

Si Zhou

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/2798012/publications.pdf>

Version: 2024-02-01

491
papers

27,543
citations

5248

83
h-index

9073

144
g-index

499
all docs

499
docs citations

499
times ranked

26867
citing authors

#	ARTICLE	IF	CITATIONS
1	Gas molecule adsorption in carbon nanotubes and nanotube bundles. <i>Nanotechnology</i> , 2002, 13, 195-200.	1.3	1,076
2	Rise of silicene: A competitive 2D material. <i>Progress in Materials Science</i> , 2016, 83, 24-151.	16.0	713
3	Metal-Organic Framework-Derived Hybrid Carbon Nanocages as a Bifunctional Electrocatalyst for Oxygen Reduction and Evolution. <i>Advanced Materials</i> , 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. <i>Nature Communications</i> , 2018, 9, 2885.	5.8	669
5	Facile Ammonia Synthesis from Electrocatalytic N ₂ Reduction under Ambient Conditions on N-Doped Porous Carbon. <i>ACS Catalysis</i> , 2018, 8, 1186-1191.	5.5	520
6	Graphene oxide: A promising nanomaterial for energy and environmental applications. <i>Nano Energy</i> , 2015, 16, 488-515.	8.2	518
7	Room-temperature metastability of multilayer graphene oxide films. <i>Nature Materials</i> , 2012, 11, 544-549.	13.3	512
8	Boosting electrocatalytic oxygen evolution by synergistically coupling layered double hydroxide with MXene. <i>Nano Energy</i> , 2018, 44, 181-190.	8.2	458
9	Co Nanoislands Rooted on Co-N-C Nanosheets as Efficient Oxygen Electrocatalyst for Zn-Air Batteries. <i>Advanced Materials</i> , 2019, 31, e1901666.	11.1	455
10	Density-functional study of Au(n=2-20) clusters: Lowest-energy structures and electronic properties. <i>Physical Review B</i> , 2002, 66, .	1.1	425
11	A Stable Bifunctional Catalyst for Rechargeable Zinc-Air Batteries: Iron-Cobalt Nanoparticles Embedded in a Nitrogen-Doped 3D Carbon Matrix. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 16166-16170.	7.2	365
12	Enhanced piezoelectric effect in Janus group-III chalcogenide monolayers. <i>Applied Physics Letters</i> , 2017, 110, .	1.5	307
13	First-Principles Study of Li-Intercalated Carbon Nanotube Ropes. <i>Physical Review Letters</i> , 2000, 85, 1706-1709.	2.9	298
14	Mechanical properties of graphene oxides. <i>Nanoscale</i> , 2012, 4, 5910.	2.8	239
15	Silicene on Substrates: A Way To Preserve or Tune Its Electronic Properties. <i>Journal of Physical Chemistry C</i> , 2013, 117, 10353-10359.	1.5	237
16	Structures, mobilities, electronic and magnetic properties of point defects in silicene. <i>Nanoscale</i> , 2013, 5, 9785.	2.8	230
17	2D covalent triazine framework: a new class of organic photocatalyst for water splitting. <i>Journal of Materials Chemistry A</i> , 2015, 3, 7750-7758.	5.2	229
18	Carbohydrate doping to enhance electromagnetic properties of MgB ₂ superconductors. <i>Applied Physics Letters</i> , 2006, 89, 142505.	1.5	226

#	ARTICLE	IF	CITATIONS
19	Toward a Reversible Mn ⁴⁺ /Mn ²⁺ Redox Reaction and Dendrite-Free Zn Anode in Near-Neutral Aqueous Zn/MnO ₂ Batteries via Salt Anion Chemistry. <i>Advanced Energy Materials</i> , 2020, 10, 1904163.	10.2	221
20	Ultrasensitive Iron-Triggered Nanosized Fe-CoOOH Integrated with Graphene for Highly Efficient Oxygen Evolution. <i>Advanced Energy Materials</i> , 2017, 7, 1602148.	10.2	216
21	Heterostructures of MXenes and N-doped graphene as highly active bifunctional electrocatalysts. <i>Nanoscale</i> , 2018, 10, 10876-10883.	2.8	215
22	Vacancy Engineering of Iron-Doped W ₁₈ O ₄₉ Nanoreactors for Low-Barrier Electrochemical Nitrogen Reduction. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 7356-7361.	7.2	215
23	From Boron Cluster to Two-Dimensional Boron Sheet on Cu(111) Surface: Growth Mechanism and Hole Formation. <i>Scientific Reports</i> , 2013, 3, 3238.	1.6	206
24	Recent progress on 2D magnets: Fundamental mechanism, structural design and modification. <i>Applied Physics Reviews</i> , 2021, 8, .	5.5	202
25	Exceptional Electrochemical HER Performance with Enhanced Electron Transfer between Ru Nanoparticles and Single Atoms Dispersed on a Carbon Substrate. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 16044-16050.	7.2	200
26	Intrinsic Strength and Failure Behaviors of Graphene Grain Boundaries. <i>ACS Nano</i> , 2012, 6, 2704-2711.	7.3	197
27	Engineering Multifunctional Collaborative Catalytic Interface Enabling Efficient Hydrogen Evolution in All pH Range and Seawater. <i>Advanced Energy Materials</i> , 2019, 9, 1901333.	10.2	196
28	Capturing the active sites of multimetallic (oxy)hydroxides for the oxygen evolution reaction. <i>Energy and Environmental Science</i> , 2020, 13, 4225-4237.	15.6	186
29	Work functions of pristine and alkali-metal intercalated carbon nanotubes and bundles. <i>Physical Review B</i> , 2002, 65, .	1.1	183
30	Initial geometries, interaction mechanism and high stability of silicene on Ag(111) surface. <i>Scientific Reports</i> , 2012, 2, 861.	1.6	183
31	Atomistic insight into the oxidation of monolayer transition metal dichalcogenides: from structures to electronic properties. <i>RSC Advances</i> , 2015, 5, 17572-17581.	1.7	183
32	MBene (MnB): a new type of 2D metallic ferromagnet with high Curie temperature. <i>Nanoscale Horizons</i> , 2018, 3, 335-341.	4.1	183
33	Tuning the Band Gap in Silicene by Oxidation. <i>ACS Nano</i> , 2014, 8, 10019-10025.	7.3	175
34	Rapid and energy-efficient microwave pyrolysis for high-yield production of highly-active bifunctional electrocatalysts for water splitting. <i>Energy and Environmental Science</i> , 2020, 13, 545-553.	15.6	169
35	Band Gap Tuning of Hydrogenated Graphene: H Coverage and Configuration Dependence. <i>Journal of Physical Chemistry C</i> , 2011, 115, 3236-3242.	1.5	167
36	Screening and Design of Novel 2D Ferromagnetic Materials with High Curie Temperature above Room Temperature. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 39032-39039.	4.0	167

#	ARTICLE	IF	CITATIONS
37	Common electronic origin of superconductivity in (Li,Fe)OHFeSe bulk superconductor and single-layer FeSe/SrTiO ₃ films. <i>Nature Communications</i> , 2016, 7, 10608.	5.8	164
38	Endohedrally Doped Cage Clusters. <i>Chemical Reviews</i> , 2020, 120, 9021-9163.	23.0	164
39	Origin of the Chemical and Kinetic Stability of Graphene Oxide. <i>Scientific Reports</i> , 2013, 3, 2484.	1.6	163
40	Evidence of Topological Surface State in Three-Dimensional Dirac Semimetal Cd ₃ As ₂ . <i>Scientific Reports</i> , 2014, 4, 6106.	1.6	159
41	Fluorescent Gold Nanoclusters with Interlocked Staples and a Fully Thiolate-Bound Kernel. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 11567-11571.	7.2	159
42	Structural Growth Sequences and Electronic Properties of Zinc Oxide Clusters (ZnO) _n (n=2-18). <i>Journal of Physical Chemistry C</i> , 2007, 111, 4956-4963.	1.5	157
43	Ultrahigh Rate and Long-Life Sodium-Ion Batteries Enabled by Engineered Surface and Near-Surface Reactions. <i>Advanced Materials</i> , 2018, 30, 1702486.	11.1	153
44	B ₈₀ and B ₁₀₁ -I ⁺ clusters: Remarkable stability of the core-shell structures established by validated density functionals. <i>Journal of Chemical Physics</i> , 2012, 136, 074302.	1.2	150
45	Multilevel Hollow MXene Tailored Low-Pt Catalyst for Efficient Hydrogen Evolution in Full-pH Range and Seawater. <i>Advanced Functional Materials</i> , 2020, 30, 1910028.	7.8	150
46	Structure of Chiral Au ₄₄ (2,4-DMBT) ₂₆ Nanocluster with an 18-Electron Shell Closure. <i>Journal of the American Chemical Society</i> , 2016, 138, 10425-10428.	6.6	149
47	Structure and electronic properties of Gen(n=2-25) clusters from density-functional theory. <i>Physical Review B</i> , 2001, 64, .	1.1	147
48	B ₈₀ and Other Medium-Sized Boron Clusters: Core-Shell Structures, Not Hollow Cages. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9969-9972.	1.1	143
49	Quasi-freestanding epitaxial silicene on Ag(111) by oxygen intercalation. <i>Science Advances</i> , 2016, 2, e1600067.	4.7	138
50	Hole Defects and Nitrogen Doping in Graphene: Implication for Supercapacitor Applications. <i>ACS Applied Materials & Interfaces</i> , 2013, 5, 11184-11193.	4.0	128
51	Nitrogen-Doped Graphene on Transition Metal Substrates as Efficient Bifunctional Catalysts for Oxygen Reduction and Oxygen Evolution Reactions. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 22578-22587.	4.0	128
52	2D Boron Sheets: Structure, Growth, and Electronic and Thermal Transport Properties. <i>Advanced Functional Materials</i> , 2020, 30, 1904349.	7.8	124
53	YN ₂ monolayer: Novel p-state Dirac half metal for high-speed spintronics. <i>Nano Research</i> , 2017, 10, 1972-1979.	5.8	120
54	Crystal and Solution Photoluminescence of MAg ₂₄ (SR) ₁₈ (M = Ag/Pd/Pt/Au) Nanoclusters and Some Implications for the Photoluminescence Mechanisms. <i>Journal of Physical Chemistry C</i> , 2017, 121, 13848-13853.	1.5	120

