De-en Jiang

List of Publications by Year in descending order

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344 papers	27,102 citations	4120 87 h-index	8599 146 g-index
386 all docs	386 docs citations	386 times ranked	24198 citing authors

#	Article	IF	Citations
1	Pseudocapacitance: From Fundamental Understanding to High Power Energy Storage Materials. Chemical Reviews, 2020, 120, 6738-6782.	23.0	1,020
2	Porous Graphene as the Ultimate Membrane for Gas Separation. Nano Letters, 2009, 9, 4019-4024.	4.5	850
3	Mechanism of Hydrogen Evolution Reaction on 1T-MoS₂ from First Principles. ACS Catalysis, 2016, 6, 4953-4961.	5.5	678
4	Tuning the Basicity of Ionic Liquids for Equimolar CO₂ Capture. Angewandte Chemie - International Edition, 2011, 50, 4918-4922.	7.2	587
5	Identification of a Highly Luminescent Au₂₂(SG)₁₈ Nanocluster. Journal of the American Chemical Society, 2014, 136, 1246-1249.	6.6	490
6	Monoplatinum Doping of Gold Nanoclusters and Catalytic Application. Journal of the American Chemical Society, 2012, 134, 16159-16162.	6.6	444
7	Carbon Dioxide Capture by Superbaseâ€Derived Protic Ionic Liquids. Angewandte Chemie - International Edition, 2010, 49, 5978-5981.	7.2	429
8	Unique chemical reactivity of a graphene nanoribbonâ€™s zigzag edge. Journal of Chemical Physics, 2007, 126, 134701.	1.2	423
9	Nickel sulfides for electrocatalytic hydrogen evolution under alkaline conditions: a case study of crystalline NiS, NiS₂, and Ni₃S₂ nanoparticles. Catalysis Science and Technology, 2016, 6, 1077-1084.	2.1	408
10	Ag₂₉(BDT)₁₂(TPP)₄: A Tetravalent Nanocluster. Journal of the American Chemical Society, 2015, 137, 11970-11975.	6.6	369
11	Stabilization and Band-Gap Tuning of the 1T-MoS₂ Monolayer by Covalent Functionalization. Chemistry of Materials, 2015, 27, 3743-3748.	3.2	297
12	Toward Understanding the Growth Mechanism: Tracing All Stable Intermediate Species from Reduction of Au(I)â€“Thiolate Complexes to Evolution of Au₂₅ Nanoclusters. Journal of the American Chemical Society, 2014, 136, 10577-10580.	6.6	294
13	Oscillation of Capacitance inside Nanopores. Nano Letters, 2011, 11, 5373-5377.	4.5	290
14	A molecule-like PtAu24(SC6H13)18 nanocluster as an electrocatalyst for hydrogen production. Nature Communications, 2017, 8, 14723.	5.8	274
15	Golden single-atomic-site platinum electrocatalysts. Nature Materials, 2018, 17, 1033-1039.	13.3	266
16	Multiâ€Molar Absorption of CO₂ by the Activation of Carboxylate Groups in Amino Acid Ionic Liquids. Angewandte Chemie - International Edition, 2016, 55, 7166-7170.	7.2	264
17	Lattice-Hydride Mechanism in Electrocatalytic CO₂ Reduction by Structurally Precise Copper-Hydride Nanoclusters. Journal of the American Chemical Society, 2017, 139, 9728-9736.	6.6	261
18	Isomerism in Au₂₈(SR)₂₀ Nanocluster and Stable Structures. Journal of the American Chemical Society, 2016, 138, 1482-1485.	6.6	246

#	Article	IF	Citations
19	Thiolate Ligands as a Double-Edged Sword for CO Oxidation on CeO₂ Supported Au₂₅(SCH₂CH₂Ph)₁₈ Nanoclusters. Journal of the American Chemical Society, 2014, 136, 6111-6122.	6.6	245
20	Electronic Ground State of Higher Acenes. Journal of Physical Chemistry A, 2008, 112, 332-335.	1.1	236
21	The â€œStapleâ€•Motif:â€‰ A Key to Stability of Thiolate-Protected Gold Nanoclusters. Journal of the American Chemical Society, 2008, 130, 2777-2779.	6.6	231
22	Understanding the MXene Pseudocapacitance. Journal of Physical Chemistry Letters, 2018, 9, 1223-1228.	2.1	231
