Xiao Cheng Zeng

List of Publications by Year in Descending Order

620 papers	36,187 citations	94 h-index	159 g-index
645 ext. papers	40,985 ext. citations	9.1 avg, IF	7.91 L-index

#	Paper	IF	Citations
620	Atomically Resolved Electrically Active Intragrain Interfaces in Perovskite Semiconductors.. *Journal of the American Chemical Society*, **2022**,	16.4	7
619	Large-Sized Au Core-Shell Clusters (= 61-66): Enduring Structure of the Icosahedral Au Core.. *Journal of Physical Chemistry Letters*, **2022**, 1389-1397	6.4	1
618	Anomalous Phase Behaviors of Monolayer NaCl Aqueous Solutions Induced by Effective Coulombic Interactions within Angstrom-Scale Slits.. *Journal of Physical Chemistry Letters*, **2022**, 2704-2710	6.4	0
617	Two-Dimensional GeC with Tunable Electronic and Carrier Transport Properties and a High Current ON/OFF Ratio. *Journal of Physical Chemistry Letters*, **2021**, 12, 11488-11496	6.4	
616	Towards complete assignment of the infrared spectrum of the protonated water cluster H(HO). *Nature Communications*, **2021**, 12, 6141	17.4	6
615	Exploration of Formation and Size-Evolution Pathways of Thiolate-Gold Nanoclusters in the CO-Directed [Au (SR)] Synthesis. *Small*, **2021**, 17, e2000627	11	5
614	Molecular Design of Three-Dimensional Metal-Free A(NH)X Perovskites for Photovoltaic Applications. *Jacs Au*, **2021**, 1, 475-483		6
613	Peroxo Species Formed in the Bulk of Silicate Cathodes. *Angewandte Chemie*, **2021**, 133, 10144-10151	3.6	0
612	Peroxo Species Formed in the Bulk of Silicate Cathodes. *Angewandte Chemie - International Edition*, **2021**, 60, 10056-10063	16.4	4
611	Directional Proton Transfer in the Reaction of the Simplest Criegee Intermediate with Water Involving the Formation of Transient HO. *Journal of Physical Chemistry Letters*, **2021**, 12, 3379-3386	6.4	3
610	Ring Model for Understanding How Interfacial Interaction Dictates the Structures of Protection Motifs and Gold Cores in Thiolate-Protected Gold Nanoclusters. *Journal of Physical Chemistry Letters*, **2021**, 12, 3006-3013	6.4	5
609	Innentitelbild: Peroxo Species Formed in the Bulk of Silicate Cathodes (Angew. Chem. 18/2021). *Angewandte Chemie*, **2021**, 133, 9814-9814	3.6	
608	How O-Binding Affects Structural Evolution of Medium Even-Sized Gold Clusters Au (= 20-34). *Journal of Physical Chemistry Letters*, **2021**, 12, 3560-3570	6.4	3
607	First-Principles Molecular Dynamics Simulations of the Spontaneous Freezing Transition of 2D Water in a Nanoslit. *Journal of the American Chemical Society*, **2021**, 143, 8177-8183	16.4	5
606	Multiple Wetting-Dewetting States of a Water Droplet on Dual-Scale Hierarchical Structured Surfaces. *Jacs Au*, **2021**, 1, 955-966		
605	Gas hydrates in confined space of nanoporous materials: new frontier in gas storage technology. *Nanoscale*, **2021**, 13, 7447-7470	7.7	11
604	Metallic surface doping of metal halide perovskites. *Nature Communications*, **2021**, 12, 7	17.4	28

603	Mechanistic Study of the Aqueous Reaction of Organic Peroxides with HSO3□on the Surface of a Water Droplet. *Angewandte Chemie*, **2021**, 133, 20362-20365	3.6	0
602	Mechanistic Study of the Aqueous Reaction of Organic Peroxides with HSO on the Surface of a Water Droplet. *Angewandte Chemie - International Edition*, **2021**, 60, 20200-20203	16.4	1
601	Two-dimensional monolayer salt nanostructures can spontaneously aggregate rather than dissolve in dilute aqueous solutions. *Nature Communications*, **2021**, 12, 5602	17.4	4
600	Two-Dimensional IV-V Monolayers with Highly Anisotropic Carrier Mobility and Electric Transport Properties. *Journal of Physical Chemistry Letters*, **2021**, 12, 1058-1065	6.4	7
599	Formation of dimethyl carbonate direct esterification of CO with methanol on reduced or stoichiometric CeO(111) and (110) surfaces. *Physical Chemistry Chemical Physics*, **2021**, 23, 16150-16156	3.6	0