#	ARTICLE	IF	CITATIONS
55	Oxidation Resistance of Monolayer Group-IV Monochalcogenides. ACS Applied Materials & Interfaces, 2017, 9, 12013-12020.	4.0	118
56	Do Composite Single-Walled Nanotubes Have Enhanced Capability for Lithium Storage?. Chemistry of Materials, 2005, 17, 992-1000.	3.2	117
57	Electron-Deficient Cu Sites on Cu ₃ Ag Catalyst Promoting CO ₂ Electroreduction to Alcohols. Advanced Energy Materials, 2020, 10, 2001987.	10.2	117
58	Amorphous structural models for graphene oxides. Carbon, 2012, 50, 1690-1698.	5.4	114
59	MBenes: emerging 2D materials as efficient electrocatalysts for the nitrogen reduction reaction. Nanoscale Horizons, 2020, 5, 1106-1115.	4.1	114
60	Physical properties and device applications of graphene oxide. Frontiers of Physics, 2020, 15, 1.	2.4	108
61	A single boron atom doped boron nitride edge as a metal-free catalyst for N ₂ fixation. Physical Chemistry Chemical Physics, 2019, 21, 1110-1116.	1.3	107
62	Melting behavior in ultrathin metallic nanowires. Physical Review B, 2002, 66, .	1.1	105
63	Strong Anisotropy of Dirac Cones in SrMnBi ₂ and CaMnBi ₂ Revealed by Angle-Resolved Photoemission Spectroscopy. Scientific Reports, 2014, 4, 5385.	1.6	105
64	Boron Nitride Nanotubes for Ammonia Synthesis: Activation by Filling Transition Metals. Journal of the American Chemical Society, 2020, 142, 308-317.	6.6	105
65	Binding energies and electronic structures of adsorbed titanium chains on carbon nanotubes. Physical Review B, 2002, 66, .	1.1	103
66	Hollow Cages versus Space-Filling Structures for Medium-Sized Gold Clusters: The Spherical Aromaticity of the Au ₅₀ Cage. Journal of Physical Chemistry A, 2005, 109, 9265-9269.	1.1	101
67	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
68	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
69	Electrocatalyzing S Cathodes via Multisulfiphilic Sites for Superior Room-Temperature Sodium-Sulfur Batteries. ACS Nano, 2020, 14, 7259-7268.	7.3	100
70	Discovery of a silicon-based ferrimagnetic wheel structure in V _x Si ₁₂ (x = 1-3) clusters: photoelectron spectroscopy and density functional theory investigation. Nanoscale, 2014, 6, 14617-14621.	2.8	99
71	Chemical-Reductant-Free Electrochemical Deuteration Reaction using Deuterium Oxide. Angewandte Chemie - International Edition, 2020, 59, 13962-13967.	7.2	99
72	Sugar Coating of Boron Powder for Efficient Carbon Doping of MgB ₂ with Enhanced Current-Carrying Performance. Advanced Materials, 2007, 19, 1373-1376.	11.1	94

#	ARTICLE	IF	CITATIONS
73	Lateral heterostructures of monolayer group-IV monochalcogenides: band alignment and electronic properties. <i>Journal of Materials Chemistry C</i> , 2017, 5, 3788-3795.	2.7	94
74	A new phase diagram of water under negative pressure: The rise of the lowest-density clathrate s-III. <i>Science Advances</i> , 2016, 2, e1501010.	4.7	92
75	Band Gap Modulated by Electronic Superlattice in Blue Phosphorene. <i>ACS Nano</i> , 2018, 12, 5059-5065.	7.3	92
76	Stabilization of body-centred cubic iron under inner-core conditions. <i>Nature Geoscience</i> , 2017, 10, 312-316.	5.4	91
77	Growth behavior and magnetic properties of $\text{Si}_n\text{Fe}(n=2\text{--}14)$ clusters. <i>Physical Review B</i> , 2006, 73, .	1.1	90
78	Inverse Capacity Growth and Pocket Effect in SnS_2 Semifilled Carbon Nanotube Anode. <i>ACS Nano</i> , 2018, 12, 8037-8047.	7.3	90
79	Structural Design Strategy and Active Site Regulation of High-Efficient Bifunctional Oxygen Reaction Electrocatalysts for Zn^{2+} Air Battery. <i>Small</i> , 2021, 17, e2006766.	5.2	89
80	Comprehensive genetic algorithm for <i>ab initio</i> global optimisation of clusters. <i>Molecular Simulation</i> , 2016, 42, 809-819.	0.9	88
81	Operando Revealing Dynamic Reconstruction of NiCo Carbonate Hydroxide for High-Rate Energy Storage. <i>Joule</i> , 2020, 4, 673-687.	11.7	88
82	Shuttle inhibition by chemical adsorption of lithium polysulfides in B and N co-doped graphene for Li^{+} /S batteries. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 25241-25248.	1.3	87
83	Electrochemical Hydrogenation with Gaseous Ammonia. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 1759-1763.	7.2	87
84	Accelerating polysulfide redox conversion on bifunctional electrocatalytic electrode for stable Li-S batteries. <i>Energy Storage Materials</i> , 2019, 20, 98-107.	9.5	87
85	Magnetic properties of atomic clusters and endohedral metallofullerenes. <i>Coordination Chemistry Reviews</i> , 2015, 289-290, 315-340.	9.5	86
86	Large Negative Thermal Expansion and Anomalous Behavior on Compression in Cubic ReO_3 -Type $\text{A}^{\text{II}}\text{B}^{\text{IV}}\text{F}_6$ and CaHfF_6 . <i>Chemistry of Materials</i> , 2015, 27, 3912-3918.	3.2	86
87	Hybrids of PtRu Nanoclusters and Black Phosphorus Nanosheets for Highly Efficient Alkaline Hydrogen Evolution Reaction. <i>ACS Catalysis</i> , 2019, 9, 10870-10875.	5.5	86
88	Controlling and Observing Sharp-Valleyed Quantum Interference Effect in Single Molecular Junctions. <i>Journal of the American Chemical Society</i> , 2018, 140, 17685-17690.	6.6	84
89	Gas adsorption on monolayer blue phosphorus: implications for environmental stability and gas sensors. <i>Nanotechnology</i> , 2017, 28, 175708.	1.3	81
90	Kernel Tuning and Nonuniform Influence on Optical and Electrochemical Gaps of Bimetal Nanoclusters. <i>Journal of the American Chemical Society</i> , 2018, 140, 3487-3490.	6.6	81

#	ARTICLE	IF	CITATIONS
91	Chemical Bonding of Partially Fluorinated Graphene. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26402-26408.	1.5	80
92	Polarimetric Convolutional Network for PolSAR Image Classification. <i>IEEE Transactions on Geoscience and Remote Sensing</i> , 2019, 57, 3040-3054.	2.7	79
93	Orbital-selective spin texture and its manipulation in a topological insulator. <i>Nature Communications</i> , 2014, 5, 3382.	5.8	78
94	Elastic coupling between layers in two-dimensional materials. <i>Nature Materials</i> , 2015, 14, 714-720.	13.3	78
95	Eighteen functional monolayer metal oxides: wide bandgap semiconductors with superior oxidation resistance and ultrahigh carrier mobility. <i>Nanoscale Horizons</i> , 2019, 4, 592-600.	4.1	78
96	Intercalation and diffusion of lithium ions in a carbon nanotube bundle by ab initio molecular dynamics simulations. <i>Energy and Environmental Science</i> , 2011, 4, 1379.	15.6	76
97	Direct evidence of interaction-induced Dirac cones in a monolayer silicene/Ag(111) system. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 14656-14661.	3.3	76
98	Quantum transport properties of ultrathin silver nanowires. <i>Nanotechnology</i> , 2003, 14, 501-504.	1.3	75
99	A new class of epitaxial porphyrin metal-organic framework thin films with extremely high photocarrier generation efficiency: promising materials for all-solid-state solar cells. <i>Journal of Materials Chemistry A</i> , 2016, 4, 12739-12747.	5.2	75
100	Cooperative Electron-Phonon Coupling and Buckled Structure in Germanene on Au(111). <i>ACS Nano</i> , 2017, 11, 3553-3559.	7.3	75
101	Structures and electronic properties of symmetric and nonsymmetric graphene grain boundaries. <i>Carbon</i> , 2013, 55, 151-159.	5.4	74
102	MXene nanoribbons as electrocatalysts for the hydrogen evolution reaction with fast kinetics. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19390-19397.	1.3	74
103	Atomic structures and covalent-to-metallic transition of lead clusters Pb_n ($n=2-22$). <i>Physical Review A</i> , 2005, 71, .	1.0	73
104	Common Fermi-surface topology and nodeless superconducting gap of K	1.1	73
105	Stabilization of fullerene-like boron cages by transition metal encapsulation. <i>Nanoscale</i> , 2015, 7, 10482-10489.	2.8	72
106	Ni_3S_2 Nanosheets in Situ Epitaxially Grown on Nanorods as High Active and Stable Homo Junction Electrocatalyst for Hydrogen Evolution Reaction. <i>ACS Sustainable Chemistry and Engineering</i> , 2018, 6, 2474-2481.	3.2	72
107	Electronic and Photonic Properties of Doped Carbon Nanotubes. <i>Journal of Nanoscience and Nanotechnology</i> , 2003, 3, 459-478.	0.9	71
108	Engineering the Electronic Structure of Single-Walled Carbon Nanotubes by Chemical Functionalization. <i>ChemPhysChem</i> , 2005, 6, 598-601.	1.0	71

#	ARTICLE	IF	CITATIONS
109	An exchange intercalation mechanism for the formation of a two-dimensional Si structure underneath graphene. <i>Nano Research</i> , 2012, 5, 352-360.	5.8	71
110	Electronic structure and superconductivity of FeSe-related superconductors. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 183201.	0.7	71
111	Graphene Oxide: Physics and Applications. <i>SpringerBriefs in Physics</i> , 2015, , .	0.2	70
112	Sensitive colorimetric detection of glucose and cholesterol by using Au@Ag core-shell nanoparticles. <i>RSC Advances</i> , 2016, 6, 35001-35007.	1.7	70
113	GeAs and SiAs monolayers: Novel 2D semiconductors with suitable band structures. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 95, 149-153.	1.3	70
114	Reverse-Graded 2D Ruddlesden-Popper Perovskites for Efficient Air-Stable Solar Cells. <i>Advanced Energy Materials</i> , 2019, 9, 1900612.	10.2	69
115	Electronic evidence of an insulator-superconductor crossover in single-layer FeSe/SrTiO ₃ films. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 18501-18506.	3.3	67
116	Melting behavior of ultrathin titanium nanowires. <i>Physical Review B</i> , 2003, 67, .	1.1	66
117	2D lateral heterostructures of group-III monochalcogenide: Potential photovoltaic applications. <i>Applied Physics Letters</i> , 2018, 112, .	1.5	66
118	Boron fullerenes with 32-56 atoms: Irregular cage configurations and electronic properties. <i>Chemical Physics Letters</i> , 2010, 501, 16-19.	1.2	65
119	B ₂₈ : the smallest all-boron cage from an ab initio global search. <i>Nanoscale</i> , 2015, 7, 15086-15090.	2.8	65
120	Label-Free Detection of Telomerase Activity in Urine Using Telomerase-Responsive Porous Anodic Alumina Nanochannels. <i>Analytical Chemistry</i> , 2016, 88, 8107-8114.	3.2	64
121	A Stable Bifunctional Catalyst for Rechargeable Zinc-Air Batteries: Iron-Cobalt Nanoparticles Embedded in a Nitrogen-Doped 3D Carbon Matrix. <i>Angewandte Chemie</i> , 2018, 130, 16398-16402.	1.6	64
122	Nonmetal-metal transition in Zn _n (n=2-20) clusters. <i>Physical Review A</i> , 2003, 68, .	1.0	63
123	Curved carbon nanotubes: From unique geometries to novel properties and peculiar applications. <i>Nano Research</i> , 2014, 7, 626-657.	5.8	63
124	Structures and Electronic Properties of V ₃ Si _n (n = 1-10) (T _j = 0 K). <i>Journal of Physical Chemistry C</i> , 2017, 121, 10987-10994.	1.5	63
125	Structural and Electronic Properties of Interfaces in Graphene and Hexagonal Boron Nitride Lateral Heterostructures. <i>Chemistry of Materials</i> , 2016, 28, 5022-5028.	3.2	63
126	Structures and Magnetic Properties of MoS ₂ Grain Boundaries with Antisite Defects. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12261-12269.	1.5	63

