Xiao Cheng Zeng

List of Publications by Year
in descending order

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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	Defect passivation in hybrid perovskite solar cells using quaternary ammonium halide anions andÂcations. Nature Energy, 2017, 2, .	39.5	1,694
2	A universal principle for a rational design of single-atom electrocatalysts. Nature Catalysis, 2018, 1, 339-348.	34.4	1,214
3	Formation of ordered ice nanotubes inside carbon nanotubes. Nature, 2001, 412, 802-805.	27.8	1,008
4	A droplet-based electricity generator with high instantaneous power density. Nature, 2020, 578, 392-396.	27.8	871
5	Bilayer Phosphorene: Effect of Stacking Order on Bandgap and Its Potential Applications in Thin-Film Solar Cells. Journal of Physical Chemistry Letters, 2014, 5, 1289-1293.	4.6	762
6	Two-Dimensional Boron Monolayer Sheets. ACS Nano, 2012, 6, 7443-7453.	14.6	690
7	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
8	Highâ€Gain and Lowâ€Drivingâ€Voltage Photodetectors Based on Organolead Triiodide Perovskites. Advanced Materials, 2015, 27, 1912-1918.	21.0	560
9	Phosphorene Nanoribbons, Phosphorus Nanotubes, and van der Waals Multilayers. Journal of Physical Chemistry C, 2014, 118, 14051-14059.	3.1	544
10	Ï€â€Conjugated Lewis Base: Efficient Trapâ€Passivation and Chargeâ€Extraction for Hybrid Perovskite Solar Cells. Advanced Materials, 2017, 29, 1604545.	21.0	543
11	Intrinsic Ferroelasticity and/or Multiferroicity in Two-Dimensional Phosphorene and Phosphorene Analogues. Nano Letters, 2016, 16, 3236-3241.	9.1	491
12	Planar-to-tubular structural transition in boron clusters: B20 as the embryo of single-walled boron nanotubes. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 961-964.	7.1	490
13	Strain-dependent electronic and magnetic properties of MoS2 monolayer, bilayer, nanoribbons and nanotubes. Physical Chemistry Chemical Physics, 2012, 14, 13035.	2.8	435
14	Simultaneously Dual Modification of Niâ€Rich Layered Oxide Cathode for Highâ€Energy Lithiumâ€Ion Batteries. Advanced Functional Materials, 2019, 29, 1808825.	14.9	430
15	Highly stable and efficient all-inorganic lead-free perovskite solar cells with native-oxide passivation. Nature Communications, 2019, 10, 16.	12.8	430
16	Cesium Titanium(IV) Bromide Thin Films Based Stable Lead-free Perovskite Solar Cells. Joule, 2018, 2, 558-570.	24.0	403
17	Coexistence and transition between Cassie and Wenzel state on pillared hydrophobic surface. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 8435-8440.	7.1	395
18	Nanosheet Supported Single-Metal Atom Bifunctional Catalyst for Overall Water Splitting. Nano Letters, 2017, 17, 5133-5139.	9.1	395

#	ARTICLE	IF	CITATIONS
19	Evidence of hollow golden cages. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 8326-8330.	7.1	361
20	Metallic Nickel Hydroxide Nanosheets Give Superior Electrocatalytic Oxidation of Urea for Fuel Cells. Angewandte Chemie - International Edition, 2016, 55, 12465-12469.	13.8	356
21	Markedly Enhanced Oxygen Reduction Activity of Single-Atom Fe Catalysts via Integration with Fe Nanoclusters. ACS Nano, 2019, 13, 11853-11862.	14.6	340
22	MoS₂/MX₂ heterobilayers: bandgap engineering <i>via</i> tensile strain or external electrical field. Nanoscale, 2014, 6, 2879-2886.	5.6	326