598	Quantitative Prediction of Aggregation-Induced Emission: A Full Quantum Mechanical Approach to the Optical Spectra. *Angewandte Chemie*, **2020**, 132, 11647-11652	3.6	3
597	New Insights into the Stability of Anhydrous 2-Imidazolium Fluoride and its High Dissolution Capability toward a Strongly Hydrogen-Bonded Compound. *Journal of the American Chemical Society*, **2020**, 142, 10314-10318	16.4	6
596	A possible unaccounted source of atmospheric sulfate formation: amine-promoted hydrolysis and non-radical oxidation of sulfur dioxide. *Chemical Science*, **2020**, 11, 2093-2102	9.4	3
595	Quantitative Prediction of Aggregation-Induced Emission: A Full Quantum Mechanical Approach to the Optical Spectra. *Angewandte Chemie - International Edition*, **2020**, 59, 11550-11555	16.4	14
594	PtSe Monolayer: A Highly Efficient Electrocatalyst toward Hydrogen and Oxygen Electrode Reactions. *ACS Applied Materials & Interfaces*, **2020**, 12, 13896-13903	9.5	15
593	PtCoNi Alloy Nanoclusters for Synergistic Catalytic Oxygen Reduction Reaction. *ACS Applied Nano Materials*, **2020**, 3, 2536-2544	5.6	6
592	Hydration, Solvation, and Isomerization of Methylglyoxal at the Air/Water Interface: New Mechanistic Pathways. *Journal of the American Chemical Society*, **2020**, 142, 5574-5582	16.4	13
591	Heterogeneous Reactions of SO on Ice: An Overlooked Sink for SO Depletion. *Journal of the American Chemical Society*, **2020**, 142, 2150-2154	16.4	4
590	Resolving the puzzle of single-atom silver dispersion on nanosized □AlO surface for high catalytic performance. *Nature Communications*, **2020**, 11, 529	17.4	43
589	High ZT 2D Thermoelectrics by Design: Strong Interlayer Vibration and Complete Band-Extrema Alignment. *Advanced Functional Materials*, **2020**, 30, 2001200	15.6	21
588	Domain Wall Conduction in Calcium-Modified Lead Titanate for Polarization Tunable Photovoltaic Devices. *Cell Reports Physical Science*, **2020**, 1, 100043	6.1	3
587	Constructing Stable and Potentially High-Performance Hybrid Organic-Inorganic Perovskites with "Unstable" Cations. *Research*, **2020**, 2020, 1986576	7.8	3
586	A droplet-based electricity generator with high instantaneous power density. *Nature*, **2020**, 578, 392-396	50.4	391

585	Directly predicting limiting potentials from easily obtainable physical properties of graphene-supported single-atom electrocatalysts by machine learning. *Journal of Materials Chemistry A*, **2020**, 8, 5663-5670	13	42
584	Chiral Au(SR): a new ligand-binding strategy for structural prediction of thiolate-protected gold nanocluster. *Chemical Communications*, **2020**, 56, 2995-2998	5.8	6
583	AgBiS2 as a low-cost and eco-friendly all-inorganic photovoltaic material: nanoscale morphology–property relationship. *Nanoscale Advances*, **2020**, 2, 770-776	5.1	4
582	Rich topologies of monolayer ices via unconventional electrowetting. *Nanoscale Horizons*, **2020**, 5, 514-522	12.8	5
581	Atomic imaging of the edge structure and growth of a two-dimensional hexagonal ice. *Nature*, **2020**, 577, 60-63	50.4	73
580	Highly efficient N fixation catalysts: transition-metal carbides MC (MXenes). *Nanoscale*, **2020**, 12, 538-547	7.7	46
579	Direct synthesis of bifunctional nanorods from a Co–adenine–MoO3 hybrid for overall water splitting. *Materials Chemistry Frontiers*, **2020**, 4, 546-554	7.8	10
578	Influence of atmospheric conditions on sulfuric acid-dimethylamine-ammonia-based new particle formation. *Chemosphere*, **2020**, 245, 125554	8.4	16
577	Reversing Interfacial Catalysis of Ambipolar WSe Single Crystal. *Advanced Science*, **2020**, 7, 1901382	13.6	75
576	Modulation of the Double-Helical Cores: A New Strategy for Structural Predictions of Thiolate-Protected Gold Nanoclusters. *Journal of Physical Chemistry Letters*, **2020**, 11, 536-540	6.4	9
