Si Zhou

List of Publications by Year in Descending Order

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	FeSi2: a two-dimensional ferromagnet containing planar hexacoordinate Fe atoms. *Nanoscale Advances*, **2022**, 4, 600-607	5.1	1
467	Eliminating Edge Electronic and Phonon States of Phosphorene Nanoribbon by Unique Edge Reconstruction (Small 2/2022). *Small*, **2022**, 18, 2270011	11	
466	Transition metal halide nanowires: A family of one-dimensional multifunctional building blocks. *Applied Physics Letters*, **2022**, 120, 023103	3.4	1
465	Photoinduced Spin Injection and Ferromagnetism in 2D Group III Monochalcogenides.. *Journal of Physical Chemistry Letters*, **2022**, 590-597	6.4	4
464	Design and implementation of a highly integrated dual hemisphere capsule robot.. *Biomedical Microdevices*, **2022**, 24, 10	3.7	0
463	Theoretical insights of structural evolution and electronic properties of Ru2Gen (n = 1□6) clusters. *European Physical Journal Plus*, **2022**, 137, 1	3.1	0
462	Evolution from superatomic AuAg monomers into molecular-like AuAg dimeric nanoclusters.. *Chemical Science*, **2022**, 13, 2778-2782	9.4	3
461	Crystal-Phase-Mediated Restructuring of Pt on TiO2 with Tunable Reactivity: Redispersion versus Reshaping. *ACS Catalysis*, **2022**, 12, 3634-3643	13.1	9
460	Inverse Design of Nanoclusters for Light-Controlled CO-HCOOH Interconversion.. *Journal of Physical Chemistry Letters*, **2022**, 2523-2532	6.4	0
459	Epitaxial growth of an atom-thin layer on a LiNiMnO cathode for stable Li-ion battery cycling.. *Nature Communications*, **2022**, 13, 1565	17.4	5
458	Strain softened bending modulus of graphene oxide. *Carbon Trends*, **2022**, 7, 100167	0	
457	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	
456	Mechanically Induced Switching between Two Discrete Conductance States: A Potential Single-Molecule Variable Resistor. *ACS Applied Materials & Interfaces*, **2021**, 13, 57646-57653	9.5	2
455	Low-dimensional non-metal catalysts: principles for regulating p-orbital-dominated reactivity. *Npj Computational Materials*, **2021**, 7,	10.9	10
454	Eliminating Edge Electronic and Phonon States of Phosphorene Nanoribbon by Unique Edge Reconstruction. *Small*, **2021**, e2105130	11	0
453	Prediction of superconductivity in bilayer borophenes.. *RSC Advances*, **2021**, 11, 40220-40227	3.7	0
452	On the photocatalysis evolution of heteroatom-doped AgM nanoclusters.. *RSC Advances*, **2021**, 11, 32526-32532	3.7	2

451	Transition of CrI from a two-dimensional network to one-dimensional chain at the monolayer limit. *Physical Chemistry Chemical Physics*, **2021**, 23, 25291-25297	3.6	0
450	Photodriven Catalytic Hydrogenation of CO to CH with Nearly 100% Selectivity over Ag Clusters. *Nano Letters*, **2021**, 21, 8693-8700	11.5	4
449	Scalable Production of Freestanding Few-Layer □Borophene Single Crystalline Sheets as Efficient Electrocatalysts for Lithium-Sulfur Batteries. *ACS Nano*, **2021**,	16.7	5
448	Electric-Field-Driven Negative Differential Conductance in 2D van der Waals Ferromagnet FeGeTe. *Nano Letters*, **2021**, 21, 9233-9239	11.5	2
447	Stability and NMR Chemical Shift of Amorphous Precursors of Methane Hydrate: Insights from Dispersion-Corrected Density Functional Theory Calculations Combined with Machine Learning. *Journal of Physical Chemistry B*, **2021**, 125, 431-441	3.4	3
446	Catalytic Hydrodenitrogenation of Pyridine under Hydrothermal Conditions: A Comprehensive Study. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 362-374	8.3	7
445	MXene and MBene as efficient catalysts for energy conversion: roles of surface, edge and interface. *JPhys Energy*, **2021**, 3, 012002	4.9	17