23	First-order transition in confined water between high-density liquid and low-density amorphous phases. Nature, 2000, 408, 564-567.	27.8	324
24	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
25	Adsorption of O₂, H₂, CO, NH₃, and NO₂ on ZnO Nanotube:â€‰ A Density Functional Theory Study. Journal of Physical Chemistry C, 2008, 112, 5747-5755.	3.1	280
26	Free-Standing Two-Dimensional Ru Nanosheets with High Activity toward Water Splitting. ACS Catalysis, 2016, 6, 1487-1492.	11.2	276
27	Nine New Phosphorene Polymorphs with Non-Honeycomb Structures: A Much Extended Family. Nano Letters, 2015, 15, 3557-3562.	9.1	275
28	Structural Prediction of Thiolate-Protected Au₃₈: A Face-Fused Bi-icosahedral Au Core. Journal of the American Chemical Society, 2008, 130, 7830-7832.	13.7	272
29	Semimetallic molybdenum disulfide ultrathin nanosheets as an efficient electrocatalyst for hydrogen evolution. Nanoscale, 2014, 6, 8359-8367.	5.6	248
30	Heterojunctionâ€Depleted Leadâ€Free Perovskite Solar Cells with Coarseâ€Grained Bâ€Î³â€CsSnI₃ Thin Films. Advanced Energy Materials, 2016, 6, 1601130.	19.5	247
31	Suppressed Ion Migration along the In-Plane Direction in Layered Perovskites. ACS Energy Letters, 2018, 3, 684-688.	17.4	240
32	Titanium Trisulfide Monolayer: Theoretical Prediction of a New Directâ€Gap Semiconductor with High and Anisotropic Carrier Mobility. Angewandte Chemie - International Edition, 2015, 54, 7572-7576.	13.8	239
33	Wetting and Interfacial Properties of Water Nanodroplets in Contact with Graphene and Monolayer Boronâ€"Nitride Sheets. ACS Nano, 2012, 6, 2401-2409.	14.6	235
34	Metallic Nickel Hydroxide Nanosheets Give Superior Electrocatalytic Oxidation of Urea for Fuel Cells. Angewandte Chemie, 2016, 128, 12653-12657.	2.0	233
35	Toward Eco-friendly and Stable Perovskite Materials for Photovoltaics. Joule, 2018, 2, 1231-1241.	24.0	224
36	Freezing of Confined Water: A Bilayer Ice Phase in Hydrophobic Nanopores. Physical Review Letters, 1997, 79, 5262-5265.	7.8	222

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37	Investigating the structural evolution of thiolate protected gold clusters from first-principles. Nanoscale, 2012, 4, 4054.	5.6	219
38	Exploration of High-Performance Single-Atom Catalysts on Support M₁/FeO_{<i>x</i>} for CO Oxidation via Computational Study. ACS Catalysis, 2015, 5, 544-552.	11.2	217
39	Lead-Free Mixed Tin and Germanium Perovskites for Photovoltaic Application. Journal of the American Chemical Society, 2017, 139, 8038-8043.	13.7	217
40	Tuning Electronic and Magnetic Properties of Early Transition-Metal Dichalcogenides via Tensile Strain. Journal of Physical Chemistry C, 2014, 118, 7242-7249.	3.1	216
41	Mechanistic Origin of the High Performance of Yolk@Shell Bi₂S₃@N-Doped Carbon Nanowire Electrodes. ACS Nano, 2018, 12, 12597-12611.	14.6	213
42	A Theoretical Study of Single-Atom Catalysis of CO Oxidation Using Au Embedded 2D h-BN Monolayer: A CO-Promoted O2 Activation. Scientific Reports, 2014, 4, 5441.	3.3	211
43	Bismuth Oxychalcogenides: A New Class of Ferroelectric/Ferroelastic Materials with Ultra High Mobility. Nano Letters, 2017, 17, 6309-6314.	9.1	208
44	On the phase diagram of water with density functional theory potentials: The melting temperature of ice Ih with the Perdewâ€"Burkeâ€"Ernzerhof and Beckeâ€"Leeâ€"Yangâ€"Parr functionals. Journal of Chemical Physics, 2009, 130, 221102.	3.0	203
