Jijun Zhao

List of Publications by Year in descending order

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		4942	9553
671	30,199	84	142
papers	citations	h-index	g-index

678	678	678	27221
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Gas molecule adsorption in carbon nanotubes and nanotube bundles. Nanotechnology, 2002, 13, 195-200.	1.3	1,076
2	Rise of silicene: A competitive 2D material. Progress in Materials Science, 2016, 83, 24-151.	16.0	713
3	Metalâ€“Organicâ€Frameworkâ€Derived Hybrid Carbon Nanocages as a Bifunctional Electrocatalyst for Oxygen Reduction and Evolution. Advanced Materials, 2017, 29, 1700874.	11.1	678
4	Atomic-level insight into super-efficient electrocatalytic oxygen evolution on iron and vanadium co-doped nickel (oxy)hydroxide. Nature Communications, 2018, 9, 2885.	5.8	669
5	Facile Ammonia Synthesis from Electrocatalytic N₂ Reduction under Ambient Conditions on N-Doped Porous Carbon. ACS Catalysis, 2018, 8, 1186-1191.	5.5	520
6	Graphene oxide: A promising nanomaterial for energy and environmental applications. Nano Energy, 2015, 16, 488-515.	8.2	518
7	Boosting electrocatalytic oxygen evolution by synergistically coupling layered double hydroxide with MXene. Nano Energy, 2018, 44, 181-190.	8.2	458
8	Density-functional study ofAun(n=2â€“20)clusters: Lowest-energy structures and electronic properties. Physical Review B, 2002, 66, .	1.1	425
9	Graphene Nucleation on Transition Metal Surface: Structure Transformation and Role of the Metal Step Edge. Journal of the American Chemical Society, 2011, 133, 5009-5015.	6.6	315
10	Enhanced piezoelectric effect in Janus group-III chalcogenide monolayers. Applied Physics Letters, 2017, 110, .	1.5	307
11	First-Principles Study of Li-Intercalated Carbon Nanotube Ropes. Physical Review Letters, 2000, 85, 1706-1709.	2.9	298
12	Electronic Properties of Carbon Nanotubes with Covalent Sidewall Functionalization. Journal of Physical Chemistry B, 2004, 108, 4227-4230.	1.2	283
13	Noncovalent functionalization of carbon nanotubes by aromatic organic molecules. Applied Physics Letters, 2003, 82, 3746-3748.	1.5	260
14	Mechanical properties of graphene oxides. Nanoscale, 2012, 4, 5910.	2.8	239
15	Silicene on Substrates: A Way To Preserve or Tune Its Electronic Properties. Journal of Physical Chemistry C, 2013, 117, 10353-10359.	1.5	237
16	Structures, mobilities, electronic and magnetic properties of point defects in silicene. Nanoscale, 2013, 5, 9785.	2.8	230
17	2D covalent triazine framework: a new class of organic photocatalyst for water splitting. Journal of Materials Chemistry A, 2015, 3, 7750-7758.	5.2	229
18	Ultrasensitive Ironâ€Triggered Nanosized Feâ€“CoOOH Integrated with Graphene for Highly Efficient Oxygen Evolution. Advanced Energy Materials, 2017, 7, 1602148.	10.2	216

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19	Heterostructures of MXenes and N-doped graphene as highly active bifunctional electrocatalysts. Nanoscale, 2018, 10, 10876-10883.	2.8	215
20	Effects of Sidewall Functionalization on Conducting Properties of Single Wall Carbon Nanotubes. Nano Letters, 2006, 6, 916-919.	4.5	213
21	First-principles calculations of second- and third-order elastic constants for single crystals of arbitrary symmetry. Physical Review B, 2007, 75, .	1.1	210
22	From Boron Cluster to Two-Dimensional Boron Sheet on Cu(111) Surface: Growth Mechanism and Hole Formation. Scientific Reports, 2013, 3, 3238.	1.6	206
23	Recent progress on 2D magnets: Fundamental mechanism, structural design and modification. Applied Physics Reviews, 2021, 8, .	5.5	202
24	Exceptional Electrochemical HER Performance with Enhanced Electron Transfer between Ru Nanoparticles and Single Atoms Dispersed on a Carbon Substrate. Angewandte Chemie - International Edition, 2021, 60, 16044-16050.	7.2	200