575	Use of Ion Exchange To Regulate the Heterogeneous Ice Nucleation Efficiency of Mica. *Journal of the American Chemical Society*, **2020**, 142, 17956-17965	16.4	12
574	Turning a Superhydrophilic Surface Weakly Hydrophilic: Topological Wetting States. *Journal of the American Chemical Society*, **2020**, 142, 18491-18502	16.4	7
573	Unraveling Molecular Mechanism on Dilute Surfactant Solution Controlled Ice Recrystallization. *Langmuir*, **2020**, 36, 1691-1698	4	2
572	Computational Prediction of Novel Ice Phases: A Perspective. *Journal of Physical Chemistry Letters*, **2020**, 11, 7449-7461	6.4	10
571	Multiturn Hollow Helices: Synthesis and Folding of Long Aromatic Oligoamides. *Organic Letters*, **2020**, 22, 6938-6942	6.2	1
570	Unraveling nucleation pathway in methane clathrate formation. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 24701-24708	11.5	16
569	Descriptor-Based Design Principle for Two-Dimensional Single-Atom Catalysts: Carbon Dioxide Electroreduction. *Journal of Physical Chemistry Letters*, **2020**, 11, 3481-3487	6.4	34
568	Markedly Enhanced Oxygen Reduction Activity of Single-Atom Fe Catalysts via Integration with Fe Nanoclusters. *ACS Nano*, **2019**, 13, 11853-11862	16.7	189

567	Facile and Versatile Functionalization of Two-Dimensional Carbon Nitrides by Design: Magnetism/Multiferroicity, Valleytronics, and Photovoltaics. *Advanced Functional Materials*, **2019**, 29, 1905752	15.6	14
566	Water desalination through rim functionalized carbon nanotubes. *Journal of Materials Chemistry A*, **2019**, 7, 3583-3591	13	28
565	Reconciling the Debate on the Existence of Pentazole HN in the Pentazolate Salt of (N)(HO)(NH)Cl. *Journal of the American Chemical Society*, **2019**, 141, 2984-2989	16.4	16
564	Reaction mechanism between small-sized Ce clusters and water molecules: an ab initio investigation on Ce + HO. *Physical Chemistry Chemical Physics*, **2019**, 21, 4006-4014	3.6	4
563	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
562	Tuning electronic structure of monolayer InP in contact with graphene or Ni: effect of a buffer layer and intrinsic In and P-vacancy. *Physical Chemistry Chemical Physics*, **2019**, 21, 1285-1293	3.6	5
561	Lead-free low-dimensional tin halide perovskites with functional organic spacers: breaking the charge-transport bottleneck. *Journal of Materials Chemistry A*, **2019**, 7, 16742-16747	13	17
560	Two-Dimensional Gold Sulfide Monolayers with Direct Band Gap and Ultrahigh Electron Mobility. *Journal of Physical Chemistry Letters*, **2019**, 10, 3773-3778	6.4	23
559	Unraveling Oxygen Evolution in Li-Rich Oxides: A Unified Modeling of the Intermediate Peroxo/Superoxo-like Dimers. *Journal of the American Chemical Society*, **2019**, 141, 10751-10759	16.4	51
558	Monolayer triphosphates MP (M = Sn, Ge) with excellent basal catalytic activity for hydrogen evolution reaction. *Nanoscale*, **2019**, 11, 12210-12219	7.7	56
557	A New Class of Bifunctional Perovskites BaMX4 (M = Co, Ni, Fe, Mn; X = F, Cl, Br, I): An n-Type Semiconductor with Combined Multiferroic and Photovoltaic Properties. *Journal of Physical Chemistry C*, **2019**, 123, 14303-14311	3.8	1
556	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
555	Method To Implement Interaction Surfaces with Virtual Companion Particles for Molecular Dynamics Simulations. *Journal of Chemical & Engineering Data*, **2019**, 64, 3693-3700	2.8	1
554	Niobium oxide dihalides NbOX2: a new family of two-dimensional van der Waals layered materials with intrinsic ferroelectricity and antiferroelectricity. *Nanoscale Horizons*, **2019**, 4, 1113-1123	10.8	19
553	Phase transitions and ferroelasticity–multiferroicity in bulk and two-dimensional silver and copper monohalides. *Nanoscale Horizons*, **2019**, 4, 1106-1112	10.8	22
