Xiao Cheng Zeng

List of Publications by Year
in descending order

627 papers	45,833 citations	1799 103 h-index	3579 181 g-index
645 all docs	645 docs citations	645 times ranked	37443 citing authors

#	Article	IF	Citations
1	Atomically Resolved Electrically Active Intragrain Interfaces in Perovskite Semiconductors. Journal of the American Chemical Society, 2022, 144, 1910-1920.	13.7	37
2	Large-Sized Au_{<i>n</i>}^{â€"} Coreâ€"Shell Clusters (<i>n</i> = 61â€"66): Enduring Structure of the Icosahedral Au₁₃ Core. Journal of Physical Chemistry Letters, 2022, 13, 1389-1397.	4.6	3
3	Generation and Release of OH Radicals from the Reaction of H₂O with O₂ over Soot. Angewandte Chemie - International Edition, 2022, 61, .	13.8	12
4	Anomalous Phase Behaviors of Monolayer NaCl Aqueous Solutions Induced by Effective Coulombic Interactions within Angstrom-Scale Slits. Journal of Physical Chemistry Letters, 2022, 13, 2704-2710.	4.6	2
5	Solvation and Hydrolysis Reaction of Isocyanic Acid at the Airâ€"Water Interface: A Computational Study. Journal of the American Chemical Society, 2022, 144, 5315-5322.	13.7	7
6	Innentitelbild: Generation and Release of OH Radicals from the Reaction of H₂O with O₂ over Soot (Angew. Chem. 21/2022). Angewandte Chemie, 2022, 134, .	2.0	1
7	Van der Waals Magnetic Heterojunctions with Giant Zeroâ€Bias Tunneling Magnetoresistance and Photoâ€Assisted Magnetic Memory. Advanced Functional Materials, 2022, 32, .	14.9	4
8	Gas hydrates in confined space of nanoporous materials: new frontier in gas storage technology. Nanoscale, 2021, 13, 7447-7470.	5.6	28
9	Metallic surface doping of metal halide perovskites. Nature Communications, 2021, 12, 7.	12.8	66
10	Molecular Design of Three-Dimensional Metal-Free A(NH₄)X₃ Perovskites for Photovoltaic Applications. Jacs Au, 2021, 1, 475-483.	7.9	19
11	Peroxo Species Formed in the Bulk of Silicate Cathodes. Angewandte Chemie, 2021, 133, 10144-10151.	2.0	2
12	Peroxo Species Formed in the Bulk of Silicate Cathodes. Angewandte Chemie - International Edition, 2021, 60, 10056-10063.	13.8	5
13	Directional Proton Transfer in the Reaction of the Simplest Criegee Intermediate with Water Involving the Formation of Transient H₃O⁺. Journal of Physical Chemistry Letters, 2021, 12, 3379-3386.	4.6	16
14	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.	4.6	17
15	Innentitelbild: Peroxo Species Formed in the Bulk of Silicate Cathodes (Angew. Chem. 18/2021). Angewandte Chemie, 2021, 133, 9814-9814.	2.0	0
16	How O₂-Binding Affects Structural Evolution of Medium Even-Sized Gold Clusters Au_{<i>n</i>}^{â€"} (<i>n</i> = 20â€"34). Journal of Physical Chemistry Letters, 2021, 12, 3560-3570.	4.6	9
17	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.	13.7	27
18	Multiple Wettingâ€"Dewetting States of a Water Droplet on Dual-Scale Hierarchical Structured Surfaces. Jacs Au, 2021, 1, 955-966.	7.9	3