45	Mechanistic Study of the Persistent Luminescence of CaAl₂O₄:Eu,Nd. Chemistry of Materials, 2015, 27, 2195-2202.	6.7	186
46	CO₂ Capture on <i>h</i>-BN Sheet with High Selectivity Controlled by External Electric Field. Journal of Physical Chemistry C, 2015, 119, 6912-6917.	3.1	183
47	Catalytic Activities of Subnanometer Gold Clusters (Au₁₆â€"Au₁₈,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T 7818-7829.	14.6	182
48	Tunable Magnetism in a Nonmetal-Substituted ZnO Monolayer: A First-Principles Study. Journal of Physical Chemistry C, 2012, 116, 11336-11342.	3.1	180
49	Type-I van der Waals heterostructure formed by MoS₂ and ReS₂ monolayers. Nanoscale Horizons, 2017, 2, 31-36.	8.0	179
50	CO Self-Promoting Oxidation on Nanosized Gold Clusters: Triangular Au₃ Active Site and CO Induced Oâ€"O Scission. Journal of the American Chemical Society, 2013, 135, 2583-2595.	13.7	178
51	Self-assembling subnanometer pores with unusual mass-transport properties. Nature Communications, 2012, 3, 949.	12.8	174
52	Long-Range Ordered Carbon Clusters: A Crystalline Material with Amorphous Building Blocks. Science, 2012, 337, 825-828.	12.6	173
53	A New Class of Folding Oligomers:â€‰ Crescent Oligoamides. Journal of the American Chemical Society, 2000, 122, 4219-4220.	13.7	168
54	Multiwalled ice helixes and ice nanotubes. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 19664-19667.	7.1	167

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55	Chemical Functionalization of Boronâ˘Nitride Nanotubes with NH3and Amino Functional Groups. Journal of the American Chemical Society, 2006, 128, 12001-12006.	13.7	165
56	Continuous Grain-Boundary Functionalization for High-Efficiency Perovskite Solar Cells with Exceptional Stability. CheM, 2018, 4, 1404-1415.	11.7	165
57	Intrinsic electronic and transport properties of graphyne sheets and nanoribbons. Nanoscale, 2013, 5, 9264.	5.6	163
58	Thiolate-Protected Au₂₀(SR)₁₆ Cluster: Prolate Au₈ Core with New [Au₃(SR)₄] Staple Motif. Journal of the American Chemical Society, 2009, 131, 13619-13621.	13.7	156
59	B₂C Graphene, Nanotubes, and Nanoribbons. Nano Letters, 2009, 9, 1577-1582.	9.1	154
60	Structures and stabilities of small silicon clusters: Ab initio molecular-orbital calculations of Si7â€"Si11. Journal of Chemical Physics, 2003, 118, 3558-3570.	3.0	153
61	Planar Pentacoordinate Carbon in CAl₅⁺: A Global Minimum. Journal of the American Chemical Society, 2008, 130, 10394-10400.	13.7	153
62	High-Level Ab Initio Electronic Structure Calculations of Water Clusters (H₂O)₁₆ and (H₂O)₁₇: A New Global Minimum for (H₂O)₁₆. Journal of Physical Chemistry Letters, 2010, 1, 3122-3127.	4.6	152
63	Measurement of Contact-Angle Hysteresis for Droplets on Nanopillared Surface and in the Cassie and Wenzel States: A Molecular Dynamics Simulation Study. ACS Nano, 2011, 5, 6834-6842.	14.6	152
64	A Nearâ€Infraredâ€Emissive Alkynylâ€Protected Au₂₄ Nanocluster. Angewandte Chemie - International Edition, 2015, 54, 9683-9686.	13.8	152
65	Controlling Catalytic Properties of Pd Nanoclusters through Their Chemical Environment at the Atomic Level Using Isoreticular Metalâ€"Organic Frameworks. ACS Catalysis, 2016, 6, 3461-3468.	11.2	152
66	Creating nanocavities of tunable sizes: Hollow helices. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 11583-11588.	7.1	149
