

# Si Zhou

## List of Publications by Citations

**Source:** <https://exaly.com/author-pdf/2798012/si-zhou-publications-by-citations.pdf>

**Version:** 2024-04-25

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

468  
papers

19,509  
citations

69  
h-index

122  
g-index

499  
ext. papers

23,588  
ext. citations

7.3  
avg, IF

7.43  
L-index

#	Paper	IF	Citations
468	Gas molecule adsorption in carbon nanotubes and nanotube bundles. <i>Nanotechnology</i> , <b>2002</b> , 13, 195-200	3.4	979
467	Rise of silicene: A competitive 2D material. <i>Progress in Materials Science</i> , <b>2016</b> , 83, 24-151	42.2	548
466	Metal-Organic-Framework-Derived Hybrid Carbon Nanocages as a Bifunctional Electrocatalyst for Oxygen Reduction and Evolution. <i>Advanced Materials</i> , <b>2017</b> , 29, 1700874	24	518
465	Room-temperature metastability of multilayer graphene oxide films. <i>Nature Materials</i> , <b>2012</b> , 11, 544-9	27	449
464	Graphene oxide: A promising nanomaterial for energy and environmental applications. <i>Nano Energy</i> , <b>2015</b> , 16, 488-515	17.1	406
463	Atomic-level insight into super-efficient electrocatalytic oxygen evolution on iron and vanadium co-doped nickel (oxy)hydroxide. <i>Nature Communications</i> , <b>2018</b> , 9, 2885	17.4	398
462	Density-functional study of Aun(n=200) clusters: Lowest-energy structures and electronic properties. <i>Physical Review B</i> , <b>2002</b> , 66,	3.3	393
461	Facile Ammonia Synthesis from Electrocatalytic N <sub>2</sub> Reduction under Ambient Conditions on N-Doped Porous Carbon. <i>ACS Catalysis</i> , <b>2018</b> , 8, 1186-1191	13.1	392
460	Boosting electrocatalytic oxygen evolution by synergistically coupling layered double hydroxide with MXene. <i>Nano Energy</i> , <b>2018</b> , 44, 181-190	17.1	304
459	First-principles study of Li-intercalated carbon nanotube ropes. <i>Physical Review Letters</i> , <b>2000</b> , 85, 1706-9	7.4	271
458	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> , <b>2018</b> , 57, 16166-16170	16.4	243
457	Co Nanoislands Rooted on Co-N-C Nanosheets as Efficient Oxygen Electrocatalyst for Zn-Air Batteries. <i>Advanced Materials</i> , <b>2019</b> , 31, e1901666	24	232
456	Carbohydrate doping to enhance electromagnetic properties of MgB <sub>2</sub> superconductors. <i>Applied Physics Letters</i> , <b>2006</b> , 89, 142505	3.4	216
455	Silicene on Substrates: A Way To Preserve or Tune Its Electronic Properties. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 10353-10359	3.8	215
454	Structures, mobilities, electronic and magnetic properties of point defects in silicene. <i>Nanoscale</i> , <b>2013</b> , 5, 9785-92	7.7	202
453	Mechanical properties of graphene oxides. <i>Nanoscale</i> , <b>2012</b> , 4, 5910-6	7.7	191
452	Enhanced piezoelectric effect in Janus group-III chalcogenide monolayers. <i>Applied Physics Letters</i> , <b>2017</b> , 110, 163102	3.4	190

451	2D covalent triazine framework: a new class of organic photocatalyst for water splitting. <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 7750-7758	13	183
450	Ultrasensitive Iron-Triggered Nanosized Fe <sub>3</sub> O <sub>4</sub> /OOH Integrated with Graphene for Highly Efficient Oxygen Evolution. <i>Advanced Energy Materials</i> , <b>2017</b> , 7, 1602148	21.8	177
449	Work functions of pristine and alkali-metal intercalated carbon nanotubes and bundles. <i>Physical Review B</i> , <b>2002</b> , 65,	3.3	174
448	Intrinsic strength and failure behaviors of graphene grain boundaries. <i>ACS Nano</i> , <b>2012</b> , 6, 2704-11	16.7	172
447	Initial geometries, interaction mechanism and high stability of silicene on Ag(111) surface. <i>Scientific Reports</i> , <b>2012</b> , 2, 861	4.9	167
446	From boron cluster to two-dimensional boron sheet on Cu(111) surface: growth mechanism and hole formation. <i>Scientific Reports</i> , <b>2013</b> , 3, 3238	4.9	162
445	Heterostructures of MXenes and N-doped graphene as highly active bifunctional electrocatalysts. <i>Nanoscale</i> , <b>2018</b> , 10, 10876-10883	7.7	154
444	Tuning the band gap in silicene by oxidation. <i>ACS Nano</i> , <b>2014</b> , 8, 10019-25	16.7	147
443	Atomistic insight into the oxidation of monolayer transition metal dichalcogenides: from structures to electronic properties. <i>RSC Advances</i> , <b>2015</b> , 5, 17572-17581	3.7	144
442	Structural Growth Sequences and Electronic Properties of Zinc Oxide Clusters (ZnO) <sub>n</sub> (n=2-18). <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 4956-4963	3.8	141
441	Origin of the chemical and kinetic stability of graphene oxide. <i>Scientific Reports</i> , <b>2013</b> , 3, 2484	4.9	139
440	Band Gap Tuning of Hydrogenated Graphene: H Coverage and Configuration Dependence. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 3236-3242	3.8	139
439	Common electronic origin of superconductivity in (Li,Fe)OHFeSe bulk superconductor and single-layer FeSe/SrTiO <sub>3</sub> films. <i>Nature Communications</i> , <b>2016</b> , 7, 10608	17.4	138
438	Structure and electronic properties of Gen (n=2-5) clusters from density-functional theory. <i>Physical Review B</i> , <b>2001</b> , 64,	3.3	138
437	Evidence of topological surface state in three-dimensional Dirac semimetal Cd <sub>3</sub> As <sub>2</sub> . <i>Scientific Reports</i> , <b>2014</b> , 4, 6106	4.9	131
436	B80 and B101-103 clusters: remarkable stability of the core-shell structures established by validated density functionals. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 074302	3.9	131
435	Ultrahigh Rate and Long-Life Sodium-Ion Batteries Enabled by Engineered Surface and Near-Surface Reactions. <i>Advanced Materials</i> , <b>2018</b> , 30, 1702486	24	130
434	Vacancy Engineering of Iron-Doped W O Nanoreactors for Low-Barrier Electrochemical Nitrogen Reduction. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 7356-7361	16.4	126

433	Fluorescent Gold Nanoclusters with Interlocked Staples and a Fully Thiolate-Bound Kernel. <i>Angewandte Chemie - International Edition</i> , <b>2016</b> , 55, 11567-71	16.4	122
432	B(80) and other medium-sized boron clusters: core-shell structures, not hollow cages. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 9969-72	2.8	121
431	Structure of Chiral Au <sub>44</sub> (2,4-DMBT) <sub>26</sub> Nanocluster with an 18-Electron Shell Closure. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 10425-8	16.4	118
430	Do Composite Single-Walled Nanotubes Have Enhanced Capability for Lithium Storage?. <i>Chemistry of Materials</i> , <b>2005</b> , 17, 992-1000	9.6	113
429	Quasi-freestanding epitaxial silicene on Ag(111) by oxygen intercalation. <i>Science Advances</i> , <b>2016</b> , 2, e1600057	10.7	112
428	Hole defects and nitrogen doping in graphene: implication for supercapacitor applications. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2013</b> , 5, 11184-93	9.5	110
427	Nitrogen-Doped Graphene on Transition Metal Substrates as Efficient Bifunctional Catalysts for Oxygen Reduction and Oxygen Evolution Reactions. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2017</b> , 9, 22578-22587	9.5	103
426	Binding energies and electronic structures of adsorbed titanium chains on carbon nanotubes. <i>Physical Review B</i> , <b>2002</b> , 66,	3.3	100
425	MBene (MnB): a new type of 2D metallic ferromagnet with high Curie temperature. <i>Nanoscale Horizons</i> , <b>2018</b> , 3, 335-341	10.8	99
424	Rapid and energy-efficient microwave pyrolysis for high-yield production of highly-active bifunctional electrocatalysts for water splitting. <i>Energy and Environmental Science</i> , <b>2020</b> , 13, 545-553	35.4	99
423	Toward a Reversible Mn <sup>4+</sup> /Mn <sup>2+</sup> Redox Reaction and Dendrite-Free Zn Anode in Near-Neutral Aqueous Zn/MnO <sub>2</sub> Batteries via Salt Anion Chemistry. <i>Advanced Energy Materials</i> , <b>2020</b> , 10, 1904163	21.8	98
422	Engineering Multifunctional Collaborative Catalytic Interface Enabling Efficient Hydrogen Evolution in All pH Range and Seawater. <i>Advanced Energy Materials</i> , <b>2019</b> , 9, 1901333	21.8	98
421	Crystal and Solution Photoluminescence of MAg <sub>24</sub> (SR) <sub>18</sub> (M = Ag/Pd/Pt/Au) Nanoclusters and Some Implications for the Photoluminescence Mechanisms. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 13848-13853	3.8	96
420	Hollow cages versus space-filling structures for medium-sized gold clusters: the spherical aromaticity of the Au <sub>50</sub> cage. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 9265-9	2.8	95
419	Melting behavior in ultrathin metallic nanowires. <i>Physical Review B</i> , <b>2002</b> , 66,	3.3	95
418	Amorphous structural models for graphene oxides. <i>Carbon</i> , <b>2012</b> , 50, 1690-1698	10.4	93
417	Screening and Design of Novel 2D Ferromagnetic Materials with High Curie Temperature above Room Temperature. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2018</b> , 10, 39032-39039	9.5	91
416	Sugar Coating of Boron Powder for Efficient Carbon Doping of MgB <sub>2</sub> with Enhanced Current-Carrying Performance. <i>Advanced Materials</i> , <b>2007</b> , 19, 1373-1376	24	89