552	Mechanistic Insight into the Reaction of Organic Acids with SO3 at the Air–Water Interface. *Angewandte Chemie*, **2019**, 131, 8439-8443	3.6	3
551	Unraveling the high-activity nature of Fe–N–C electrocatalysts for the oxygen reduction reaction: the extraordinary synergy between Fe–N4 and Fe4N. *Journal of Materials Chemistry A*, **2019**, 7, 11792-11801	13	55
550	Room temperature electrofreezing of water yields a missing dense ice phase in the phase diagram. *Nature Communications*, **2019**, 10, 1925	17.4	13

549	Tailoring Passivation Molecular Structures for Extremely Small Open-Circuit Voltage Loss in Perovskite Solar Cells. *Journal of the American Chemical Society*, **2019**, 141, 5781-5787	16.4	368
548	SLIPS-TENG: robust triboelectric nanogenerator with optical and charge transparency using a slippery interface. *National Science Review*, **2019**, 6, 540-550	10.8	54
547	Rational design of one-dimensional hybrid organic□inorganic perovskites with room-temperature ferroelectricity and strong piezoelectricity. *Materials Horizons*, **2019**, 6, 1463-1473	14.4	10
546	Mechanistic Insight into the Reaction of Organic Acids with SO at the Air-Water Interface. *Angewandte Chemie - International Edition*, **2019**, 58, 8351-8355	16.4	22
545	Au: The Smallest Gold Cluster with the High-Symmetry Icosahedral Core Au. *Journal of Physical Chemistry Letters*, **2019**, 10, 1820-1827	6.4	12
544	Reaction mechanism between small-sized Ce clusters and water molecules II: an ab initio investigation on Ce (n = 1-3) + mHO (m = 2-6). *Physical Chemistry Chemical Physics*, **2019**, 21, 8945-8955	3.6	3
543	Simultaneously Dual Modification of Ni-Rich Layered Oxide Cathode for High-Energy Lithium-Ion Batteries. *Advanced Functional Materials*, **2019**, 29, 1808825	15.6	287
542	Bi(Sb)NCa3: Expansion of Perovskite Photovoltaics into All-Inorganic Anti-Perovskite Materials. *Journal of Physical Chemistry C*, **2019**, 123, 6363-6369	3.8	5
541	Theoretical studies on tunable electronic structures and potential applications of two-dimensional arsenene-based materials. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1387	7.9	12
540	Direct observation of 2-dimensional ices on different surfaces near room temperature without confinement. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 16723-16728	11.5	17
539	Graphene/antimonene/graphene heterostructure: A potential anode for sodium-ion batteries. *Carbon*, **2019**, 153, 767-775	10.4	28
538	Carbon fragments as highly active metal-free catalysts for the oxygen reduction reaction: a mechanistic study. *Nanoscale*, **2019**, 11, 19422-19428	7.7	11
537	Magnetism in bimetallic PtxNi clusters via cross-atomic coupling. *Journal of Materials Chemistry C*, **2019**, 7, 9293-9300	7.1	1
536	B-Doped MnN4-G Nanosheets as Bifunctional Electrocatalysts for Both Oxygen Reduction and Oxygen Evolution Reactions. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 18711-18717	8.3	25
535	Diisopropylammonium Bromide Based Two-Dimensional Ferroelectric Monolayer Molecular Crystal with Large In-Plane Spontaneous Polarization. *Journal of the American Chemical Society*, **2019**, 141, 1452-1456	16.4	9
534	Unraveling a New Chemical Mechanism of Missing Sulfate Formation in Aerosol Haze: Gaseous NO with Aqueous HSO/SO. *Journal of the American Chemical Society*, **2019**, 141, 19312-19320	16.4	23
533	Understanding Hygroscopic Nucleation of Sulfate Aerosols: Combination of Molecular Dynamics Simulation with Classical Nucleation Theory. *Journal of Physical Chemistry Letters*, **2019**, 10, 1126-1132	6.4	3
532	Structural and Electronic Properties of Binary Clusters SiGe (+ = 6-13). *Journal of Nanoscience and Nanotechnology*, **2019**, 19, 7879-7885	1.3	1