444	Temperature-dependent hardness of zinc-blende structured covalent materials. *Science China Materials*, **2021**, 64, 2280-2288	7.1	3
443	Single O Atom Doped Ag Cluster Cations for CO Oxidation: An O-Doped Superatom Ag15O+ with Remarkable Stability. *Journal of Physical Chemistry C*, **2021**, 125, 7067-7076	3.8	3
442	Precisely Constructed Silver Active Sites in Gold Nanoclusters for Chemical Fixation of CO. *Angewandte Chemie - International Edition*, **2021**, 60, 10573-10576	16.4	16
441	Precisely Constructed Silver Active Sites in Gold Nanoclusters for Chemical Fixation of CO2. *Angewandte Chemie*, **2021**, 133, 10667-10670	3.6	6
440	Transition metal-doped Bn (n = 7□10) clusters: confirmation of a circular disk Jellium model. *European Physical Journal Plus*, **2021**, 136, 1	3.1	4
439	Progress of tubulin polymerization activity detection methods. *Bioorganic and Medicinal Chemistry Letters*, **2021**, 37, 127698	2.9	9
438	Computational high-throughput screening of alloy nanoclusters for electrocatalytic hydrogen evolution. *Npj Computational Materials*, **2021**, 7,	10.9	17
437	New boron nitride monolith phases from high-pressure compression of double-walled boron nitride nanotubes. *Journal of Chemical Physics*, **2021**, 154, 134702	3.9	1
436	First-Principles Study of the Atomic Structures and Catalytic Properties of Monolayer TaS2 with Intrinsic Defects. *Journal of Physical Chemistry C*, **2021**, 125, 10362-10369	3.8	1
435	Thermal properties of energetic materials from quasi-harmonic first-principles calculations. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	1
434	Architecting Freestanding Sulfur Cathodes for Superior Room-Temperature Na□S Batteries. *Advanced Functional Materials*, **2021**, 31, 2102280	15.6	13

433	Structural Design Strategy and Active Site Regulation of High-Efficient Bifunctional Oxygen Reaction Electrocatalysts for Zn-Air Battery. *Small*, **2021**, 17, e2006766	11	24
432	Insight on the active sites of CoNi alloy embedded in N-doped carbon nanotubes for oxygen reduction reaction. *Science China Materials*, **2021**, 64, 2719-2728	7.1	2
431	Exceptional Electrochemical HER Performance with Enhanced Electron Transfer between Ru Nanoparticles and Single Atoms Dispersed on a Carbon Substrate. *Angewandte Chemie - International Edition*, **2021**, 60, 16044-16050	16.4	65
430	Ground-State Structures of Hydrated Calcium Ion Clusters From Comprehensive Genetic Algorithm Search. *Frontiers in Chemistry*, **2021**, 9, 637750	5	2
429	Exceptional Electrochemical HER Performance with Enhanced Electron Transfer between Ru Nanoparticles and Single Atoms Dispersed on a Carbon Substrate. *Angewandte Chemie*, **2021**, 133, 16180-16186	3.6	6
428	Dithiol Self-Assembled Monolayer Based Electrochemical Surface Plasmon Resonance Optical Fiber Sensor for Selective Heavy Metal Ions Detection. *Journal of Lightwave Technology*, **2021**, 39, 4034-4040	4	3
427	Enhanced Valley Polarization of Bilayer MoSe with Variable Stacking Order and Interlayer Coupling. *Journal of Physical Chemistry Letters*, **2021**, 12, 5879-5888	6.4	2
426	Searching for cluster Lego blocks for three-dimensional and two-dimensional assemblies. *Physical Review Materials*, **2021**, 5,	3.2	2
425	Phase Diagrams for sII Clathrate Hydrates of CO from First-Principles Thermodynamics. *Journal of Physical Chemistry A*, **2021**, 125, 5956-5962	2.8	1
424	Compression behavior of energetic □CL-20 crystals from density functional theory calculations. *Journal of Raman Spectroscopy*, **2021**, 52, 1764	2.3	1
423	Visible-light overall water splitting on g-C3N4 decorated by subnanometer oxide clusters. *Materials Today Physics*, **2021**, 16, 100312	8	11