415	Oxidation Resistance of Monolayer Group-IV Monochalcogenides. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2017</b> , 9, 12013-12020	9.5	88
414	Structure and structural evolution of () clusters using a genetic algorithm and density functional theory method. <i>Solid State Communications</i> , <b>2007</b> , 144, 174-179	1.6	86
413	A single boron atom doped boron nitride edge as a metal-free catalyst for N fixation. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 1110-1116	3.6	84
412	YN2 monolayer: Novel p-state Dirac half metal for high-speed spintronics. <i>Nano Research</i> , <b>2017</b> , 10, 1972-1979	4.1	82
411	Growth behavior and magnetic properties of SinFe (n=2-4) clusters. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	82
410	Discovery of a silicon-based ferrimagnetic wheel structure in V(x)Si(12)(-) (x = 1-3) clusters: photoelectron spectroscopy and density functional theory investigation. <i>Nanoscale</i> , <b>2014</b> , 6, 14617-21	7.7	76
409	Endohedrally Doped Cage Clusters. <i>Chemical Reviews</i> , <b>2020</b> , 120, 9021-9163	68.1	76
408	N-doped graphitic carbon materials hybridized with transition metals (compounds) for hydrogen evolution reaction: Understanding the synergistic effect from atomistic level. <i>Carbon</i> , <b>2018</b> , 133, 260-266	10.4	75
407	A new phase diagram of water under negative pressure: The rise of the lowest-density clathrate s-III. <i>Science Advances</i> , <b>2016</b> , 2, e1501010	14.3	75
406	Lateral heterostructures of monolayer group-IV monochalcogenides: band alignment and electronic properties. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 3788-3795	7.1	73
405	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> , <b>2016</b> , 18, 25241-25248	3.6	72
404	Strong anisotropy of Dirac cones in SrMnBi2 and CaMnBi2 revealed by angle-resolved photoemission spectroscopy. <i>Scientific Reports</i> , <b>2014</b> , 4, 5385	4.9	71
403	Capturing the active sites of multimetallic (oxy)hydroxides for the oxygen evolution reaction. <i>Energy and Environmental Science</i> , <b>2020</b> , 13, 4225-4237	35.4	71
402	Common Fermi-surface topology and nodeless superconducting gap of K0.68Fe1.79Se2 and (Ti0.45K0.34)Fe1.84Se2 superconductors revealed via angle-resolved photoemission. <i>Physical Review B</i> , <b>2011</b> , 83,	3.3	70
401	Magnetic properties of atomic clusters and endohedral metallofullerenes. <i>Coordination Chemistry Reviews</i> , <b>2015</b> , 289-290, 315-340	23.2	69
400	2D Boron Sheets: Structure, Growth, and Electronic and Thermal Transport Properties. <i>Advanced Functional Materials</i> , <b>2020</b> , 30, 1904349	15.6	69
399	Orbital-selective spin texture and its manipulation in a topological insulator. <i>Nature Communications</i> , <b>2014</b> , 5, 3382	17.4	68
398	Intercalation and diffusion of lithium ions in a carbon nanotube bundle by ab initio molecular dynamics simulations. <i>Energy and Environmental Science</i> , <b>2011</b> , 4, 1379	35.4	68

397	Gas adsorption on monolayer blue phosphorus: implications for environmental stability and gas sensors. <i>Nanotechnology</i> , <b>2017</b> , 28, 175708	3.4	67
396	Atomic structures and covalent-to-metallic transition of lead clusters $Pb_n(n=2\bar{2}2)$ . <i>Physical Review A</i> , <b>2005</b> , 71,	2.6	67
395	Quantum transport properties of ultrathin silver nanowires. <i>Nanotechnology</i> , <b>2003</b> , 14, 501-504	3.4	67
394	Electronic and photonic properties of doped carbon nanotubes. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2003</b> , 3, 459-78	1.3	67
393	Engineering the electronic structure of single-walled carbon nanotubes by chemical functionalization. <i>ChemPhysChem</i> , <b>2005</b> , 6, 598-601	3.2	67
392	Multilevel Hollow MXene Tailored Low-Pt Catalyst for Efficient Hydrogen Evolution in Full-pH Range and Seawater. <i>Advanced Functional Materials</i> , <b>2020</b> , 30, 1910028	15.6	66
391	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> , <b>2021</b> , 60, 16044-16050	16.4	65
390	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> , <b>2016</b> , 4, 12739-12747	13	64
389	Melting behavior of ultrathin titanium nanowires. <i>Physical Review B</i> , <b>2003</b> , 67,	3.3	64
388	Structures and electronic properties of symmetric and nonsymmetric graphene grain boundaries. <i>Carbon</i> , <b>2013</b> , 55, 151-159	10.4	63
387	Electronic evidence of an insulator-superconductor crossover in single-layer FeSe/SrTiO <sub>3</sub> films. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2014</b> , 111, 18501-6	11.5	62
386	An exchange intercalation mechanism for the formation of a two-dimensional Si structure underneath graphene. <i>Nano Research</i> , <b>2012</b> , 5, 352-360	10	62
385	Boron fullerenes with $32\bar{6}$ atoms: Irregular cage configurations and electronic properties. <i>Chemical Physics Letters</i> , <b>2010</b> , 501, 16-19	2.5	62
384	Kernel Tuning and Nonuniform Influence on Optical and Electrochemical Gaps of Bimetal Nanoclusters. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 3487-3490	16.4	61
383	Inverse Capacity Growth and Pocket Effect in SnS Semifilled Carbon Nanotube Anode. <i>ACS Nano</i> , <b>2018</b> , 12, 8037-8047	16.7	61
382	Band Gap Modulated by Electronic Superlattice in Blue Phosphorene. <i>ACS Nano</i> , <b>2018</b> , 12, 5059-5065	16.7	61
381	Electrocatalyzing S Cathodes Multisulfiphilic Sites for Superior Room-Temperature Sodium-Sulfur Batteries. <i>ACS Nano</i> , <b>2020</b> , 14, 7259-7268	16.7	61
380	Boron Nitride Nanotubes for Ammonia Synthesis: Activation by Filling Transition Metals. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 308-317	16.4	61

379	B28: the smallest all-boron cage from an ab initio global search. <i>Nanoscale</i> , <b>2015</b> , 7, 15086-90	7.7	60
378	Chemical Bonding of Partially Fluorinated Graphene. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 26402-26408	6.4	60
377	Controlling and Observing Sharp-Valleyed Quantum Interference Effect in Single Molecular Junctions. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 17685-17690	16.4	60
376	Stabilization of body-centred cubic iron under inner-core conditions. <i>Nature Geoscience</i> , <b>2017</b> , 10, 312-316	16.3	59
375	Stabilization of fullerene-like boron cages by transition metal encapsulation. <i>Nanoscale</i> , <b>2015</b> , 7, 10482-9	9.7	59
374	Large Negative Thermal Expansion and Anomalous Behavior on Compression in Cubic ReO <sub>3</sub> -Type AIBiVF <sub>6</sub> : CaZrF <sub>6</sub> and CaHfF <sub>6</sub> . <i>Chemistry of Materials</i> , <b>2015</b> , 27, 3912-3918	9.6	59
373	Comprehensive genetic algorithm for ab initio global optimisation of clusters. <i>Molecular Simulation</i> , <b>2016</b> , 42, 809-819	2	59
372	Elastic coupling between layers in two-dimensional materials. <i>Nature Materials</i> , <b>2015</b> , 14, 714-20	27	58
371	Sensitive colorimetric detection of glucose and cholesterol by using Au@Ag core-shell nanoparticles. <i>RSC Advances</i> , <b>2016</b> , 6, 35001-35007	3.7	58
370	Electronic structure and superconductivity of FeSe-related superconductors. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 183201	1.8	56
369	Ni <sub>3</sub> S <sub>2</sub> Nanosheets in Situ Epitaxially Grown on Nanorods as High Active and Stable Homojunction Electrocatalyst for Hydrogen Evolution Reaction. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2018</b> , 6, 2474-2481	8.3	56
368	Cage and tube structures of medium-sized zinc oxide clusters (ZnO) <sub>n</sub> (n=24, 28, 36, and 48). <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 144710	3.9	56
367	Physical properties and device applications of graphene oxide. <i>Frontiers of Physics</i> , <b>2020</b> , 15, 1	3.7	56
366	Nonmetal-metal transition in Zn <sub>n</sub> (n=20) clusters. <i>Physical Review A</i> , <b>2003</b> , 68,	2.6	55
365	Structure and electronic properties of cobalt atoms encapsulated in Si <sub>n</sub> (n = 103) clusters. <i>Chemical Physics Letters</i> , <b>2005</b> , 411, 279-284	2.5	55
364	A simple, fast, label-free colorimetric method for detection of telomerase activity in urine by using hemin-graphene conjugates. <i>Biosensors and Bioelectronics</i> , <b>2017</b> , 87, 600-606	11.8	54
363	Curved carbon nanotubes: From unique geometries to novel properties and peculiar applications. <i>Nano Research</i> , <b>2014</b> , 7, 626-657	10	53
362	MXene nanoribbons as electrocatalysts for the hydrogen evolution reaction with fast kinetics. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 19390-19397	3.6	53

361	Dichotomy of the electronic structure and superconductivity between single-layer and double-layer FeSe/SrTiO <sub>3</sub> films. <i>Nature Communications</i> , <b>2014</b> , 5, 5047	17.4	52
360	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> , <b>2016</b> , 113, 14656-14661	11.5	52
359	Eighteen functional monolayer metal oxides: wide bandgap semiconductors with superior oxidation resistance and ultrahigh carrier mobility. <i>Nanoscale Horizons</i> , <b>2019</b> , 4, 592-600	10.8	51
358	Structure and magnetic properties of Co-Cu bimetallic clusters. <i>Physical Review B</i> , <b>2002</b> , 66,	3.3	51
357	Structural and Electronic Properties of Interfaces in Graphene and Hexagonal Boron Nitride Lateral Heterostructures. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 5022-5028	9.6	51
356	Polarimetric Convolutional Network for PolSAR Image Classification. <i>IEEE Transactions on Geoscience and Remote Sensing</i> , <b>2019</b> , 57, 3040-3054	8.1	51
355	Structures and Electronic Properties of V <sub>3</sub> Si <sub>n</sub> (n = 3-4) Clusters: A Combined Ab Initio and Experimental Study. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 10987-10994	3.8	50
354	Structure and magnetic properties of cobalt doped Si <sub>n</sub> (n=2-4) clusters. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2007</b> , 367, 335-344	2.3	50
353	Accelerating polysulfide redox conversion on bifunctional electrocatalytic electrode for stable Li-S batteries. <i>Energy Storage Materials</i> , <b>2019</b> , 20, 98-107	19.4	50
352	Tunable Assembly of sp <sup>3</sup> Cross-Linked 3D Graphene Monoliths: A First-Principles Prediction. <i>Advanced Functional Materials</i> , <b>2013</b> , 23, 5846-5853	15.6	49
351	Cooperative Electron-Phonon Coupling and Buckled Structure in Germanene on Au(111). <i>ACS Nano</i> , <b>2017</b> , 11, 3553-3559	16.7	48
350	Operando Revealing Dynamic Reconstruction of NiCo Carbonate Hydroxide for High-Rate Energy Storage. <i>Joule</i> , <b>2020</b> , 4, 673-687	27.8	48
349	A novel double-helical-kernel evolution pattern of gold nanoclusters: alternate single-stranded growth at both ends. <i>Nanoscale</i> , <b>2017</b> , 9, 3742-3746	7.7	47
348	Phosphorus quantum dots as visible-light photocatalyst for water splitting. <i>Computational Materials Science</i> , <b>2017</b> , 130, 56-63	3.2	47
347	Reverse-Graded 2D Ruddlesden-Popper Perovskites for Efficient Air-Stable Solar Cells. <i>Advanced Energy Materials</i> , <b>2019</b> , 9, 1900612	21.8	47
346	Label-Free Detection of Telomerase Activity in Urine Using Telomerase-Responsive Porous Anodic Alumina Nanochannels. <i>Analytical Chemistry</i> , <b>2016</b> , 88, 8107-14	7.8	46
345	First-principles study of molecular hydrogen dissociation on doped Al <sub>12</sub> X (X = B, Al, C, Si, P, Mg, and Ca) clusters. <i>Journal of Computational Chemistry</i> , <b>2009</b> , 30, 2509-14	3.5	46
344	A Stable Bifunctional Catalyst for Rechargeable Zinc-Air Batteries: Iron-Cobalt Nanoparticles Embedded in a Nitrogen-Doped 3D Carbon Matrix. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 16398-16402	3.6	46