531	Two-dimensional MgXSe (X = Al, Ga) monolayers with tunable electronic properties for optoelectronic and photocatalytic applications. *Nanoscale*, **2019**, 11, 19806-19813	7.7	10
530	Unexpected quenching effect on new particle formation from the atmospheric reaction of methanol with SO. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 24966-24971	11.5	17
529	Copper(i) sulfide: a two-dimensional semiconductor with superior oxidation resistance and high carrier mobility. *Nanoscale Horizons*, **2019**, 4, 223-230	10.8	32
528	Iron Clusters Embedded in Graphene Nanocavities: Heat-Induced Structural Evolution and Catalytic C□ Bond Breaking. *ACS Applied Nano Materials*, **2019**, 2, 535-545	5.6	2
527	Highly stable and efficient all-inorganic lead-free perovskite solar cells with native-oxide passivation. *Nature Communications*, **2019**, 10, 16	17.4	283
526	Design of Single-Molecule Multiferroics for Efficient Ultrahigh-Density Nonvolatile Memories. *Advanced Science*, **2019**, 6, 1801572	13.6	26
525	PbTiO3 as Electron-Selective Layer for High-Efficiency Perovskite Solar Cells: Enhanced Electron Extraction via Tunable Ferroelectric Polarization. *Advanced Functional Materials*, **2019**, 29, 1806427	15.6	16
524	Lead-Free Dion□acobson Tin Halide Perovskites for Photovoltaics. *ACS Energy Letters*, **2019**, 4, 276-277	20.1	73
523	Water transport through subnanopores in the ultimate size limit: Mechanism from molecular dynamics. *Nano Research*, **2019**, 12, 587-592	10	15
522	Hydrogen Production via Efficient Formic Acid Decomposition: Engineering the Surface Structure of Pd-Based Alloy Catalysts by Design. *ACS Catalysis*, **2019**, 9, 781-790	13.1	33
521	Aluminum and Nitrogen Codoped Graphene: Highly Active and Durable Electrocatalyst for Oxygen Reduction Reaction. *ACS Catalysis*, **2019**, 9, 610-619	13.1	33
520	Water Confined in Nanocapillaries: Two-Dimensional Bilayer Squarelike Ice and Associated Solid□iquid□olid Transition. *Journal of Physical Chemistry C*, **2018**, 122, 6704-6712	3.8	21
519	Structural Evolution of Gold-Doped Bismuth Clusters AuBi□(n = 4□). *Journal of Physical Chemistry C*, **2018**, 122, 6947-6954	3.8	13
518	Hybrid nanobud-array structures (C24)n/MoS2 and (C24V)n/MoS2: two-dimensional half metallic and ferromagnetic materials. *Journal of Materials Chemistry C*, **2018**, 6, 3373-3386	7.1	1
517	Continuous Grain-Boundary Functionalization for High-Efficiency Perovskite Solar Cells with Exceptional Stability. *CheM*, **2018**, 4, 1404-1415	16.2	124
516	Nitric Acid-Amine Chemistry in the Gas Phase and at the Air-Water Interface. *Journal of the American Chemical Society*, **2018**, 140, 6456-6466	16.4	31
515	Two-Dimensional AuMX (M = Al, Ga, In; X = S, Se) Monolayers Featuring Intracrystalline Aurophilic Interactions with Novel Electronic and Optical Properties. *ACS Applied Materials & Interfaces*, **2018**, 10, 16739-16746	9.5	7
514	Phase behaviors of deeply supercooled bilayer water unseen in bulk water. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 4839-4844	11.5	10

513	Tuning the Stereoselectivity and Solvation Selectivity at Interfacial and Bulk Environments by Changing Solvent Polarity: Isomerization of Glyoxal in Different Solvent Environments. *Journal of the American Chemical Society*, **2018**, 140, 5535-5543	16.4	17
512	Insight into Chemistry on Cloud/Aerosol Water Surfaces. *Accounts of Chemical Research*, **2018**, 51, 1229-1237	24.3	67
511	Suppressed Ion Migration along the In-Plane Direction in Layered Perovskites. *ACS Energy Letters*, **2018**, 3, 684-688	20.1	166
510	Cesium Titanium(IV) Bromide Thin Films Based Stable Lead-free Perovskite Solar Cells. *Joule*, **2018**, 2, 558-570	27.8	260
509	Monolayer and bilayer polyaniline CN: two-dimensional semiconductors with high thermal conductivity. *Nanoscale*, **2018**, 10, 4301-4310	7.7	72