422	Compositionally Designed 2D Ruddlesden□Popper Perovskites for Efficient and Stable Solar Cells. *Solar Rrl*, **2021**, 5, 2000661	7.1	3
421	Sustainable S cathodes with synergic electrocatalysis for room-temperature Na□S batteries. *Journal of Materials Chemistry A*, **2021**, 9, 566-574	13	19
420	Electrocatalytic and photocatalytic applications of atomically precise gold-based nanoclusters. *Science China Chemistry*, **2021**, 64, 1065-1075	7.9	3
419	Atomic Wires of Transition Metal Chalcogenides: A Family of 1D Materials for Flexible Electronics and Spintronics. *Jacs Au*, **2021**, 1, 147-155		3
418	Selective CO2 conversion tuned by periodicities in Au8n+4(TBBT)4n+8 nanoclusters. *Nano Research*, **2021**, 14, 807-813	10	2
417	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	1	2
416	Ring-contraction of hantzsch esters and their derivatives to pyrroles via electrochemical extrusion of ethyl acetate out of aromatic rings. *Green Chemistry*, **2021**, 23, 3468-3473	10	3

415	Multiscale simulations of the hydration shells surrounding spherical FeO nanoparticles and effect on magnetic properties. *Nanoscale*, **2021**, 13, 9293-9302	7.7	2
414	Distinct structure assembly driven by metal-ligand binding in Au nanoclusters and its relation to photocatalysis. *Chemical Communications*, **2021**, 57, 2176-2179	5.8	4
413	Effects of spin-phonon coupling on two-dimensional ferromagnetic semiconductors: a case study of iron and ruthenium trihalides. *Nanoscale*, **2021**, 13, 7714-7722	7.7	2
412	The cooperation of Fe3C nanoparticles with isolated single iron atoms to boost the oxygen reduction reaction for Zn□ir batteries. *Journal of Materials Chemistry A*, **2021**, 9, 6831-6840	13	28
411	First-principles explorations on P8 and N2 assembled nanowire and nanosheet. *Nano Express*, **2021**, 2, 010004	2	2
410	Robust charge spatial separation and linearly tunable band gap of low-energy tube-edge phosphorene nanoribbon. *Nanoscale Advances*, **2021**, 3, 4416-4423	5.1	0
409	MBLT: Learning Motion and Background for Vehicle Tracking in Satellite Videos. *IEEE Transactions on Geoscience and Remote Sensing*, **2021**, 1-15	8.1	3
408	Imaging Vacancy Defects in Single-Layer Chromium Triiodide. *Journal of Physical Chemistry Letters*, **2021**, 12, 2199-2205	6.4	1
407	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	6.4	7
406	Magnetic field modulated photoelectric devices in ferromagnetic semiconductor CrXh (X = S/Se, h = Cl/Br/I) van der Waals heterojunctions. *Applied Physics Letters*, **2021**, 119, 032103	3.4	1
405	Kondo Holes in the Two-Dimensional Itinerant Ising Ferromagnet FeGeTe. *Nano Letters*, **2021**, 21, 6117-6123	11.5	3
404	Remote Passivation in Two-Dimensional Materials: The Case of the Monolayer-Bilayer Lateral Junction of MoSe. *Journal of Physical Chemistry Letters*, **2021**, 12, 8046-8052	6.4	0
403	Distinct chemical fixation of CO enabled by exotic gold nanoclusters. *Journal of Chemical Physics*, **2021**, 155, 054305	3.9	0
402	Universal Zigzag Edge Reconstruction of an □Phase Puckered Monolayer and Its Resulting Robust Spatial Charge Separation. *Nano Letters*, **2021**, 21, 8095-8102	11.5	0
401	Active-Site Tailoring of Gold Cluster Catalysts for Electrochemical CO2 Reduction. *ACS Catalysis*, **2021**, 11, 11551-11560	13.1	10
400	Methane conversion by transition metal-doped vanadium oxide clusters. *Chemical Physics Letters*, **2021**, 779, 138829	2.5	1
399	Recent progress on 2D magnets: Fundamental mechanism, structural design and modification. *Applied Physics Reviews*, **2021**, 8, 031305	17.3	35