343	MBenes: emerging 2D materials as efficient electrocatalysts for the nitrogen reduction reaction. <i>Nanoscale Horizons</i> , <b>2020</b> , 5, 1106-1115	10.8	45
342	Hybrids of PtRu Nanoclusters and Black Phosphorus Nanosheets for Highly Efficient Alkaline Hydrogen Evolution Reaction. <i>ACS Catalysis</i> , <b>2019</b> , 9, 10870-10875	13.1	45
341	Direct synthesis and in situ characterization of monolayer parallelogrammic rhenium diselenide on gold foil. <i>Communications Chemistry</i> , <b>2018</b> , 1,	6.3	44
340	Substituted Hantzsch Esters as Versatile Radical Reservoirs in Photoredox Reactions. <i>Advanced Synthesis and Catalysis</i> , <b>2018</b> , 360, 925-931	5.6	44
339	Structures and Magnetic Properties of MoS <sub>2</sub> Grain Boundaries with Antisite Defects. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 12261-12269	3.8	43
338	2D lateral heterostructures of group-III monochalcogenide: Potential photovoltaic applications. <i>Applied Physics Letters</i> , <b>2018</b> , 112, 143902	3.4	43
337	Monolayer group-III monochalcogenides by oxygen functionalization: a promising class of two-dimensional topological insulators. <i>Npj Quantum Materials</i> , <b>2018</b> , 3,	5	43
336	GeAs and SiAs monolayers: Novel 2D semiconductors with suitable band structures. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2018</b> , 95, 149-153	3	43
335	Electron-Deficient Cu Sites on Cu <sub>3</sub> Ag <sub>1</sub> Catalyst Promoting CO <sub>2</sub> Electroreduction to Alcohols. <i>Advanced Energy Materials</i> , <b>2020</b> , 10, 2001987	21.8	43
334	Electrochemical Hydrogenation with Gaseous Ammonia. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 1759-1763	16.4	43
333	Atomic structures and electronic properties of phosphorene grain boundaries. <i>2D Materials</i> , <b>2016</b> , 3, 025008	5.9	42
332	Chemical-Reductant-Free Electrochemical Deuteration Reaction using Deuterium Oxide. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 13962-13967	16.4	41
331	Atomic Sulfur Anchored on Silicene, Phosphorene, and Borophene for Excellent Cycle Performance of Li-S Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2017</b> , 9, 42836-42844	9.5	41
330	Synthesis and characteristics of form-stable n-octadecane/expanded graphite composite phase change materials. <i>Applied Physics A: Materials Science and Processing</i> , <b>2010</b> , 100, 1143-1148	2.6	41
329	True nanocable assemblies with insulating BN nanotube sheaths and conducting Cu nanowire cores. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 2529-32	3.4	40
328	Two-dimensional ZnO for the selective photoreduction of CO <sub>2</sub> . <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 16294-16303	13	39
327	A Silver Nanocluster Containing Interstitial Sulfur and Unprecedented Chemical Bonds. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 11273-11277	16.4	39
326	Elastic properties of vanadium-based alloys from first-principles theory. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	38

325	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> , <b>2020</b> , 8, 3071-3082	13	38
324	Is the kernel-staples match a key-lock match?. <i>Chemical Science</i> , <b>2018</b> , 9, 2437-2442	9.4	37
323	Fluorescent Gold Nanoclusters with Interlocked Staples and a Fully Thiolate-Bound Kernel. <i>Angewandte Chemie</i> , <b>2016</b> , 128, 11739-11743	3.6	37
322	What is the best density functional to describe water clusters: evaluation of widely used density functionals with various basis sets for (H <sub>2</sub> O) <sub>n</sub> (n = 1-10). <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 130, 341-352	1.9	37
321	Cubic imidazolate frameworks-derived CoFe alloy nanoparticles-embedded N-doped graphitic carbon for discharging reaction of Zn-air battery. <i>Science China Materials</i> , <b>2020</b> , 63, 327-338	7.1	37
320	Adaptive Multiscale Deep Fusion Residual Network for Remote Sensing Image Classification. <i>IEEE Transactions on Geoscience and Remote Sensing</i> , <b>2019</b> , 57, 8506-8521	8.1	36
319	Electronic Structures of Germanene on MoS <sub>2</sub> : Effect of Substrate and Molecular Adsorption. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 21691-21698	3.8	36
318	Synthesis of shape-stabilized paraffin/silicon dioxide composites as phase change material for thermal energy storage. <i>Journal of Materials Science</i> , <b>2010</b> , 45, 1672-1676	4.3	36
317	Magic structures of helical multishell zirconium nanowires. <i>Physical Review B</i> , <b>2002</b> , 65,	3.3	36
316	Boron clusters with 46, 48, and 50 atoms: competition among the core-shell, bilayer and quasi-planar structures. <i>Nanoscale</i> , <b>2017</b> , 9, 13905-13909	7.7	35
315	Initial Growth Mechanism of Blue Phosphorene on Au(111) Surface. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 17893-17899	3.8	35
314	Tunable optical properties of icosahedral, dodecahedral, and tetrahedral clusters. <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	35
313	Recent progress on 2D magnets: Fundamental mechanism, structural design and modification. <i>Applied Physics Reviews</i> , <b>2021</b> , 8, 031305	17.3	35
312	A Molecular-Cage Strategy Enabling Efficient Chemisorption/Electrocatalytic Interface in Nanostructured Li <sub>2</sub> S Cathode for Li Metal-Free Rechargeable Cells with High Energy. <i>Advanced Functional Materials</i> , <b>2019</b> , 29, 1905986	15.6	33
311	Density functional theory modeling of multilayer "epitaxial" graphene oxide. <i>Accounts of Chemical Research</i> , <b>2014</b> , 47, 3331-9	24.3	33
310	Ab initio-predicted micro-mechanical performance of refractory high-entropy alloys. <i>Scientific Reports</i> , <b>2015</b> , 5, 12334	4.9	33
309	Copper(i) sulfide: a two-dimensional semiconductor with superior oxidation resistance and high carrier mobility. <i>Nanoscale Horizons</i> , <b>2019</b> , 4, 223-230	10.8	32
308	Point defects in epitaxial silicene on Ag(111) surfaces. <i>2D Materials</i> , <b>2016</b> , 3, 025034	5.9	31

307	Graphene Oxide: Physics and Applications. <i>SpringerBriefs in Physics</i> , <b>2015</b> ,	0.6	30
306	Optimally stuffed fullerene structures of silicon nanoclusters. <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	30
305	Unique Transformation from Graphene to Carbide on Re(0001) Induced by Strong Carbon-Metal Interaction. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 17574-17581	16.4	29
304	Electronic and transport gaps of graphene opened by grain boundaries. <i>Journal of Applied Physics</i> , <b>2012</b> , 112, 053713	2.5	29
303	B,N-Doped Defective Carbon Entangled Fe <sub>3</sub> C Nanoparticles as the Superior Oxygen Reduction Electrocatalyst for Zn/Air Batteries. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2019</b> , 7, 19104-19112	8.3	28
302	First-principles study of transition metal doped Li <sub>2</sub> S as cathode materials in lithium batteries. <i>Journal of Renewable and Sustainable Energy</i> , <b>2012</b> , 4, 063128	2.5	28
301	Controllable Conversion of CO on Non-Metallic Gold Clusters. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 1919-1924	16.4	28
300	The cooperation of Fe <sub>3</sub> C nanoparticles with isolated single iron atoms to boost the oxygen reduction reaction for Zn/Air batteries. <i>Journal of Materials Chemistry A</i> , <b>2021</b> , 9, 6831-6840	13	28
299	Graphene oxide and lithium amidoborane: a new way to bridge chemical and physical approaches for hydrogen storage. <i>Journal of Materials Chemistry A</i> , <b>2013</b> , 1, 8016	13	27
298	Cluster-assembled materials based on Na <sub>6</sub> Pb. <i>Physical Review B</i> , <b>2003</b> , 68,	3.3	27
297	Structural, Electronic, and Magnetic Properties of Small Vanadium Clusters. <i>Physica Status Solidi (B): Basic Research</i> , <b>1999</b> , 215, 1127-1135	1.3	27
296	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> , <b>2020</b> , 8, 21189-21198	13	27
295	Point defects in group III nitrides: A comparative first-principles study. <i>Journal of Applied Physics</i> , <b>2019</b> , 125, 215705	2.5	26
294	Mechanical properties of bilayer graphene with twist and grain boundaries. <i>Journal of Applied Physics</i> , <b>2013</b> , 113, 043514	2.5	26
293	Mass spectrometric and first principles study of AlnCl <sub>n</sub> clusters. <i>Solid State Communications</i> , <b>2002</b> , 122, 543-547	1.6	26
292	Structural and electronic properties of Sbn (n=2-10) clusters using density-functional theory. <i>Physical Review A</i> , <b>2005</b> , 72,	2.6	26
291	Growth control, interface behavior, band alignment, and potential device applications of 2D lateral heterostructures. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2018</b> , 8, e1353	7.9	26
290	Giant magnetic anisotropy of a 5d transition metal decorated two-dimensional polyphthalocyanine framework. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 2147-2154	7.1	25

