Jijun Zhao

List of Publications by Year in Descending Order

650 papers	23,162 citations	72 h-index	125 g-index
678 ext. papers	26,673 ext. citations	5.3 avg, IF	7.47 L-index

#	Paper	IF	Citations
650	FeSi2: a two-dimensional ferromagnet containing planar hexacoordinate Fe atoms. *Nanoscale Advances*, **2022**, 4, 600-607	5.1	1
649	Transition metal halide nanowires: A family of one-dimensional multifunctional building blocks. *Applied Physics Letters*, **2022**, 120, 023103	3.4	1
648	Photoinduced Spin Injection and Ferromagnetism in 2D Group III Monochalcogenides.. *Journal of Physical Chemistry Letters*, **2022**, 590-597	6.4	4
647	Theoretical insights of structural evolution and electronic properties of Ru2Gen (n = 1□16) clusters. *European Physical Journal Plus*, **2022**, 137, 1	3.1	0
646	Crystal-Phase-Mediated Restructuring of Pt on TiO2 with Tunable Reactivity: Redispersion versus Reshaping. *ACS Catalysis*, **2022**, 12, 3634-3643	13.1	9
645	Inverse Design of Nanoclusters for Light-Controlled CO-HCOOH Interconversion.. *Journal of Physical Chemistry Letters*, **2022**, 2523-2532	6.4	0
644	First-principles calculations of transition elements interaction with hydrogen in vanadium. *Journal of Nuclear Materials*, **2022**, 153710	3.3	1
643	Strain softened bending modulus of graphene oxide. *Carbon Trends*, **2022**, 7, 100167	0	
642	Modeling irradiation-induced intragranular gas bubble in tungsten under external tensile loading. *International Journal of Refractory Metals and Hard Materials*, **2022**, 105, 105824	4.1	0
641	Heat transfer analysis of irradiation-induced gas bubble in tungsten from a fractal dimension perspective. *International Journal of Heat and Mass Transfer*, **2022**, 193, 122965	4.9	1
640	Low-dimensional non-metal catalysts: principles for regulating p-orbital-dominated reactivity. *Npj Computational Materials*, **2021**, 7,	10.9	10
639	Eliminating Edge Electronic and Phonon States of Phosphorene Nanoribbon by Unique Edge Reconstruction. *Small*, **2021**, e2105130	11	0
638	Prediction of superconductivity in bilayer borophenes.. *RSC Advances*, **2021**, 11, 40220-40227	3.7	0
637	Scalable Production of Freestanding Few-Layer □Borophene Single Crystalline Sheets as Efficient Electrocatalysts for Lithium-Sulfur Batteries. *ACS Nano*, **2021**,	16.7	5
636	Electric-Field-Driven Negative Differential Conductance in 2D van der Waals Ferromagnet FeGeTe. *Nano Letters*, **2021**, 21, 9233-9239	11.5	2
635	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
634	MXene and MBene as efficient catalysts for energy conversion: roles of surface, edge and interface. *JPhys Energy*, **2021**, 3, 012002	4.9	17

633	Temperature-dependent hardness of zinc-blende structured covalent materials. *Science China Materials*, **2021**, 64, 2280-2288	7.1	3
632	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
631	Ultra-high hydrogen storage capacity of holey graphyne. *Nanotechnology*, **2021**,	3.4	5
630	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
629	Computational high-throughput screening of alloy nanoclusters for electrocatalytic hydrogen evolution. *Npj Computational Materials*, **2021**, 7,	10.9	17
628	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
627	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
626	Thermal properties of energetic materials from quasi-harmonic first-principles calculations. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	1
625	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
624	Ground-State Structures of Hydrated Calcium Ion Clusters From Comprehensive Genetic Algorithm Search. *Frontiers in Chemistry*, **2021**, 9, 637750	5	2
623	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
622	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
621	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
620	Ab initio modelling of helium behavior in Fe/TaC interface. *Nuclear Materials and Energy*, **2021**, 27, 100956	2.1	1
619	Searching for cluster Lego blocks for three-dimensional and two-dimensional assemblies. *Physical Review Materials*, **2021**, 5,	3.2	2
618	Phase Diagrams for sII Clathrate Hydrates of CO from First-Principles Thermodynamics. *Journal of Physical Chemistry A*, **2021**, 125, 5956-5962	2.8	1
617	Compression behavior of energetic CL-20 crystals from density functional theory calculations. *Journal of Raman Spectroscopy*, **2021**, 52, 1764	2.3	1
616	Effects of Cr and Ti additions on the stability and migration of C, N and O in vanadium: A first-principles study. *Fusion Engineering and Design*, **2021**, 168, 112604	1.7	2