23	Insights into Interfaces, Stability, Electronic Properties, and Catalytic Activities of Atomically Precise Metal Nanoclusters from First Principles. Accounts of Chemical Research, 2018, 51, 2793-2802.	7.6	231
24	Understanding seed-mediated growth of gold nanoclusters at molecular level. Nature Communications, 2017, 8, 927.	5.8	228
25	Single rhodium atoms anchored in micropores for efficient transformation of methane under mild conditions. Nature Communications, 2018, 9, 1231.	5.8	213
26	Quantum Mechanical Basis for Kinetic Diameters of Small Gaseous Molecules. Journal of Physical Chemistry A, 2014, 118, 1150-1154.	1.1	212
27	Electrode materialâ€“ionic liquid coupling for electrochemical energy storage. Nature Reviews Materials, 2020, 5, 787-808.	23.3	210
28	Universal Surface Engineering of Transition Metals for Superior Electrocatalytic Hydrogen Evolution in Neutral Water. Journal of the American Chemical Society, 2017, 139, 12283-12290.	6.6	207
29	Au₁₉ Nanocluster Featuring a V-Shaped Alkynylâ€“Gold Motif. Journal of the American Chemical Society, 2015, 137, 652-655.	6.6	206
30	First principles assessment of ideal fracture energies of materials with mobile impurities: implications for hydrogen embrittlement of metals. Acta Materialia, 2004, 52, 4801-4807.	3.8	191
31	How Do Aryl Groups Attach to a Graphene Sheet?. Journal of Physical Chemistry B, 2006, 110, 23628-23632.	1.2	191
32	First principles study of magnetism in nanographenes. Journal of Chemical Physics, 2007, 127, 124703.	1.2	191
33	Interconversion between Superatomic 6-Electron and 8-Electron Configurations of M@Au₂₄(SR)₁₈ Clusters (M = Pd, Pt). Journal of the American Chemical Society, 2015, 137, 10833-10840.	6.6	183
34	Solvent Effect on the Pore-Size Dependence of an Organic Electrolyte Supercapacitor. Journal of Physical Chemistry Letters, 2012, 3, 1727-1731.	2.1	182
35	Sulfate Recognition by Persistent Crystalline Capsules with Rigidified Hydrogenâ€Bonding Cavities. Angewandte Chemie - International Edition, 2008, 47, 1866-1870.	7.2	179
36	Computational Insights into Materials and Interfaces for Capacitive Energy Storage. Advanced Science, 2017, 4, 1700059.	5.6	176

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37	A classical density functional theory for interfacial layering of ionic liquids. Soft Matter, 2011, 7, 11222.	1.2	170
38	From Superatomic Au₂₅(SR)₁₈^{â^'} to Superatomic M@Au₂₄(SR)₁₈^q Coreâ^'Shell Clusters. Inorganic Chemistry, 2009, 48, 2720-2722.	1.9	167
39	Adsorption and diffusion energetics of hydrogen atoms on Fe(110) from first principles. Surface Science, 2003, 547, 85-98.	0.8	161
40	The expanding universe of thiolated gold nanoclusters and beyond. Nanoscale, 2013, 5, 7149.	2.8	159
41	Insights into CO2/N2 separation through nanoporous graphene from molecular dynamics. Nanoscale, 2013, 5, 9984.	2.8	155
42	B80 and B101â€“103 clusters: Remarkable stability of the core-shell structures established by validated density functionals. Journal of Chemical Physics, 2012, 136, 074302.	1.2	150
43	Three-orders-of-magnitude variation of carrier lifetimes with crystal phase of gold nanoclusters. Science, 2019, 364, 279-282.	6.0	149
44	Open-Shell Singlet Character of Cyclacenes and Short Zigzag Nanotubes. Organic Letters, 2007, 9, 5449-5452.	2.4	147
45	Gold Nanowired: A Linear (Au₂₅)_n Polymer from Au₂₅ Molecular Clusters. ACS Nano, 2014, 8, 8505-8512.	7.3	146
46	Enhancing the Capacitive Performance of Electric Double-Layer Capacitors with Ionic Liquid Mixtures. ACS Energy Letters, 2016, 1, 21-26.	8.8	146