289	Structures and electronic properties of BSi (n = 4-10) clusters: A combined ab initio and experimental study. <i>Journal of Chemical Physics</i> , <b>2017</b> , 146, 044306	3.9	24
288	Low-Energy Structures of Binary Pt <sub>n</sub> Clusters from Global Search Using Genetic Algorithm and Density Functional Theory. <i>Journal of Cluster Science</i> , <b>2015</b> , 26, 389-409	3	24
287	Density-functional study of structural and electronic properties of Al <sub>n</sub> N(n=2-12) clusters. <i>Physical Review A</i> , <b>2005</b> , 72,	2.6	24
286	Structural Design Strategy and Active Site Regulation of High-Efficient Bifunctional Oxygen Reaction Electrocatalysts for Zn-Air Battery. <i>Small</i> , <b>2021</b> , 17, e2006766	11	24
285	Long life rechargeable Li-O <sub>2</sub> batteries enabled by enhanced charge transfer in nanocable-like Fe@N-doped carbon nanotube catalyst. <i>Science China Materials</i> , <b>2017</b> , 60, 415-426	7.1	23
284	Controlling the synthesis of uniform electron-deficient Pd clusters for superior hydrogen production from formic acid. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 10363-10371	13	23
283	Immobilized trimeric metal clusters: A family of the smallest catalysts for selective CO <sub>2</sub> reduction toward multi-carbon products. <i>Nano Energy</i> , <b>2020</b> , 76, 105049	17.1	23
282	Excitonic AuRu(PPh)(SCHPh) cluster for light-driven dinitrogen fixation. <i>Chemical Science</i> , <b>2020</b> , 11, 2440-2447	9.4	23
281	Stability and magnetic properties of transition metal atoms endohedral B <sub>n</sub> N <sub>n</sub> (n=12-28) cages. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 084306	3.9	23
280	N-doped carbon-coated Co <sub>3</sub> O <sub>4</sub> nanosheet array/carbon cloth for stable rechargeable Zn-air batteries. <i>Science China Materials</i> , <b>2019</b> , 62, 624-632	7.1	23
279	Strong Adlayer-Substrate Interactions "Break" the Patching Growth of h-BN onto Graphene on Re(0001). <i>ACS Nano</i> , <b>2017</b> , 11, 1807-1815	16.7	22
278	Realization of Strained Stanene by Interface Engineering. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 1558-1565	6.4	22
277	Selecting electrode materials for monolayer ReS <sub>2</sub> with an Ohmic contact. <i>Journal of Materials Chemistry C</i> , <b>2018</b> , 6, 6764-6770	7.1	22
276	Band gap opening in bilayer silicene by alkali metal intercalation. <i>Journal of Physics Condensed Matter</i> , <b>2014</b> , 26, 475303	1.8	22
275	Defects and oxidation of group-III monochalcogenide monolayers. <i>Journal of Chemical Physics</i> , <b>2017</b> , 147, 104709	3.9	22
274	Nanocables made of a transition metal wire and boron nitride sheath: Density functional calculations. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	22
273	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> , <b>2016</b> , 183, 2941-2948	5.8	22
272	2D lateral heterostructures of monolayer and bilayer phosphorene. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 2291-2300	7.1	21

271	Two-dimensional spin-valley-coupled Dirac semimetals in functionalized SbAs monolayers. <i>Materials Horizons</i> , <b>2019</b> , 6, 781-787	14.4	21
270	De novo design of Au(SR) nanoclusters. <i>Nature Communications</i> , <b>2020</b> , 11, 3349	17.4	21
269	Selective C-C Coupling by Spatially Confined Dimeric Metal Centers. <i>IScience</i> , <b>2020</b> , 23, 101051	6.1	21
268	The Evolution in Catalytic Activity Driven by Periodic Transformation in the Inner Sites of Gold Clusters. <i>Advanced Functional Materials</i> , <b>2019</b> , 29, 1904242	15.6	21
267	Structure, Electrode Voltage and Activation Energy of LiMnxCoyNi1-x-yO2 Solid Solutions as Cathode Materials for Li Batteries from First-Principles. <i>Journal of the Electrochemical Society</i> , <b>2012</b> , 159, A1203-A1208	3.9	21
266	Structural growth sequences and electronic properties of manganese-doped germanium clusters: MnGe <sub>n</sub> (2n-5). <i>Journal of Physics Condensed Matter</i> , <b>2008</b> , 20, 335223	1.8	21
265	Electronic and magnetic properties of manganese and iron-doped Ga <sub>n</sub> As <sub>n</sub> nanocages (n=7-12). <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 044908	3.9	21
264	Interaction between Post-Graphene Group-IV Honeycomb Monolayers and Metal Substrates: Implication for Synthesis and Structure Control. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 5123-5129	3.8	20
263	Which Density Functional Should Be Used to Describe Protonated Water Clusters?. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 3117-3127	2.8	20
262	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> , <b>2016</b> , 120, 14699-14705	3.8	20
261	Design of three-shell icosahedral matryoshka clusters A@B@A <sub>2</sub> (A = Sn, Pb; B = Mg, Zn, Cd, Mn). <i>Scientific Reports</i> , <b>2014</b> , 4, 6915	4.9	20
260	Improved stability of water clusters (H <sub>2</sub> O) <sub>30</sub> : a Monte Carlo search coupled with DFT computations. <i>Theoretical Chemistry Accounts</i> , <b>2012</b> , 131, 1	1.9	20
259	Ideal strength of random alloys from first principles. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	20
258	Magnetic properties of transition-metal impurities in silicon quantum dots. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	20
257	A Silver Nanocluster Containing Interstitial Sulfur and Unprecedented Chemical Bonds. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 11443-11447	3.6	20
256	Gold-Doping of Double-Crown Pd Nanoclusters. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 18187-18192	4.8	19
255	Silicene catalysts for CO hydrogenation: the number of layers controls selectivity. <i>Nanoscale</i> , <b>2019</b> , 11, 7734-7743	7.7	19
254	The isolable matryoshka nesting doll icosahedral cluster [As@Ni <sub>12</sub> @As <sub>20</sub> ] <sup>3-</sup> as a "superatom": analogy with the jellium cluster Al <sub>13</sub> - generated in the gas phase by laser vaporization. <i>Chemical Communications</i> , <b>2006</b> , 4204-5	5.8	19

253	Sustainable S cathodes with synergic electrocatalysis for room-temperature NaS batteries. <i>Journal of Materials Chemistry A</i> , <b>2021</b> , 9, 566-574	13	19
252	Atomistic understanding of the lateral growth of graphene from the edge of an h-BN domain: towards a sharp in-plane junction. <i>Nanoscale</i> , <b>2017</b> , 9, 3585-3592	7.7	18
251	Interaction between helium and intrinsic point defects in 3C-SiC single crystal. <i>Journal of Applied Physics</i> , <b>2017</b> , 121, 225111	2.5	18
250	Oxygen Evolution Reaction over the Au/YSZ Interface at High Temperature. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 4617-4621	16.4	18
249	Ag Au (PET) Nanocluster: Dimeric Assembly of Au (PET) Enabled by Silver Atoms. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 13941-13946	16.4	18
248	Ionic and superionic phases in ammonia dihydrate NH <sub>3</sub> D <sub>2</sub> H <sub>2</sub> O under high pressure. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	18
247	Adsorption of selected gases on metal-organic frameworks and covalent organic frameworks: A comparative grand canonical Monte Carlo simulation. <i>Journal of Applied Physics</i> , <b>2012</b> , 111, 112628	2.5	18
246	Combining Machine Learning Potential and Structure Prediction for Accelerated Materials Design and Discovery. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 8710-8720	6.4	18
245	Accurate electronic properties and non-linear optical response of two-dimensional MA <sub>2</sub> Z <sub>4</sub> . <i>Nanoscale</i> , <b>2021</b> , 13, 5479-5488	7.7	18
244	Reactions of Copper and Silver Cations with Carbon Dioxide: An Infrared Photodissociation Spectroscopic and Theoretical Study. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 3220-3226	2.8	17
243	Defective Graphene on the Transition-Metal Surface: Formation of Efficient Bifunctional Catalysts for Oxygen Evolution/Reduction Reactions in Alkaline Media. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 17410-17415	9.5	17
242	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> , <b>2018</b> , 12, 417-424	4.5	17
241	Engineering magnetic anisotropy in two-dimensional magnetic materials. <i>Advances in Physics: X</i> , <b>2018</b> , 3, 1432415	5.1	17
240	Halogen-doping in LiCoO <sub>2</sub> cathode materials for Li-ion batteries: insights from ab initio calculations. <i>RSC Advances</i> , <b>2015</b> , 5, 107326-107332	3.7	17
239	MXene and MBene as efficient catalysts for energy conversion: roles of surface, edge and interface. <i>JPhys Energy</i> , <b>2021</b> , 3, 012002	4.9	17
238	Computational high-throughput screening of alloy nanoclusters for electrocatalytic hydrogen evolution. <i>Npj Computational Materials</i> , <b>2021</b> , 7,	10.9	17
237	Two-dimensional B-C-O alloys: a promising class of 2D materials for electronic devices. <i>Nanoscale</i> , <b>2016</b> , 8, 8910-8	7.7	17
236	A Ternary Alloy Substrate to Synthesize Monolayer Graphene with Liquid Carbon Precursor. <i>ACS Nano</i> , <b>2017</b> , 11, 1371-1379	16.7	16