615	Oxygen interaction with alloying elements (Cr/Ni) and vacancies in dilute austenitic iron alloys: A first-principles study. *Fusion Engineering and Design*, **2021**, 163, 112123	1.7	2
614	Compositionally Designed 2D Ruddlesden□Popper Perovskites for Efficient and Stable Solar Cells. *Solar Rrl*, **2021**, 5, 2000661	7.1	3
613	Atomic Wires of Transition Metal Chalcogenides: A Family of 1D Materials for Flexible Electronics and Spintronics. *Jacs Au*, **2021**, 1, 147-155		3
612	A first-principles study of helium diffusion in quartz and coesite under high pressure up to 12GPa. *Geoscience Frontiers*, **2021**, 12, 1001-1009	6	0
611	The influence of temperature on the elastic properties of body-centered cubic reduced activation steels. *Materials and Design*, **2021**, 197, 109282	8.1	4
610	Numerical simulations of thermal conductivity in void-containing tungsten: Topological feature of voids. *Journal of Nuclear Materials*, **2021**, 543, 152601	3.3	4
609	Selective CO2 conversion tuned by periodicities in Au8n+4(TBBT)4n+8 nanoclusters. *Nano Research*, **2021**, 14, 807-813	10	2
608	Intrinsic spin-valley-coupled Dirac state in Janus functionalized □BiAs monolayer. *Nanoscale Horizons*, **2021**, 6, 283-289	10.8	2
607	Ferromagnetic Dirac half-metallicity in transition metal embedded honeycomb borophene. *Physical Chemistry Chemical Physics*, **2021**, 23, 17150-17157	3.6	3
606	Multiscale simulations of the hydration shells surrounding spherical FeO nanoparticles and effect on magnetic properties. *Nanoscale*, **2021**, 13, 9293-9302	7.7	2
605	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
604	First-principles explorations on P8 and N2 assembled nanowire and nanosheet. *Nano Express*, **2021**, 2, 010004	2	2
603	Imaging Vacancy Defects in Single-Layer Chromium Triiodide. *Journal of Physical Chemistry Letters*, **2021**, 12, 2199-2205	6.4	1
602	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
601	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
600	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
599	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
598	Methane conversion by transition metal-doped vanadium oxide clusters. *Chemical Physics Letters*, **2021**, 779, 138829	2.5	1