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19	Formation of porous ice frameworks at room temperature. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	7
20	Mechanistic Study of the Aqueous Reaction of Organic Peroxides with HSO 3 âˆ’ on the Surface of a Water Droplet. Angewandte Chemie, 2021, 133, 20362-20365.	2.0	2
21	Mechanistic Study of the Aqueous Reaction of Organic Peroxides with HSO₃^{âˆ’} on the Surface of a Water Droplet. Angewandte Chemie - International Edition, 2021, 60, 20200-20203.	13.8	9
22	Anisotropic Properties of Quasiâ€1D In₄Se₃: Mechanical Exfoliation, Electronic Transport, and Polarizationâ€Dependent Photoresponse. Advanced Functional Materials, 2021, 31, 2106459.	14.9	11
23	Two-dimensional monolayer salt nanostructures can spontaneously aggregate rather than dissolve in dilute aqueous solutions. Nature Communications, 2021, 12, 5602.	12.8	12
24	Two-Dimensional IVâ€“V Monolayers with Highly Anisotropic Carrier Mobility and Electric Transport Properties. Journal of Physical Chemistry Letters, 2021, 12, 1058-1065.	4.6	23
25	Formation of dimethyl carbonate<i>via</i>direct esterification of CO₂with methanol on reduced or stoichiometric CeO₂(111) and (110) surfaces. Physical Chemistry Chemical Physics, 2021, 23, 16150-16156.	2.8	5
26	Towards complete assignment of the infrared spectrum of the protonated water cluster H+(H2O)21. Nature Communications, 2021, 12, 6141.	12.8	35
27	Two-Dimensional GeC₂ with Tunable Electronic and Carrier Transport Properties and a High Current ON/OFF Ratio. Journal of Physical Chemistry Letters, 2021, 12, 11488-11496.	4.6	6
28	AgBiS₂ as a low-cost and eco-friendly all-inorganic photovoltaic material: nanoscale morphologyâ€“property relationship. Nanoscale Advances, 2020, 2, 770-776.	4.6	15
29	Rich topologies of monolayer ices <i>via</i> unconventional electrowetting. Nanoscale Horizons, 2020, 5, 514-522.	8.0	7
30	Atomic imaging of the edge structure and growth of a two-dimensional hexagonal ice. Nature, 2020, 577, 60-63.	27.8	149
31	Highly efficient N₂ fixation catalysts: transition-metal carbides M₂C (MXenes). Nanoscale, 2020, 12, 538-547.	5.6	71
32	Direct synthesis of bifunctional nanorods from a Coâ€“adenineâ€“MoO₃ hybrid for overall water splitting. Materials Chemistry Frontiers, 2020, 4, 546-554.	5.9	17
33	Influence of atmospheric conditions on sulfuric acid-dimethylamine-ammonia-based new particle formation. Chemosphere, 2020, 245, 125554.	8.2	30
34	Reversing Interfacial Catalysis of Ambipolar WSe₂ Single Crystal. Advanced Science, 2020, 7, 1901382.	11.2	100
35	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.	4.6	16
36	Use of Ion Exchange To Regulate the Heterogeneous Ice Nucleation Efficiency of Mica. Journal of the American Chemical Society, 2020, 142, 17956-17965.	13.7	26

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37	Turning a Superhydrophilic Surface Weakly Hydrophilic: Topological Wetting States. Journal of the American Chemical Society, 2020, 142, 18491-18502.	13.7	25
38	Unraveling Molecular Mechanism on Dilute Surfactant Solution Controlled Ice Recrystallization. Langmuir, 2020, 36, 1691-1698.	3.5	8
39	Exploration of Formation and Sizeâ€Evolution Pathways of Thiolateâ€Gold Nanoclusters in the COâ€Directed [Au 25 (SR) 18] â^’ Synthesis. Small, 2020, 17, 2000627.	10.0	9
40	Computational Prediction of Novel Ice Phases: A Perspective. Journal of Physical Chemistry Letters, 2020, 11, 7449-7461.	4.6	17
41	Multiturn Hollow Helices: Synthesis and Folding of Long Aromatic Oligoamides. Organic Letters, 2020, 22, 6938-6942.	4.6	10
42	Unraveling nucleation pathway in methane clathrate formation. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 24701-24708.	7.1	49
43	Quantitative Prediction of Aggregationâ€Induced Emission: A Full Quantum Mechanical Approach to the Optical Spectra. Angewandte Chemie, 2020, 132, 11647-11652.	2.0	3
44	New Insights into the Stability of Anhydrous 2<i>H</i>-Imidazolium Fluoride and its High Dissolution Capability toward a Strongly Hydrogen-Bonded Compound. Journal of the American Chemical Society, 2020, 142, 10314-10318.	13.7	8
45	A possible unaccounted source of atmospheric sulfate formation: amine-promoted hydrolysis and non-radical oxidation of sulfur dioxide. Chemical Science, 2020, 11, 2093-2102.	7.4	11
46	Quantitative Prediction of Aggregationâ€Induced Emission: A Full Quantum Mechanical Approach to the Optical Spectra. Angewandte Chemie - International Edition, 2020, 59, 11550-11555.	13.8	23
47	Pt₅Se₄ Monolayer: A Highly Efficient Electrocatalyst toward Hydrogen and Oxygen Electrode Reactions. ACS Applied Materials & Interfaces, 2020, 12, 13896-13903.	8.0	26
48	PtCoNi Alloy Nanoclusters for Synergistic Catalytic Oxygen Reduction Reaction. ACS Applied Nano Materials, 2020, 3, 2536-2544.	5.0	18
49	Hydration, Solvation, and Isomerization of Methylglyoxal at the Air/Water Interface: New Mechanistic Pathways. Journal of the American Chemical Society, 2020, 142, 5574-5582.	13.7	26
50	Heterogeneous Reactions of SO3 on Ice: An Overlooked Sink for SO3 Depletion. Journal of the American Chemical Society, 2020, 142, 2150-2154.	13.7	8
51	Resolving the puzzle of single-atom silver dispersion on nanosized Î³-Al2O3 surface for high catalytic performance. Nature Communications, 2020, 11, 529.	12.8	111
52	High ZT 2D Thermoelectrics by Design: Strong Interlayer Vibration and Complete Bandâ€Extrema Alignment. Advanced Functional Materials, 2020, 30, 2001200.	14.9	32
53	Domain Wall Conduction in Calcium-Modified Lead Titanate for Polarization Tunable Photovoltaic Devices. Cell Reports Physical Science, 2020, 1, 100043.	5.6	4
54	Descriptor-Based Design Principle for Two-Dimensional Single-Atom Catalysts: Carbon Dioxide Electroreduction. Journal of Physical Chemistry Letters, 2020, 11, 3481-3487.	4.6	65