25	Magnetism of Transition-Metal/Carbon-Nanotube Hybrid Structures. Physical Review Letters, 2003, 90, 257203.	2.9	198
26	Intrinsic Strength and Failure Behaviors of Graphene Grain Boundaries. ACS Nano, 2012, 6, 2704-2711.	7.3	197
27	Engineering Multifunctional Collaborative Catalytic Interface Enabling Efficient Hydrogen Evolution in All pH Range and Seawater. Advanced Energy Materials, 2019, 9, 1901333.	10.2	196
28	Fe-Anchored Graphene Oxide: A Low-Cost and Easily Accessible Catalyst for Low-Temperature CO Oxidation. Journal of Physical Chemistry C, 2012, 116, 2507-2514.	1.5	189
29	Novel Structures and Properties of Gold Nanowires. Physical Review Letters, 2001, 86, 2046-2049.	2.9	186
30	Work functions of pristine and alkali-metal intercalated carbon nanotubes and bundles. Physical Review B, 2002, 65, .	1.1	183
31	Initial geometries, interaction mechanism and high stability of silicene on Ag(111) surface. Scientific Reports, 2012, 2, 861.	1.6	183
32	Atomistic insight into the oxidation of monolayer transition metal dichalcogenides: from structures to electronic properties. RSC Advances, 2015, 5, 17572-17581.	1.7	183
33	MBene (MnB): a new type of 2D metallic ferromagnet with high Curie temperature. Nanoscale Horizons, 2018, 3, 335-341.	4.1	183
34	Tuning the Band Gap in Silicene by Oxidation. ACS Nano, 2014, 8, 10019-10025.	7.3	175
35	Rapid and energy-efficient microwave pyrolysis for high-yield production of highly-active bifunctional electrocatalysts for water splitting. Energy and Environmental Science, 2020, 13, 545-553.	15.6	169
36	Band Gap Tuning of Hydrogenated Graphene: H Coverage and Configuration Dependence. Journal of Physical Chemistry C, 2011, 115, 3236-3242.	1.5	167

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37	Screening and Design of Novel 2D Ferromagnetic Materials with High Curie Temperature above Room Temperature. ACS Applied Materials & Interfaces, 2018, 10, 39032-39039.	4.0	167
38	Probing the Electronic Effect of Carbon Nanotubes in Catalysis: NH₃ Synthesis with Ru Nanoparticles. Chemistry - A European Journal, 2010, 16, 5379-5384.	1.7	164
39	Endohedrally Doped Cage Clusters. Chemical Reviews, 2020, 120, 9021-9163.	23.0	164
40	Correlation between hardness and elastic moduli of the covalent crystals. Computational Materials Science, 2011, 50, 2287-2290.	1.4	163
41	Comparative Study of Hydrogen Adsorption on Carbon and BN Nanotubes. Journal of Physical Chemistry B, 2006, 110, 13363-13369.	1.2	157
42	Structural Growth Sequences and Electronic Properties of Zinc Oxide Clusters (ZnO)n(n=2-18). Journal of Physical Chemistry C, 2007, 111, 4956-4963.	1.5	157
43	Ultrahigh Rate and Longâ€Life Sodiumâ€Ion Batteries Enabled by Engineered Surface and Nearâ€Surface Reactions. Advanced Materials, 2018, 30, 1702486.	11.1	153
44	B80 and B101â€“103 clusters: Remarkable stability of the core-shell structures established by validated density functionals. Journal of Chemical Physics, 2012, 136, 074302.	1.2	150
45	Multilevel Hollow MXene Tailored Lowâ€Pt Catalyst for Efficient Hydrogen Evolution in Fullâ€pH Range and Seawater. Advanced Functional Materials, 2020, 30, 1910028.	7.8	150
46	Chemical environment and magnetic moment effects on point defect formations in CoCrNi-based concentrated solid-solution alloys. Acta Materialia, 2020, 187, 122-134.	3.8	149
47	Structure and electronic properties ofGen(n=2â€“25)clusters from density-functional theory. Physical Review B, 2001, 64, .	1.1	147
48	B₈₀ and Other Medium-Sized Boron Clusters: Coreâ”Shell Structures, Not Hollow Cages. Journal of Physical Chemistry A, 2010, 114, 9969-9972.	1.1	143
49	Magic Carbon Clusters in the Chemical Vapor Deposition Growth of Graphene. Journal of the American Chemical Society, 2012, 134, 2970-2975.	6.6	138
50	Quasi-freestanding epitaxial silicene on Ag(111) by oxygen intercalation. Science Advances, 2016, 2, e1600067.	4.7	138
