37
110	Valley-selective circular dichroism and high carrier mobility of graphene-like BC₆N. Nanoscale, 2018, 10, 13179-13186.	5.6	37
111	First-principles study of ZnS nanostructures: nanotubes, nanowires and nanosheets. Nanotechnology, 2008, 19, 305708.	2.6	36
112	Chemical Reactivity of Single-Walled Carbon Nanotubes to Amidogen from Density Functional Calculations. Journal of Physical Chemistry B, 2004, 108, 9599-9603.	2.6	35
113	Density-functional theory calculations of XH3-decorated SiC nanotubes (X={C,Si}): Structures, energetics, and electronic structures. Journal of Applied Physics, 2005, 97, 104311.	2.5	35
114	First-principles prediction of a new Dirac-fermion material: silicon germanide monolayer. Journal of Physics Condensed Matter, 2013, 25, 395501.	1.8	35
115	Low-energy transmission electron diffraction and imaging of large-area graphene. Science Advances, 2017, 3, e1603231.	10.3	35
116	Electronic properties of BN/C nanotube heterostructures. Journal of Applied Physics, 2010, 107, .	2.5	34
117	Dirac cones and highly anisotropic electronic structure of super-graphyne. Carbon, 2017, 113, 40-45.	10.3	34
118	Synergistic trifunctional electrocatalysis of pyridinic nitrogen and single transition-metal atoms anchored on pyrazine-modified graphdiyne. Science Bulletin, 2020, 65, 995-1002.	9.0	34
119	Regulating polysulfide intermediates by ultrathin Co-Bi nanosheet electrocatalyst in lithiumâ˜sulfur batteries. Nano Today, 2021, 40, 101246.	11.9	34
120	Ultrafine zirconium boride nanoparticles constructed bidirectional catalyst for ultrafast and long-lived lithium-sulfur batteries. Energy Storage Materials, 2022, 45, 130-141.	18.0	34
121	Plasma properties of a laser-ablated aluminum target in air. Laser and Particle Beams, 2003, 21, 97-101.	1.0	33
122	A scheme for the economical use of numerical basis sets in calculations with SIESTA. Theoretical Chemistry Accounts, 2004, 112, 158.	1.4	33
123	Faceted Silicon Nanotubes:â€‰ Structure, Energetic, and Passivation Effects. Journal of Physical Chemistry C, 2007, 111, 1234-1238.	3.1	32
124	Graphyne-based carbon allotropes with tunable properties: From Dirac fermion to semiconductor. Diamond and Related Materials, 2014, 41, 65-72.	3.9	32
125	High-efficiency helium separation through an inorganic graphenylene membrane: a theoretical study. Physical Chemistry Chemical Physics, 2020, 22, 9789-9795.	2.8	32
126	Stable multifunctional single-atom catalysts adsorbed on pyrazine-modified graphyne. Applied Surface Science, 2021, 553, 149464.	6.1	32

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127	Screening of Transition-Metal Single-Atom Catalysts Anchored on Covalentâ€“Organic Frameworks for Efficient Nitrogen Fixation. ACS Applied Materials & Interfaces, 2022, 14, 1024-1033.	8.0	32
128	Hydrogen storage capacity in single-walled carbon nanotubes. Physical Review B, 2002, 65, .	3.2	31
129	Proton stopping power in a group of bioorganic compounds over the energy range of 0.05â€“10MeV. Nuclear Instruments & Methods in Physics Research B, 2006, 248, 1-6.	1.4	31
130	Hydrogen saturation stabilizes vacancy-induced ferromagnetic ordering in graphene. Physical Chemistry Chemical Physics, 2010, 12, 13699.	2.8	31
131	Gas Adsorption Effects on the Electronic Properties of Two-Dimensional Nickel Bis(dithiolene) Complex. Journal of Physical Chemistry C, 2016, 120, 3846-3852.	3.1	31
132	Collision of hydrogen atom with single-walled carbon nanotube: Adsorption, insertion, and healing. Journal of Chemical Physics, 2001, 115, 8152-8156.	3.0	30
133	Theoretical study of the OH reaction with cytosine. Computational and Theoretical Chemistry, 2005, 723, 123-129.	1.5	30
134	Tuning the electronic structures of semiconducting SiC nanotubes by N and NHx (x=1,2) groups. Journal of Chemical Physics, 2006, 125, 194710.	3.0	30
135	Manifold electronic structure transition of BNC biribbons. Journal of Applied Physics, 2011, 110, .	2.5	30
136	Characterization of the effects of 3-MeV proton irradiation on fine-grained isotropic nuclear graphite. Carbon, 2014, 77, 311-318.	10.3	30
137	Large-Scale Synthesis of Few-Layer F-BN Nanocages with Zigzag-Edge Triangular Antidot Defects and Investigation of the Advanced Ferromagnetism. Nano Letters, 2015, 15, 8122-8128.	9.1	30
138	Chern Insulator and Chern Half-Metal States in the Two-Dimensional Spin-Gapless Semiconductor Mn₂C₆S₁₂. Journal of Physical Chemistry Letters, 2017, 8, 3770-3775.	4.6	30
139	Robust half-metallicity and topological aspects in two-dimensional Cu-TPyB. Scientific Reports, 2015, 5, 14098.	3.3	29
140	Cu₃N and its analogs: a new class of electrodes for lithium ion batteries. Journal of Materials Chemistry A, 2017, 5, 8762-8768.	10.3	29
141	Orientational DNA binding and directed transport on nanomaterial heterojunctions. Nanoscale, 2020, 12, 5217-5226.	5.6	29
142	Cross sections of electron inelastic interactions in DNA. Radiation and Environmental Biophysics, 2004, 43, 173-182.	1.4	28
143	Stable and extendable cage containing nanosize silica clusters based on three-membered rings. Physical Review B, 2004, 69, .	3.2	28
144	Electron stopping power and inelastic mean free path in amino acids and protein over the energy range of 20â€“20,000ÂeV. Radiation and Environmental Biophysics, 2006, 45, 135-143.	1.4	28