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55	A droplet-based electricity generator with high instantaneous power density. Nature, 2020, 578, 392-396.	27.8	871
56	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.	10.3	112
57	Chiral Au₂₂(SR)₁₇^{âˆ’}: a new ligand-binding strategy for structural prediction of thiolate-protected gold nanocluster. Chemical Communications, 2020, 56, 2995-2998.	4.1	10
58	Constructing Stable and Potentially High-Performance Hybrid Organic-Inorganic Perovskites with â€œUnstableâ€•Cations. Research, 2020, 2020, 1986576.	5.7	4
59	Theoretical studies on tunable electronic structures and potential applications of twoâ€dimensional arseneneâ€based materials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1387.	14.6	33
60	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.	7.1	33
61	Graphene/antimonene/graphene heterostructure: A potential anode for sodium-ion batteries. Carbon, 2019, 153, 767-775.	10.3	45
62	Carbon fragments as highly active metal-free catalysts for the oxygen reduction reaction: a mechanistic study. Nanoscale, 2019, 11, 19422-19428.	5.6	20
63	Magnetism in bimetallic PtxNiNâˆ’x clusters via cross-atomic coupling. Journal of Materials Chemistry C, 2019, 7, 9293-9300.	5.5	1
64	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.	6.7	48
65	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.	13.7	10
66	Unraveling a New Chemical Mechanism of Missing Sulfate Formation in Aerosol Haze: Gaseous NO₂ with Aqueous HSO₃^{â€“}/SO₃^{2â€“}. Journal of the American Chemical Society, 2019, 141, 19312-19320.	13.7	36
67	Markedly Enhanced Oxygen Reduction Activity of Single-Atom Fe Catalysts via Integration with Fe Nanoclusters. ACS Nano, 2019, 13, 11853-11862.	14.6	340
68	Facile and Versatile Functionalization of Twoâ€Dimensional Carbon Nitrides by Design: Magnetism/Multiferroicity, Valleytronics, and Photovoltaics. Advanced Functional Materials, 2019, 29, 1905752.	14.9	19
69	Water desalination through rim functionalized carbon nanotubes. Journal of Materials Chemistry A, 2019, 7, 3583-3591.	10.3	56
70	Reconciling the Debate on the Existence of Pentazole HN₅ in the Pentazolate Salt of (N₅)₆(H₃O)₃(NH₄)₄Cl. Journal of the American Chemical Society, 2019, 141, 2984-2989.	13.7	21
71	Reaction mechanism between small-sized Ce clusters and water molecules: an <i>ab initio</i> investigation on Ce_n + H₂O. Physical Chemistry Chemical Physics, 2019, 21, 4006-4014.	2.8	8
72	Eighteen functional monolayer metal oxides: wide bandgap semiconductors with superior oxidation resistance and ultrahigh carrier mobility. Nanoscale Horizons, 2019, 4, 592-600.	8.0	78