#	ARTICLE	IF	CITATIONS
127	A simple, fast, label-free colorimetric method for detection of telomerase activity in urine by using hemin-graphene conjugates. <i>Biosensors and Bioelectronics</i> , 2017, 87, 600-606.	5.3	63
128	Substituted Hantzsch Esters as Versatile Radical Reservoirs in Photoredox Reactions. <i>Advanced Synthesis and Catalysis</i> , 2018, 360, 925-931.	2.1	63
129	N-Doped carbon coating enhances the bifunctional oxygen reaction activity of CoFe nanoparticles for a highly stable Zn-air battery. <i>Journal of Materials Chemistry A</i> , 2020, 8, 21189-21198.	5.2	63
130	Two-dimensional ZnO for the selective photoreduction of CO ₂ . <i>Journal of Materials Chemistry A</i> , 2019, 7, 16294-16303.	5.2	62
131	Structure and electronic properties of cobalt atoms encapsulated in Sin (n=1-13) clusters. <i>Chemical Physics Letters</i> , 2005, 411, 279-284.	1.2	61
132	Adaptive Multiscale Deep Fusion Residual Network for Remote Sensing Image Classification. <i>IEEE Transactions on Geoscience and Remote Sensing</i> , 2019, 57, 8506-8521.	2.7	61
133	Accurate electronic properties and non-linear optical response of two-dimensional MA2Z4. <i>Nanoscale</i> , 2021, 13, 5479-5488.	2.8	61
134	Cage and tube structures of medium-sized zinc oxide clusters (ZnO) _n (n=24, 28, 36, and 48). <i>Journal of Chemical Physics</i> , 2008, 128, 144710.	1.2	60
135	Precisely Constructed Silver Active Sites in Gold Nanoclusters for Chemical Fixation of CO ₂ . <i>Angewandte Chemie - International Edition</i> , 2021, 60, 10573-10576.	7.2	60
136	Tunable Assembly of sp ³ Cross-Linked 3D Graphene Monoliths: A First-Principles Prediction. <i>Advanced Functional Materials</i> , 2013, 23, 5846-5853.	7.8	59
137	The cooperation of Fe ₃ C nanoparticles with isolated single iron atoms to boost the oxygen reduction reaction for Zn-air batteries. <i>Journal of Materials Chemistry A</i> , 2021, 9, 6831-6840.	5.2	59
138	Excellent HER and OER Catalyzing Performance of Se Vacancies in Defects-Engineered PtSe ₂ : From Simulation to Experiment. <i>Advanced Energy Materials</i> , 2022, 12, 2102359.	10.2	59
139	A novel double-helical-kernel evolution pattern of gold nanoclusters: alternate single-stranded growth at both ends. <i>Nanoscale</i> , 2017, 9, 3742-3746.	2.8	58
140	Direct synthesis and in situ characterization of monolayer parallelogrammic rhenium diselenide on gold foil. <i>Communications Chemistry</i> , 2018, 1, .	2.0	58
141	Monolayer group-III monochalcogenides by oxygen functionalization: a promising class of two-dimensional topological insulators. <i>Npj Quantum Materials</i> , 2018, 3, .	1.8	58
142	Dichotomy of the electronic structure and superconductivity between single-layer and double-layer FeSe/SrTiO ₃ films. <i>Nature Communications</i> , 2014, 5, 5047.	5.8	57
143	A Silver Nanocluster Containing Interstitial Sulfur and Unprecedented Chemical Bonds. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 11273-11277.	7.2	57
144	Immobilized trimeric metal clusters: A family of the smallest catalysts for selective CO ₂ reduction toward multi-carbon products. <i>Nano Energy</i> , 2020, 76, 105049.	8.2	56

#	ARTICLE	IF	CITATIONS
145	Controllable Conversion of CO ₂ on Non-Metallic Gold Clusters. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 1919-1924.	7.2	55
146	De novo design of Au ₃₆ (SR) ₂₄ nanoclusters. <i>Nature Communications</i> , 2020, 11, 3349.	5.8	54
147	Structure and magnetic properties of cobalt doped () clusters. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2007, 367, 335-344.	0.9	53
148	Phosphorus quantum dots as visible-light photocatalyst for water splitting. <i>Computational Materials Science</i> , 2017, 130, 56-63.	1.4	53
149	Atomic Sulfur Anchored on Silicene, Phosphorene, and Borophene for Excellent Cycle Performance of Li-S Batteries. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 42836-42844.	4.0	53
150	Active-Site Tailoring of Gold Cluster Catalysts for Electrochemical CO ₂ Reduction. <i>ACS Catalysis</i> , 2021, 11, 11551-11560.	5.5	53
151	Structure and magnetic properties of Co-Cu bimetallic clusters. <i>Physical Review B</i> , 2002, 66, .	1.1	52
152	A Molecular-Cage Strategy Enabling Efficient Chemisorption-Free Electrochemical Interface in Nanostructured Li ₂ S Cathode for Li Metal-Free Rechargeable Cells with High Energy. <i>Advanced Functional Materials</i> , 2019, 29, 1905986.	7.8	51
153	Copper(II) sulfide: a two-dimensional semiconductor with superior oxidation resistance and high carrier mobility. <i>Nanoscale Horizons</i> , 2019, 4, 223-230.	4.1	51
154	Cubic imidazolate frameworks-derived CoFe alloy nanoparticles-embedded N-doped graphitic carbon for discharging reaction of Zn-air battery. <i>Science China Materials</i> , 2020, 63, 327-338.	3.5	51
155	First-principles study of molecular hydrogen dissociation on doped Al ₁₂ X (X = B, Al, C, Si). <i>Tj ETQq1 1.0.784314 rgBT / Ov</i>	1.5	50
156	Synthesis and characteristics of form-stable n-octadecane/expanded graphite composite phase-change materials. <i>Applied Physics A: Materials Science and Processing</i> , 2010, 100, 1143-1148.	1.1	49
157	Atomic structures and electronic properties of phosphorene grain boundaries. <i>2D Materials</i> , 2016, 3, 025008.	2.0	49
158	Initial Growth Mechanism of Blue Phosphorene on Au(111) Surface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 17893-17899.	1.5	48
159	Is the kernel "staples match a key" lock match?. <i>Chemical Science</i> , 2018, 9, 2437-2442.	3.7	48
160	B,N-Doped Defective Carbon Entangled Fe ₃ C Nanoparticles as the Superior Oxygen Reduction Electrocatalyst for Zn-Air Batteries. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 19104-19112.	3.2	48
161	A sacrificial Zn strategy enables anchoring of metal single atoms on the exposed surface of holey 2D molybdenum carbide nanosheets for efficient electrocatalysis. <i>Journal of Materials Chemistry A</i> , 2020, 8, 3071-3082.	5.2	48
162	Boron clusters with 46, 48, and 50 atoms: competition among the core-shell, bilayer and quasi-planar structures. <i>Nanoscale</i> , 2017, 9, 13905-13909.	2.8	47

#	ARTICLE	IF	CITATIONS
163	What is the best density functional to describe water clusters: evaluation of widely used density functionals with various basis sets for (H ₂ O) _n (n=1-10). <i>Theoretical Chemistry Accounts</i> , 2011, 130, 341-352.	0.5	46
164	Ag ₂ Au ₅₀ (PET) ₃₆ Nanocluster: Dimeric Assembly of Au ₂₅ (PET) ₁₈ Enabled by Silver Atoms. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 13941-13946.	7.2	46
165	Computational high-throughput screening of alloy nanoclusters for electrocatalytic hydrogen evolution. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	46
166	Architecting Freestanding Sulfur Cathodes for Superior Room-Temperature Na-S Batteries. <i>Advanced Functional Materials</i> , 2021, 31, 2102280.	7.8	46
167	True Nanocable Assemblies with Insulating BN Nanotube Sheaths and Conducting Cu Nanowire Cores. <i>Journal of Physical Chemistry B</i> , 2006, 110, 2529-2532.	1.2	45
168	Combining Machine Learning Potential and Structure Prediction for Accelerated Materials Design and Discovery. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8710-8720.	2.1	45
169	Elastic properties of vanadium-based alloys from first-principles theory. <i>Physical Review B</i> , 2012, 86, .	1.1	44
170	Crystal-Phase-Mediated Restructuring of Pt on TiO ₂ with Tunable Reactivity: Redispersion versus Reshaping. <i>ACS Catalysis</i> , 2022, 12, 3634-3643.	5.5	44
171	Fluorescent Gold Nanoclusters with Interlocked Staples and a Fully Thiolate-Bound Kernel. <i>Angewandte Chemie</i> , 2016, 128, 11739-11743.	1.6	42
172	Synthesis of shape-stabilized paraffin/silicon dioxide composites as phase change material for thermal energy storage. <i>Journal of Materials Science</i> , 2010, 45, 1672-1676.	1.7	41
173	Point defects in group III nitrides: A comparative first-principles study. <i>Journal of Applied Physics</i> , 2019, 125, .	1.1	41
174	Excitonic Au ₄ Ru ₂ (PPh ₃) ₂ (SC ₂ H ₄ Ph) ₈ cluster for light-driven dinitrogen fixation. <i>Chemical Science</i> , 2020, 11, 2440-2447.	1.7	41
175	Low-dimensional non-metal catalysts: principles for regulating p-orbital-dominated reactivity. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	41
176	Ab initio-predicted micro-mechanical performance of refractory high-entropy alloys. <i>Scientific Reports</i> , 2015, 5, 12334.	1.6	40
177	Electronic Structures of Germanene on MoS ₂ : Effect of Substrate and Molecular Adsorption. <i>Journal of Physical Chemistry C</i> , 2016, 120, 21691-21698.	1.5	40
178	Scalable Production of Freestanding Few-Layer 12-Borophene Single Crystalline Sheets as Efficient Electrocatalysts for Lithium-Sulfur Batteries. <i>ACS Nano</i> , 2021, 15, 17327-17336.	7.3	40
179	Density Functional Theory Modeling of Multilayer Epitaxial-Graphene Oxide. <i>Accounts of Chemical Research</i> , 2014, 47, 3331-3339.	7.6	39
180	Sustainable S cathodes with synergic electrocatalysis for room-temperature Na-S batteries. <i>Journal of Materials Chemistry A</i> , 2021, 9, 566-574.	5.2	39