398	A Full CMOS Quenching Circuit With Fuse Protection for InGaAs/InP Single Photon Detectors. *IEEE Transactions on Circuits and Systems II: Express Briefs*, **2021**, 68, 3224-3228	3.5	

397	Superior flexibility of planar graphene allotropes with pentagons and heptagons. *Applied Surface Science*, **2021**, 569, 151048	6.7	0
396	Evolution of Water Layer Adsorption on the GaN(0001) Surface and Its Influence on Electronic Properties. *Journal of Physical Chemistry C*, **2021**, 125, 667-674	3.8	0
395	Accurate electronic properties and non-linear optical response of two-dimensional MA2Z4. *Nanoscale*, **2021**, 13, 5479-5488	7.7	18
394	Cd-driven surface reconstruction and photodynamics in gold nanoclusters. *Chemical Science*, **2021**, 12, 3290-3294	9.4	13
393	Wavelength-Tunable Optical Fiber Localized Surface Plasmon Resonance Biosensor a Diblock Copolymer-Templated Nanorod Monolayer. *ACS Applied Materials & Interfaces*, **2020**, 12, 50929-50940	9.5	9
392	Competition between tubular, planar and cage geometries: a complete picture of structural evolution of B (n = 31-50) clusters. *Physical Chemistry Chemical Physics*, **2020**, 22, 12959-12966	3.6	11
391	Matching vacancy formation energy and defect levels with the density of amorphous Ga2O3. *Journal of Materials Science*, **2020**, 55, 9343-9353	4.3	1
390	Ag Au (PET) Nanocluster: Dimeric Assembly of Au (PET) Enabled by Silver Atoms. *Angewandte Chemie - International Edition*, **2020**, 59, 13941-13946	16.4	18
389	Chemical-Reductant-Free Electrochemical Deuteration Reaction using Deuterium Oxide. *Angewandte Chemie - International Edition*, **2020**, 59, 13962-13967	16.4	41
388	MBenes: emerging 2D materials as efficient electrocatalysts for the nitrogen reduction reaction. *Nanoscale Horizons*, **2020**, 5, 1106-1115	10.8	45
387	2D Palladium Diselenide: Giant Thickness-Tunable Bandgap and Robust Air Stability of 2D Palladium Diselenide (Small 19/2020). *Small*, **2020**, 16, 2070106	11	
386	Ag2Au50(PET)36 Nanocluster: Dimeric Assembly of Au25(PET)18 Enabled by Silver Atoms. *Angewandte Chemie*, **2020**, 132, 14045-14050	3.6	2
385	Chemical-Reductant-Free Electrochemical Deuteration Reaction using Deuterium Oxide. *Angewandte Chemie*, **2020**, 132, 14066-14071	3.6	12
384	Experimental Realization of Two-Dimensional Buckled Lieb Lattice. *Nano Letters*, **2020**, 20, 2537-2543	11.5	2
383	Oxidation Behaviors of Two-dimensional Metal Chalcogenides. *ChemNanoMat*, **2020**, 6, 838-849	3.5	4
382	Tuning the electronic properties of bilayer black phosphorene with the twist angle. *Journal of Materials Chemistry C*, **2020**, 8, 6264-6272	7.1	14
381	Structures and vertical detachment energies of water cluster anions (H2O)□ with n = 6□11. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	4
380	Distributed Robust Filtering for Wireless Sensor Networks with Markov Switching Topologies and Deception Attacks. *Sensors*, **2020**, 20,	3.8	3

379	Structure Evolution of Transition Metal-doped Gold Clusters M@Au12 (M = 3d–5d): Across the Periodic Table. *Journal of Physical Chemistry C*, **2020**, 124, 7449-7457	3.8	10
378	2D tetragonal transition-metal phosphides: an ideal platform to screen metal shrouded crystals for multifunctional applications. *Nanoscale*, **2020**, 12, 6776-6784	7.7	11
377	Immobilized trimeric metal clusters: A family of the smallest catalysts for selective CO2 reduction toward multi-carbon products. *Nano Energy*, **2020**, 76, 105049	17.1	23
376	Anionic Copper Clusters Reacting with NO: An Open-Shell Superatom Cu. *Journal of Physical Chemistry Letters*, **2020**, 11, 5807-5814	6.4	13
375	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. *Inorganic Chemistry*, **2020**, 59, 10253-10261	5.1	3