47	Quantum Effects on the Capacitance of Graphene-Based Electrodes. Journal of Physical Chemistry C, 2015, 119, 22297-22303.	1.5	144
48	Transformation Strategy for Highly Crystalline Covalent Triazine Frameworks: From Staggered AB to Eclipsed AA Stacking. Journal of the American Chemical Society, 2020, 142, 6856-6860.	6.6	136
49	Understanding the High Solubility of CO₂ in an Ionic Liquid with the Tetracyanoborate Anion. Journal of Physical Chemistry B, 2011, 115, 9789-9794.	1.2	132
50	Structure and Bonding between an Aryl Group and Metal Surfaces. Journal of the American Chemical Society, 2006, 128, 6030-6031.	6.6	131
51	Density functional theory for differential capacitance of planar electric double layers in ionic liquids. Chemical Physics Letters, 2011, 504, 153-158.	1.2	130
52	The strategies for improving carbon dioxide chemisorption by functionalized ionic liquids. RSC Advances, 2013, 3, 15518.	1.7	127
53	Structure of Au₁₅(SR)₁₃ and Its Implication for the Origin of the Nucleus in Thiolated Gold Nanoclusters. Journal of the American Chemical Society, 2013, 135, 8786-8789.	6.6	126
54	Curvature Effect on the Capacitance of Electric Double Layers at Ionic Liquid/Onion-Like Carbon Interfaces. Journal of Chemical Theory and Computation, 2012, 8, 1058-1063.	2.3	125

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55	Functionalizing Porous Aromatic Frameworks with Polar Organic Groups for High-Capacity and Selective CO₂ Separation: A Molecular Simulation Study. Langmuir, 2011, 27, 3451-3460.	1.6	124
56	Size Dependence of Atomically Precise Gold Nanoclusters in Chemoselective Hydrogenation and Active Site Structure. ACS Catalysis, 2014, 4, 2463-2469.	5.5	123
57	Superatomic Orbitals under Spinâ€"Orbit Coupling. Journal of Physical Chemistry Letters, 2014, 5, 3286-3289.	2.1	122
58	Precise control of alloying sites of bimetallic nanoclusters via surface motif exchange reaction. Nature Communications, 2017, 8, 1555.	5.8	122
59	Steric Effects in the Reaction of Aryl Radicals on Surfaces. Langmuir, 2009, 25, 286-293.	1.6	121
60	The role of low-coordinate oxygen on Co₃O₄(110) in catalyticCO oxidation. Physical Chemistry Chemical Physics, 2011, 13, 978-984.	1.3	121
61	Alkynylâ€Protected Au₂₃ Nanocluster: A 12â€Electron System. Angewandte Chemie - International Edition, 2015, 54, 5977-5980.	7.2	121
62	Effects of interlayer confinement and hydration on capacitive charge storage in birnessite. Nature Materials, 2021, 20, 1689-1694.	13.3	119
63	Adsorption and dissociation of CO on Fe(110) from first principles. Surface Science, 2004, 570, 167-177.	0.8	118
64	Accurate Static and Dynamic Properties of Liquid Electrolytes for Li-Ion Batteries from ab initio Molecular Dynamics. Journal of Physical Chemistry B, 2011, 115, 3085-3090.	1.2	115
65	Electrochemical Windows of Sulfone-Based Electrolytes for High-Voltage Li-Ion Batteries. Journal of Physical Chemistry B, 2011, 115, 12120-12125.	1.2	113
66	Microscopic Insights into the Electrochemical Behavior of Nonaqueous Electrolytes in Electric Double-Layer Capacitors. Journal of Physical Chemistry Letters, 2013, 4, 1260-1267.	2.1	113
67	First principles study of the graphene/Ru(0001) interface. Journal of Chemical Physics, 2009, 130, 074705.	1.2	111
68	Solidâ€"Electrolyte Interphase Formation and Electrolyte Reduction at Li-Ion Battery Graphite Anodes: Insights from First-Principles Molecular Dynamics. Journal of Physical Chemistry C, 2012, 116, 24476-24481.	1.5	111