#	ARTICLE	IF	CITATIONS
181	Magic structures of helical multishell zirconium nanowires. <i>Physical Review B</i> , 2002, 65, .	1.1	38
182	Tunable optical properties of icosahedral, dodecahedral, and tetrahedral clusters. <i>Physical Review B</i> , 2005, 71, .	1.1	38
183	Unique Transformation from Graphene to Carbide on Re(0001) Induced by Strong Carbon-Metal Interaction. <i>Journal of the American Chemical Society</i> , 2017, 139, 17574-17581.	6.6	38
184	Two-dimensional spin-valley-coupled Dirac semimetals in functionalized SbAs monolayers. <i>Materials Horizons</i> , 2019, 6, 781-787.	6.4	38
185	Controlling the synthesis of uniform electron-deficient Pd clusters for superior hydrogen production from formic acid. <i>Journal of Materials Chemistry A</i> , 2019, 7, 10363-10371.	5.2	38
186	Growth control, interface behavior, band alignment, and potential device applications of 2D lateral heterostructures. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1353.	6.2	37
187	Selective C-C Coupling by Spatially Confined Dimeric Metal Centers. <i>IScience</i> , 2020, 23, 101051.	1.9	37
188	Point defects in epitaxial silicene on Ag(111) surfaces. <i>2D Materials</i> , 2016, 3, 025034.	2.0	35
189	Giant magnetic anisotropy of a 5d transition metal decorated two-dimensional polyphthalocyanine framework. <i>Journal of Materials Chemistry C</i> , 2016, 4, 2147-2154.	2.7	35
190	Defects and oxidation of group-III monochalcogenide monolayers. <i>Journal of Chemical Physics</i> , 2017, 147, 104709.	1.2	35
191	Mass spectrometric and first principles study of Aln clusters. <i>Solid State Communications</i> , 2002, 122, 543-547.	0.9	34
192	Electronic and transport gaps of graphene opened by grain boundaries. <i>Journal of Applied Physics</i> , 2012, 112, .	1.1	34
193	Mechanical properties of bilayer graphene with twist and grain boundaries. <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	34
194	Low-Energy Structures of Binary Pt-Sn Clusters from Global Search Using Genetic Algorithm and Density Functional Theory. <i>Journal of Cluster Science</i> , 2015, 26, 389-409.	1.7	34
195	Selecting electrode materials for monolayer ReS ₂ with an Ohmic contact. <i>Journal of Materials Chemistry C</i> , 2018, 6, 6764-6770.	2.7	34
196	Defective Graphene on the Transition-Metal Surface: Formation of Efficient Bifunctional Catalysts for Oxygen Evolution/Reduction Reactions in Alkaline Media. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 17410-17415.	4.0	34
197	N-doped carbon-coated Co ₃ O ₄ nanosheet array/carbon cloth for stable rechargeable Zn-air batteries. <i>Science China Materials</i> , 2019, 62, 624-632.	3.5	34
198	The Evolution in Catalytic Activity Driven by Periodic Transformation in the Inner Sites of Gold Clusters. <i>Advanced Functional Materials</i> , 2019, 29, 1904242.	7.8	33

#	ARTICLE	IF	CITATIONS
199	Oxygen Evolution Reaction over the Au/YSZ Interface at High Temperature. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 4617-4621.	7.2	33
200	Optimally stuffed fullerene structures of silicon nanoclusters. <i>Physical Review B</i> , 2005, 71, .	1.1	32
201	First-principles study of transition metal doped Li ₂ S as cathode materials in lithium batteries. <i>Journal of Renewable and Sustainable Energy</i> , 2012, 4, .	0.8	32
202	Two-dimensional intrinsic ferromagnets with high Curie temperatures: synthesis, physical properties and device applications. <i>Journal of Materials Chemistry C</i> , 2021, 9, 6103-6121.	2.7	32
203	Epitaxial growth of an atom-thin layer on a LiNi _{0.5} Mn _{1.5} O ₄ cathode for stable Li-ion battery cycling. <i>Nature Communications</i> , 2022, 13, 1565.	5.8	32
204	Application of Hantzsch Ester and Meyer Nitrile in Radical Alkynylation Reactions. <i>Organic Letters</i> , 2018, 20, 6906-6909.	2.4	31
205	Exceptional Electrochemical HER Performance with Enhanced Electron Transfer between Ru Nanoparticles and Single Atoms Dispersed on a Carbon Substrate. <i>Angewandte Chemie</i> , 2021, 133, 16180-16186.	1.6	31
206	MXene and MBene as efficient catalysts for energy conversion: roles of surface, edge and interface. <i>JPhys Energy</i> , 2021, 3, 012002.	2.3	31
207	Band gap opening in bilayer silicene by alkali metal intercalation. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 475303.	0.7	30
208	Mo Concentration Controls the Morphological Transitions from Dendritic to Semicompact, and to Compact Growth of Monolayer Crystalline MoS ₂ on Various Substrates. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 42751-42759.	4.0	30
209	Electrochemical Hydrogenation with Gaseous Ammonia. <i>Angewandte Chemie</i> , 2019, 131, 1773-1777.	1.6	30
210	Structure, Electrode Voltage and Activation Energy of LiMn _x Co _y Ni _{1-x-y} O ₂ Solid Solutions as Cathode Materials for Li Batteries from First-Principles. <i>Journal of the Electrochemical Society</i> , 2012, 159, A1203-A1208.	1.3	29
211	Goldâ€ƒDoping of Doubleâ€ƒCrown Pd Nanoclusters. <i>Chemistry - A European Journal</i> , 2017, 23, 18187-18192.	1.7	29
212	Cd-driven surface reconstruction and photodynamics in gold nanoclusters. <i>Chemical Science</i> , 2021, 12, 3290-3294.	3.7	29
213	Cluster-assembled materials based onNa ₆ Pb. <i>Physical Review B</i> , 2003, 68, .	1.1	28
214	Stability and magnetic properties of transition metal atoms endohedral B _n N _n â€ƒ(n=12â€ƒ28) cages. <i>Journal of Chemical Physics</i> , 2008, 128, 084306.	1.2	28
215	Ultrasensitive photometric and visual determination of organophosphorus pesticides based on the inhibition of enzyme-triggered formation of core-shell gold-silver nanoparticles. <i>Mikrochimica Acta</i> , 2016, 183, 2941-2948.	2.5	28
216	3D Network nanostructured NiCoP nanosheets supported on N-doped carbon coated Ni foam as a highly active bifunctional electrocatalyst for hydrogen and oxygen evolution reactions. <i>Frontiers of Chemical Science and Engineering</i> , 2018, 12, 417-424.	2.3	28

#	ARTICLE	IF	CITATIONS
217	Engineering magnetic anisotropy in two-dimensional magnetic materials. <i>Advances in Physics: X</i> , 2018, 3, 1432415.	1.5	28
218	Silicene catalysts for CO ₂ hydrogenation: the number of layers controls selectivity. <i>Nanoscale</i> , 2019, 11, 7734-7743.	2.8	28
219	Wavelength-Tunable Optical Fiber Localized Surface Plasmon Resonance Biosensor via a Diblock Copolymer-Templated Nanorod Monolayer. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 50929-50940.	4.0	28
220	Tuning the electronic properties of bilayer black phosphorene with the twist angle. <i>Journal of Materials Chemistry C</i> , 2020, 8, 6264-6272.	2.7	28
221	Superatomic Signature and Reactivity of Silver Clusters with Oxygen: Double Magic Ag ₁₇ with Geometric and Electronic Shell Closure. <i>CCS Chemistry</i> , 2021, 3, 219-229.	4.6	28
222	Structural, Electronic, and Magnetic Properties of Small Vanadium Clusters. <i>Physica Status Solidi (B): Basic Research</i> , 1999, 215, 1127-1135.	0.7	27
223	Structural and electronic properties of Sbn (n=2-10) clusters using density-functional theory. <i>Physical Review A</i> , 2005, 72, .	1.0	27
224	Graphene oxide and lithium amidoborane: a new way to bridge chemical and physical approaches for hydrogen storage. <i>Journal of Materials Chemistry A</i> , 2013, 1, 8016.	5.2	27
225	Strong Adlayer-Substrate Interactions Break the Patching Growth of h-BN onto Graphene on Re(0001). <i>ACS Nano</i> , 2017, 11, 1807-1815.	7.3	27
226	Structures and electronic properties of B ₃ Si ⁿ (n = 4-10) clusters: A combined ab initio and experimental study. <i>Journal of Chemical Physics</i> , 2017, 146, 044306.	1.2	27
227	Which Density Functional Should Be Used to Describe Protonated Water Clusters?. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3117-3127.	1.1	27
228	Photodriven Catalytic Hydrogenation of CO ₂ to CH ₄ with Nearly 100% Selectivity over Ag ₂₅ Clusters. <i>Nano Letters</i> , 2021, 21, 8693-8700.	4.5	27
229	Density-functional study of structural and electronic properties of Al _n N (n=2-12) clusters. <i>Physical Review A</i> , 2005, 72, .	1.0	26
230	The isolable matryoshka nesting doll icosahedral cluster [As@Ni ₁₂ @As ₂₀] ³⁺ as a "superatom" analogy with the jellium cluster Al ₁₃ ⁺ generated in the gas phase by laser vaporization. <i>Chemical Communications</i> , 2006, , 4204-4205.	2.2	26
231	Halogen-doping in LiCoO ₂ cathode materials for Li-ion batteries: insights from ab initio calculations. <i>RSC Advances</i> , 2015, 5, 107326-107332.	1.7	26
232	Tunable Thermal Conductivity of Silicene by Germanium Doping. <i>Journal of Superconductivity and Novel Magnetism</i> , 2016, 29, 717-720.	0.8	26
233	Long life rechargeable Li-O ₂ batteries enabled by enhanced charge transfer in nanocable-like Fe@N-doped carbon nanotube catalyst. <i>Science China Materials</i> , 2017, 60, 415-426.	3.5	26
234	Optimization of photocarrier dynamics and activity in phosphorene with intrinsic defects for nitrogen fixation. <i>Journal of Materials Chemistry A</i> , 2020, 8, 20570-20580.	5.2	26