67	Unraveling the Mechanisms of O₂ Activation by Size-Selected Gold Clusters: Transition from Superoxo to Peroxo Chemisorption. Journal of the American Chemical Society, 2012, 134, 9438-9445.	13.7	149
68	Atomic imaging of the edge structure and growth of a two-dimensional hexagonal ice. Nature, 2020, 577, 60-63.	27.8	149
69	Detection of Novel Gaseous States at the Highly Oriented Pyrolytic Graphiteâ˘Water Interface. Langmuir, 2007, 23, 1778-1783.	3.5	148
70	A grand unified model for liganded gold clusters. Nature Communications, 2016, 7, 13574.	12.8	148
71	Gold-Caged Metal Clusters with Large HOMOâ˘LUMO Gap and High Electron Affinity. Journal of the American Chemical Society, 2005, 127, 15680-15681.	13.7	137
72	Structures and relative stability of neutral gold clusters: Aun (n=15â€"19). Journal of Chemical Physics, 2006, 125, 154303.	3.0	136

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73	Thermal conductivity of a two-dimensional phosphorene sheet: a comparative study with graphene. Nanoscale, 2015, 7, 18716-18724.	5.6	132
74	Distinct ice patterns on solid surfaces with various wettabilities. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 11285-11290.	7.1	132
75	Endohedral Silicon Fullerenes SiN(27 â‰¤Nâ‰¤ 39). Journal of the American Chemical Society, 2004, 126, 13845-13849.	13.7	129
76	Perovskite Chalcogenides with Optimal Bandgap and Desired Optical Absorption for Photovoltaic Devices. Advanced Energy Materials, 2017, 7, 1700216.	19.5	128
77	CO Oxidation on TiO₂ (110) Supported Subnanometer Gold Clusters: Size and Shape Effects. Journal of the American Chemical Society, 2013, 135, 19336-19346.	13.7	127
78	Metallic single-walled silicon nanotubes. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 2664-2668.	7.1	124
79	Interlocked Catenane-Like Structure Predicted in Au₂₄(SR)₂₀: Implication to Structural Evolution of Thiolated Gold Clusters from Homoleptic Gold(I) Thiolates to Core-Stacked Nanoparticles. Journal of the American Chemical Society, 2012, 134, 3015-3024.	13.7	123
80	Band-Gap Engineering <i>via</i> Tailored Line Defects in Boron-Nitride Nanoribbons, Sheets, and Nanotubes. ACS Nano, 2012, 6, 4104-4112.	14.6	121
81	Validity of Tolmanâ€™s equation: How large should a droplet be?. Journal of Chemical Physics, 1998, 109, 4063-4070.	3.0	120
82	Structures and stability of medium silicon clusters. II. Ab initio molecular orbital calculations of Si12â€"Si20. Journal of Chemical Physics, 2004, 120, 8985-8995.	3.0	120
83	Efficient Kinetic Macrocyclization. Journal of the American Chemical Society, 2009, 131, 2629-2637.	13.7	120
84	Polymorphism and polyamorphism in bilayer water confined to slit nanopore under high pressure. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 21240-21245.	7.1	120
85	Tunable Optical Properties and Charge Separation in CH₃NH₃Sn_{<i>x</i>}Pb_{1â€"<i>x</i>}I₃/TiO₂-Based Planar Perovskites Cells. Journal of the American Chemical Society, 2015, 137, 8227-8236.	13.7	119
86	Probing the Structural Evolution of Medium-Sized Gold Clusters: Aunâ^' (n = 27â^'35). Journal of the American Chemical Society, 2010, 132, 6596-6605.	13.7	118
87	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.	4.6	118
88	Icosahedral Crown Gold Nanocluster Au₄₃Cu₁₂ with High Catalytic Activity. Nano Letters, 2010, 10, 1055-1062.	9.1	115