51	In situ capture of active species and oxidation mechanism of RhB and MB dyes over sunlight-driven Ag/Ag3PO4 plasmonic nanocatalyst. Applied Catalysis B: Environmental, 2012, 125, 538-545.	10.8	137
52	Structures and electronic properties of Cu20, Ag20, and Au20 clusters with density functional method. Chemical Physics Letters, 2003, 380, 716-720.	1.2	129
53	Endohedral Silicon Fullerenes SiN(27 â‰Nâ‰ 39). Journal of the American Chemical Society, 2004, 126, 13845-13849.	6.6	129
54	Hole Defects and Nitrogen Doping in Graphene: Implication for Supercapacitor Applications. ACS Applied Materials & Interfaces, 2013, 5, 11184-11193.	4.0	128

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55	Nitrogen-Doped Graphene on Transition Metal Substrates as Efficient Bifunctional Catalysts for Oxygen Reduction and Oxygen Evolution Reactions. ACS Applied Materials & Interfaces, 2017, 9, 22578-22587.	4.0	128
56	Transition Metal Surface Passivation Induced Graphene Edge Reconstruction. Journal of the American Chemical Society, 2012, 134, 6204-6209.	6.6	127
57	2D Boron Sheets: Structure, Growth, and Electronic and Thermal Transport Properties. Advanced Functional Materials, 2020, 30, 1904349.	7.8	124
58	YN2 monolayer: Novel p-state Dirac half metal for high-speed spintronics. Nano Research, 2017, 10, 1972-1979.	5.8	120
59	Formation of Carbon Clusters in the Initial Stage of Chemical Vapor Deposition Graphene Growth on Ni(111) Surface. Journal of Physical Chemistry C, 2011, 115, 17695-17703.	1.5	119
60	Oxidation Resistance of Monolayer Group-IV Monochalcogenides. ACS Applied Materials & Interfaces, 2017, 9, 12013-12020.	4.0	118
61	Do Composite Single-Walled Nanotubes Have Enhanced Capability for Lithium Storage?. Chemistry of Materials, 2005, 17, 992-1000.	3.2	117
62	Graphene oxide as a chemically tunable 2-D material for visible-light photocatalyst applications. Journal of Catalysis, 2013, 299, 204-209.	3.1	115
63	Amorphous structural models for graphene oxides. Carbon, 2012, 50, 1690-1698.	5.4	114
64	MBenes: emerging 2D materials as efficient electrocatalysts for the nitrogen reduction reaction. Nanoscale Horizons, 2020, 5, 1106-1115.	4.1	114
65	Appropriate description of intermolecular interactions in the methane hydrates: An assessment of DFT methods. Journal of Computational Chemistry, 2013, 34, 121-131.	1.5	111
66	Melting behavior in ultrathin metallic nanowires. Physical Review B, 2002, 66, .	1.1	105
67	Boron Nitride Nanotubes for Ammonia Synthesis: Activation by Filling Transition Metals. Journal of the American Chemical Society, 2020, 142, 308-317.	6.6	105
68	Binding energies and electronic structures of adsorbed titanium chains on carbon nanotubes. Physical Review B, 2002, 66, .	1.1	103
69	Hollow Cages versus Space-Filling Structures for Medium-Sized Gold Clusters:â€‰ The Spherical Aromaticity of the Au50 Cage. Journal of Physical Chemistry A, 2005, 109, 9265-9269.	1.1	101
70	Structure and structural evolution of () clusters using a genetic algorithm and density functional theory method. Solid State Communications, 2007, 144, 174-179.	0.9	101
71	N-doped graphitic carbon materials hybridized with transition metals (compounds) for hydrogen evolution reaction: Understanding the synergistic effect from atomistic level. Carbon, 2018, 133, 260-266.	5.4	100
72	Genetic Algorithms for the Geometry Optimization of Atomic and Molecular Clusters. Journal of Computational and Theoretical Nanoscience, 2004, 1, 117-131.	0.4	99

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73	Discovery of a silicon-based ferrimagnetic wheel structure in V_xSi₁₂^{â^'} (x = 1â€“3) clusters: photoelectron spectroscopy and density functional theory investigation. Nanoscale, 2014, 6, 14617-14621.	2.8	99
74	Lateral heterostructures of monolayer group-IV monochalcogenides: band alignment and electronic properties. Journal of Materials Chemistry C, 2017, 5, 3788-3795.	2.7	94