#	ARTICLE	IF	CITATIONS
235	Vacancy Engineering of Iron-Doped $W_{18}O_{49}$ Nanoreactors for Low-Barrier Electrochemical Nitrogen Reduction. <i>Angewandte Chemie</i> , 2020, 132, 7426-7431.	1.6	26
236	2D lateral heterostructures of monolayer and bilayer phosphorene. <i>Journal of Materials Chemistry C</i> , 2017, 5, 2291-2300.	2.7	25
237	Interaction between helium and intrinsic point defects in 3C-SiC single crystal. <i>Journal of Applied Physics</i> , 2017, 121, .	1.1	25
238	Identifying the Non-Identical Outermost Selenium Atoms and Invariable Band Gaps across the Grain Boundary of Anisotropic Rhenium Diselenide. <i>ACS Nano</i> , 2018, 12, 10095-10103.	7.3	25
239	Realization of Strained Stanene by Interface Engineering. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1558-1565.	2.1	25
240	Reactivity and Lability Modulated by a Valence Electron Moving in and out of 25-Atom Gold Nanoclusters. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 21135-21142.	7.2	25
241	Enhanced Ferromagnetism of Cr_3 Bilayer by Self-Intercalation*. <i>Chinese Physics Letters</i> , 2020, 37, 107506.	1.3	25
242	Evolution from superatomic $Au_{24}Ag_{20}$ monomers into molecular-like $Au_{43}Ag_{38}$ dimeric nanoclusters. <i>Chemical Science</i> , 2022, 13, 2778-2782.	3.7	25
243	Nanocables made of a transition metal wire and boron nitride sheath: Density functional calculations. <i>Physical Review B</i> , 2006, 74, .	1.1	24
244	Possible Formation of Graphyne on Transition Metal Surfaces: A Competition with Graphene from the Chemical Potential Point of View. <i>Journal of Physical Chemistry C</i> , 2016, 120, 14699-14705.	1.5	24
245	Reactions of Copper and Silver Cations with Carbon Dioxide: An Infrared Photodissociation Spectroscopic and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3220-3226.	1.1	24
246	A Silver Nanocluster Containing Interstitial Sulfur and Unprecedented Chemical Bonds. <i>Angewandte Chemie</i> , 2018, 130, 11443-11447.	1.6	24
247	Hydrated Sodium Ion Clusters $[Na+(H_2O)_n]$ ($n = 1-6$): An ab initio Study on Structures and Non-covalent Interaction. <i>Frontiers in Chemistry</i> , 2019, 7, 624.	1.8	24
248	High-Curie-temperature ferromagnetism in bilayer Cr_3 on bulk semiconducting substrates. <i>Physical Review Materials</i> , 2020, 4, .	0.9	24
249	Magnetic properties of transition-metal impurities in silicon quantum dots. <i>Physical Review B</i> , 2007, 75, .	1.1	23
250	Structural growth sequences and electronic properties of manganese-doped germanium clusters: $MnGe_n$ ($2 \leq n \leq 15$). <i>Journal of Physics Condensed Matter</i> , 2008, 20, 335223.	0.7	23
251	Design of Three-shell Icosahedral Matryoshka Clusters $A@B_{12}@A_{20}$ ($A = Sn, Pb; B = Mg, Zn, Cd, Mn$). <i>Scientific Reports</i> , 2014, 4, 6915.	1.6	23
252	Two-dimensional CaO alloys: a promising class of 2D materials for electronic devices. <i>Nanoscale</i> , 2016, 8, 8910-8918.	2.8	23

#	ARTICLE	IF	CITATIONS
253	Structural Evolution and Superatoms in Molybdenum Atom Stabilized Boron Clusters: MoBn ($n=10-24$). Journal of Cluster Science, 2018, 29, 847-852.	1.7	23
254	Two-Dimensional AXenes: A New Family of Room-Temperature d^0 Ferromagnets and Their Structural Phase Transitions. Journal of Physical Chemistry Letters, 2019, 10, 7753-7759.	2.1	23
255	Manipulating the assembled structure of atomically thin CoSe ₂ nanomaterials for enhanced water oxidation catalysis. Nano Energy, 2019, 57, 371-378.	8.2	23
256	Efficient Photoexcited Charge Separation at the Interface of a Novel 0D/2D Heterojunction: A Time-Dependent Ultrafast Dynamic Study. Journal of Physical Chemistry Letters, 2021, 12, 2312-2319.	2.1	23
257	Kondo Holes in the Two-Dimensional Itinerant Ising Ferromagnet Fe ₃ GeTe ₂ . Nano Letters, 2021, 21, 6117-6123.	4.5	23
258	Electronic and magnetic properties of manganese and iron-doped GaAs nanocages ($n=7-12$). Journal of Chemical Physics, 2008, 129, 044908.	1.2	22
259	First-principles studies on the thermal decomposition behavior of FOX-7. High Pressure Research, 2010, 30, 301-309.	0.4	22
260	Ideal strength of random alloys from first principles. Physical Review B, 2013, 87, .	1.1	22
261	The precise editing of surface sites on a molecular-like gold catalyst for modulating regioselectivity. Chemical Science, 2020, 11, 8000-8004.	3.7	22
262	Anionic Copper Clusters Reacting with NO: An Open-Shell Superatom Cu ₁₈ . Journal of Physical Chemistry Letters, 2020, 11, 5807-5814.	2.1	22
263	Progress of tubulin polymerization activity detection methods. Bioorganic and Medicinal Chemistry Letters, 2021, 37, 127698.	1.0	22
264	First-Principles Study of the Atomic Structures and Catalytic Properties of Monolayer TaS ₂ with Intrinsic Defects. Journal of Physical Chemistry C, 2021, 125, 10362-10369.	1.5	22
265	A-Site Cation Substitutions in Strained Y-Doped BaZrO ₃ Multilayer Films Leading to Fast Proton Transport Pathways. Journal of Physical Chemistry C, 2016, 120, 8387-8391.	1.5	21
266	A Ternary Alloy Substrate to Synthesize Monolayer Graphene with Liquid Carbon Precursor. ACS Nano, 2017, 11, 1371-1379.	7.3	21
267	Interaction between Post-Graphene Group-IV Honeycomb Monolayers and Metal Substrates: Implication for Synthesis and Structure Control. Journal of Physical Chemistry C, 2017, 121, 5123-5129.	1.5	21
268	Ionic and superionic phases in ammonia dihydrate $NH_3 \cdot H_2O$ under high pressure. Physical Review B, 2017, 95, 041111.	1.1	21
269	Silicon Nanocages for Selective Carbon Dioxide Conversion under Visible Light. Journal of Physical Chemistry C, 2019, 123, 9973-9980.	1.5	21
270	Hollow Co ₃ O ₄ Nanosphere Surrounded by N-Doped Graphitic Carbon Filled within Multilayer-Sandwiched Graphene Network: A High-Performance Anode for Lithium Storage. Inorganic Chemistry, 2019, 58, 3416-3424.	1.9	21

#	ARTICLE	IF	CITATIONS
271	Core-Shell MnO ₂ Nanotubes@Nickel-Cobalt-Zinc Hydroxide Nanosheets for Supercapacitive Energy Storage. ACS Applied Nano Materials, 2020, 3, 7462-7473.	2.4	21
272	Dual-Constrained Sulfur in FeS ₂ @C Nanostructured Lithium-Sulfide Batteries. ACS Applied Energy Materials, 2020, 3, 10950-10960.	2.5	21
273	Competition between tubular, planar and cage geometries: a complete picture of structural evolution of B _n (n = 31-50) clusters. Physical Chemistry Chemical Physics, 2020, 22, 12959-12966.	1.3	21
274	2D tetragonal transition-metal phosphides: an ideal platform to screen metal shrouded crystals for multifunctional applications. Nanoscale, 2020, 12, 6776-6784.	2.8	21
275	Precisely Constructed Silver Active Sites in Gold Nanoclusters for Chemical Fixation of CO ₂ . Angewandte Chemie, 2021, 133, 10667-10670.	1.6	21
276	Layer-dependent magnetic phase diagram in FenGeTe2 (3 ≤ n ≤ 7) ultrathin films. Communications Physics, 2022, 5, .	2.0	21
277	Adsorption of selected gases on metal-organic frameworks and covalent organic frameworks: A comparative grand canonical Monte Carlo simulation. Journal of Applied Physics, 2012, 111, 112628.	1.1	20
278	Improved stability of water clusters (H ₂ O) ₃₀₋₄₈ : a Monte Carlo search coupled with DFT computations. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	20
279	Chemical Structure of Oxidized Multilayer Epitaxial Graphene: A Density Functional Theory Study. Journal of Physical Chemistry C, 2013, 117, 6267-6274.	1.5	20
280	Structural evolution and magnetic properties of anionic clusters Cr ₂ Ge _n (n = 14): photoelectron spectroscopy and density functional theory computation. Journal of Physics Condensed Matter, 2018, 30, 335501.		20
281	Room temperature electrofreezing of water yields a missing dense ice phase in the phase diagram. Nature Communications, 2019, 10, 1925.	5.8	20
282	Chemical-Free Electrochemical Deuteration Reaction using Deuterium Oxide. Angewandte Chemie, 2020, 132, 14066-14071.	1.6	20
283	CO ₂ reduction on p-block metal oxide overlayers on metal substrates: 2D MgO as a prototype. Journal of Materials Chemistry A, 2020, 8, 5688-5698.	5.2	20
284	Visible-light overall water splitting on g-C ₃ N ₄ decorated by subnanometer oxide clusters. Materials Today Physics, 2021, 16, 100312.	2.9	20
285	Stability and Vibrations of Guest Molecules in the Type II Clathrate Hydrate: A First-Principles Study of Solid Phase. Journal of Physical Chemistry A, 2015, 119, 7063-7069.	1.1	19
286	Atomistic understanding of the lateral growth of graphene from the edge of an h-BN domain: towards a sharp in-plane junction. Nanoscale, 2017, 9, 3585-3592.	2.8	19
287	Tuning Schottky barriers for monolayer GaSe FETs by exploiting a weak Fermi level pinning effect. Physical Chemistry Chemical Physics, 2018, 20, 21732-21738.	1.3	19
288	Giant Thickness-Tunable Bandgap and Robust Air Stability of 2D Palladium Diselenide. Small, 2020, 16, e2000754.	5.2	19

#	ARTICLE	IF	CITATIONS
289	Catalytic Hydrodenitrogenation of Pyridine under Hydrothermal Conditions: A Comprehensive Study. ACS Sustainable Chemistry and Engineering, 2021, 9, 362-374.	3.2	19
290	Film Structure of Epitaxial Graphene Oxide on SiC: Insight on the Relationship Between Interlayer Spacing, Water Content, and Intralayer Structure. Advanced Materials Interfaces, 2014, 1, 1300106.	1.9	18
291	An Electrochemical Cinnamyl C-H Amination Reaction Using Carbonyl Sulfamate. Chinese Journal of Chemistry, 2019, 37, 570-574.	2.6	18
292	Structure Evolution of Transition Metal-doped Gold Clusters M@Au ₁₂ (M = 3d-5d): Across the Periodic Table. Journal of Physical Chemistry C, 2020, 124, 7449-7457.	1.5	18
293	Electrocatalytic and photocatalytic applications of atomically precise gold-based nanoclusters. Science China Chemistry, 2021, 64, 1065-1075.	4.2	18
294	Tacrolimus Enhances the Invasion Potential of Hepatocellular Carcinoma Cells and Promotes Lymphatic Metastasis in a Rat Model of Hepatocellular Carcinoma: Involvement of Vascular Endothelial Growth Factor-C. Transplantation Proceedings, 2011, 43, 2747-2754.	0.3	17
295	Anomalous High-Energy Waterfall-Like Electronic Structure in 5d Transition Metal Oxide Sr ₂ IrO ₄ with a Strong Spin-Orbit Coupling. Scientific Reports, 2015, 5, 13036.	1.6	17
296	Novel Magnetic Monolayers of Transition Metal Silicide. Journal of Superconductivity and Novel Magnetism, 2015, 28, 1755-1758.	0.8	17
297	Electric field and strain tunable electronic structures in monolayer Black Phosphorus. Computational Materials Science, 2016, 112, 297-303.	1.4	17
298	Magnetism in the p-type Monolayer II-VI semiconductors SrS and SrSe. Scientific Reports, 2017, 7, 45869.	1.6	17
299	CoWO ₄ nanoparticles wrapped by RGO as high capacity anode material for lithium ion batteries. Rare Metals, 2017, 36, 411-417.	3.6	17
300	Revisit of large-gap Si ₁₆ clusters encapsulating group IV metal atoms (Ti, Zr, Hf). Journal of Computational Chemistry, 2018, 39, 2268-2272.	1.5	17
301	Foreign atom encapsulated Au ₁₂ golden cages for catalysis of CO oxidation. Physical Chemistry Chemical Physics, 2019, 21, 10587-10593.	1.3	17
302	Precisely modulating the surface sites on atomically monodispersed gold-based nanoclusters for controlling their catalytic performances. Nanoscale, 2020, 12, 18004-18012.	2.8	17
303	Robust spin manipulation in 2D organometallic Kagome lattices: a first-principles study. Physical Chemistry Chemical Physics, 2020, 22, 11045-11052.	1.3	17
304	Surface thermal stability of nickel clusters. Physica Status Solidi (B): Basic Research, 1996, 193, 355-361.	0.7	16
305	Confining a bi-enzyme inside the nanochannels of a porous aluminum oxide membrane for accelerating the enzymatic reactions. Chemical Communications, 2017, 53, 2673-2676.	2.2	16
306	An electrocatalyst with anti-oxidized capability for overall water splitting. Nano Research, 2018, 11, 3411-3418.	5.8	16