69	Oxide-supported atomically precise gold nanocluster for catalyzing Sonogashira cross-coupling. Journal of Catalysis, 2013, 306, 177-183.	3.1	110
70	Enhancing graphene capacitance by nitrogen: effects of doping configuration and concentration. Physical Chemistry Chemical Physics, 2016, 18, 4668-4674.	1.3	110
71	High CO2 solubility, permeability and selectivity in ionic liquids with the tetracyanoborate anion. RSC Advances, 2012, 2, 11813.	1.7	109
72	Ion-Gated Gas Separation through Porous Graphene. Nano Letters, 2017, 17, 1802-1807.	4.5	109

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73	Simulating the Initial Stage of Phenolic Resin Carbonization via the ReaxFF Reactive Force Field. Journal of Physical Chemistry A, 2009, 113, 6891-6894.	1.1	107
74	Selective Deposition of Ru Nanoparticles on TiSi₂ Nanonet and Its Utilization for Li₂O₂ Formation and Decomposition. Journal of the American Chemical Society, 2014, 136, 8903-8906.	6.6	106
75	Computational Discovery and Design of MXenes for Energy Applications: Status, Successes, and Opportunities. ACS Applied Materials & Interfaces, 2019, 11, 24885-24905.	4.0	105
76	Facile Cr³⁺-Doping Strategy Dramatically Promoting Ru/CeO₂ for Low-Temperature CO₂ Methanation: Unraveling the Roles of Surface Oxygen Vacancies and Hydroxyl Groups. ACS Catalysis, 2021, 11, 5762-5775.	5.5	105
77	Atomically Precise Bimetallic Au₁₉Cu₃₀ Nanocluster with an Icosidodecahedral Cu₃₀ Shell and an Alkynylâ€“Cu Interface. Journal of the American Chemical Society, 2017, 139, 9451-9454.	6.6	104
78	Circumacenes versus periacenes: HOMOâ€“LUMO gap and transition from nonmagnetic to magnetic ground state with size. Chemical Physics Letters, 2008, 466, 72-75.	1.2	103
79	Adsorption, Diffusion, and Dissociation of H2S on Fe(100) from First Principles. Journal of Physical Chemistry B, 2004, 108, 19140-19145.	1.2	101
80	Selective Charging Behavior in an Ionic Mixture Electrolyte-Supercapacitor System for Higher Energy and Power. Journal of the American Chemical Society, 2017, 139, 18681-18687.	6.6	101
81	Transforming Porous Organic Cages into Porous Ionic Liquids via a Supramolecular Complexation Strategy. Angewandte Chemie - International Edition, 2020, 59, 2268-2272.	7.2	101
82	Selectivity trend of gas separation through nanoporous graphene. Journal of Solid State Chemistry, 2015, 224, 2-6.	1.4	97
83	Understanding controls on interfacial wetting at epitaxial graphene: Experiment and theory. Physical Review B, 2012, 85, .	1.1	95
84	Advanced Liquid Membranes Based on Novel Ionic Liquids for Selective Separation of Olefin/Paraffin via Olefin-Facilitated Transport. Industrial & Engineering Chemistry Research, 2008, 47, 881-888.	1.8	94
85	Taâ€“TiOx nanoparticles as radical scavengers to improve the durability of Feâ€“Nâ€“C oxygen reduction catalysts. Nature Energy, 2022, 7, 281-289.	19.8	93
86	Global minimization of gold clusters by combining neural network potentials and the basin-hopping method. Nanoscale, 2015, 7, 14817-14821.	2.8	90
87	Synthesis of Water-Soluble [Au₂₅(SR)₁₈]^{â^'} Using a Stoichiometric Amount of NaBH₄. Journal of the American Chemical Society, 2018, 140, 11370-11377.	6.6	90
88	Diphosphine-Protected Au₂₂ Nanoclusters on Oxide Supports Are Active for Gas-Phase Catalysis without Ligand Removal. Nano Letters, 2016, 16, 6560-6567.	4.5	88
89	Revealing isoelectronic size conversion dynamics of metal nanoclusters by a noncrystallization approach. Nature Communications, 2018, 9, 1979.	5.8	88