374	An Au Cluster Fortified by Four Ferrocenes. *Journal of Physical Chemistry A*, **2020**, 124, 6061-6067	2.8	7
373	New refractory MAB phases and their 2D derivatives: insight into the effects of valence electron concentration and chemical composition. *RSC Advances*, **2020**, 10, 25836-25847	3.7	1
372	Toward a Reversible Mn4+/Mn2+ Redox Reaction and Dendrite-Free Zn Anode in Near-Neutral Aqueous Zn/MnO2 Batteries via Salt Anion Chemistry. *Advanced Energy Materials*, **2020**, 10, 1904163	21.8	98
371	De novo design of Au(SR) nanoclusters. *Nature Communications*, **2020**, 11, 3349	17.4	21
370	First-Principles Calculations for Stable □TiM Alloys Using Cluster-Plus-Glue-Atom Model. *Acta Metallurgica Sinica (English Letters)*, **2020**, 33, 968-974	2.5	1
369	CO2 reduction on p-block metal oxide overlayers on metal substrates□2D MgO as a prototype. *Journal of Materials Chemistry A*, **2020**, 8, 5688-5698	13	9
368	Numerical simulation of flow past a triangular prism with fluid□tructure interaction. *Engineering Applications of Computational Fluid Mechanics*, **2020**, 14, 462-476	4.5	4
367	Multilevel Hollow MXene Tailored Low-Pt Catalyst for Efficient Hydrogen Evolution in Full-pH Range and Seawater. *Advanced Functional Materials*, **2020**, 30, 1910028	15.6	66
366	Vacancy Engineering of Iron-Doped W O Nanoreactors for Low-Barrier Electrochemical Nitrogen Reduction. *Angewandte Chemie - International Edition*, **2020**, 59, 7356-7361	16.4	126
365	Operando Revealing Dynamic Reconstruction of NiCo Carbonate Hydroxide for High-Rate Energy Storage. *Joule*, **2020**, 4, 673-687	27.8	48
364	Vacancy Engineering of Iron-Doped W18O49 Nanoreactors for Low-Barrier Electrochemical Nitrogen Reduction. *Angewandte Chemie*, **2020**, 132, 7426-7431	3.6	15
363	Aminomethyl-Functionalized Carbon Nanotubes as a Host of Small Sulfur Clusters for High-Performance Lithium-Sulfur Batteries. *ChemSusChem*, **2020**, 13, 2761-2768	8.3	8
362	Excitonic AuRu(PPh)(SCHPh) cluster for light-driven dinitrogen fixation. *Chemical Science*, **2020**, 11, 2440-2447	9.4	23

361	R□ktitelbild: Vacancy Engineering of Iron-Doped W18O49 Nanoreactors for Low-Barrier Electrochemical Nitrogen Reduction (Angew. Chem. 19/2020). *Angewandte Chemie*, **2020**, 132, 7696-7696	3.6	1
360	Selective C-C Coupling by Spatially Confined Dimeric Metal Centers. *IScience*, **2020**, 23, 101051	6.1	21
359	High-Curie-temperature ferromagnetism in bilayer CrI3 on bulk semiconducting substrates. *Physical Review Materials*, **2020**, 4,	3.2	12
358	Surface-enhanced resonance Raman detection of 1,1-diamino-2,2-dinitroethylene (FOX-7) on metal-doped Au 12 and Ag 12 clusters. *Journal of Raman Spectroscopy*, **2020**, 51, 2425-2434	2.3	0
357	Electrocatalyzing S Cathodes Multisulfiphilic Sites for Superior Room-Temperature Sodium-Sulfur Batteries. *ACS Nano*, **2020**, 14, 7259-7268	16.7	61
356	analytic calculation of point defects in AlGaN/GaN heterointerfaces. *Journal of Physics Condensed Matter*, **2020**,	1.8	2
355	Cubic imidazolate frameworks-derived CoFe alloy nanoparticles-embedded N-doped graphitic carbon for discharging reaction of Zn-air battery. *Science China Materials*, **2020**, 63, 327-338	7.1	37
354	Tunable bending modulus and bending limit of oxidized graphene. *Nanoscale*, **2020**, 12, 1623-1628	7.7	6
353	Physical properties and device applications of graphene oxide. *Frontiers of Physics*, **2020**, 15, 1	3.7	56
352	Rapid and energy-efficient microwave pyrolysis for high-yield production of highly-active bifunctional electrocatalysts for water splitting. *Energy and Environmental Science*, **2020**, 13, 545-553	35.4	99
351	Controllable Conversion of CO on Non-Metallic Gold Clusters. *Angewandte Chemie - International Edition*, **2020**, 59, 1919-1924	16.4	28