508	Abnormal phase transition between two-dimensional high-density liquid crystal and low-density crystalline solid phases. *Nature Communications*, **2018**, 9, 198	17.4	5
507	Earth-Abundant Nontoxic Titanium(IV)-based Vacancy-Ordered Double Perovskite Halides with Tunable 1.0 to 1.8 eV Bandgaps for Photovoltaic Applications. *ACS Energy Letters*, **2018**, 3, 297-304	20.1	192
506	Phonon thermal transport in a graphene/MoSe van der Waals heterobilayer. *Physical Chemistry Chemical Physics*, **2018**, 20, 2637-2645	3.6	23
505	Anatase (101) Reconstructed Surface with Novel Functionalities: Desired Bandgap for Visible Light Absorption and High Chemical Reactivity. *Advanced Functional Materials*, **2018**, 28, 1705529	15.6	9
504	Formation of aqueous-phase sulfate during the haze period in China: Kinetics and atmospheric implications. *Atmospheric Environment*, **2018**, 177, 93-99	5.3	15
503	Argon Plasma Treatment to Tune Perovskite Surface Composition for High Efficiency Solar Cells and Fast Photodetectors. *Advanced Materials*, **2018**, 30, 1705176	24	60
502	A universal principle for a rational design of single-atom electrocatalysts. *Nature Catalysis*, **2018**, 1, 339-348	36.5	739
501	Thermal transport in phosphorene and phosphorene-based materials: A review on numerical studies. *Chinese Physics B*, **2018**, 27, 036501	1.2	12
500	CaP: A New Two-Dimensional Functional Material with Desirable Band Gap and Ultrahigh Carrier Mobility. *Journal of Physical Chemistry Letters*, **2018**, 9, 1728-1733	6.4	71
499	Reaction of Criegee Intermediate with Nitric Acid at the Air-Water Interface. *Journal of the American Chemical Society*, **2018**, 140, 4913-4921	16.4	35
498	The structural isomerism in gold nanoclusters. *Nanoscale*, **2018**, 10, 9476-9483	7.7	29
497	Co-mixing hydrogen and methane may double the energy storage capacity. *Journal of Materials Chemistry A*, **2018**, 6, 8916-8922	13	11
496	Formation of CO2 Hydrates within Single-Walled Carbon Nanotubes at Ambient Pressure: CO2 Capture and Selective Separation of a CO2/H2 Mixture in Water. *Journal of Physical Chemistry C*, **2018**, 122, 7951-7958	3.8	15

495	Perovskite Solar Cells: Stable Formamidinium-Based Perovskite Solar Cells via In Situ Grain Encapsulation (Adv. Energy Mater. 22/2018). *Advanced Energy Materials*, **2018**, 8, 1870101	21.8	1
494	Zero-Dimensional Organic-Inorganic Perovskite Variant: Transition between Molecular and Solid Crystal. *Journal of the American Chemical Society*, **2018**, 140, 10456-10463	16.4	54
493	Transition-Metal Dihydride Monolayers: A New Family of Two-Dimensional Ferromagnetic Materials with Intrinsic Room-Temperature Half-Metallicity. *Journal of Physical Chemistry Letters*, **2018**, 9, 4260-4266	6.4	87
492	Monolayered semiconducting GeAsSe and SnSbTe with ultrahigh hole mobility. *Frontiers of Physics*, **2018**, 13, 1	3.7	9
491	Structural evolution and magnetic properties of anionic clusters CrGe (n = 3-14): photoelectron spectroscopy and density functional theory computation. *Journal of Physics Condensed Matter*, **2018**, 30, 335501	1.8	15
490	Toward Eco-friendly and Stable Perovskite Materials for Photovoltaics. *Joule*, **2018**, 2, 1231-1241	27.8	126
489	Self-Catalytic Reaction of SO and NH To Produce Sulfamic Acid and Its Implication to Atmospheric Particle Formation. *Journal of the American Chemical Society*, **2018**, 140, 11020-11028	16.4	58
488	Tin and germanium based two-dimensional Ruddlesden-Popper hybrid perovskites for potential lead-free photovoltaic and photoelectronic applications. *Nanoscale*, **2018**, 10, 11314-11319	7.7	51
487	Integration of a functionalized graphene nano-network into a planar perovskite absorber for high-efficiency large-area solar cells. *Materials Horizons*, **2018**, 5, 868-873	14.4	21