#	ARTICLE	IF	CITATIONS
307	An ultralow-density porous ice with the largest internal cavity identified in the water phase diagram. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 12684-12691.	3.3	16
308	Evolution of atomic structures of Sn _N , Sn _N ⁺ , and Sn _N Cl ⁺ clusters (N = 1-10). <i>Journal of Chemical Physics</i> , 2019, 150, 124701.	1.2	16
309	Tunable bending modulus and bending limit of oxidized graphene. <i>Nanoscale</i> , 2020, 12, 1623-1628.	2.8	16
310	Atomic Wires of Transition Metal Chalcogenides: A Family of 1D Materials for Flexible Electronics and Spintronics. <i>JACS</i> , 2021, 143, 147-155.	3.6	16
311	Temperature-dependent hardness of zinc-blende structured covalent materials. <i>Science China Materials</i> , 2021, 64, 2280-2288.	3.5	16
312	Insight on the active sites of CoNi alloy embedded in N-doped carbon nanotubes for oxygen reduction reaction. <i>Science China Materials</i> , 2021, 64, 2719-2728.	3.5	16
313	Mechanically Induced Switching between Two Discrete Conductance States: A Potential Single-Molecule Variable Resistor. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 57646-57653.	4.0	16
314	Regulating the Electronic Configuration of Supported Iron Nanoparticles for Electrochemical Catalytic Nitrogen Fixation. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	16
315	Electronic properties and chemical trends of the arsenic and silicon impurities in CdTe . <i>Physical Review B</i> , 2007, 76, .	1.1	15
316	Stability and magnetic properties of Fe encapsulating in silicon nanotubes. <i>Nanotechnology</i> , 2007, 18, 235705.	1.3	15
317	Insight into the initial oxidation of H_2Si from first-principles thermodynamics. <i>Physical Review B</i> , 2013, 87, .	1.1	15
318	Structures and Spectroscopic Properties of $\text{F}_2\text{H}_2\text{O}$ Clusters from a Global Search Based On Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3413-3422.	1.1	15
319	Three-dimensional phase field simulation of intragranular void formation and thermal conductivity in irradiated Fe . <i>Journal of Materials Science</i> , 2018, 53, 11002-11014.	1.7	15
320	Revisit the landscape of protonated water clusters $\text{H}^+(\text{H}_2\text{O})_n$ with $n = 10-17$: An <i>ab initio</i> global search. <i>Journal of Chemical Physics</i> , 2018, 148, 174305.	1.2	15
321	Numerical simulation of flow past stationary and oscillating deformable circles with fluid-structure interaction. <i>Experimental and Computational Multiphase Flow</i> , 2020, 2, 151-161.	1.9	15
322	MBLT: Learning Motion and Background for Vehicle Tracking in Satellite Videos. <i>IEEE Transactions on Geoscience and Remote Sensing</i> , 2022, 60, 1-15.	2.7	15
323	Dithiol Self-Assembled Monolayer Based Electrochemical Surface Plasmon Resonance Optical Fiber Sensor for Selective Heavy Metal Ions Detection. <i>Journal of Lightwave Technology</i> , 2021, 39, 4034-4040.	2.7	15
324	<i>Ab initio</i> global optimization of clusters. <i>Chemical Modelling</i> , 2015, , 249-292.	0.2	15

#	ARTICLE	IF	CITATIONS
325	Ag ₂₄ Au cluster decorated mesoporous Co ₃ O ₄ for highly selective and efficient photothermal CO ₂ hydrogenation. <i>Nano Research</i> , 2022, 15, 4965-4972.	5.8	15
326	Enhanced thermoelectric properties of graphene oxide patterned by nanoroads. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 10607-10615.	1.3	14
327	The Synthesis of Chiral Ag ₄ Pd ₂ (SR) ₈ by Nonreplaced Galvanic Reaction. <i>Particle and Particle Systems Characterization</i> , 2019, 36, 1900003.	1.2	14
328	Structures, stabilities and electronic properties of TimSi ^m n (m = 1, 2, n = 14, 20) clusters: a combined ab initio and experimental study. <i>European Physical Journal Plus</i> , 2020, 135, 1.	1.2	14
329	Imaging Vacancy Defects in Single-Layer Chromium Triiodide. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2199-2205.	2.1	14
330	Density functional study of onion-skin-like [As@Ni ₁₂ As ₂₀] ³⁺ and [Sb@Pd ₁₂ Sb ₂₀] ³⁺ cluster ions. <i>Chemical Physics Letters</i> , 2004, 396, 161-166.	1.2	13
331	Thermal decomposition behaviour of RDX by first-principles molecular dynamics simulation. <i>Molecular Simulation</i> , 2008, 34, 961-965.	0.9	13
332	Temperature and coverage effects on the stability of epitaxial silicene on Ag(111) surfaces. <i>Applied Surface Science</i> , 2017, 409, 97-101.	3.1	13
333	Medium-sized $\{m\text{Si}_n\}$ ($n = 14, 20$) clusters: a combined study of photoelectron spectroscopy and DFT calculations. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 354002.	0.7	13
334	Dual transition metal doped germanium clusters for catalysis of CO oxidation. <i>Journal of Alloys and Compounds</i> , 2019, 806, 698-704.	2.8	13
335	Atomically Sharp Dual Grain Boundaries in 2D WS ₂ Bilayers. <i>Small</i> , 2019, 15, e1902590.	5.2	13
336	Carrier Dynamics and Transfer across the CdS/MoS ₂ Interface upon Optical Excitation. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 6544-6550.	2.1	13
337	Control of Photocarrier Separation and Recombination at Bismuth Oxyhalide Interface for Nitrogen Fixation. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 9304-9312.	2.1	13
338	Effects of spin-phonon coupling on two-dimensional ferromagnetic semiconductors: a case study of iron and ruthenium trihalides. <i>Nanoscale</i> , 2021, 13, 7714-7722.	2.8	13
339	Ag Doped Au ₄₄ Nanoclusters for Electrocatalytic Conversion of CO ₂ to CO. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	13
340	Electronic properties of a silicon carbide nanotube under uniaxial tensile strain: a density function theory study. <i>Journal of Nanoparticle Research</i> , 2010, 12, 2919-2928.	0.8	12
341	Novel electronic structures of superlattice composed of graphene and silicene. <i>Materials Research Bulletin</i> , 2014, 50, 268-272.	2.7	12
342	A new family of multifunctional silicon clathrates: Optoelectronic and thermoelectric applications. <i>Journal of Applied Physics</i> , 2017, 121, .	1.1	12

#	ARTICLE	IF	CITATIONS
343	Design of superhalogens using a core-shell structure model. <i>Nanoscale</i> , 2017, 9, 18781-18787.	2.8	12
344	Mechanism of Ce promoting SO ₂ resistance of MnO _x / γ -Al ₂ O ₃ : An experimental and DFT study. <i>Korean Journal of Chemical Engineering</i> , 2017, 34, 2065-2071.	1.2	12
345	Metal-Encapsulated Boron Nitride Nanocages for Solar-Driven Nitrogen Fixation. <i>Journal of Physical Chemistry C</i> , 2020, 124, 23798-23806.	1.5	12
346	Experimental Realization of Two-Dimensional Buckled Lieb Lattice. <i>Nano Letters</i> , 2020, 20, 2537-2543.	4.5	12
347	First-principles calculations of elastic moduli of Ti-Mo-Nb alloys using a cluster-plus-glue-atom model for stable solid solutions. <i>Journal of Materials Science</i> , 2013, 48, 3138-3146.	1.7	11
348	Evolution of boron clusters in iron tetraborides under high pressure: semiconducting and ferromagnetic superhard materials. <i>RSC Advances</i> , 2015, 5, 48012-48023.	1.7	11
349	A strain or electric field induced direct bandgap in ultrathin silicon film and its application in photovoltaics or photocatalysis. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7156-7162.	1.3	11
350	Large magnetic anisotropy in chemically engineered iridium dimer. <i>Communications Physics</i> , 2018, 1, .	2.0	11
351	Monolayered semiconducting GeAsSe and SnSbTe with ultrahigh hole mobility. <i>Frontiers of Physics</i> , 2018, 13, 1.	2.4	11
352	Performance Evaluation of Asphalt Mixture with Nanosized Volcanic Ash Filler. <i>Journal of Transportation Engineering Part B: Pavements</i> , 2018, 144, 04018028.	0.8	11
353	Rational design of two-dimensional hybrid Co/N-doped carbon nanosheet arrays for efficient bi-functional electrocatalysis. <i>Sustainable Energy and Fuels</i> , 2019, 3, 1757-1763.	2.5	11
354	Ligand-protected Au ₄ Ru ₂ and Au ₅ Ru ₂ nanoclusters: distinct structures and implications for site-cooperation catalysis. <i>Chemical Communications</i> , 2020, 56, 12833-12836.	2.2	11
355	Remarkable Role of Grain Boundaries in the Thermal Transport Properties of Phosphorene. <i>ACS Omega</i> , 2020, 5, 17416-17422.	1.6	11
356	Oxidation Behaviors of Two-dimensional Metal Chalcogenides. <i>ChemNanoMat</i> , 2020, 6, 838-849.	1.5	11
357	Enhanced Valley Polarization of Bilayer MoSe ₂ with Variable Stacking Order and Interlayer Coupling. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5879-5888.	2.1	11
358	AB ₂ N monolayer: a direct band gap semiconductor with high and highly anisotropic carrier mobility. <i>Nanoscale</i> , 2022, 14, 930-938.	2.8	11
359	Photoinduced Spin Injection and Ferromagnetism in 2D Group III Monochalcogenides. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 590-597.	2.1	11
360	A first-principle study of the structural and electronic properties of amorphous Cu-Zr alloys. <i>Science China: Physics, Mechanics and Astronomy</i> , 2011, 54, 249-255.	2.0	10