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145	Energetic Minimum Structures of Imogolite Nanotubes: A First-Principles Prediction. Journal of Physical Chemistry C, 2009, 113, 14834-14837.	3.1	28
146	Can cation vacancy defects induce room temperature ferromagnetism in GaN?. Applied Physics Letters, 2013, 102, 062411.	3.3	28
147	Study of the plasma produced from laser ablation of a KTP crystal. Applied Surface Science, 2003, 207, 227-235.	6.1	27
148	Orientation-Dependent Stability and Quantum-Confinement Effects of Silicon Carbide Nanowires. Journal of Physical Chemistry C, 2009, 113, 12731-12735.	3.1	27
149	A comparative first-principles study of the electronic, mechanical, defect and acoustic properties of Ti₂AlC and Ti₃AlC. Journal Physics D: Applied Physics, 2014, 47, 215301.	2.8	27
150	Photo-assisted high performance single atom electrocatalysis of the N₂ reduction reaction by a Mo-embedded covalent organic framework. Journal of Materials Chemistry A, 2021, 9, 19949-19957.	10.3	27
151	Reactions of Â·OH with thymine studied using density functional theory. International Journal of Quantum Chemistry, 2005, 101, 211-218.	2.0	26
152	Neutral vacancy-defect-induced magnetism in SiC monolayer. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 42, 2451-2454.	2.7	26
153	Protection of nuclear graphite toward liquid fluoride salt by isotropic pyrolytic carbon coating. Journal of Nuclear Materials, 2013, 442, 306-308.	2.7	26
154	Prediction of quantum anomalous Hall effect on graphene nanomesh. RSC Advances, 2015, 5, 9875-9880.	3.6	26
155	Band inversion and topological aspects in a TiNI monolayer. Physical Chemistry Chemical Physics, 2016, 18, 22154-22159.	2.8	26
156	Honeycomb-Patterned Quantum Dots beyond Graphene. Journal of Physical Chemistry C, 2011, 115, 17743-17749.	3.1	25
157	Spin-polarization of VGaON center in GaN and its application in spin qubit. Applied Physics Letters, 2012, 100, 192401.	3.3	25
158	Dumbbell stanane: a large-gap quantum spin hall insulator. Physical Chemistry Chemical Physics, 2015, 17, 16624-16629.	2.8	25
159	Kane Fermion in a Two-Dimensional Ï€-Conjugated Bis(iminothiolato)nickel Monolayer. Journal of Physical Chemistry Letters, 2018, 9, 614-619.	4.6	25
160	Bi-atom active sites embedded in a two-dimensional covalent organic framework for efficient nitrogen reduction reaction. Applied Surface Science, 2021, 563, 150352.	6.1	25
161	Structures of hydrogen molecules in single-walled carbon nanotubes. Chemical Physics Letters, 2002, 357, 97-102.	2.6	24
162	Ab initio study of base-functionalized single walled carbon nanotubes. Chemical Physics Letters, 2005, 415, 183-187.	2.6	24

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163	Lattice match and lattice mismatch models of graphene on hexagonal boron nitride from first principles. Journal of Physics Condensed Matter, 2014, 26, 095002.	1.8	24
164	Two-Dimensional Metalâ€“Organic Half-metallic Antiferromagnet: CoFePz. Journal of Physical Chemistry C, 2018, 122, 1846-1851.	3.1	24
165	Two- and Three-Membered-Ring Hybrid Structures of Silica Nanoclusters. Journal of Physical Chemistry B, 2004, 108, 18451-18454.	2.6	23
166	Selectable functionalization of single-walled carbon nanotubes resulting fromCHn(n=1â€“3)adsorption. Physical Review B, 2004, 69, .	3.2	23
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