89	CO Oxidation Catalyzed by Single-Walled Helical Gold Nanotube. Nano Letters, 2008, 8, 195-202.	9.1	113
90	Quantized Water Transport: Ideal Desalination through Graphyne-4 Membrane. Scientific Reports, 2013, 3, 3163.	3.3	113

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91	Highly Confined Water: Two-Dimensional Ice, Amorphous Ice, and Clathrate Hydrates. Accounts of Chemical Research, 2014, 47, 2505-2513.	15.6	113
92	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
93	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
94	Motif Transition in Growth Patterns of Small to Medium-Sized Silicon Clusters. Angewandte Chemie - International Edition, 2005, 44, 1491-1494.	13.8	111
95	van der Waals trilayers and superlattices: modification of electronic structures of MoS₂ by intercalation. Nanoscale, 2014, 6, 4566-4571.	5.6	111
96	New Mechanistic Pathways for Criegeeâ€“Water Chemistry at the Air/Water Interface. Journal of the American Chemical Society, 2016, 138, 11164-11169.	13.7	111
97	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
98	Adsorption and Surface Reactivity on Single-Walled Boron Nitride Nanotubes Containing Stoneâ^'Wales Defects. Journal of Physical Chemistry C, 2007, 111, 14105-14112.	3.1	110
99	Doping Golden Buckyballs: Cu@Au16â^' and Cu@Au17â^' Cluster Anions. Angewandte Chemie - International Edition, 2007, 46, 2915-2918.	13.8	110
100	SLIPS-TENG: robust triboelectric nanogenerator with optical and charge transparency using a slippery interface. National Science Review, 2019, 6, 540-550.	9.5	110
101	Au42:Â An Alternative Icosahedral Golden Fullerene Cage. Journal of the American Chemical Society, 2005, 127, 3698-3699.	13.7	109
102	Periodic Graphene Nanobuds. Nano Letters, 2009, 9, 250-256.	9.1	108
103	Metalâ€“organic Kagome lattices M₃(2,3,6,7,10,11-hexaiminotriphenylene)₂ (M =) Tj ETQq1 1 0.784314 rgBT Physics, 2015, 17, 5954-5958.	2.8	108
104	Hydrogen Storage in Pillared Li-Dispersed Boron Carbide Nanotubes. Journal of Physical Chemistry C, 2008, 112, 8458-8463.	3.1	105
105	Exploration of Half Metallicity in Edge-Modified Graphene Nanoribbons. Journal of Physical Chemistry C, 2010, 114, 3937-3944.	3.1	105
106	Application of Electronic Counting Rules for Ligand-Protected Gold Nanoclusters. Accounts of Chemical Research, 2018, 51, 2739-2747.	15.6	105
107	Au34-:â€‰ A Fluxional Coreâ^'Shell Cluster. Journal of Physical Chemistry C, 2007, 111, 8228-8232.	3.1	103
108	Structural Transition of Gold Nanoclusters: From the Golden Cage to the Golden Pyramid. ACS Nano, 2009, 3, 1225-1230.	14.6	103

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109	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
110	Self-Assembly and Properties of Nonmetalated Tetraphenyl-Porphyrin on Metal Substrates. Journal of Physical Chemistry C, 2010, 114, 9408-9415.	3.1	101
111	Lead-Free Dionâ€"Jacobson Tin Halide Perovskites for Photovoltaics. ACS Energy Letters, 2019, 4, 276-277.	17.4	101
112	Relative stability of planar versus double-ring tubular isomers of neutral and anionic boron cluster B20 and B20â^'. Journal of Chemical Physics, 2006, 124, 154310.	3.0	100
113	Materials design of half-metallic graphene and graphene nanoribbons. Applied Physics Letters, 2009, 94, .	3.3	100
114	Hydroxyl-decorated graphene systems as candidates for organic metal-free ferroelectrics, multiferroics, and high-performance proton battery cathode materials. Physical Review B, 2013, 87, .	3.2	100