90	Confined Interlayer Water Promotes Structural Stability for High-Rate Electrochemical Proton Intercalation in Tungsten Oxide Hydrates. ACS Energy Letters, 2019, 4, 2805-2812.	8.8	88

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91	Mechanochemical synthesis of pillar[5]quinone derived multi-microporous organic polymers for radioactive organic iodide capture and storage. Nature Communications, 2020, 11, 1086.	5.8	87
92	A Heteroleptic Gold Hydride Nanocluster for Efficient and Selective Electrocatalytic Reduction of CO₂ to CO. Journal of the American Chemical Society, 2022, 144, 5258-5262.	6.6	87
93	CoP for hydrogen evolution: implications from hydrogen adsorption. Physical Chemistry Chemical Physics, 2016, 18, 23864-23871.	1.3	84
94	Harnessing strong metalâ€“support interactions via a reverse route. Nature Communications, 2020, 11, 3042.	5.8	84
95	Highly Efficient Carbon Monoxide Capture by Carbanionâ€Functionalized Ionic Liquids through Câ€Site Interactions. Angewandte Chemie - International Edition, 2017, 56, 6843-6847.	7.2	83
96	Monolayer dispersion of MoO3, NiO and their precursors on Î³-Al2O3. Applied Catalysis A: General, 1999, 188, 201-209.	2.2	82
97	What Protects the Core When the Thiolated Au Cluster is Extremely Small?. Journal of Physical Chemistry C, 2009, 113, 16983-16987.	1.5	82
98	The Smallest Thiolated Gold Superatom Complexes. Journal of Physical Chemistry C, 2009, 113, 17291-17295.	1.5	82
99	Porous liquid zeolites: hydrogen bonding-stabilized H-ZSM-5 in branched ionic liquids. Nanoscale, 2019, 11, 1515-1519.	2.8	82
100	Acidâ€“Base Reactivity of Perovskite Catalysts Probed via Conversion of 2-Propanol over Titanates and Zirconates. ACS Catalysis, 2017, 7, 4423-4434.	5.5	81
101	Effects of Metal-Doping on Hydrogen Evolution Reaction Catalyzed by MAu₂₄ and M₂Au₃₆ Nanoclusters (M = Pt, Pd). ACS Applied Materials & Interfaces, 2018, 10, 44645-44653.	4.0	81
102	Stabilizing gold clusters by heterostructured transition-metal oxideâ€“mesoporous silica supports for enhanced catalytic activities for CO oxidation. Chemical Communications, 2012, 48, 11413.	2.2	80
103	Interstaple Dithiol Cross-Linking in Au₂₅(SR)₁₈ Nanomolecules: A Combined Mass Spectrometric and Computational Study. Journal of the American Chemical Society, 2011, 133, 20258-20266.	6.6	79
104	SO₂absorption in EmimClâ€“TEG deep eutectic solvents. Physical Chemistry Chemical Physics, 2018, 20, 15168-15173.	1.3	76
105	First principles study of H2S adsorption and dissociation on Fe(110). Surface Science, 2005, 583, 60-68.	0.8	75
106	Boron Supercapacitors. ACS Energy Letters, 2016, 1, 1241-1246.	8.8	75
107	Descriptors for Hydrogen Evolution on Single Atom Catalysts in Nitrogen-Doped Graphene. Journal of Physical Chemistry C, 2020, 124, 19571-19578.	1.5	75
108	CO₂ Adsorption As a Flat-Lying, Tridentate Carbonate on CeO₂(100). Journal of Physical Chemistry C, 2014, 118, 9042-9050.	1.5	73

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109	A Generic Model for Electric Double Layers in Porous Electrodes. Journal of Physical Chemistry C, 2016, 120, 8704-8710.	1.5	73
110	Alkynyl-protected silver nanoclusters featuring an anticuboctahedral kernel. Nanoscale, 2017, 9, 11405-11409.	2.8	73
111	Real Time Monitoring of the Dynamic Intracluster Diffusion of Single Gold Atoms into Silver Nanoclusters. Journal of the American Chemical Society, 2019, 141, 18977-18983.	6.6	73
112	Surpassing Robeson Upper Limit for CO2/N2 Separation with Fluorinated Carbon Molecular Sieve Membranes. CheM, 2020, 6, 631-645.	5.8	73