597	Recent progress on 2D magnets: Fundamental mechanism, structural design and modification. *Applied Physics Reviews*, **2021**, 8, 031305	17.3	35
596	Interactions of solute atoms with self-interstitial atoms/clusters in vanadium: A first-principles study. *Journal of Nuclear Materials*, **2021**, 553, 153055	3.3	5
595	Examining deformation localization of irradiated tungsten under uniaxial compression with crystal plasticity. *International Journal of Refractory Metals and Hard Materials*, **2021**, 100, 105637	4.1	
594	Superior flexibility of planar graphene allotropes with pentagons and heptagons. *Applied Surface Science*, **2021**, 569, 151048	6.7	0
593	Investigation of electronic and vibrational properties of dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate under high-pressure conditions. *Physical Chemistry Chemical Physics*, **2021**, 23, 7442-7448	3.6	0
592	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
591	A valence balancing rule for the design of bimetallic phosphides targeting high thermoelectric performance. *Physical Chemistry Chemical Physics*, **2021**, 23, 18916-18924	3.6	1
590	Accurate electronic properties and non-linear optical response of two-dimensional MA2Z4. *Nanoscale*, **2021**, 13, 5479-5488	7.7	18
589	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
588	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
587	Matching vacancy formation energy and defect levels with the density of amorphous Ga2O3. *Journal of Materials Science*, **2020**, 55, 9343-9353	4.3	1
586	Materials selection for nuclear applications in view of divacancy energies by comprehensive first-principles calculations. *Journal of Nuclear Materials*, **2020**, 538, 152253	3.3	2
585	MBenes: emerging 2D materials as efficient electrocatalysts for the nitrogen reduction reaction. *Nanoscale Horizons*, **2020**, 5, 1106-1115	10.8	45
584	Two-Dimensional Metallic NiTe with Ultrahigh Environmental Stability, Conductivity, and Electrocatalytic Activity. *ACS Nano*, **2020**, 14, 9011-9020	16.7	27
583	Charge effect on the irradiation damage of silicon: Insights from phase-field simulation. *Materials Today Communications*, **2020**, 24, 101187	2.5	
582	Experimental Realization of Two-Dimensional Buckled Lieb Lattice. *Nano Letters*, **2020**, 20, 2537-2543	11.5	2
581	Oxidation Behaviors of Two-dimensional Metal Chalcogenides. *ChemNanoMat*, **2020**, 6, 838-849	3.5	4
580	Tuning the electronic properties of bilayer black phosphorene with the twist angle. *Journal of Materials Chemistry C*, **2020**, 8, 6264-6272	7.1	14

579	Structures and vertical detachment energies of water cluster anions (H2O)□ with n = 6□11. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	4
578	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
577	2D tetragonal transition-metal phosphides: an ideal platform to screen metal shrouded crystals for multifunctional applications. *Nanoscale*, **2020**, 12, 6776-6784	7.7	11
576	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
575	Anionic Copper Clusters Reacting with NO: An Open-Shell Superatom Cu. *Journal of Physical Chemistry Letters*, **2020**, 11, 5807-5814	6.4	13
574	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
573	First-principles investigations of intrinsic point defects and helium impurities in vanadium monocarbide. *Nuclear Instruments & Methods in Physics Research B*, **2020**, 479, 163-170	1.2	1
572	First-Principles Calculations for Stable □TiMo Alloys Using Cluster-Plus-Glue-Atom Model. *Acta Metallurgica Sinica (English Letters)*, **2020**, 33, 968-974	2.5	1
571	First-principles study of the □(112) grain boundary in Fe-rich Fe-Cr alloys. *Scripta Materialia*, **2020**, 181, 140-143	5.6	2
570	CO2 reduction on p-block metal oxide overlayers on metal substrates□D MgO as a prototype. *Journal of Materials Chemistry A*, **2020**, 8, 5688-5698	13	9
569	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
568	Operando Revealing Dynamic Reconstruction of NiCo Carbonate Hydroxide for High-Rate Energy Storage. *Joule*, **2020**, 4, 673-687	27.8	48
567	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
566	Two-dimensional cyclohexane methylamine based perovskites as stable light absorbers for solar cells. *Solar Energy*, **2020**, 201, 13-20	6.8	4
565	A mechanism-based quantitative multi-scale framework for investigating irradiation hardening of tungsten at low temperature. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2020**, 774, 138941	5.3	3
564	Chemical environment and magnetic moment effects on point defect formations in CoCrNi-based concentrated solid-solution alloys. *Acta Materialia*, **2020**, 187, 122-134	8.4	57
563	Excitonic AuRu(PPh)(SCHPh) cluster for light-driven dinitrogen fixation. *Chemical Science*, **2020**, 11, 2440-2447	9.4	23
562	Selective C-C Coupling by Spatially Confined Dimeric Metal Centers. *IScience*, **2020**, 23, 101051	6.1	21