75	A new phase diagram of water under negative pressure: The rise of the lowest-density clathrate s-III. Science Advances, 2016, 2, e1501010.	4.7	92
76	Band Gap Modulated by Electronic Superlattice in Blue Phosphorene. ACS Nano, 2018, 12, 5059-5065.	7.3	92
77	Stabilization of body-centred cubic iron under inner-core conditions. Nature Geoscience, 2017, 10, 312-316.	5.4	91
78	Growth behavior and magnetic properties ofSinFe(n=2â€“14)clusters. Physical Review B, 2006, 73, .	1.1	90
79	Inverse Capacity Growth and Pocket Effect in SnS₂ Semifilled Carbon Nanotube Anode. ACS Nano, 2018, 12, 8037-8047.	7.3	90
80	Comprehensive genetic algorithm forab initioglobal optimisation of clusters. Molecular Simulation, 2016, 42, 809-819.	0.9	88
81	Operando Revealing Dynamic Reconstruction of NiCo Carbonate Hydroxide for High-Rate Energy Storage. Joule, 2020, 4, 673-687.	11.7	88
82	Shuttle inhibition by chemical adsorption of lithium polysulfides in B and N co-doped graphene for Liâ€“S batteries. Physical Chemistry Chemical Physics, 2016, 18, 25241-25248.	1.3	87
83	Accelerating polysulfide redox conversion on bifunctional electrocatalytic electrode for stable Li-S batteries. Energy Storage Materials, 2019, 20, 98-107.	9.5	87
84	Magnetic properties of atomic clusters and endohedral metallofullerenes. Coordination Chemistry Reviews, 2015, 289-290, 315-340.	9.5	86
85	Hybrids of PtRu Nanoclusters and Black Phosphorus Nanosheets for Highly Efficient Alkaline Hydrogen Evolution Reaction. ACS Catalysis, 2019, 9, 10870-10875.	5.5	86
86	Alloying effect on the elastic properties of refractory high-entropy alloys. Materials and Design, 2017, 114, 243-252.	3.3	85
87	Structural and vibrational properties of solid nitromethane under high pressure by density functional theory. Journal of Chemical Physics, 2006, 124, 124501.	1.2	82
88	Band alignment of two-dimensional lateral heterostructures. 2D Materials, 2017, 4, 015038.	2.0	80
89	Niâ€“Ta binary bulk metallic glasses. Scripta Materialia, 2010, 63, 178-180.	2.6	79
90	Eighteen functional monolayer metal oxides: wide bandgap semiconductors with superior oxidation resistance and ultrahigh carrier mobility. Nanoscale Horizons, 2019, 4, 592-600.	4.1	78

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91	Body-centered tetragonal B2N2: a novel sp3 bonding boron nitride polymorph. Physical Chemistry Chemical Physics, 2011, 13, 14565.	1.3	77
92	Energetics and electronic structures of AlN nanotubes/wires and their potential application as ammonia sensors. Nanotechnology, 2007, 18, 424023.	1.3	76
93	Intercalation and diffusion of lithium ions in a carbon nanotube bundle by ab initio molecular dynamics simulations. Energy and Environmental Science, 2011, 4, 1379.	15.6	76
94	Quantum transport properties of ultrathin silver nanowires. Nanotechnology, 2003, 14, 501-504.	1.3	75
95	Complete Spin Polarization for a Carbon Nanotube with an Adsorbed Atomic Transition-Metal Chain. Nano Letters, 2004, 4, 561-563.	4.5	75
96	A new class of epitaxial porphyrin metalâ€“organic framework thin films with extremely high photocarrier generation efficiency: promising materials for all-solid-state solar cells. Journal of Materials Chemistry A, 2016, 4, 12739-12747.	5.2	75
97	Cooperative Electronâ€“Phonon Coupling and Buckled Structure in Germanene on Au(111). ACS Nano, 2017, 11, 3553-3559.	7.3	75
98	Structures and electronic properties of symmetric and nonsymmetric graphene grain boundaries. Carbon, 2013, 55, 151-159.	5.4	74
99	MXene nanoribbons as electrocatalysts for the hydrogen evolution reaction with fast kinetics. Physical Chemistry Chemical Physics, 2018, 20, 19390-19397.	1.3	74
100	Tailorable AcceptorC60â^'nBnand DonorC60â^'mNmPairs for Molecular Electronics. Physical Review Letters, 2003, 90, 206602.	2.9	73