235	Stability and Vibrations of Guest Molecules in the Type II Clathrate Hydrate: A First-Principles Study of Solid Phase. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 7063-9	2.8	16
234	Structural Evolution and Superatoms in Molybdenum Atom Stabilized Boron Clusters: MoBn (n = 10-14). <i>Journal of Cluster Science</i> , <b>2018</b> , 29, 847-852	3	16
233	Tunable Thermal Conductivity of Silicene by Germanium Doping. <i>Journal of Superconductivity and Novel Magnetism</i> , <b>2016</b> , 29, 717-720	1.5	16
232	Mo Concentration Controls the Morphological Transitions from Dendritic to Semicompact, and to Compact Growth of Monolayer Crystalline MoS on Various Substrates. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 42751-42759	9.5	16
231	Film Structure of Epitaxial Graphene Oxide on SiC: Insight on the Relationship Between Interlayer Spacing, Water Content, and Intralayer Structure. <i>Advanced Materials Interfaces</i> , <b>2014</b> , 1, 1300106	4.6	16
230	Novel Magnetic Monolayers of Transition Metal Silicide. <i>Journal of Superconductivity and Novel Magnetism</i> , <b>2015</b> , 28, 1755-1758	1.5	16
229	Chemical Structure of Oxidized Multilayer Epitaxial Graphene: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 6267-6274	3.8	16
228	Precisely Constructed Silver Active Sites in Gold Nanoclusters for Chemical Fixation of CO. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 10573-10576	16.4	16
227	Manipulating the assembled structure of atomically thin CoSe <sub>2</sub> nanomaterials for enhanced water oxidation catalysis. <i>Nano Energy</i> , <b>2019</b> , 57, 371-378	17.1	16
226	Silicon Nanocages for Selective Carbon Dioxide Conversion under Visible Light. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 9973-9980	3.8	15
225	Vacancy Engineering of Iron-Doped W <sub>18</sub> O <sub>49</sub> Nanoreactors for Low-Barrier Electrochemical Nitrogen Reduction. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 7426-7431	3.6	15
224	Structural evolution and magnetic properties of anionic clusters CrGe (n = 3-14): photoelectron spectroscopy and density functional theory computation. <i>Journal of Physics Condensed Matter</i> , <b>2018</b> , 30, 335501	1.8	15
223	Anomalous High-Energy Waterfall-Like Electronic Structure in 5 d Transition Metal Oxide Sr <sub>2</sub> IrO <sub>4</sub> with a Strong Spin-Orbit Coupling. <i>Scientific Reports</i> , <b>2015</b> , 5, 13036	4.9	15
222	First-principles studies on the thermal decomposition behavior of FOX-7. <i>High Pressure Research</i> , <b>2010</b> , 30, 301-309	1.6	15
221	Surface thermal stability of nickel clusters. <i>Physica Status Solidi (B): Basic Research</i> , <b>1996</b> , 193, 355-361	1.3	15
220	Identifying the Non-Identical Outermost Selenium Atoms and Invariable Band Gaps across the Grain Boundary of Anisotropic Rhenium Diselenide. <i>ACS Nano</i> , <b>2018</b> , 12, 10095-10103	16.7	15
219	An Electrochemical Cinnamyl C <sub>H</sub> Amination Reaction Using Carbonyl Sulfamate. <i>Chinese Journal of Chemistry</i> , <b>2019</b> , 37, 570-574	4.9	14
218	Hollow CoO Nanosphere Surrounded by N-Doped Graphitic Carbon Filled within Multilayer-Sandwiched Graphene Network: A High-Performance Anode for Lithium Storage. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 3416-3424	5.1	14

217	Tuning the electronic properties of bilayer black phosphorene with the twist angle. <i>Journal of Materials Chemistry C</i> , <b>2020</b> , 8, 6264-6272	7.1	14
216	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. <i>Transplantation Proceedings</i> , <b>2011</b> , 43, 2747-54	1.1	14
215	Reactivity and Lability Modulated by a Valence Electron Moving in and out of 25-Atom Gold Nanoclusters. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 21135-21142	16.4	14
214	A-Site Cation Substitutions in Strained Y-Doped BaZrO <sub>3</sub> Multilayer Films Leading to Fast Proton Transport Pathways. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 8387-8391	3.8	14
213	Electrochemical Hydrogenation with Gaseous Ammonia. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 1773-1777	3.6	14
212	Application of Hantzsch Ester and Meyer Nitrile in Radical Alkynylation Reactions. <i>Organic Letters</i> , <b>2018</b> , 20, 6906-6909	6.2	14
211	Foreign atom encapsulated Au golden cages for catalysis of CO oxidation. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 10587-10593	3.6	13
210	Room temperature electrofreezing of water yields a missing dense ice phase in the phase diagram. <i>Nature Communications</i> , <b>2019</b> , 10, 1925	17.4	13
209	Anionic Copper Clusters Reacting with NO: An Open-Shell Superatom Cu. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 5807-5814	6.4	13
208	Stability and magnetic properties of Fe encapsulating in silicon nanotubes. <i>Nanotechnology</i> , <b>2007</b> , 18, 235705	3.4	13
207	Electronic properties and chemical trends of the arsenic in situ impurities in Hg <sub>1-x</sub> Cd <sub>x</sub> Te: First-principles study. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	13
206	Enhanced Ferromagnetism of CrI <sub>3</sub> Bilayer by Self-Intercalation. <i>Chinese Physics Letters</i> , <b>2020</b> , 37, 107506	1.8	13
205	Architecting Freestanding Sulfur Cathodes for Superior Room-Temperature Na <sup>+</sup> Batteries. <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2102280	15.6	13
204	Cd-driven surface reconstruction and photodynamics in gold nanoclusters. <i>Chemical Science</i> , <b>2021</b> , 12, 3290-3294	9.4	13
203	Confining a bi-enzyme inside the nanochannels of a porous aluminum oxide membrane for accelerating the enzymatic reactions. <i>Chemical Communications</i> , <b>2017</b> , 53, 2673-2676	5.8	12
202	Magnetism in the p-type Monolayer II-VI semiconductors SrS and SrSe. <i>Scientific Reports</i> , <b>2017</b> , 7, 45869	4.9	12
201	Chemical-Reductant-Free Electrochemical Deuteration Reaction using Deuterium Oxide. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 14066-14071	3.6	12
200	Revisit the landscape of protonated water clusters H(H <sub>2</sub> O) <sub>n</sub> with n = 10-17: An ab initio global search. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 174305	3.9	12



199	Density functional study of onion-skin-like [As@Ni <sub>12</sub> As <sub>20</sub> ] <sub>3</sub> and [Sb@Pd <sub>12</sub> Sb <sub>20</sub> ] <sub>3</sub> cluster ions. <i>Chemical Physics Letters</i> , <b>2004</b> , 396, 161-166	2.5	12
198	High-Curie-temperature ferromagnetism in bilayer CrI <sub>3</sub> on bulk semiconducting substrates. <i>Physical Review Materials</i> , <b>2020</b> , 4,	3.2	12
197	Ab initio global optimization of clusters. <i>Chemical Modelling</i> , <b>2015</b> , 249-292	2	12
196	Two-Dimensional AXenes: A New Family of Room-Temperature d Ferromagnets and Their Structural Phase Transitions. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 7753-7759	6.4	12
195	A new family of multifunctional silicon clathrates: Optoelectronic and thermoelectric applications. <i>Journal of Applied Physics</i> , <b>2017</b> , 121, 085107	2.5	11
194	Competition between tubular, planar and cage geometries: a complete picture of structural evolution of B (n = 31-50) clusters. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 12959-12966	3.6	11
193	2D tetragonal transition-metal phosphides: an ideal platform to screen metal shrouded crystals for multifunctional applications. <i>Nanoscale</i> , <b>2020</b> , 12, 6776-6784	7.7	11
192	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> , <b>2016</b> , 18, 7156-62	3.6	11
191	Tuning Schottky barriers for monolayer GaSe FETs by exploiting a weak Fermi level pinning effect. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 21732-21738	3.6	11
190	Electronic properties of a silicon carbide nanotube under uniaxial tensile strain: a density function theory study. <i>Journal of Nanoparticle Research</i> , <b>2010</b> , 12, 2919-2928	2.3	11
189	Core-shell MnO <sub>2</sub> Nanotubes@NickelCobaltZinc Hydroxide Nanosheets for Supercapacitive Energy Storage. <i>ACS Applied Nano Materials</i> , <b>2020</b> , 3, 7462-7473	5.6	11
188	Precisely modulating the surface sites on atomically monodispersed gold-based nanoclusters for controlling their catalytic performances. <i>Nanoscale</i> , <b>2020</b> , 12, 18004-18012	7.7	11
187	Giant Thickness-Tunable Bandgap and Robust Air Stability of 2D Palladium Diselenide. <i>Small</i> , <b>2020</b> , 16, e2000754	11	11
186	Visible-light overall water splitting on g-C <sub>3</sub> N <sub>4</sub> decorated by subnanometer oxide clusters. <i>Materials Today Physics</i> , <b>2021</b> , 16, 100312	8	11
185	CoWO <sub>4</sub> nanoparticles wrapped by RGO as high capacity anode material for lithium ion batteries. <i>Rare Metals</i> , <b>2017</b> , 36, 411-417	5.5	10
184	An ultralow-density porous ice with the largest internal cavity identified in the water phase diagram. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2019</b> , 116, 12684-12691	11.5	10
183	Structure Evolution of Transition Metal-doped Gold Clusters M@Au <sub>12</sub> (M = 3d <sub>5</sub> ): Across the Periodic Table. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 7449-7457	3.8	10
182	Structures and Spectroscopic Properties of F(HO) with n = 1-10 Clusters from a Global Search Based On Density Functional Theory. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 3413-3422	2.8	10

181	Electric field and strain tunable electronic structures in monolayer Black Phosphorus. <i>Computational Materials Science</i> , <b>2016</b> , 112, 297-303	3.2	10
180	Novel electronic structures of superlattice composed of graphene and silicene. <i>Materials Research Bulletin</i> , <b>2014</b> , 50, 268-272	5.1	10
179	A first-principle study of the structural and electronic properties of amorphous Cu-Zr alloys. <i>Science China: Physics, Mechanics and Astronomy</i> , <b>2011</b> , 54, 249-255	3.6	10
178	Thermal decomposition behaviour of RDX by first-principles molecular dynamics simulation. <i>Molecular Simulation</i> , <b>2008</b> , 34, 961-965	2	10
177	Low-dimensional non-metal catalysts: principles for regulating p-orbital-dominated reactivity. <i>Npj Computational Materials</i> , <b>2021</b> , 7,	10.9	10
176	The precise editing of surface sites on a molecular-like gold catalyst for modulating regioselectivity. <i>Chemical Science</i> , <b>2020</b> , 11, 8000-8004	9.4	10
175	Control of Photocarrier Separation and Recombination at Bismuth Oxyhalide Interface for Nitrogen Fixation. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 9304-9312	6.4	10
174	The Synthesis of Chiral Ag <sub>4</sub> Pd <sub>2</sub> (SR) <sub>8</sub> by Nonreplaced Galvanic Reaction. <i>Particle and Particle Systems Characterization</i> , <b>2019</b> , 36, 1900003	3.1	10
173	Revisit of large-gap Si clusters encapsulating group-IV metal atoms (Ti, Zr, Hf). <i>Journal of Computational Chemistry</i> , <b>2018</b> , 39, 2268-2272	3.5	10
172	Active-Site Tailoring of Gold Cluster Catalysts for Electrochemical CO <sub>2</sub> Reduction. <i>ACS Catalysis</i> , <b>2021</b> , 11, 11551-11560	13.1	10
171	Superatomic Signature and Reactivity of Silver Clusters with Oxygen: Double Magic Ag <sub>17</sub> with Geometric and Electronic Shell Closure. <i>CCS Chemistry</i> , 219-229	7.2	10
170	Hydrated Sodium Ion Clusters [Na(H <sub>2</sub> O) <sub>n</sub> ] <sup>+</sup> (n = 1-6): An Study on Structures and Non-covalent Interaction. <i>Frontiers in Chemistry</i> , <b>2019</b> , 7, 624	5	9
169	Rational design of two-dimensional hybrid Co/N-doped carbon nanosheet arrays for efficient bi-functional electrocatalysis. <i>Sustainable Energy and Fuels</i> , <b>2019</b> , 3, 1757-1763	5.8	9
168	Wavelength-Tunable Optical Fiber Localized Surface Plasmon Resonance Biosensor a Diblock Copolymer-Templated Nanorod Monolayer. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 50929-50945	9	9
167	CO <sub>2</sub> reduction on p-block metal oxide overlayers on metal substrates—D MgO as a prototype. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 5688-5698	13	9
166	An electrocatalyst with anti-oxidized capability for overall water splitting. <i>Nano Research</i> , <b>2018</b> , 11, 3411-3418	9	9
165	Enhanced thermoelectric properties of graphene oxide patterned by nanoroads. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 10607-15	3.6	9
164	Medium-sized [Formula: see text] (n = 14-20) clusters: a combined study of photoelectron spectroscopy and DFT calculations. <i>Journal of Physics Condensed Matter</i> , <b>2018</b> , 30, 354002	1.8	9