561	Helium behaviors at Mn6Ni16Si7 precipitate in □Fe: Insights from ab initio modeling. *Computational Materials Science*, **2020**, 181, 109735	3.2	1
560	Ab initio study of He, Ne, Ar, Kr incorporation in zirconium carbide. *Journal of Nuclear Materials*, **2020**, 534, 152154	3.3	1
559	High-Curie-temperature ferromagnetism in bilayer CrI3 on bulk semiconducting substrates. *Physical Review Materials*, **2020**, 4,	3.2	12
558	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
557	analytic calculation of point defects in AlGaN/GaN heterointerfaces. *Journal of Physics Condensed Matter*, **2020**,	1.8	2
556	Tunable bending modulus and bending limit of oxidized graphene. *Nanoscale*, **2020**, 12, 1623-1628	7.7	6
555	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
554	Controllable Conversion of CO on Non-Metallic Gold Clusters. *Angewandte Chemie - International Edition*, **2020**, 59, 1919-1924	16.4	28
553	Boron Nitride Nanotubes for Ammonia Synthesis: Activation by Filling Transition Metals. *Journal of the American Chemical Society*, **2020**, 142, 308-317	16.4	61
552	Understanding the thermal conductivity of pristine W and W□Re alloys from a physics-based model. *Journal of Nuclear Materials*, **2020**, 529, 151931	3.3	4
551	Metal-Encapsulated Boron Nitride Nanocages for Solar-Driven Nitrogen Fixation. *Journal of Physical Chemistry C*, **2020**, 124, 23798-23806	3.8	8
550	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
549	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
548	Carrier Dynamics and Transfer across the CdS/MoS Interface upon Optical Excitation. *Journal of Physical Chemistry Letters*, **2020**, 11, 6544-6550	6.4	7
547	Remarkable Role of Grain Boundaries in the Thermal Transport Properties of Phosphorene. *ACS Omega*, **2020**, 5, 17416-17422	3.9	1
546	Electronic structures and charge carrier mobilities of boron-graphdiyne sheet and nanoribbons. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 124, 114354	3	1
545	Compressive behavior and electronic properties of ammonia ice: a first-principles study.. *RSC Advances*, **2020**, 10, 26579-26587	3.7	1
544	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

543	Solar driven CO hydrogenation on transition metal doped ZnO cluster. *Journal of Chemical Physics*, **2020**, 153, 164306	3.9	4
542	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
541	Dual-Constrained Sulfur in FeS2@C Nanostructured Lithium-Sulfide Batteries. *ACS Applied Energy Materials*, **2020**, 3, 10950-10960	6.1	5
540	Enhanced Ferromagnetism of CrI3 Bilayer by Self-Intercalation. *Chinese Physics Letters*, **2020**, 37, 107506	1.8	13
539	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
538	Endohedrally Doped Cage Clusters. *Chemical Reviews*, **2020**, 120, 9021-9163	68.1	76
537	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
536	2D Boron Sheets: Structure, Growth, and Electronic and Thermal Transport Properties. *Advanced Functional Materials*, **2020**, 30, 1904349	15.6	69
535	Robust spin manipulation in 2D organometallic Kagome lattices: a first-principles study. *Physical Chemistry Chemical Physics*, **2020**, 22, 11045-11052	3.6	7
534	Giant Thickness-Tunable Bandgap and Robust Air Stability of 2D Palladium Diselenide. *Small*, **2020**, 16, e2000754	11	11
533	Hydrated Sodium Ion Clusters [Na(HO) (= 1-6)]: An Study on Structures and Non-covalent Interaction. *Frontiers in Chemistry*, **2019**, 7, 624	5	9
532	First-principles investigation of hydrogen behavior in different oxides in ODS steels. *International Journal of Hydrogen Energy*, **2019**, 44, 17105-17113	6.7	2
531	Two-dimensional spin valley-coupled Dirac semimetals in functionalized SbAs monolayers. *Materials Horizons*, **2019**, 6, 781-787	14.4	21
530	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
529	Insight into void formation near grain boundary from phase-field simulations. *Nuclear Instruments & Methods in Physics Research B*, **2019**, 453, 50-55	1.2	
528	Two-dimensional ZnO for the selective photoreduction of CO2. *Journal of Materials Chemistry A*, **2019**, 7, 16294-16303	13	39
527	Point defects in group III nitrides: A comparative first-principles study. *Journal of Applied Physics*, **2019**, 125, 215705	2.5	26
526	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