350	A sacrificial Zn strategy enables anchoring of metal single atoms on the exposed surface of holey 2D molybdenum carbide nanosheets for efficient electrocatalysis. *Journal of Materials Chemistry A*, **2020**, 8, 3071-3082	13	38
349	Solar Driven CO2 Hydrogenation on Ti-Doped Silicon Nanocages. *Journal of Cluster Science*, **2020**, 31, 627-635	3	5
348	Boron Nitride Nanotubes for Ammonia Synthesis: Activation by Filling Transition Metals. *Journal of the American Chemical Society*, **2020**, 142, 308-317	16.4	61
347	Numerical simulation of flow past stationary and oscillating deformable circles with fluid-structure interaction. *Experimental and Computational Multiphase Flow*, **2020**, 2, 151-161	4.2	9
346	Metal-Encapsulated Boron Nitride Nanocages for Solar-Driven Nitrogen Fixation. *Journal of Physical Chemistry C*, **2020**, 124, 23798-23806	3.8	8
345	Three-dimensional borophene: A light-element topological nodal-line semimetal with direction-dependent type-II Weyl fermions. *Physical Review B*, **2020**, 102,	3.3	4
344	Ligand-protected AuRu and AuRu nanoclusters: distinct structures and implications for site-cooperation catalysis. *Chemical Communications*, **2020**, 56, 12833-12836	5.8	3

343	N-Doped carbon coating enhances the bifunctional oxygen reaction activity of CoFe nanoparticles for a highly stable Zn□air battery. *Journal of Materials Chemistry A*, **2020**, 8, 21189-21198	13	27
342	Optimization of photocarrier dynamics and activity in phosphorene with intrinsic defects for nitrogen fixation. *Journal of Materials Chemistry A*, **2020**, 8, 20570-20580	13	8
341	Core□Shell MnO2 Nanotubes@Nickel□Cobalt□Zinc Hydroxide Nanosheets for Supercapacitive Energy Storage. *ACS Applied Nano Materials*, **2020**, 3, 7462-7473	5.6	11
340	Carrier Dynamics and Transfer across the CdS/MoS Interface upon Optical Excitation. *Journal of Physical Chemistry Letters*, **2020**, 11, 6544-6550	6.4	7
339	Remarkable Role of Grain Boundaries in the Thermal Transport Properties of Phosphorene. *ACS Omega*, **2020**, 5, 17416-17422	3.9	1
338	Compressive behavior and electronic properties of ammonia ice: a first-principles study.. *RSC Advances*, **2020**, 10, 26579-26587	3.7	1
337	Rational design of 2D organic magnets with giant magnetic anisotropy based on two-coordinate 5d transition metals. *APL Materials*, **2020**, 8, 071105	5.7	2
336	The precise editing of surface sites on a molecular-like gold catalyst for modulating regioselectivity. *Chemical Science*, **2020**, 11, 8000-8004	9.4	10
335	Reactivity and Lability Modulated by a Valence Electron Moving in and out of 25-Atom Gold Nanoclusters. *Angewandte Chemie*, **2020**, 132, 21321-21328	3.6	2
334	Reactivity and Lability Modulated by a Valence Electron Moving in and out of 25-Atom Gold Nanoclusters. *Angewandte Chemie - International Edition*, **2020**, 59, 21135-21142	16.4	14
333	Solar driven CO hydrogenation on transition metal doped ZnO cluster. *Journal of Chemical Physics*, **2020**, 153, 164306	3.9	4
332	Control of Photocarrier Separation and Recombination at Bismuth Oxyhalide Interface for Nitrogen Fixation. *Journal of Physical Chemistry Letters*, **2020**, 11, 9304-9312	6.4	10
331	Dual-Constrained Sulfur in FeS2@C Nanostructured Lithium-Sulfide Batteries. *ACS Applied Energy Materials*, **2020**, 3, 10950-10960	6.1	5
330	Enhanced Ferromagnetism of CrI3 Bilayer by Self-Intercalation. *Chinese Physics Letters*, **2020**, 37, 107506	1.8	13
329	Precisely modulating the surface sites on atomically monodispersed gold-based nanoclusters for controlling their catalytic performances. *Nanoscale*, **2020**, 12, 18004-18012	7.7	11