163	Monolayered semiconducting GeAsSe and SnSbTe with ultrahigh hole mobility. <i>Frontiers of Physics</i> , <b>2018</b> , 13, 1	3.7	9
162	Three-dimensional phase field simulation of intragranular void formation and thermal conductivity in irradiated Fe. <i>Journal of Materials Science</i> , <b>2018</b> , 53, 11002-11014	4.3	9
161	Dual transition metal doped germanium clusters for catalysis of CO oxidation. <i>Journal of Alloys and Compounds</i> , <b>2019</b> , 806, 698-704	5.7	9
160	First-principles calculations of elastic moduli of TiMoNb alloys using a cluster-plus-glue-atom model for stable solid solutions. <i>Journal of Materials Science</i> , <b>2013</b> , 48, 3138-3146	4.3	9
159	Insight into the initial oxidation of 4H-SiC from first-principles thermodynamics. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	9
158	Numerical simulation of flow past stationary and oscillating deformable circles with fluid-structure interaction. <i>Experimental and Computational Multiphase Flow</i> , <b>2020</b> , 2, 151-161	4.2	9
157	Progress of tubulin polymerization activity detection methods. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2021</b> , 37, 127698	2.9	9
156	Crystal-Phase-Mediated Restructuring of Pt on TiO <sub>2</sub> with Tunable Reactivity: Redispersion versus Reshaping. <i>ACS Catalysis</i> , <b>2022</b> , 12, 3634-3643	13.1	9
155	Atomically Sharp Dual Grain Boundaries in 2D WS <sub>2</sub> Bilayers. <i>Small</i> , <b>2019</b> , 15, e1902590	11	8
154	Aminomethyl-Functionalized Carbon Nanotubes as a Host of Small Sulfur Clusters for High-Performance Lithium-Sulfur Batteries. <i>ChemSusChem</i> , <b>2020</b> , 13, 2761-2768	8.3	8
153	Anomalous ideal tensile strength of ferromagnetic Fe and Fe-rich alloys. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	8
152	Mechanical anisotropy and strain-tailored band structures of pentagonal boron nitride monolayers. <i>Journal of Applied Physics</i> , <b>2017</b> , 122, 094302	2.5	8
151	Metal-Encapsulated Boron Nitride Nanocages for Solar-Driven Nitrogen Fixation. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 23798-23806	3.8	8
150	Optimization of photocarrier dynamics and activity in phosphorene with intrinsic defects for nitrogen fixation. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 20570-20580	13	8
149	Temperature and coverage effects on the stability of epitaxial silicene on Ag(111) surfaces. <i>Applied Surface Science</i> , <b>2017</b> , 409, 97-101	6.7	7
148	An Au Cluster Fortified by Four Ferrocenes. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 6061-6067	2.8	7
147	Three dimensional porous SiC for lithium polysulfide trapping. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 4005-4011	3.6	7
146	Tuning the structures of two-dimensional cuprous oxide confined on Au(111). <i>Nano Research</i> , <b>2018</b> , 11, 5957-5967	10	7

145	Performance Evaluation of Asphalt Mixture with Nanosized Volcanic Ash Filler. <i>Journal of Transportation Engineering Part B: Pavements</i> , <b>2018</b> , 144, 04018028	1.4	7
144	Design of superhalogens using a core-shell structure model. <i>Nanoscale</i> , <b>2017</b> , 9, 18781-18787	7.7	7
143	Mechanism of Ce promoting SO <sub>2</sub> resistance of MnO <sub>x</sub> /Al <sub>2</sub> O <sub>3</sub> : An experimental and DFT study. <i>Korean Journal of Chemical Engineering</i> , <b>2017</b> , 34, 2065-2071	2.8	7
142	Tensile strain-induced softening of iron at high temperature. <i>Scientific Reports</i> , <b>2015</b> , 5, 16654	4.9	7
141	Evolution of boron clusters in iron tetraborides under high pressure: semiconducting and ferromagnetic superhard materials. <i>RSC Advances</i> , <b>2015</b> , 5, 48012-48023	3.7	7
140	Ground state structures, electronic and optical properties of medium-sized Nan + (n = 9, 15, 21, 26, 31, 36, 41, 50 and 59) clusters from ab initio genetic algorithm. <i>European Physical Journal D</i> , <b>2013</b> , 67, 1	1.3	7
139	Quantum conductance of armchair carbon nanocoils: roles of geometry effects. <i>Science China: Physics, Mechanics and Astronomy</i> , <b>2011</b> , 54, 841-845	3.6	7
138	Catalytic Hydrodenitrogenation of Pyridine under Hydrothermal Conditions: A Comprehensive Study. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2021</b> , 9, 362-374	8.3	7
137	Carrier Dynamics and Transfer across the CdS/MoS Interface upon Optical Excitation. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 6544-6550	6.4	7
136	Robust spin manipulation in 2D organometallic Kagome lattices: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 11045-11052	3.6	7
135	Efficient Photoexcited Charge Separation at the Interface of a Novel 0D/2D Heterojunction: A Time-Dependent Ultrafast Dynamic Study. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 2312-2319	6.4	7
134	Large magnetic anisotropy in chemically engineered iridium dimer. <i>Communications Physics</i> , <b>2018</b> , 1,	5.4	7
133	Solvent-Based Atomistic Theory for Doping Colloidal-Synthesized Quantum Dots via Cation Exchange. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 27085-27090	3.8	6
132	Tunable bending modulus and bending limit of oxidized graphene. <i>Nanoscale</i> , <b>2020</b> , 12, 1623-1628	7.7	6
131	Precisely Constructed Silver Active Sites in Gold Nanoclusters for Chemical Fixation of CO <sub>2</sub> . <i>Angewandte Chemie</i> , <b>2021</b> , 133, 10667-10670	3.6	6
130	Exceptional Electrochemical HER Performance with Enhanced Electron Transfer between Ru Nanoparticles and Single Atoms Dispersed on a Carbon Substrate. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 16180-16186	3.6	6
129	Revisit of Sin (n = 21-29) Clusters by Ab Initio Global Search. <i>Journal of Cluster Science</i> , <b>2017</b> , 28, 1729-1737		5
128	Quantum oscillation in carrier transport in two-dimensional junctions. <i>Nanoscale</i> , <b>2018</b> , 10, 7912-7917	7.7	5

127	Ab initio molecular dynamics study of fluid H <sub>2</sub> O-CO <sub>2</sub> mixture in broad pressure-temperature range. <i>AIP Advances</i> , <b>2017</b> , 7, 115217	1.5	5
126	Tuning the electronic and optical properties of hydrogen-terminated Si nanocluster by uniaxial compression. <i>Journal of Nanoparticle Research</i> , <b>2012</b> , 14, 1	2.3	5
125	Carbon clusters near the step of Rh surface: implication for the initial stage of graphene nucleation. <i>European Physical Journal D</i> , <b>2013</b> , 67, 1	1.3	5
124	Oxidation of step edges on vicinal 4H-SiC(0001) surfaces. <i>Applied Physics Letters</i> , <b>2013</b> , 103, 211603	3.4	5
123	Effect of iron on high pressure elasticity of hydrous wadsleyite and ringwoodite by first-principles simulation. <i>High Pressure Research</i> , <b>2012</b> , 32, 385-395	1.6	5
122	Calculations of electronic structure of Ge <sub>44</sub> Mn <sub>2</sub> Ba <sub>8</sub> and Ge <sub>42</sub> Mn <sub>4</sub> Ba <sub>8</sub> clathrates. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	5
121	Topologically protected states and half-metal behaviors: Defect-strain synergy effects in two-dimensional antimonene. <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	5
120	Excellent HER and OER Catalyzing Performance of Se-Vacancies in Defects-Engineered PtSe <sub>2</sub> : From Simulation to Experiment. <i>Advanced Energy Materials</i> , 2102359	21.8	5
119	Scalable Production of Freestanding Few-Layer Borophene Single Crystalline Sheets as Efficient Electrocatalysts for Lithium-Sulfur Batteries. <i>ACS Nano</i> , <b>2021</b> ,	16.7	5
118	Solar Driven CO <sub>2</sub> Hydrogenation on Ti-Doped Silicon Nanocages. <i>Journal of Cluster Science</i> , <b>2020</b> , 31, 627-635	3	5
117	Dual-Constrained Sulfur in FeS <sub>2</sub> @C Nanostructured Lithium-Sulfide Batteries. <i>ACS Applied Energy Materials</i> , <b>2020</b> , 3, 10950-10960	6.1	5
116	Epitaxial growth of an atom-thin layer on a LiNiMnO cathode for stable Li-ion battery cycling.. <i>Nature Communications</i> , <b>2022</b> , 13, 1565	17.4	5
115	Ultra-thin Ga nanosheets: analogues of high pressure Ga(iii). <i>Nanoscale</i> , <b>2019</b> , 11, 17201-17205	7.7	4
114	Evolution of atomic structures of Sn, Sn <sub>n</sub> , and SnCl clusters (N = 4-20): Insight from ab initio calculations. <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 174304	3.9	4
113	Dissociation mechanism of gas hydrates (I, II, H) of alkane molecules: a comparative molecular dynamics simulation. <i>Molecular Simulation</i> , <b>2015</b> , 41, 1086-1094	2	4
112	Oxidation Behaviors of Two-dimensional Metal Chalcogenides. <i>ChemNanoMat</i> , <b>2020</b> , 6, 838-849	3.5	4
111	Structures and vertical detachment energies of water cluster anions (H <sub>2</sub> O) <sub>n</sub> <sup>-</sup> with n = 6-11. <i>Theoretical Chemistry Accounts</i> , <b>2020</b> , 139, 1	1.9	4
110	Numerical simulation of flow past a triangular prism with fluid-structure interaction. <i>Engineering Applications of Computational Fluid Mechanics</i> , <b>2020</b> , 14, 462-476	4.5	4