#	ARTICLE	IF	CITATIONS
361	Three dimensional porous SiC for lithium polysulfide trapping. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4005-4011.	1.3	10
362	Rational design of 2D organic magnets with giant magnetic anisotropy based on two-coordinate 5d transition metals. <i>APL Materials</i> , 2020, 8, .	2.2	10
363	Ring-contraction of hantzsch esters and their derivatives to pyrroles <i>via</i> electrochemical extrusion of ethyl acetate out of aromatic rings. <i>Green Chemistry</i> , 2021, 23, 3468-3473.	4.6	10
364	Electric-Field-Driven Negative Differential Conductance in 2D van der Waals Ferromagnet Fe ₃ GeTe ₂ . <i>Nano Letters</i> , 2021, 21, 9233-9239.	4.5	10
365	Transition metal halide nanowires: A family of one-dimensional multifunctional building blocks. <i>Applied Physics Letters</i> , 2022, 120, .	1.5	10
366	Enhanced Fluorescence with Tunable Color in Doped Diphosphine-Protected Gold Nanoclusters. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 5873-5880.	2.1	10
367	Anomalous ideal tensile strength of ferromagnetic Fe and Fe-rich alloys. <i>Physical Review B</i> , 2014, 90, .	1.1	9
368	Tensile strain-induced softening of iron at high temperature. <i>Scientific Reports</i> , 2015, 5, 16654.	1.6	9
369	Mechanical anisotropy and strain-tailored band structures of pentagonal boron nitride monolayers. <i>Journal of Applied Physics</i> , 2017, 122, 094302.	1.1	9
370	Strongly Hole-Doped and Highly Decoupled Graphene on Platinum by Water Intercalation. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3998-4002.	2.1	9
371	Atomic Structures and Electronic Properties of Large-Sized GeN Clusters (N=45, 50, 55, 60, 65, 70) by First-Principles Global Search. <i>Journal of Cluster Science</i> , 2019, 30, 371-377.	1.7	9
372	Three-dimensional borophene: A light-element topological nodal-line semimetal with direction-dependent type-II Weyl fermions. <i>Physical Review B</i> , 2020, 102, .	1.1	9
373	New refractory MAB phases and their 2D derivatives: insight into the effects of valence electron concentration and chemical composition. <i>RSC Advances</i> , 2020, 10, 25836-25847.	1.7	9
374	Aminomethyl-Functionalized Carbon Nanotubes as a Host of Small Sulfur Clusters for High-Performance Lithium-Sulfur Batteries. <i>ChemSusChem</i> , 2020, 13, 2761-2768.	3.6	9
375	Single O Atom Doped Ag Cluster Cations for CO Oxidation: An O-Doped Superatom Ag ₁₅ O ⁺ with Remarkable Stability. <i>Journal of Physical Chemistry C</i> , 2021, 125, 7067-7076.	1.5	9
376	Eliminating Edge Electronic and Phonon States of Phosphorene Nanoribbon by Unique Edge Reconstruction. <i>Small</i> , 2022, 18, e2105130.	5.2	9
377	Prediction of superconductivity in bilayer borophenes. <i>RSC Advances</i> , 2021, 11, 40220-40227.	1.7	9
378	Transition-Metal Interlink Neural Network: Machine Learning of 2D Metal-Organic Frameworks with High Magnetic Anisotropy. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 33726-33733.	4.0	9

#	ARTICLE	IF	CITATIONS
379	Tuning the structures of two-dimensional cuprous oxide confined on Au(111). <i>Nano Research</i> , 2018, 11, 5957-5967.	5.8	8
380	Solar Driven CO ₂ Hydrogenation on Ti-Doped Silicon Nanocages. <i>Journal of Cluster Science</i> , 2020, 31, 627-635.	1.7	8
381	Numerical simulation of flow past a triangular prism with fluid-structure interaction. <i>Engineering Applications of Computational Fluid Mechanics</i> , 2020, 14, 462-476.	1.5	8
382	Compositionally Designed 2D Ruddlesden-Popper Perovskites for Efficient and Stable Solar Cells. <i>Solar Rrl</i> , 2021, 5, 2000661.	3.1	8
383	Selective CO ₂ conversion tuned by periodicities in Au _{8n+4} (TBBT) _{4n+8} nanoclusters. <i>Nano Research</i> , 2021, 14, 807-813.	5.8	8
384	New boron nitride monolith phases from high-pressure compression of double-walled boron nitride nanotubes. <i>Journal of Chemical Physics</i> , 2021, 154, 134702.	1.2	8
385	Ab initio analytic calculation of point defects in AlGa _N /Ga _N heterointerfaces. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 035002.	0.7	8
386	Electrical Conductance of Graphene with Point Defects. <i>Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica</i> , 2019, 35, 1142-1149.	2.2	8
387	FeSi ₂ : a two-dimensional ferromagnet containing planar hexacoordinate Fe atoms. <i>Nanoscale Advances</i> , 2022, 4, 600-607.	2.2	8
388	Dramatically Enhanced Second Harmonic Generation in Janus Group-III Chalcogenide Monolayers. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	8
389	Quantum conductance of armchair carbon nanocoils: roles of geometry effects. <i>Science China: Physics, Mechanics and Astronomy</i> , 2011, 54, 841-845.	2.0	7
390	Effect of iron on high pressure elasticity of hydrous wadsleyite and ringwoodite by first-principles simulation. <i>High Pressure Research</i> , 2012, 32, 385-395.	0.4	7
391	Ground state structures, electronic and optical properties of medium-sized Nan + (n = 9, 15, 21, 26, 31). <i>Tj ETQq1 1 0.784314 rgBT / 0.6</i>	0.6	7
392	Oxidation of step edges on vicinal 4H-SiC(0001) surfaces. <i>Applied Physics Letters</i> , 2013, 103, 211603.	1.5	7
393	Dissociation mechanism of gas hydrates (I, II, H) of alkane molecules: a comparative molecular dynamics simulation. <i>Molecular Simulation</i> , 2015, 41, 1086-1094.	0.9	7
394	Magnetic Anisotropy of Small Irn Clusters (n=5). <i>Journal of Cluster Science</i> , 2016, 27, 935-946.	1.7	7
395	Surface-functionalized cation exchange membrane by covalent immobilization of polyelectrolyte multilayer for effective separation of mono- and multivalent cations. <i>Separation Science and Technology</i> , 2016, 51, 2823-2832.	1.3	7
396	Ultra-thin Ga nanosheets: analogues of high pressure Ga(III). <i>Nanoscale</i> , 2019, 11, 17201-17205.	2.8	7

#	ARTICLE	IF	CITATIONS
397	Reactivity and Lability Modulated by a Valence Electron Moving in and out of 25-Atom Gold Nanoclusters. <i>Angewandte Chemie</i> , 2020, 132, 21321-21328.	1.6	7
398	An Au ₈ Cluster Fortified by Four Ferrocenes. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6061-6067.	1.1	7
399	Searching for cluster Lego blocks for three-dimensional and two-dimensional assemblies. <i>Physical Review Materials</i> , 2021, 5, .	0.9	7
400	The reactivity of O ₂ with copper cluster anions Cu ⁿ⁻ (n=7-20): Leveling effect of spin accommodation. <i>Chinese Chemical Letters</i> , 2022, 33, 995-1000.	4.8	7
401	Topologically protected states and half-metal behaviors: Defect-strain synergy effects in two-dimensional antimonene. <i>Physical Review Materials</i> , 2019, 3, .	0.9	7
402	Tuning the electronic and optical properties of hydrogen-terminated Si nanocluster by uniaxial compression. <i>Journal of Nanoparticle Research</i> , 2012, 14, 1.	0.8	6
403	Carbon clusters near the step of Rh surface: implication for the initial stage of graphene nucleation. <i>European Physical Journal D</i> , 2013, 67, 1.	0.6	6
404	Solvent-Based Atomistic Theory for Doping Colloidal-Synthesized Quantum Dots via Cation Exchange. <i>Journal of Physical Chemistry C</i> , 2016, 120, 27085-27090.	1.5	6
405	Ab initio molecular dynamics study of fluid H ₂ O-CO ₂ mixture in broad pressure-temperature range. <i>AIP Advances</i> , 2017, 7, .	0.6	6
406	Low-Energy Structures and Electronic Properties of Large-Sized Si _N Clusters (N = 60, 80, 100, 120, 150, 170). <i>Journal of Physical Chemistry C</i> , 2018, 122, 11086-11095.	1.5	6
407	Interaction Mechanisms of Insensitive Explosive FOX-7 and Graphene Oxides from Ab Initio Calculations. <i>Nanomaterials</i> , 2019, 9, 1290.	1.9	6
408	Solar driven CO ₂ hydrogenation on transition metal doped Zn ₁₂ O ₁₂ cluster. <i>Journal of Chemical Physics</i> , 2020, 153, 164306.	1.2	6
409	Distinct structure assembly driven by metal-ligand binding in Au ₂₃ nanoclusters and its relation to photocatalysis. <i>Chemical Communications</i> , 2021, 57, 2176-2179.	2.2	6
410	Ground-State Structures of Hydrated Calcium Ion Clusters From Comprehensive Genetic Algorithm Search. <i>Frontiers in Chemistry</i> , 2021, 9, 637750.	1.8	6
411	Magnetic field modulated photoelectric devices in ferromagnetic semiconductor CrXh (X = Mn, Fe, Co, Ni) Tj ETQq1 1 0.784314 rgBT / Over	1.5	6
412	Intrinsic Multiferroic in VNI Monolayer. <i>ACS Applied Electronic Materials</i> , 2022, 4, 3177-3182.	2.0	6
413	Optical and thermal properties of a cyanine dye medium for next-generation DVD-Rs. <i>Imaging Science Journal</i> , 1999, 47, 113-117.	0.2	5
414	Calculations of electronic structure of Ge ₄₄ Mn ₂ Ba ₈ and Ge ₄₂ Mn ₄ Ba ₈ clathrates. <i>Physical Review B</i> , 2004, 70, .	1.1	5