525	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
524	Foreign atom encapsulated Au golden cages for catalysis of CO oxidation. *Physical Chemistry Chemical Physics*, **2019**, 21, 10587-10593	3.6	13
523	Reverse-Graded 2D RuddlesdenPopper Perovskites for Efficient Air-Stable Solar Cells. *Advanced Energy Materials*, **2019**, 9, 1900612	21.8	47
522	Uniaxial compression behavior and spectroscopic properties of energetic 1,1-diamino-2,2-dinitroethylene (FOX-7) crystals from density functional theory calculations. *Progress in Natural Science: Materials International*, **2019**, 29, 329-334	3.6	3
521	Room temperature electrofreezing of water yields a missing dense ice phase in the phase diagram. *Nature Communications*, **2019**, 10, 1925	17.4	13
520	Defect stability and electronic structure of doped Ga2O3: A comprehensive ab initio study. *Journal of Alloys and Compounds*, **2019**, 794, 374-384	5.7	12
519	Silicene catalysts for CO hydrogenation: the number of layers controls selectivity. *Nanoscale*, **2019**, 11, 7734-7743	7.7	19
518	Controlling the synthesis of uniform electron-deficient Pd clusters for superior hydrogen production from formic acid. *Journal of Materials Chemistry A*, **2019**, 7, 10363-10371	13	23
517	Realization of Strained Stanene by Interface Engineering. *Journal of Physical Chemistry Letters*, **2019**, 10, 1558-1565	6.4	22
516	The pressure effects and vibrational properties of energetic material: Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX). *Journal of Raman Spectroscopy*, **2019**, 50, 889-898	2.3	9
515	Silicon Nanocages for Selective Carbon Dioxide Conversion under Visible Light. *Journal of Physical Chemistry C*, **2019**, 123, 9973-9980	3.8	15
514	Vanadium carbide coating as hydrogen permeation barrier: A DFT study. *International Journal of Hydrogen Energy*, **2019**, 44, 6093-6102	6.7	14
513	Oxygen Evolution Reaction over the Au/YSZ Interface at High Temperature. *Angewandte Chemie - International Edition*, **2019**, 58, 4617-4621	16.4	18
512	The effect of Cr on He segregation and diffusion at (1 1 2) grain boundary in Fe. *Nuclear Instruments & Methods in Physics Research B*, **2019**, 456, 7-11	1.2	1
511	Engineering Multifunctional Collaborative Catalytic Interface Enabling Efficient Hydrogen Evolution in All pH Range and Seawater. *Advanced Energy Materials*, **2019**, 9, 1901333	21.8	98
510	Dual transition metal doped germanium clusters for catalysis of CO oxidation. *Journal of Alloys and Compounds*, **2019**, 806, 698-704	5.7	9
509	Strongly Hole-Doped and Highly Decoupled Graphene on Platinum by Water Intercalation. *Journal of Physical Chemistry Letters*, **2019**, 10, 3998-4002	6.4	3
508	Mo Concentration Controls the Morphological Transitions from Dendritic to Semicompact, and to Compact Growth of Monolayer Crystalline MoS on Various Substrates. *ACS Applied Materials & Interfaces*, **2019**, 11, 42751-42759	9.5	16