486	PtPd(111) Surface versus PtAu(111) Surface: Which One Is More Active for Methanol Oxidation?. *ACS Catalysis*, **2018**, 8, 132-143	13.1	41
485	Unravelling the Role of Topological Defects on Catalytic Unzipping of Single-Walled Carbon Nanotubes by Single Transition Metal Atom. *Journal of Physical Chemistry Letters*, **2018**, 9, 6801-6807	6.4	4
484	Insights into High Conductivity of the Two-Dimensional Iodine-Oxidized sp-c-COF. *ACS Applied Materials & Interfaces*, **2018**, 10, 43595-43602	9.5	17
483	Large magnetic anisotropy in chemically engineered iridium dimer. *Communications Physics*, **2018**, 1,	5.4	7
482	Mechanistic Origin of the High Performance of Yolk@Shell BiS@N-Doped Carbon Nanowire Electrodes. *ACS Nano*, **2018**, 12, 12597-12611	16.7	166
481	Quasi-1D TiS Nanoribbons: Mechanical Exfoliation and Thickness-Dependent Raman Spectroscopy. *ACS Nano*, **2018**, 12, 12713-12720	16.7	41
480	Application of Electronic Counting Rules for Ligand-Protected Gold Nanoclusters. *Accounts of Chemical Research*, **2018**, 51, 2739-2747	24.3	75
479	Two-dimensional dry ices with rich polymorphic and polyamorphic phase behavior. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 10263-10268	11.5	5
478	PCl: A Unique Post-Phosphorene 2D Material with Superior Properties against Oxidation. *Journal of Physical Chemistry Letters*, **2018**, 9, 6568-6575	6.4	12

477	Determination of CO Adsorption Sites on Gold Clusters Au (n = 21-25): A Size Region That Bridges the Pyramidal and Core-Shell Structures. *Journal of Physical Chemistry Letters*, **2018**, 9, 5430-5439	6.4	5
476	Fabrication and understanding of CuSi-Si@carbon@graphene nanocomposites as high-performance anodes for lithium-ion batteries. *Nanoscale*, **2018**, 10, 22203-22214	7.7	72
475	Inch-Scale Grain Boundary Free Organic Crystals Developed by Nucleation Seed-Controlled Shearing Method. *ACS Applied Materials & Interfaces*, **2018**, 10, 35395-35403	9.5	37
474	Assessment of Catalytic Activities of Gold Nanoclusters with Simple Structure Descriptors. *ACS Catalysis*, **2018**, 8, 9702-9710	13.1	26
473	Machine learning and artificial neural network prediction of interfacial thermal resistance between graphene and hexagonal boron nitride. *Nanoscale*, **2018**, 10, 19092-19099	7.7	55
472	Self-scrolling MoS metallic wires. *Nanoscale*, **2018**, 10, 18178-18185	7.7	70
471	A type-I van der Waals heterobilayer of WSe/MoTe. *Nanotechnology*, **2018**, 29, 335203	3.4	20
470	Multifunctional Binary Monolayers Ge P : Tunable Band Gap, Ferromagnetism, and Photocatalyst for Water Splitting. *ACS Applied Materials & Interfaces*, **2018**, 10, 19897-19905	9.5	36
469	Understanding the quenching nature of Mn in wide band gap inorganic compounds: design principles for Mn phosphors with higher efficiency. *Physical Chemistry Chemical Physics*, **2018**, 20, 16992-16999	3.6	24
468	Stable Formamidinium-Based Perovskite Solar Cells via In Situ Grain Encapsulation. *Advanced Energy Materials*, **2018**, 8, 1800232	21.8	59
467	A molecular perspective for global modeling of upper atmospheric NH from freezing clouds. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 6147-6152	11.5	20
466	Criegee intermediate inside fullerene cage: Evidence for size-dependent reactivity. *Journal of Chemical Physics*, **2018**, 148, 244301	3.9	2
465	Formation of HONO from the NH-promoted hydrolysis of NO dimers in the atmosphere. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 7236-7241	11.5	39
464	Prediction of a new ice clathrate with record low density: A potential candidate as ice XIX in guest-free form. *Chemical Physics Letters*, **2017**, 671, 186-191	2.5	29
463	Lateral and flexural phonon thermal transport in graphene and stanene bilayers. *Physical Chemistry Chemical Physics*, **2017**, 19, 6554-6562	3.6	31
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