109	First-principles study of the effect of water on the phase transitions in Mg <sub>2</sub> SiO <sub>4</sub> forsterite. <i>High Pressure Research</i> , <b>2010</b> , 30, 318-324	1.6	4
108	Optical and thermal properties of a cyanine dye medium for next-generation DVD-Rs. <i>Imaging Science Journal</i> , <b>1999</b> , 47, 113-117	0.9	4
107	Photoinduced Spin Injection and Ferromagnetism in 2D Group III Monochalcogenides.. <i>Journal of Physical Chemistry Letters</i> , <b>2022</b> , 590-597	6.4	4
106	Photodriven Catalytic Hydrogenation of CO to CH with Nearly 100% Selectivity over Ag Clusters. <i>Nano Letters</i> , <b>2021</b> , 21, 8693-8700	11.5	4
105	Three-dimensional borophene: A light-element topological nodal-line semimetal with direction-dependent type-II Weyl fermions. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	4
104	Solar driven CO hydrogenation on transition metal doped ZnO cluster. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 164306	3.9	4
103	Transition metal-doped B <sub>n</sub> (n = 7-10) clusters: confirmation of a circular disk Jellium model. <i>European Physical Journal Plus</i> , <b>2021</b> , 136, 1	3.1	4
102	Magnetic Anisotropy of Small Irn Clusters (n = 2-8). <i>Journal of Cluster Science</i> , <b>2016</b> , 27, 935-946	3	4
101	Atomic Structures and Electronic Properties of Large-Sized Ge <sub>N</sub> Clusters (N = 45, 50, 55, 60, 65, 70) by First-Principles Global Search. <i>Journal of Cluster Science</i> , <b>2019</b> , 30, 371-377	3	4
100	Two-dimensional intrinsic ferromagnets with high Curie temperatures: synthesis, physical properties and device applications. <i>Journal of Materials Chemistry C</i> ,	7.1	4
99	Distinct structure assembly driven by metal-ligand binding in Au nanoclusters and its relation to photocatalysis. <i>Chemical Communications</i> , <b>2021</b> , 57, 2176-2179	5.8	4
98	Elastic anharmonicity of bcc Fe and Fe-based random alloys from first-principles calculations. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	3
97	ThermalMechanical Responses of the First Wall in CFETR Under Transient Events. <i>Journal of Fusion Energy</i> , <b>2017</b> , 36, 49-57	1.6	3
96	Distributed Robust Filtering for Wireless Sensor Networks with Markov Switching Topologies and Deception Attacks. <i>Sensors</i> , <b>2020</b> , 20,	3.8	3
95	Surfactant-Free Approach for Engineering an Ultrathin Ti-Doped Ni(OH) Nanosheet on Carbon Cloth: Experimental and Theoretical Insight into Boosted Alkaline Water Oxidation Activity. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 10253-10261	5.1	3
94	Low-Energy Structures and Electronic Properties of Large-Sized Si <sub>N</sub> Clusters (N = 60, 80, 100, 120, 150, 170). <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 11086-11095	3.8	3
93	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> , <b>2016</b> , 51, 2823-2832	2.5	3
92	Strongly Hole-Doped and Highly Decoupled Graphene on Platinum by Water Intercalation. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 3998-4002	6.4	3

91	Effect of Hydrogen in a Vanadium Grain Boundary by First Principles. <i>Fusion Science and Technology</i> , <b>2014</b> , 66, 106-111	1.1	3
90	Self-assembly 2D zinc-phthalocyanine heterojunction: An ideal platform for high efficiency solar cell. <i>Applied Physics Letters</i> , <b>2017</b> , 111, 253904	3.4	3
89	Hexanuclear cobalt carbonyl carbide clusters: the interplay between octahedral and trigonal prismatic structures. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 9314-20	5.1	3
88	Tuning Optical Absorption and Emission of Sub-Nanometer Gold-Caged Metal Systems M@Au <sub>14</sub> by Substitutional Doping. <i>Journal of Computational and Theoretical Nanoscience</i> , <b>2006</b> , 3, 312-314	0.3	3
87	Electrical Conductance of Graphene with Point Defects. <i>Wuli Huaxue Xuebao/Acta Physico - Chimica Sinica</i> , <b>2019</b> , 35, 1142-1149	3.8	3
86	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> , <b>2021</b> , 125, 431-441	3.4	3
85	Structural Modeling and Physical Properties. <i>SpringerBriefs in Physics</i> , <b>2015</b> , 31-56	0.6	3
84	Ligand-protected AuRu and AuRu nanoclusters: distinct structures and implications for site-cooperation catalysis. <i>Chemical Communications</i> , <b>2020</b> , 56, 12833-12836	5.8	3
83	Structures, stabilities and electronic properties of TimSi <sub>m</sub> (m = 1-2, n = 14-20) clusters: a combined ab initio and experimental study. <i>European Physical Journal Plus</i> , <b>2020</b> , 135, 1	3.1	3
82	Temperature-dependent hardness of zinc-blende structured covalent materials. <i>Science China Materials</i> , <b>2021</b> , 64, 2280-2288	7.1	3
81	Single O Atom Doped Ag Cluster Cations for CO Oxidation: An O-Doped Superatom Ag <sub>150+</sub> with Remarkable Stability. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 7067-7076	3.8	3
80	Dithiol Self-Assembled Monolayer Based Electrochemical Surface Plasmon Resonance Optical Fiber Sensor for Selective Heavy Metal Ions Detection. <i>Journal of Lightwave Technology</i> , <b>2021</b> , 39, 4034-4040	4	3
79	Compositionally Designed 2D Ruddlesden-Popper Perovskites for Efficient and Stable Solar Cells. <i>Solar Rrl</i> , <b>2021</b> , 5, 2000661	7.1	3
78	Electrocatalytic and photocatalytic applications of atomically precise gold-based nanoclusters. <i>Science China Chemistry</i> , <b>2021</b> , 64, 1065-1075	7.9	3
77	Atomic Wires of Transition Metal Chalcogenides: A Family of 1D Materials for Flexible Electronics and Spintronics. <i>Jacs Au</i> , <b>2021</b> , 1, 147-155		3
76	Ring-contraction of hantzsch esters and their derivatives to pyrroles via electrochemical extrusion of ethyl acetate out of aromatic rings. <i>Green Chemistry</i> , <b>2021</b> , 23, 3468-3473	10	3
75	MBLT: Learning Motion and Background for Vehicle Tracking in Satellite Videos. <i>IEEE Transactions on Geoscience and Remote Sensing</i> , <b>2021</b> , 1-15	8.1	3
74	Kondo Holes in the Two-Dimensional Itinerant Ising Ferromagnet FeGeTe. <i>Nano Letters</i> , <b>2021</b> , 21, 6117-6123	6.123	3

73	Evolution from superatomic AuAg monomers into molecular-like AuAg dimeric nanoclusters.. <i>Chemical Science</i> , <b>2022</b> , 13, 2778-2782	9.4	3
72	Ag <sub>2</sub> Au <sub>50</sub> (PET) <sub>36</sub> Nanocluster: Dimeric Assembly of Au <sub>25</sub> (PET) <sub>18</sub> Enabled by Silver Atoms. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 14045-14050	3.6	2
71	Experimental Realization of Two-Dimensional Buckled Lieb Lattice. <i>Nano Letters</i> , <b>2020</b> , 20, 2537-2543	11.5	2
70	Electronic and magnetic properties of transition metal decorated monolayer GaS. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2018</b> , 101, 131-138	3	2
69	Interaction Mechanisms of Insensitive Explosive FOX-7 and Graphene Oxides from Ab Initio Calculations. <i>Nanomaterials</i> , <b>2019</b> , 9,	5.4	2
68	Optical property of amorphous semiconductor mercury cadmium telluride from first-principles study. <i>Science in China Series D: Earth Sciences</i> , <b>2009</b> , 52, 1928-1932		2
67	Gas Molecules Adsorption on Carbon Nanotubes. <i>Materials Research Society Symposia Proceedings</i> , <b>2000</b> , 633, 13481		2
66	Mechanically Induced Switching between Two Discrete Conductance States: A Potential Single-Molecule Variable Resistor. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> , 13, 57646-57653	9.5	2
65	Electric-Field-Driven Negative Differential Conductance in 2D van der Waals Ferromagnet FeGeTe. <i>Nano Letters</i> , <b>2021</b> , 21, 9233-9239	11.5	2
64	analytic calculation of point defects in AlGa <sub>n</sub> /Ga <sub>n</sub> heterointerfaces. <i>Journal of Physics Condensed Matter</i> , <b>2020</b> ,	1.8	2
63	Rational design of 2D organic magnets with giant magnetic anisotropy based on two-coordinate 5d transition metals. <i>APL Materials</i> , <b>2020</b> , 8, 071105	5.7	2
62	Reactivity and Lability Modulated by a Valence Electron Moving in and out of 25-Atom Gold Nanoclusters. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 21321-21328	3.6	2
61	Insight on the active sites of CoNi alloy embedded in N-doped carbon nanotubes for oxygen reduction reaction. <i>Science China Materials</i> , <b>2021</b> , 64, 2719-2728	7.1	2
60	Ground-State Structures of Hydrated Calcium Ion Clusters From Comprehensive Genetic Algorithm Search. <i>Frontiers in Chemistry</i> , <b>2021</b> , 9, 637750	5	2
59	Enhanced Valley Polarization of Bilayer MoSe with Variable Stacking Order and Interlayer Coupling. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 5879-5888	6.4	2
58	Searching for cluster Lego blocks for three-dimensional and two-dimensional assemblies. <i>Physical Review Materials</i> , <b>2021</b> , 5,	3.2	2
57	Selective CO <sub>2</sub> conversion tuned by periodicities in Au <sub>8n+4</sub> (TBBT) <sub>4n+8</sub> nanoclusters. <i>Nano Research</i> , <b>2021</b> , 14, 807-813	10	2
56	Comparison of flows and heat transfers in reactor cores with spherical-particle fuels and cylindrical-rod fuels. <i>Journal of Nuclear Science and Technology</i> , <b>2021</b> , 58, 226-240	1	2