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73	Tuning electronic structure of monolayer InP₃ 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.	2.8	7
74	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.	10.3	24
75	Two-Dimensional Gold Sulfide Monolayers with Direct Band Gap and Ultrahigh Electron Mobility. Journal of Physical Chemistry Letters, 2019, 10, 3773-3778.	4.6	34
76	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.	13.7	82
77	Monolayer triphosphates MP₃ (M = Sn, Ge) with excellent basal catalytic activity for hydrogen evolution reaction. Nanoscale, 2019, 11, 12210-12219.	5.6	76
78	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.	3.1	1
79	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.	7.1	16
80	Method To Implement Interaction Surfaces with Virtual Companion Particles for Molecular Dynamics Simulations. Journal of Chemical & Engineering Data, 2019, 64, 3693-3700.	1.9	1
81	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.	8.0	43
82	Phase transitions and ferroelasticityâ€“multiferroicity in bulk and two-dimensional silver and copper monohalides. Nanoscale Horizons, 2019, 4, 1106-1112.	8.0	32
83	Mechanistic Insight into the Reaction of Organic Acids with SO₃ at the Airâ€“Water Interface. Angewandte Chemie, 2019, 131, 8439-8443.	2.0	9
84	Unraveling the high-activity nature of Feâ€“Nâ€“C electrocatalysts for the oxygen reduction reaction: the extraordinary synergy between Feâ€“N₄ and Fe₄N. Journal of Materials Chemistry A, 2019, 7, 11792-11801.	10.3	84
85	Room temperature electrofreezing of water yields a missing dense ice phase in the phase diagram. Nature Communications, 2019, 10, 1925.	12.8	20
86	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.	13.7	585
87	SLIPS-TENG: robust triboelectric nanogenerator with optical and charge transparency using a slippery interface. National Science Review, 2019, 6, 540-550.	9.5	110
88	Rational design of one-dimensional hybrid organicâ€“inorganic perovskites with room-temperature ferroelectricity and strong piezoelectricity. Materials Horizons, 2019, 6, 1463-1473.	12.2	16
89	Mechanistic Insight into the Reaction of Organic Acids with SO₃ at the Airâ€“Water Interface. Angewandte Chemie - International Edition, 2019, 58, 8351-8355.	13.8	30
90	Au₆₀^{â€“}: The Smallest Gold Cluster with the High-Symmetry Icosahedral Core Au₁₃. Journal of Physical Chemistry Letters, 2019, 10, 1820-1827.	4.6	17

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91	Reaction mechanism between small-sized Ce clusters and water molecules II: an<i>ab initio</i>investigation on Ce_n(<i>n</i>= 1â€“3) +<i>m</i>H₂O (<i>m</i>= 2â€“6). Physical Chemistry Chemical Physics, 2019, 21, 8945-8955.	2.8	8
92	Simultaneously Dual Modification of Niâ€Rich Layered Oxide Cathode for Highâ€Energy Lithiumâ€Ion Batteries. Advanced Functional Materials, 2019, 29, 1808825.	14.9	430
93	Bi(Sb)NCa₃: Expansion of Perovskite Photovoltaics into All-Inorganic Anti-Perovskite Materials. Journal of Physical Chemistry C, 2019, 123, 6363-6369.	3.1	10
94	Understanding Hygroscopic Nucleation of Sulfate Aerosols: Combination of Molecular Dynamics Simulation with Classical Nucleation Theory. Journal of Physical Chemistry Letters, 2019, 10, 1126-1132.	4.6	13
95	Structural and Electronic Properties of Binary Clusters Si_{<i>m</i>}Ge_{<i>n</i>} (<i>m</i> + <i>n</i> = 6â€“13). Journal of Nanoscience and Nanotechnology, 2019, 19, 7879-7885.	0.9	1
96	Two-dimensional MgX₂Se₄ (X = Al, Ga) monolayers with tunable electronic properties for optoelectronic and photocatalytic applications. Nanoscale, 2019, 11, 19806-19813.	5.6	21
97	Unexpected quenching effect on new particle formation from the atmospheric reaction of methanol with SO ₃. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 24966-24971.	7.1	32
98	Copper(<scp>i</scp>) sulfide: a two-dimensional semiconductor with superior oxidation resistance and high carrier mobility. Nanoscale Horizons, 2019, 4, 223-230.	8.0	51
99	Iron Clusters Embedded in Graphene Nanocavities: Heat-Induced Structural Evolution and Catalytic Câ€“C Bond Breaking. ACS Applied Nano Materials, 2019, 2, 535-545.	5.0	5
100	Highly stable and efficient all-inorganic lead-free perovskite solar cells with native-oxide passivation. Nature Communications, 2019, 10, 16.	12.8	430
101	Design of Singleâ€Molecule Multiferroics for Efficient Ultrahighâ€Density Nonvolatile Memories. Advanced Science, 2019, 6, 1801572.	11.2	41
102	PbTiO₃ as Electronâ€Selective Layer for Highâ€Efficiency Perovskite Solar Cells: Enhanced Electron Extraction via Tunable Ferroelectric Polarization. Advanced Functional Materials, 2019, 29, 1806427.	14.9	23
103	Lead-Free Dionâ€“Jacobson Tin Halide Perovskites for Photovoltaics. ACS Energy Letters, 2019, 4, 276-277.	17.4	101
104	Water transport through subnanopores in the ultimate size limit: Mechanism from molecular dynamics. Nano Research, 2019, 12, 587-592.	10.4	25
105	Hydrogen Production via Efficient Formic Acid Decomposition: Engineering the Surface Structure of Pd-Based Alloy Catalysts by Design. ACS Catalysis, 2019, 9, 781-790.	11.2	62
106	Aluminum and Nitrogen Codoped Graphene: Highly Active and Durable Electrocatalyst for Oxygen Reduction Reaction. ACS Catalysis, 2019, 9, 610-619.	11.2	56
107	Water Confined in Nanocapillaries: Two-Dimensional Bilayer Squarelike Ice and Associated Solidâ€“Liquidâ€“Solid Transition. Journal of Physical Chemistry C, 2018, 122, 6704-6712.	3.1	27
108	Structural Evolution of Gold-Doped Bismuth Clusters AuBi_{<i>n</i>}^{â€“} (<i>n</i> = 4â€“8). Journal of Physical Chemistry C, 2018, 122, 6947-6954.	3.1	16