113	All-Carboxylate-Protected Superatomic Silver Nanocluster with an Unprecedented Rhombohedral Ag₈ Core. Journal of the American Chemical Society, 2020, 142, 16905-16909.	6.6	72
114	Theoretical Advances in Understanding and Designing the Active Sites for Hydrogen Evolution Reaction. ACS Catalysis, 2022, 12, 8404-8433.	5.5	72
115	Unusual effects of solvent polarity on capacitance for organic electrolytes in a nanoporous electrode. Nanoscale, 2014, 6, 5545-5550.	2.8	70
116	Metallic Hydrogen in Atomically Precise Gold Nanoclusters. Chemistry of Materials, 2017, 29, 4840-4847.	3.2	70
117	Computational Screening of MXene Electrodes for Pseudocapacitive Energy Storage. Journal of Physical Chemistry C, 2019, 123, 315-321.	1.5	69
118	Windowed Carbon Nanotubes for Efficient CO₂ Removal from Natural Gas. Journal of Physical Chemistry Letters, 2012, 3, 3343-3347.	2.1	68
119	Structure and basicity of Î³-Al2O3-supported MgO and its application to mercaptan oxidation. Applied Catalysis A: General, 2001, 219, 69-78.	2.2	67
120	Efficient Absorption of SO₂ by Deep Eutectic Solvents Formed by Biobased Aprotic Organic Compound Succinonitrile and 1-Ethyl-3-methylimidazolium Chloride. ACS Sustainable Chemistry and Engineering, 2019, 7, 9086-9091.	3.2	67
121	Highly soluble alkoxide magnesium salts for rechargeable magnesium batteries. Journal of Materials Chemistry A, 2014, 2, 581-584.	5.2	66
122	Understanding Selective Hydrogenation of Î±,Î²-Unsaturated Ketones to Unsaturated Alcohols on the Au₂₅(SR)₁₈ Cluster. ACS Catalysis, 2015, 5, 6624-6629.	5.5	66
123	Magnetic doping of a thiolated-gold superatom: First-principles density functional theory calculations. Physical Review B, 2009, 80, .	1.1	64
124	Oxidation Potentials of Functionalized Sulfone Solvents for High-Voltage Li-Ion Batteries: A Computational Study. Journal of Physical Chemistry B, 2012, 116, 3235-3238.	1.2	63
125	Stronger-than-Pt hydrogen adsorption in a Au₂₂ nanocluster for the hydrogen evolution reaction. Journal of Materials Chemistry A, 2018, 6, 7532-7537.	5.2	63
126	Control of single-ligand chemistry on thiolated Au25 nanoclusters. Nature Communications, 2020, 11, 5498.	5.8	63

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127	In Search of a Structural Model for a Thiolate-protected Au₃₈ Cluster. Journal of Physical Chemistry C, 2008, 112, 13905-13910.	1.5	62
128	Kinetic Charging Inversion in Ionic Liquid Electric Double Layers. Journal of Physical Chemistry Letters, 2014, 5, 2195-2200.	2.1	62
129	Expanded Porphyrins as Two-Dimensional Porous Membranes for CO₂ Separation. ACS Applied Materials & Interfaces, 2015, 7, 13073-13079.	4.0	62
130	General Structureâ€“Reactivity Relationship for Oxygen on Transition-Metal Oxides. Journal of Physical Chemistry Letters, 2017, 8, 2206-2211.	2.1	62
131	Low-temperature activation of methane on doped single atoms: descriptor and prediction. Physical Chemistry Chemical Physics, 2018, 20, 22909-22914.	1.3	62
132	The ligand effect on the isomer stability of Au₂₄(SR)₂₀ clusters. Nanoscale, 2015, 7, 2225-2229.	2.8	61
133	Universal molecular-confined synthesis of interconnected porous metal oxides-N-C frameworks for electrocatalytic water splitting. Nano Energy, 2018, 48, 600-606.	8.2	61
134	Highly Polar but Amorphous Polymers with Robust Membrane CO2/N2 Separation Performance. Joule, 2019, 3, 1881-1894.	11.7	60
135	Elucidation of the Reaction Mechanism for High-Temperature Water Gas Shift over an Industrial-Type Copperâ€“Chromiumâ€“Iron Oxide Catalyst. Journal of the American Chemical Society, 2019, 141, 7990-7999.	6.6	60