#	ARTICLE	IF	CITATIONS
415	Hexanuclear Cobalt Carbonyl Carbide Clusters: The Interplay between Octahedral and Trigonal Prismatic Structures. <i>Inorganic Chemistry</i> , 2008, 47, 9314-9320.	1.9	5
416	Revisit of S_{2n} ($n=21$) Clusters by Ab Initio Global Search. <i>Journal of Cluster Science</i> , 2017, 28, 1729-1737.	1.7	5
417	Quantum oscillation in carrier transport in two-dimensional junctions. <i>Nanoscale</i> , 2018, 10, 7912-7917.	2.8	5
418	Electronic and magnetic properties of transition metal decorated monolayer GaS. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 101, 131-138.	1.3	5
419	Phase Diagram of Methane Hydrates and Discovery of MH-VI Hydrate. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6007-6013.	1.1	5
420	Distributed Robust Filtering for Wireless Sensor Networks with Markov Switching Topologies and Deception Attacks. <i>Sensors</i> , 2020, 20, 1948.	2.1	5
421	Surfactant-Free Approach for Engineering an Ultrathin Ti-Doped Ni(OH) ₂ Nanosheet on Carbon Cloth: Experimental and Theoretical Insight into Boosted Alkaline Water Oxidation Activity. <i>Inorganic Chemistry</i> , 2020, 59, 10253-10261.	1.9	5
422	First-Principles Calculations for Stable $\hat{\nu}$ -Ti $\hat{\nu}$ -Mo Alloys Using Cluster-Plus-Glue-Atom Model. <i>Acta Metallurgica Sinica (English Letters)</i> , 2020, 33, 968-974.	1.5	5
423	Multiscale simulations of the hydration shells surrounding spherical Fe ₃ O ₄ nanoparticles and effect on magnetic properties. <i>Nanoscale</i> , 2021, 13, 9293-9302.	2.8	5
424	Posture Dynamic Modeling and Stability Analysis of a Magnetic Driven Dual-Spin Spherical Capsule Robot. <i>Micromachines</i> , 2021, 12, 238.	1.4	5
425	Transition metal-doped Bn ($n=7$) clusters: confirmation of a circular disk Jellium model. <i>European Physical Journal Plus</i> , 2021, 136, 1.	1.2	5
426	Universal Zigzag Edge Reconstruction of an $\hat{\nu}$ -Phase Puckered Monolayer and Its Resulting Robust Spatial Charge Separation. <i>Nano Letters</i> , 2021, 21, 8095-8102.	4.5	5
427	Methane conversion by transition metal-doped vanadium oxide clusters. <i>Chemical Physics Letters</i> , 2021, 779, 138829.	1.2	5
428	Evolution of Water Layer Adsorption on the GaN(0001) Surface and Its Influence on Electronic Properties. <i>Journal of Physical Chemistry C</i> , 2021, 125, 667-674.	1.5	5
429	Stability and NMR Chemical Shift of Amorphous Precursors of Methane Hydrate: Insights from Dispersion-Corrected Density Functional Theory Calculations Combined with Machine Learning. <i>Journal of Physical Chemistry B</i> , 2021, 125, 431-441.	1.2	5
430	A comprehensive study of indole catalytic hydrodenitrogenation under hydrothermal conditions. <i>AIChE Journal</i> , 2022, 68, e17531.	1.8	5
431	Robust Dirac spin gapless semiconductors in a two-dimensional oxalate based organic honeycomb-kagome lattice. <i>Nanoscale</i> , 2022, 14, 2023-2029.	2.8	5
432	Two-dimensional oxides assembled by clusters ($\hat{\nu}$) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 62 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML") <mml:msub><mml:mi>M</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math> clusters (<mml:math>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 62 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML") <mml:mrow>	1.3	5
	Review Research, 2021, 3, .		

#	ARTICLE	IF	CITATIONS
---	---------	----	-----------

433			
-----	--	--	--

[Zbl](#) [inl](#) [math](#)

#	ARTICLE	IF	CITATIONS
451	Tuning Optical Absorption and Emission of Sub-Nanometer Gold-Caged Metal Systems M@Au ₁₄ by Substitutional Doping. Journal of Computational and Theoretical Nanoscience, 2006, 3, 312-314.	0.4	3
452	On the photocatalysis evolution of heteroatom-doped Ag ₄ M ₂ nanoclusters. RSC Advances, 2021, 11, 32526-32532.	1.7	3
453	Transition of CrI ₂ from a two-dimensional network to one-dimensional chain at the monolayer limit. Physical Chemistry Chemical Physics, 2021, 23, 25291-25297.	1.3	3
454	Compression Behavior and Vibrational Properties of New Energetic Material LLM-105 Analyzed Using the Dispersion-Corrected Density Functional Theory. Molecules, 2021, 26, 6831.	1.7	3
455	Phase Diagrams and Spectral Characteristics of Hydrofluorocarbon Hydrates: Insights from First-Principles Thermodynamics. ACS Sustainable Chemistry and Engineering, 2021, 9, 16347-16355.	3.2	3
456	Theoretical insights of structural evolution and electronic properties of Ru ₂ Gen (n=16) clusters. European Physical Journal Plus, 2022, 137, 1.	1.2	3
457	Design and implementation of a highly integrated dual hemisphere capsule robot. Biomedical Microdevices, 2022, 24, 10.	1.4	3
458	Manipulating the organic-inorganic interface of atomically precise Au ₃₆ (SR) ₂₄ catalysts for CO oxidation. Chemical Communications, 2022, 58, 3003-3006.	2.2	3
459	Intramolecular hydroamination of alkynes driven by isomeric Au ₃₆ (SR) ₂₄ nanocluster catalysts. Nano Research, 2023, 16, 3641-3648.	5.8	3
460	Inverse Design of Nanoclusters for Light-Controlled CO ₂ →HCOOH Interconversion. Journal of Physical Chemistry Letters, 2022, 13, 2523-2532.	2.1	3
461	Asymmetrically Doping a Platinum Atom into a Au ₃₈ Nanocluster for Changing the Electron Configuration and Reactivity in Electrocatalysis. Angewandte Chemie, 0, , .	1.6	3
462	Advanced catalytic CO ₂ hydrogenation on Ni/ZrO ₂ with light induced oxygen vacancy formation in photothermal conditions at medium-low temperatures. Catalysis Science and Technology, 2022, 12, 4740-4752.	2.1	3
463	Gas Molecules Adsorption on Carbon Nanotubes. Materials Research Society Symposia Proceedings, 2000, 633, 13481.	0.1	2
464	Optical property of amorphous semiconductor mercury cadmium telluride from first-principles study. Science in China Series D: Earth Sciences, 2009, 52, 1928-1932.	0.9	2
465	First-Principles Study of Lithium Adsorption, Storage and Diffusion Properties for Graphite Oxides. Journal of Nanoscience and Nanotechnology, 2016, 16, 8106-8112.	0.9	2
466	Pressure dependence on electronic structures, charge distribution and bond orders of solid nitromethane using nonlocal DFT functional. Molecular Simulation, 2018, 44, 1454-1460.	0.9	2
467	Comparison of flows and heat transfers in reactor cores with spherical-particle fuels and cylindrical-rod fuels. Journal of Nuclear Science and Technology, 2021, 58, 226-240.	0.7	2
468	Compression behavior of energetic μ -CL ₂₀ crystals from density functional theory calculations. Journal of Raman Spectroscopy, 2021, 52, 1764.	1.2	2

#	ARTICLE	IF	CITATIONS
469	Effects of vacancy defects on the magnetic properties of vanadium diselenide monolayers: a first principle investigation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 17615-17622.	1.3	2
470	STRUCTURAL AND RAMAN SPECTRA STUDIES OF SUPPORTED LiF CLUSTERS. <i>Surface Review and Letters</i> , 1996, 03, 157-160.	0.5	1
471	Chemical stability of epoxy functionalizations of graphene: A density functional theory study. <i>Materials Research Society Symposia Proceedings</i> , 2013, 1549, 19-24.	0.1	1
472	Perovskite Solar Cells: Reverse-Graded 2D Ruddlesden-Popper Perovskites for Efficient Air-Stable Solar Cells (<i>Adv. Energy Mater.</i> 21/2019). <i>Advanced Energy Materials</i> , 2019, 9, 1970075.	10.2	1
473	Structural and Electronic Properties of Binary Clusters Si_mGe_n ($m+n=6-13$). <i>Journal of Nanoscience and Nanotechnology</i> , 2019, 19, 7879-7885.	0.9	1
474	Vacancy Engineering of Iron-Doped $\text{W}_{18}\text{O}_{49}$ Nanoreactors for Low-Barrier Electrochemical Nitrogen Reduction (<i>Angew. Chem.</i> 19/2020). <i>Angewandte Chemie</i> , 2020, 132, 7696-7696.	1.6	1
475	Phase Diagrams for all Clathrate Hydrates of CO_2 from First-Principles Thermodynamics. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5956-5962.	1.1	1
476	Remote Passivation in Two-Dimensional Materials: The Case of the Monolayer-Bilayer Lateral Junction of MoSe_2 . <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8046-8052.	2.1	1
477	A Full CMOS Quenching Circuit With Fuse Protection for InGaAs/InP Single Photon Detectors. <i>IEEE Transactions on Circuits and Systems II: Express Briefs</i> , 2021, 68, 3224-3228.	2.2	1
478	Surface-enhanced resonance Raman detection of 1,1-diamino-2,2-dinitroethylene (FOX-7) on metal-doped Au 12 and Ag 12 clusters. <i>Journal of Raman Spectroscopy</i> , 2020, 51, 2425-2434.	1.2	1
479	Eliminating Edge Electronic and Phonon States of Phosphorene Nanoribbon by Unique Edge Reconstruction (<i>Small</i> 2/2022). <i>Small</i> , 2022, 18, .	5.2	1
480	Strain modulation of the exciton anisotropy and carrier lifetime in black phosphorene. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	1.3	1
481	Cluster- and energy-separated extreme states in a synthesized superatomic solid. <i>Physical Review B</i> , 2022, 105, .	1.1	1
482	Strain softened bending modulus of graphene oxide. <i>Carbon Trends</i> , 2022, 7, 100167.	1.4	1
483	Fabricating and Modulating Robust Multi-Photoaddressable Systems with the Derivatives of Diarylethylene and Donor-Acceptor Stenhouse Adducts. <i>Journal of Physical Chemistry Letters</i> , 2022, , 3611-3620.	2.1	1
484	Thermo-chemical metastability of multilayer epitaxial graphene oxide: Experiments and density functional theory calculations. <i>Materials Research Society Symposia Proceedings</i> , 2012, 1451, 39-44.	0.1	0
485	Microspotting: Film Structure of Epitaxial Graphene Oxide on SiC: Insight on the Relationship Between Interlayer Spacing, Water Content, and Intralayer Structure (<i>Adv. Mater. Interfaces</i> 3/2014). <i>Advanced Materials Interfaces</i> , 2014, 1, n/a-n/a.	1.9	0
486	Characterization and on-line adjustment of the sagittal-bent Laue crystal profile. <i>Journal of Synchrotron Radiation</i> , 2018, 25, 1346-1353.	1.0	0

#	ARTICLE	IF	CITATIONS
487	2D Palladium Diselenide: Giant Thickness-Tunable Bandgap and Robust Air Stability of 2D Palladium Diselenide (Small 19/2020). Small, 2020, 16, 2070106.	5.2	0
488	First-Principles Study of the Effects of Carbon, Nitrogen, and Oxygen on Helium Behavior in Body-Centered-Cubic Vanadium. Fusion Science and Technology, 0, , 1-10.	0.6	0
489	First-principles study of crystal-face specificity in surface properties of Fe-rich Fe-Cr alloys. Physical Review Materials, 2019, 3, .	0.9	0
490	A novel method for measuring the focal point of a sagittal-focusing Laue crystal monochromator. Journal of Synchrotron Radiation, 2019, 26, 1826-1829.	1.0	0
491	Interlayer Hopping Kinetics of Vacancies in CrI ₃ Layers Leading to Monolayer/Bilayer Heterostructures. Advanced Materials Interfaces, 0, , 2200626.	1.9	0