115	Group <scp>IVB</scp> transition metal trichalcogenides: a new class of <scp>2D</scp> layered materials beyond graphene. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 211-222.	14.6	100
116	Reversing Interfacial Catalysis of Ambipolar WSe₂ Single Crystal. Advanced Science, 2020, 7, 1901382.	11.2	100
117	The Tolman Length:â€‰ Is It Positive or Negative?. Journal of the American Chemical Society, 2005, 127, 15346-15347.	13.7	99
118	Ferroelectricity in Covalently functionalized Two-dimensional Materials: Integration of High-mobility Semiconductors and Nonvolatile Memory. Nano Letters, 2016, 16, 7309-7315.	9.1	99
119	Thermal Conductivity of Monolayer MoSe₂ and MoS₂. Journal of Physical Chemistry C, 2016, 120, 26067-26075.	3.1	99
120	Stable Three-Center Hydrogen Bonding in a Partially Rigidified Structure. Chemistry - A European Journal, 2001, 7, 4352-4357.	3.3	98
121	Icosahedral B12-containing coreâ€"shell structures of B80. Chemical Communications, 2010, 46, 3878.	4.1	96
122	Half-Metallicity in Hybrid Graphene/Boron Nitride Nanoribbons with Dihydrogenated Edges. Journal of Physical Chemistry C, 2011, 115, 9442-9450.	3.1	96
123	Tuning the electronic properties of monolayer and bilayer PtSe₂via strain engineering. Journal of Materials Chemistry C, 2016, 4, 3106-3112.	5.5	96
124	Insight into Chemistry on Cloud/Aerosol Water Surfaces. Accounts of Chemical Research, 2018, 51, 1229-1237.	15.6	96
125	Probing the Planar Tetra-, Penta-, and Hexacoordinate Carbon in Carbonâ^'Boron Mixed Clusters. Journal of the American Chemical Society, 2008, 130, 2580-2592.	13.7	95
126	Al_{<i>x</i>}C Monolayer Sheets: Two-Dimensional Networks with Planar Tetracoordinate Carbon and Potential Applications as Donor Materials in Solar Cell. Journal of Physical Chemistry Letters, 2014, 5, 2058-2065.	4.6	95

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127	The melting temperature of proton-disordered hexagonal ice: A computer simulation of 4-site transferable intermolecular potential model of water. Journal of Chemical Physics, 2000, 112, 8534-8538.	3.0	94
128	First-principles study of methane dehydrogenation on a bimetallic Cu/Ni(111) surface. Journal of Chemical Physics, 2009, 131, 174702.	3.0	94
129	Transition from one-dimensional water to ferroelectric ice within a supramolecular architecture. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3481-3486.	7.1	94
130	Strong Aggregation and Directional Assembly of Aromatic Oligoamide Macrocycles. Journal of the American Chemical Society, 2011, 133, 18590-18593.	13.7	94
131	Ferroelectric hexagonal and rhombic monolayer ice phases. Chemical Science, 2014, 5, 1757-1764.	7.4	94
132	Nanoscale Hydrophobic Interaction and Nanobubble Nucleation. Physical Review Letters, 2004, 93, 185701.	7.8	93
133	Guest-free monolayer clathrate and its coexistence with two-dimensional high-density ice. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 5718-5722.	7.1	93
134	Near-Barrierless Ammonium Bisulfate Formation via a Loop-Structure Promoted Proton-Transfer Mechanism on the Surface of Water. Journal of the American Chemical Society, 2016, 138, 1816-1819.	13.7	93
135	Twoâ€Dimensional Singleâ€Layer Organicâ€"Inorganic Hybrid Perovskite Semiconductors. Advanced Energy Materials, 2017, 7, 1601731.	19.5	93