507	Interaction Mechanisms of Insensitive Explosive FOX-7 and Graphene Oxides from Ab Initio Calculations. *Nanomaterials*, **2019**, 9,	5.4	2
506	A Molecular-Cage Strategy Enabling Efficient Chemisorption–Electrocatalytic Interface in Nanostructured Li2S Cathode for Li Metal-Free Rechargeable Cells with High Energy. *Advanced Functional Materials*, **2019**, 29, 1905986	15.6	33
505	Hybrids of PtRu Nanoclusters and Black Phosphorus Nanosheets for Highly Efficient Alkaline Hydrogen Evolution Reaction. *ACS Catalysis*, **2019**, 9, 10870-10875	13.1	45
504	Topologically protected states and half-metal behaviors: Defect-strain synergy effects in two-dimensional antimonene. *Physical Review Materials*, **2019**, 3,	3.2	5
503	Electrical Conductance of Graphene with Point Defects. *Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica*, **2019**, 35, 1142-1149	3.8	3
502	Determination of second- and third-order elastic constants for energetic materials. *Computational Materials Science*, **2019**, 161, 379-384	3.2	4
501	First principles investigations of hydrogen interaction with vacancy-oxygen complexes in vanadium alloys. *International Journal of Hydrogen Energy*, **2019**, 44, 26637-26645	6.7	8
500	Structural and Electronic Properties of Binary Clusters SiGe (+ = 6-13). *Journal of Nanoscience and Nanotechnology*, **2019**, 19, 7879-7885	1.3	1
499	Two-Dimensional AXenes: A New Family of Room-Temperature d Ferromagnets and Their Structural Phase Transitions. *Journal of Physical Chemistry Letters*, **2019**, 10, 7753-7759	6.4	12
498	Copper(i) sulfide: a two-dimensional semiconductor with superior oxidation resistance and high carrier mobility. *Nanoscale Horizons*, **2019**, 4, 223-230	10.8	32
497	Atomistic understanding of helium behaviors at grain boundaries in vanadium. *Computational Materials Science*, **2019**, 158, 296-306	3.2	9
496	Atomic Structures and Electronic Properties of Large-Sized GeN Clusters (N = 45, 50, 55, 60, 65, 70) by First-Principles Global Search. *Journal of Cluster Science*, **2019**, 30, 371-377	3	4
495	First-principles calculations of vacancy-O-He and vacancy-N-He complexes in vanadium. *Computational Materials Science*, **2019**, 160, 180-185	3.2	10
494	Energetics of helium-vacancy complexes in Fe-9Cr alloys from first-principles calculations. *Journal of Nuclear Materials*, **2019**, 513, 143-151	3.3	19
493	All-Silicon Topological Semimetals with Closed Nodal Line. *Journal of Physical Chemistry Letters*, **2019**, 10, 244-250	6.4	14
492	Accelerating polysulfide redox conversion on bifunctional electrocatalytic electrode for stable Li-S batteries. *Energy Storage Materials*, **2019**, 20, 98-107	19.4	50
491	Interactions between helium, hydrogen and intrinsic point defects in TaC crystal. *Journal of Alloys and Compounds*, **2018**, 741, 900-907	5.7	8
490	Understanding the mechanical properties of reduced activation steels. *Materials and Design*, **2018**, 146, 260-272	8.1	6

489	Stability of X-C-vacancy complexes (X=H, He) in vanadium from first principles investigations. *Journal of Nuclear Materials*, **2018**, 505, 119-126	3.3	9
488	Quantum oscillation in carrier transport in two-dimensional junctions. *Nanoscale*, **2018**, 10, 7912-7917	7.7	5
487	Electronic and magnetic properties of transition metal decorated monolayer GaS. *Physica E: Low-Dimensional Systems and Nanostructures*, **2018**, 101, 131-138	3	2
486	2D lateral heterostructures of group-III monochalcogenide: Potential photovoltaic applications. *Applied Physics Letters*, **2018**, 112, 143902	3.4	43
485	Structural Evolution and Superatoms in Molybdenum Atom Stabilized Boron Clusters: MoBn (n = 10–14). *Journal of Cluster Science*, **2018**, 29, 847-852	3	16
484	MBene (MnB): a new type of 2D metallic ferromagnet with high Curie temperature. *Nanoscale Horizons*, **2018**, 3, 335-341	10.8	99
483	An electrocatalyst with anti-oxidized capability for overall water splitting. *Nano Research*, **2018**, 11, 3411-3418	10	9
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