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109	Hybrid nanobud-array structures (C₂₄)_n/MoS₂and (C₂₄V)_n/MoS₂: two-dimensional half metallic and ferromagnetic materials. Journal of Materials Chemistry C, 2018, 6, 3373-3386.	5.5	1
110	Continuous Grain-Boundary Functionalization for High-Efficiency Perovskite Solar Cells with Exceptional Stability. CheM, 2018, 4, 1404-1415.	11.7	165
111	Nitric Acidâ€“Amine Chemistry in the Gas Phase and at the Airâ€“Water Interface. Journal of the American Chemical Society, 2018, 140, 6456-6466.	13.7	51
112	Two-Dimensional AuMX2 (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.	8.0	11
113	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.	7.1	13
114	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.	13.7	23
115	Insight into Chemistry on Cloud/Aerosol Water Surfaces. Accounts of Chemical Research, 2018, 51, 1229-1237.	15.6	96
116	Suppressed Ion Migration along the In-Plane Direction in Layered Perovskites. ACS Energy Letters, 2018, 3, 684-688.	17.4	240
117	Cesium Titanium(IV) Bromide Thin Films Based Stable Lead-free Perovskite Solar Cells. Joule, 2018, 2, 558-570.	24.0	403
118	Monolayer and bilayer polyaniline C₃N: two-dimensional semiconductors with high thermal conductivity. Nanoscale, 2018, 10, 4301-4310.	5.6	87
119	Abnormal phase transition between two-dimensional high-density liquid crystal and low-density crystalline solid phases. Nature Communications, 2018, 9, 198.	12.8	9
120	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.	17.4	314
121	Phonon thermal transport in a graphene/MoSe₂ van der Waals heterobilayer. Physical Chemistry Chemical Physics, 2018, 20, 2637-2645.	2.8	32
122	Anatase (101) Reconstructed Surface with Novel Functionalities: Desired Bandgap for Visible Light Absorption and High Chemical Reactivity. Advanced Functional Materials, 2018, 28, 1705529.	14.9	9
123	Formation of aqueous-phase sulfate during the haze period in China: Kinetics and atmospheric implications. Atmospheric Environment, 2018, 177, 93-99.	4.1	23
124	Argon Plasma Treatment to Tune Perovskite Surface Composition for High Efficiency Solar Cells and Fast Photodetectors. Advanced Materials, 2018, 30, 1705176.	21.0	81
125	A universal principle for a rational design of single-atom electrocatalysts. Nature Catalysis, 2018, 1, 339-348.	34.4	1,214
126	Thermal transport in phosphorene and phosphorene-based materials: A review on numerical studies. Chinese Physics B, 2018, 27, 036501.	1.4	23