136	Compression Limit of Two-Dimensional Water Constrained in Graphene Nanocapillaries. ACS Nano, 2015, 9, 12197-12204.	14.6	92
137	Magic-Number Gold Nanoclusters with Diameters from 1 to 3.5 nm: Relative Stability and Catalytic Activity for CO Oxidation. Nano Letters, 2015, 15, 682-688.	9.1	92
138	A new phase diagram of water under negative pressure: The rise of the lowest-density clathrate s-III. Science Advances, 2016, 2, e1501010.	10.3	92
139	Doping the Golden Cage Au16- with Si, Ge, and Sn. Journal of the American Chemical Society, 2007, 129, 15136-15137.	13.7	90
140	Oxidation of a two-dimensional hexagonal boron nitride monolayer: a first-principles study. Physical Chemistry Chemical Physics, 2012, 14, 5545.	2.8	90
141	How does water freeze inside carbon nanotubes?. Physica A: Statistical Mechanics and Its Applications, 2002, 314, 462-469.	2.6	89
142	Structural Evolution of Doped Gold Clusters: MAuxâˆ' (M = Si, Ge, Sn; x = 5âˆ'8). Journal of the American Chemical Society, 2009, 131, 3396-3404.	13.7	89
143	Self-Assembly of Surfactants and Polymorphic Transition in Nanotubes. Journal of the American Chemical Society, 2008, 130, 7916-7920.	13.7	87
144	Characterizing hydrophobicity of amino acid side chains in a protein environment via measuring contact angle of a water nanodroplet on planar peptide network. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 12946-12951.	7.1	87

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145	Double Perovskite Cs₂BBiX₆ (B = Ag, Cu; X = Br, Cl)/TiO₂ Heterojunction: An Efficient Pb-Free Perovskite Interface for Charge Extraction. Journal of Physical Chemistry C, 2017, 121, 4471-4480.	3.1	87
146	Monolayer and bilayer polyaniline C₃N: two-dimensional semiconductors with high thermal conductivity. Nanoscale, 2018, 10, 4301-4310.	5.6	87
147	Ice nanotube: What does the unit cell look like?. Journal of Chemical Physics, 2000, 113, 5037.	3.0	86
148	Isomer identification and resolution in small gold clusters. Journal of Chemical Physics, 2010, 132, 054305.	3.0	86
149	Self-Catalytic Reaction of SO₃ and NH₃ To Produce Sulfamic Acid and Its Implication to Atmospheric Particle Formation. Journal of the American Chemical Society, 2018, 140, 11020-11028.	13.7	86
150	Structural Transitions from Pyramidal to Fused Planar to Tubular to Core/Shell Compact in Gold Clusters:â€‰ Aun- (n = 21â^'25). Journal of Physical Chemistry C, 2007, 111, 4190-4198.	3.1	85
151	Magnetic doping of the golden cage cluster<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>M</mml:mi><mml:mo>@</mml:mo><mml:msubsup><mml:mrow><mml:mtext>Au</mml:mtex Physical Review B, 2009, 79, .	3.2	85
152	Tuning thermal contact conductance at grapheneâ€"copper interface<i>via</i>surface nanoengineering. Nanoscale, 2015, 7, 6286-6294.	5.6	85
153	Signature of coexistence of superconductivity and ferromagnetism in two-dimensional NbSe2 triggered by surface molecular adsorption. Nature Communications, 2016, 7, 11210.	12.8	85
154	Ab initio calculation of bowl, cage, and ring isomers of C20 and C20â^'. Journal of Chemical Physics, 2005, 122, 204109.	3.0	84
155	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
156	A Global Search of Highly Stable Gold-Covered Bimetallic Clusters M@Aun (n=8â€"17): Endohedral Gold Clusters. ChemPhysChem, 2006, 7, 2275-2278.	2.1	83
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