101	Atomic structures and covalent-to-metallic transition of lead clustersPbn(n=2â€“22). Physical Review A, 2005, 71, .	1.0	73
102	First-principles calculations of structural, electronic, vibrational, and magnetic properties of C60 and C48N12: A comparative study. Journal of Chemical Physics, 2003, 118, 8621-8635.	1.2	72
103	Stabilization of fullerene-like boron cages by transition metal encapsulation. Nanoscale, 2015, 7, 10482-10489.	2.8	72
104	Electronic and Photonic Properties of Doped Carbon Nanotubes. Journal of Nanoscience and Nanotechnology, 2003, 3, 459-478.	0.9	71
105	Engineering the Electronic Structure of Single-Walled Carbon Nanotubes by Chemical Functionalization. ChemPhysChem, 2005, 6, 598-601.	1.0	71
106	An exchange intercalation mechanism for the formation of a two-dimensional Si structure underneath graphene. Nano Research, 2012, 5, 352-360.	5.8	71
107	Graphene Oxide: Physics and Applications. SpringerBriefs in Physics, 2015, , .	0.2	70
108	GeAs and SiAs monolayers: Novel 2D semiconductors with suitable band structures. Physica E: Low-Dimensional Systems and Nanostructures, 2018, 95, 149-153.	1.3	70

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109	High-pressure behavior of crystalline FOX-7 by density functional theory calculations. Computational Materials Science, 2008, 42, 698-703.	1.4	69
110	Reverseâ€Graded 2D Ruddlesdenâ€“Popper Perovskites for Efficient Airâ€Stable Solar Cells. Advanced Energy Materials, 2019, 9, 1900612.	10.2	69
111	A novel CuTi-containing catalyst derived from hydrotalcite-like compounds for selective catalytic reduction of NO with C3H6 under lean-burn conditions. Journal of Catalysis, 2014, 309, 268-279.	3.1	68
112	Atomic and Electronic Structures of Fluorinated BN Nanotubes:Â Computational Study. Journal of Physical Chemistry B, 2006, 110, 25678-25685.	1.2	67
113	Melting behavior of ultrathin titanium nanowires. Physical Review B, 2003, 67, .	1.1	66
114	2D lateral heterostructures of group-III monochalcogenide: Potential photovoltaic applications. Applied Physics Letters, 2018, 112, .	1.5	66
115	Boron fullerenes with 32â€“56 atoms: Irregular cage configurations and electronic properties. Chemical Physics Letters, 2010, 501, 16-19.	1.2	65
116	B₂₈: the smallest all-boron cage from an ab initio global search. Nanoscale, 2015, 7, 15086-15090.	2.8	65
117	The stability and electronic structure of single-walled ZnO nanotubes by density functional theory. Nanotechnology, 2007, 18, 345706.	1.3	64
118	Nonmetal-metal transition inZnn(n=2â€“20)clusters. Physical Review A, 2003, 68, .	1.0	63
119	Curved carbon nanotubes: From unique geometries to novel properties and peculiar applications. Nano Research, 2014, 7, 626-657.	5.8	63
120	Structures and Electronic Properties of V₃Si_n^{â€“} (n =) Tj ETQq0 0 0 rgBT /Overlock 10987-10994.	1.5	63
121	Structural and Electronic Properties of Interfaces in Graphene and Hexagonal Boron Nitride Lateral Heterostructures. Chemistry of Materials, 2016, 28, 5022-5028.	3.2	63
122	Structures and Magnetic Properties of MoS₂ Grain Boundaries with Antisite Defects. Journal of Physical Chemistry C, 2017, 121, 12261-12269.	1.5	63
123	Two-dimensional ZnO for the selective photoreduction of CO₂. Journal of Materials Chemistry A, 2019, 7, 16294-16303.	5.2	62
124	Geometric and electronic properties of titanium clusters studied by ultrasoft pseudopotential. Solid State Communications, 2001, 118, 157-161.	0.9	61
125	Structure and electronic properties of cobalt atoms encapsulated in Sin (n=1â€“13) clusters. Chemical Physics Letters, 2005, 411, 279-284.	1.2	61
126	Distinct properties of single-wall carbon nanotubes with monovalent sidewall additions. Nanotechnology, 2005, 16, 635-638.	1.3	61

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127	First-principles studies of diamond polytypes. Diamond and Related Materials, 2008, 17, 356-364.	1.8	61