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127	CaP₃: A New Two-Dimensional Functional Material with Desirable Band Gap and Ultrahigh Carrier Mobility. Journal of Physical Chemistry Letters, 2018, 9, 1728-1733.	4.6	112
128	Reaction of Criegee Intermediate with Nitric Acid at the Airâ€"Water Interface. Journal of the American Chemical Society, 2018, 140, 4913-4921.	13.7	53
129	The structural isomerism in gold nanoclusters. Nanoscale, 2018, 10, 9476-9483.	5.6	37
130	Co-mixing hydrogen and methane may double the energy storage capacity. Journal of Materials Chemistry A, 2018, 6, 8916-8922.	10.3	22
131	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.	3.1	21
132	PtPd(111) Surface versus PtAu(111) Surface: Which One Is More Active for Methanol Oxidation?. ACS Catalysis, 2018, 8, 132-143.	11.2	56
133	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.	4.6	7
134	Insights into High Conductivity of the Two-Dimensional Iodine-Oxidized sp²-c-COF. ACS Applied Materials & Interfaces, 2018, 10, 43595-43602.	8.0	37
135	Large magnetic anisotropy in chemically engineered iridium dimer. Communications Physics, 2018, 1, .	5.3	11
136	Mechanistic Origin of the High Performance of Yolk@Shell Bi₂S₃@N-Doped Carbon Nanowire Electrodes. ACS Nano, 2018, 12, 12597-12611.	14.6	213
137	Quasi-1D TiS₃ Nanoribbons: Mechanical Exfoliation and Thickness-Dependent Raman Spectroscopy. ACS Nano, 2018, 12, 12713-12720.	14.6	77
138	Application of Electronic Counting Rules for Ligand-Protected Gold Nanoclusters. Accounts of Chemical Research, 2018, 51, 2739-2747.	15.6	105
139	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.	7.1	6
140	P3Cl2: A Unique Post-Phosphorene 2D Material with Superior Properties against Oxidation. Journal of Physical Chemistry Letters, 2018, 9, 6568-6575.	4.6	16
141	Determination of CO Adsorption Sites on Gold Clusters Au_{<i>n</i>}^{â€"} (<i>n</i>) Tj ETQq1 1 0.784314 rgBT Chemistry Letters, 2018, 9, 5430-5439.	4.6	9
142	Fabrication and understanding of Cu₃Si-Si@carbon@graphene nanocomposites as high-performance anodes for lithium-ion batteries. Nanoscale, 2018, 10, 22203-22214.	5.6	103
143	Inch-Scale Grain Boundary Free Organic Crystals Developed by Nucleation Seed-Controlled Shearing Method. ACS Applied Materials & Interfaces, 2018, 10, 35395-35403.	8.0	48
144	Assessment of Catalytic Activities of Gold Nanoclusters with Simple Structure Descriptors. ACS Catalysis, 2018, 8, 9702-9710.	11.2	38

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145	Machine learning and artificial neural network prediction of interfacial thermal resistance between graphene and hexagonal boron nitride. Nanoscale, 2018, 10, 19092-19099.	5.6	75
146	Self-scrolling MoS₂ metallic wires. Nanoscale, 2018, 10, 18178-18185.	5.6	83
147	A type-I van der Waals heterobilayer of WSe₂/MoTe₂. Nanotechnology, 2018, 29, 335203.	2.6	24
148	Multifunctional Binary Monolayers Ge_{<i>x</i>}P_{<i>y</i>}: Tunable Band Gap, Ferromagnetism, and Photocatalyst for Water Splitting. ACS Applied Materials & Interfaces, 2018, 10, 19897-19905.	8.0	48
149	Understanding the quenching nature of Mn⁴⁺in wide band gap inorganic compounds: design principles for Mn⁴⁺phosphors with higher efficiency. Physical Chemistry Chemical Physics, 2018, 20, 16992-16999.	2.8	30
150	Stable Formamidiniumâ€Based Perovskite Solar Cells via In Situ Grain Encapsulation. Advanced Energy Materials, 2018, 8, 1800232.	19.5	78
151	A molecular perspective for global modeling of upper atmospheric NH ₃ from freezing clouds. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6147-6152.	7.1	27
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