55	Multiscale simulations of the hydration shells surrounding spherical FeO nanoparticles and effect on magnetic properties. <i>Nanoscale</i> , <b>2021</b> , 13, 9293-9302	7.7	2
54	Effects of spin-phonon coupling on two-dimensional ferromagnetic semiconductors: a case study of iron and ruthenium trihalides. <i>Nanoscale</i> , <b>2021</b> , 13, 7714-7722	7.7	2
53	First-principles explorations on P8 and N2 assembled nanowire and nanosheet. <i>Nano Express</i> , <b>2021</b> , 2, 010004	2	2
52	Pressure dependence on electronic structures, charge distribution and bond orders of solid nitromethane using nonlocal DFT functional. <i>Molecular Simulation</i> , <b>2018</b> , 44, 1454-1460	2	2
51	Phase Diagram of Methane Hydrates and Discovery of MH-VI Hydrate. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 6007-6013	2.8	2
50	Matching vacancy formation energy and defect levels with the density of amorphous Ga <sub>2</sub> O <sub>3</sub> . <i>Journal of Materials Science</i> , <b>2020</b> , 55, 9343-9353	4.3	1
49	New refractory MAB phases and their 2D derivatives: insight into the effects of valence electron concentration and chemical composition. <i>RSC Advances</i> , <b>2020</b> , 10, 25836-25847	3.7	1
48	First-Principles Calculations for Stable TiMo Alloys Using Cluster-Plus-Glue-Atom Model. <i>Acta Metallurgica Sinica (English Letters)</i> , <b>2020</b> , 33, 968-974	2.5	1
47	Röntgenbild: Vacancy Engineering of Iron-Doped W <sub>18</sub> O <sub>49</sub> Nanoreactors for Low-Barrier Electrochemical Nitrogen Reduction (Angew. Chem. 19/2020). <i>Angewandte Chemie</i> , <b>2020</b> , 132, 7696-7698	3.6	1
46	Chemical stability of epoxy functionalizations of graphene: A density functional theory study. <i>Materials Research Society Symposia Proceedings</i> , <b>2013</b> , 1549, 19-24		1
45	STRUCTURAL AND RAMAN SPECTRA STUDIES OF SUPPORTED LiF CLUSTERS. <i>Surface Review and Letters</i> , <b>1996</b> , 03, 157-160	1.1	1
44	FeSi <sub>2</sub> : a two-dimensional ferromagnet containing planar hexacoordinate Fe atoms. <i>Nanoscale Advances</i> , <b>2022</b> , 4, 600-607	5.1	1
43	Transition metal halide nanowires: A family of one-dimensional multifunctional building blocks. <i>Applied Physics Letters</i> , <b>2022</b> , 120, 023103	3.4	1
42	Regulating the Electronic Configuration of Supported Iron Nanoparticles for Electrochemical Catalytic Nitrogen Fixation. <i>Advanced Functional Materials</i> , 2111733	15.6	1
41	Phase Diagrams and Spectral Characteristics of Hydrofluorocarbon Hydrates: Insights from First-Principles Thermodynamics. <i>ACS Sustainable Chemistry and Engineering</i> ,	8.3	1
40	On the photocatalysis evolution of heteroatom-doped AgM nanoclusters.. <i>RSC Advances</i> , <b>2021</b> , 11, 32526-32532	9.7	1
39	Remarkable Role of Grain Boundaries in the Thermal Transport Properties of Phosphorene. <i>ACS Omega</i> , <b>2020</b> , 5, 17416-17422	3.9	1
38	Compressive behavior and electronic properties of ammonia ice: a first-principles study.. <i>RSC Advances</i> , <b>2020</b> , 10, 26579-26587	3.7	1

37	New boron nitride monolith phases from high-pressure compression of double-walled boron nitride nanotubes. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 134702	3.9	1
36	First-Principles Study of the Atomic Structures and Catalytic Properties of Monolayer TaS <sub>2</sub> with Intrinsic Defects. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 10362-10369	3.8	1
35	Thermal properties of energetic materials from quasi-harmonic first-principles calculations. <i>Journal of Physics Condensed Matter</i> , <b>2021</b> , 33,	1.8	1
34	Phase Diagrams for all Clathrate Hydrates of CO from First-Principles Thermodynamics. <i>Journal of Physical Chemistry A</i> , <b>2021</b> , 125, 5956-5962	2.8	1
33	Compression behavior of energetic ECL-20 crystals from density functional theory calculations. <i>Journal of Raman Spectroscopy</i> , <b>2021</b> , 52, 1764	2.3	1
32	First-Principles Study of Lithium Adsorption, Storage and Diffusion Properties for Graphite Oxides. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2016</b> , 16, 8106-8112	1.3	1
31	Structural and Electronic Properties of Binary Clusters SiGe (+ = 6-13). <i>Journal of Nanoscience and Nanotechnology</i> , <b>2019</b> , 19, 7879-7885	1.3	1
30	Imaging Vacancy Defects in Single-Layer Chromium Triiodide. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 2199-2205	6.4	1
29	Magnetic field modulated photoelectric devices in ferromagnetic semiconductor CrXh (X = S/Se, h = Cl/Br/I) van der Waals heterojunctions. <i>Applied Physics Letters</i> , <b>2021</b> , 119, 032103	3.4	1
28	Methane conversion by transition metal-doped vanadium oxide clusters. <i>Chemical Physics Letters</i> , <b>2021</b> , 779, 138829	2.5	1
27	Intramolecular hydroamination of alkynes driven by isomeric Au <sub>36</sub> (SR) <sub>24</sub> nanocluster catalysts. <i>Nano Research</i> , 1	10	1
26	Ag <sub>24</sub> Au cluster decorated mesoporous Co <sub>3</sub> O <sub>4</sub> for highly selective and efficient photothermal CO <sub>2</sub> hydrogenation. <i>Nano Research</i> , 1	10	1
25	Dramatically Enhanced Second Harmonic Generation in Janus Group-III Chalcogenide Monolayers. <i>Advanced Optical Materials</i> , 2200076	8.1	1
24	Perovskite Solar Cells: Reverse-Graded 2D Ruddlesden-Popper Perovskites for Efficient Air-Stable Solar Cells (Adv. Energy Mater. 21/2019). <i>Advanced Energy Materials</i> , <b>2019</b> , 9, 1970075	21.8	0
23	Design and implementation of a highly integrated dual hemisphere capsule robot.. <i>Biomedical Microdevices</i> , <b>2022</b> , 24, 10	3.7	0
22	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> , <b>2020</b> , 51, 2425-2434	2.3	0
21	Eliminating Edge Electronic and Phonon States of Phosphorene Nanoribbon by Unique Edge Reconstruction. <i>Small</i> , <b>2021</b> , e2105130	11	0
20	A comprehensive study of indole catalytic hydrodenitrogenation under hydrothermal conditions. <i>AICHE Journal</i> , e17531	3.6	0

19	Prediction of superconductivity in bilayer borophenes.. <i>RSC Advances</i> , <b>2021</b> , 11, 40220-40227	3.7	o
18	Theoretical insights of structural evolution and electronic properties of Ru <sub>2</sub> Gen (n = 1-6) clusters. <i>European Physical Journal Plus</i> , <b>2022</b> , 137, 1	3.1	o
17	Transition of CrI from a two-dimensional network to one-dimensional chain at the monolayer limit. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 25291-25297	3.6	o
16	Robust charge spatial separation and linearly tunable band gap of low-energy tube-edge phosphorene nanoribbon. <i>Nanoscale Advances</i> , <b>2021</b> , 3, 4416-4423	5.1	o
15	Remote Passivation in Two-Dimensional Materials: The Case of the Monolayer-Bilayer Lateral Junction of MoSe. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 8046-8052	6.4	o
14	Distinct chemical fixation of CO enabled by exotic gold nanoclusters. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 054305	3.9	o
13	Universal Zigzag Edge Reconstruction of an $\Phi$ Phase Puckered Monolayer and Its Resulting Robust Spatial Charge Separation. <i>Nano Letters</i> , <b>2021</b> , 21, 8095-8102	11.5	o
12	Superior flexibility of planar graphene allotropes with pentagons and heptagons. <i>Applied Surface Science</i> , <b>2021</b> , 569, 151048	6.7	o
11	Evolution of Water Layer Adsorption on the GaN(0001) Surface and Its Influence on Electronic Properties. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 667-674	3.8	o
10	Inverse Design of Nanoclusters for Light-Controlled CO-HCOOH Interconversion.. <i>Journal of Physical Chemistry Letters</i> , <b>2022</b> , 2523-2532	6.4	o
9	2D Palladium Diselenide: Giant Thickness-Tunable Bandgap and Robust Air Stability of 2D Palladium Diselenide (Small 19/2020). <i>Small</i> , <b>2020</b> , 16, 2070106	11	
8	Thermo-chemical metastability of multilayer epitaxial graphene oxide: Experiments and density functional theory calculations. <i>Materials Research Society Symposia Proceedings</i> , <b>2012</b> , 1451, 39-44		
7	Eliminating Edge Electronic and Phonon States of Phosphorene Nanoribbon by Unique Edge Reconstruction (Small 2/2022). <i>Small</i> , <b>2022</b> , 18, 2270011	11	
6	A novel method for measuring the focal point of a sagittal-focusing Laue crystal monochromator. <i>Journal of Synchrotron Radiation</i> , <b>2019</b> , 26, 1826-1829	2.4	
5	First-Principles Study of the Effects of Carbon, Nitrogen, and Oxygen on Helium Behavior in Body-Centered-Cubic Vanadium. <i>Fusion Science and Technology</i> , 1-10	1.1	
4	Characterization and on-line adjustment of the sagittal-bent Laue crystal profile. <i>Journal of Synchrotron Radiation</i> , <b>2018</b> , 25, 1346-1353	2.4	
3	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> , <b>2021</b> , 68, 3224-3228	3.5	
2	Strain softened bending modulus of graphene oxide. <i>Carbon Trends</i> , <b>2022</b> , 7, 100167	o	

- 1 Fabricating and Modulating Robust Multi-Photoaddressable Systems with the Derivatives of Diarylethylene and Donor-Acceptor Stenhouse Adducts.. *Journal of Physical Chemistry Letters*, **2022**, 3611-3620 6.4