128	Accurate electronic properties and non-linear optical response of two-dimensional MA2Z4. Nanoscale, 2021, 13, 5479-5488.	2.8	61
129	Cage and tube structures of medium-sized zinc oxide clusters (ZnO)n (n=24, 28, 36, and 48). Journal of Chemical Physics, 2008, 128, 144710.	1.2	60
130	Two-Dimensional Metallic NiTe₂ with Ultrahigh Environmental Stability, Conductivity, and Electrocatalytic Activity. ACS Nano, 2020, 14, 9011-9020.	7.3	60
131	Tunable Assembly of sp³ Crossâ€Linked 3D Graphene Monoliths: A Firstâ€Principles Prediction. Advanced Functional Materials, 2013, 23, 5846-5853.	7.8	59
132	Excellent HER and OER Catalyzing Performance of Seâ€Vacancies in Defectsâ€Engineered PtSe₂: From Simulation to Experiment. Advanced Energy Materials, 2022, 12, 2102359.	10.2	59
133	Direct synthesis and in situ characterization of monolayer parallelogrammic rhenium diselenide on gold foil. Communications Chemistry, 2018, 1, .	2.0	58
134	Monolayer group-III monochalcogenides by oxygen functionalization: a promising class of two-dimensional topological insulators. Npj Quantum Materials, 2018, 3, .	1.8	58
135	Structure and stability of bilayer borophene: The roles of hexagonal holes and interlayer bonding. FlatChem, 2018, 7, 48-54.	2.8	58
136	Immobilized trimeric metal clusters: A family of the smallest catalysts for selective CO2 reduction toward multi-carbon products. Nano Energy, 2020, 76, 105049.	8.2	56
137	Effect of surface Lewis acidity on selective catalytic reduction of NO by C3H6 over calcined hydrotalcite. Applied Catalysis A: General, 2013, 451, 176-183.	2.2	55
138	Controllable Conversion of CO₂on Nonâ€Metallic Gold Clusters. Angewandte Chemie - International Edition, 2020, 59, 1919-1924.	7.2	55
139	Structures and electronic properties of ultrathin titanium nanowires. Journal of Physics Condensed Matter, 2001, 13, L403-L408.	0.7	53
140	Structure and magnetic properties of cobalt doped () clusters. Physics Letters, Section A: General, Atomic and Solid State Physics, 2007, 367, 335-344.	0.9	53
141	Phosphorus quantum dots as visible-light photocatalyst for water splitting. Computational Materials Science, 2017, 130, 56-63.	1.4	53
142	Atomic Sulfur Anchored on Silicene, Phosphorene, and Borophene for Excellent Cycle Performance of Liâ€“S Batteries. ACS Applied Materials & Interfaces, 2017, 9, 42836-42844.	4.0	53
143	Structure and magnetic properties of Co-Cu bimetallic clusters. Physical Review B, 2002, 66, .	1.1	52
144	Functionalization of BN nanotubes with dichlorocarbenes. Nanotechnology, 2008, 19, 015202.	1.3	52

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145	Titanium-decorated graphene oxide for carbon monoxide capture and separation. Physical Chemistry Chemical Physics, 2011, 13, 21126.	1.3	52
146	Mechanical and electronic properties of B₁₂-based ternary crystals of orthorhombic phase. Journal of Physics Condensed Matter, 2010, 22, 315503.	0.7	51
147	Stability and dissolution of heliumâ€“vacancy complexes in vanadium solid. Journal of Nuclear Materials, 2011, 419, 1-8.	1.3	51
148	A Molecularâ€Cage Strategy Enabling Efficient Chemisorptionâ€“Electrocatalytic Interface in Nanostructured Li₂S Cathode for Li Metalâ€Free Rechargeable Cells with High Energy. Advanced Functional Materials, 2019, 29, 1905986.	7.8	51
149	Copper(<scp>i</scp>) sulfide: a two-dimensional semiconductor with superior oxidation resistance and high carrier mobility. Nanoscale Horizons, 2019, 4, 223-230.	4.1	51
150	Pressure-induced metallization in solid boron. Physical Review B, 2002, 66, .	1.1	50
151	Firstâ€principles study of molecular hydrogen dissociation on doped Al₁₂X (X = B, Al, C, Si,) Tj ETQq1 1 0.784314 rgBT /Ov	1.5	50
152	Atomic structures and electronic properties of phosphorene grain boundaries. 2D Materials, 2016, 3, 025008.	2.0	49
153	Structures, electronic properties, and hydrogen-storage capacity of single-walled TiO2 nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2009, 41, 838-842.	1.3	48