328	Combining Machine Learning Potential and Structure Prediction for Accelerated Materials Design and Discovery. *Journal of Physical Chemistry Letters*, **2020**, 11, 8710-8720	6.4	18
327	Electron-Deficient Cu Sites on Cu3Ag1 Catalyst Promoting CO2 Electroreduction to Alcohols. *Advanced Energy Materials*, **2020**, 10, 2001987	21.8	43
326	Endohedrally Doped Cage Clusters. *Chemical Reviews*, **2020**, 120, 9021-9163	68.1	76

325	Structures, stabilities and electronic properties of TimSi n (m = 1-2, n = 14-20) clusters: a combined ab initio and experimental study. *European Physical Journal Plus*, **2020**, 135, 1	3.1	3
324	Capturing the active sites of multimetallic (oxy)hydroxides for the oxygen evolution reaction. *Energy and Environmental Science*, **2020**, 13, 4225-4237	35.4	71
323	2D Boron Sheets: Structure, Growth, and Electronic and Thermal Transport Properties. *Advanced Functional Materials*, **2020**, 30, 1904349	15.6	69
322	Robust spin manipulation in 2D organometallic Kagome lattices: a first-principles study. *Physical Chemistry Chemical Physics*, **2020**, 22, 11045-11052	3.6	7
321	Giant Thickness-Tunable Bandgap and Robust Air Stability of 2D Palladium Diselenide. *Small*, **2020**, 16, e2000754	11	11
320	Atomically Sharp Dual Grain Boundaries in 2D WS Bilayers. *Small*, **2019**, 15, e1902590	11	8
319	Ultra-thin Ga nanosheets: analogues of high pressure Ga(iii). *Nanoscale*, **2019**, 11, 17201-17205	7.7	4
318	Hydrated Sodium Ion Clusters [Na(HO) (= 1-6)]: An Study on Structures and Non-covalent Interaction. *Frontiers in Chemistry*, **2019**, 7, 624	5	9
317	A single boron atom doped boron nitride edge as a metal-free catalyst for N fixation. *Physical Chemistry Chemical Physics*, **2019**, 21, 1110-1116	3.6	84
316	Two-dimensional spin□alley-coupled Dirac semimetals in functionalized SbAs monolayers. *Materials Horizons*, **2019**, 6, 781-787	14.4	21
315	Eighteen functional monolayer metal oxides: wide bandgap semiconductors with superior oxidation resistance and ultrahigh carrier mobility. *Nanoscale Horizons*, **2019**, 4, 592-600	10.8	51
314	Adaptive Multiscale Deep Fusion Residual Network for Remote Sensing Image Classification. *IEEE Transactions on Geoscience and Remote Sensing*, **2019**, 57, 8506-8521	8.1	36
313	Two-dimensional ZnO for the selective photoreduction of CO2. *Journal of Materials Chemistry A*, **2019**, 7, 16294-16303	13	39
312	Point defects in group III nitrides: A comparative first-principles study. *Journal of Applied Physics*, **2019**, 125, 215705	2.5	26
311	Perovskite Solar Cells: Reverse-Graded 2D Ruddlesden□opper Perovskites for Efficient Air-Stable Solar Cells (Adv. Energy Mater. 21/2019). *Advanced Energy Materials*, **2019**, 9, 1970075	21.8	0
310	Co Nanoislands Rooted on Co-N-C Nanosheets as Efficient Oxygen Electrocatalyst for Zn-Air Batteries. *Advanced Materials*, **2019**, 31, e1901666	24	232
309	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	11.5	19
308	Rational design of two-dimensional hybrid Co/N-doped carbon nanosheet arrays for efficient bi-functional electrocatalysis. *Sustainable Energy and Fuels*, **2019**, 3, 1757-1763	5.8	9

307	Evolution of atomic structures of Sn, Sn , and SnCl clusters (N = 4-20): Insight from ab initio calculations. *Journal of Chemical Physics*, **2019**, 150, 174304	3.9	4
306	Foreign atom encapsulated Au golden cages for catalysis of CO oxidation. *Physical Chemistry Chemical Physics*, **2019**, 21, 10587-10593	3.6	13
305	Reverse-Graded 2D RuddlesdenPopper Perovskites for Efficient Air-Stable Solar Cells. *Advanced Energy Materials*, **2019**, 9, 1900612	21.8	47
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