154	He-induced vacancy formation in bcc Fe solid from first-principles simulation. Journal of Nuclear Materials, 2014, 444, 147-152.	1.3	48
155	Initial Growth Mechanism of Blue Phosphorene on Au(111) Surface. Journal of Physical Chemistry C, 2017, 121, 17893-17899.	1.5	48
156	Characteristics of Raman spectra for graphene oxide from ab initio simulations. Journal of Chemical Physics, 2011, 135, 184503.	1.2	47
157	Boron clusters with 46, 48, and 50 atoms: competition among the coreâ€“shell, bilayer and quasi-planar structures. Nanoscale, 2017, 9, 13905-13909.	2.8	47
158	Structural transition of Si clusters and their thermodynamics. Chemical Physics Letters, 2001, 341, 529-534.	1.2	46
159	Vibrational properties of molecule and crystal of TATB: A comparative density functional study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2006, 358, 63-69.	0.9	46
160	Transformation from chemisorption to physisorption with tube diameter and gas concentration: Computational studies on NH3 adsorption in BN nanotubes. Journal of Chemical Physics, 2007, 127, 184705.	1.2	46
161	Improving hydrogen storage properties of covalent organic frameworks by substitutional doping. International Journal of Hydrogen Energy, 2010, 35, 266-271.	3.8	46
162	What is the best density functional to describe water clusters: evaluation of widely used density functionals with various basis sets for (H2O) n (nÂ=Â1â€“10). Theoretical Chemistry Accounts, 2011, 130, 341-352.	0.5	46

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163	Computational high-throughput screening of alloy nanoclusters for electrocatalytic hydrogen evolution. Npj Computational Materials, 2021, 7, .	3.5	46
164	Structural, electronic, and magnetic properties of heterofullerene C48B12. Chemical Physics Letters, 2003, 375, 445-451.	1.2	45
165	True Nanocable Assemblies with Insulating BN Nanotube Sheaths and Conducting Cu Nanowire Cores. Journal of Physical Chemistry B, 2006, 110, 2529-2532.	1.2	45
166	Structure and electronic properties of medium-sized GanNn clusters (n=4â€“12). Chemical Physics Letters, 2006, 422, 170-173.	1.2	45
167	First-Principles Study of Water Chains Encapsulated in Single-Walled Carbon Nanotube. Journal of Physical Chemistry C, 2009, 113, 5368-5375.	1.5	45
168	Atomic structures and electronic properties of small Auâ€“Ag binary clusters: Effects of size and composition. Computational and Theoretical Chemistry, 2012, 993, 36-44.	1.1	45
169	Combining Machine Learning Potential and Structure Prediction for Accelerated Materials Design and Discovery. Journal of Physical Chemistry Letters, 2020, 11, 8710-8720.	2.1	45
170	Elastic properties of vanadium-based alloys from first-principles theory. Physical Review B, 2012, 86, .	1.1	44
171	Crystal-Phase-Mediated Restructuring of Pt on TiO₂ with Tunable Reactivity: Redispersion versus Reshaping. ACS Catalysis, 2022, 12, 3634-3643.	5.5	44
172	Dual Relationship between Large Gold Clusters (Antifullerenes) and Carbon Fullerenes:â€‰ A New Lowest-Energy Cage Structure for Au50. Journal of Physical Chemistry A, 2007, 111, 411-414.	1.1	43
173	High-pressure behavior of TATB crystal by density functional theory. Physics Letters, Section A: General, Atomic and Solid State Physics, 2007, 367, 383-388.	0.9	43
174	Atomic Structure of the Magic (ZnO)₆₀ Cluster: First-Principles Prediction of a Sodalite Motif for ZnO Nanoclusters. Journal of Physical Chemistry C, 2010, 114, 5741-5744.	1.5	43
175	Ab initio molecular dynamics simulation of binary Cu64Zr36 bulk metallic glass: Validation of the cluster-plus-glue-atom model. Journal of Applied Physics, 2011, 109, .	1.1	43
176	A novel superhard BN allotrope under cold compression of h-BN. Journal of Physics Condensed Matter, 2013, 25, 122204.	0.7	43
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