136	Solubility of Gases in a Common Ionic Liquid from Molecular Dynamics Based Free Energy Calculations. Journal of Physical Chemistry B, 2014, 118, 2719-2725.	1.2	59
137	The Nâ€“B Interaction through a Water Bridge: Understanding the Chemoselectivity of a Fluorescent Protein Based Probe for Peroxynitrite. Journal of the American Chemical Society, 2016, 138, 4900-4907.	6.6	59
138	Comprehensive View of the Ligandâ€“Gold Interface from First Principles. Chemistry of Materials, 2017, 29, 6908-6915.	3.2	59
139	Permeance of H2 through porous graphene from molecular dynamics. Solid State Communications, 2013, 175-176, 101-105.	0.9	58
140	A Poly(acrylonitrile)-Functionalized Porous Aromatic Framework Synthesized by Atom-Transfer Radical Polymerization for the Extraction of Uranium from Seawater. Industrial & Engineering Chemistry Research, 2016, 55, 4125-4129.	1.8	58
141	Thiolated Gold Nanowires: Metallic versus Semiconducting. ACS Nano, 2009, 3, 2351-2357.	7.3	57
142	Au<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>40</mml:mn></mml:msub></mml:math>: A large tetrahedral magic cluster. Physical Review B, 2011, 84, .	1.1	57
143	Selective CO Production by Photoelectrochemical Methane Oxidation on TiO₂. ACS Central Science, 2018, 4, 631-637.	5.3	56
144	First-Principles Insight into Electrocatalytic Reduction of CO₂ to CH₄ on a Copper Nanoparticle. Journal of Physical Chemistry C, 2018, 122, 11392-11398.	1.5	56

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145	Titanium Carbide MXene Shows an Electrochemical Anomaly in Water-in-Salt Electrolytes. ACS Nano, 2021, 15, 15274-15284.	7.3	56
146	Rational design and synthesis of a porous, task-specific polycarbazole for efficient CO₂ capture. Chemical Communications, 2016, 52, 4454-4457.	2.2	55
147	Dopant-Dependent Electronic Structures Observed for M₂Au₃₆(SC₆H₁₃)₂₄ Clusters (M = Pt, Pd). Journal of Physical Chemistry Letters, 2018, 9, 982-989.	2.1	55
148	Thiolate-Protected Trimetallic Au_{â¼20}Ag_{â¼4}Pd and Au_{â¼20}Ag_{â¼4}Pt Alloy Clusters with Controlled Chemical Composition and Metal Positions. Journal of Physical Chemistry Letters, 2018, 9, 2590-2594.	2.1	55
149	On the Structure of a Thiolated Gold Cluster: Au₄₄(SR)₂₈^{2â»}. Journal of Physical Chemistry C, 2010, 114, 15883-15889.	1.5	54
150	Highly efficient electrocatalytic hydrogen evolution promoted by Oâ€“Moâ€“C interfaces of ultrafine Î²-Mo₂C nanostructures. Chemical Science, 2020, 11, 3523-3530.	3.7	54
151	The surface structure of silver-coated gold nanocrystals and its influence on shape control. Nature Communications, 2015, 6, 7664.	5.8	53
152	Interfacial and electronic properties of heterostructures of MXene and graphene. Physical Review B, 2019, 99, .	1.1	53
153	Proton Redox and Transport in MXene-Confined Water. ACS Applied Materials & Interfaces, 2020, 12, 763-770.	4.0	53
154	Interface Engineering of Earth-Abundant Transition Metals Using Boron Nitride for Selective Electroreduction of CO₂. ACS Applied Materials & Interfaces, 2018, 10, 6694-6700.	4.0	52
155	Computational Investigation of Reactive to Nonreactive Capture of Carbon Dioxide by Oxygen-Containing Lewis Bases. Journal of Physical Chemistry A, 2010, 114, 11761-11767.	1.1	51
156	Identify the Removable Substructure in Carbon Activation. Chemistry of Materials, 2017, 29, 7288-7295.	3.2	51
157	Hetero-biicosahedral [Au₂₄Pd(PPh₃)₁₀(SC₂H₄Ph)₅Cl₂]<sup> nanocluster: selective synthesis and optical and electrochemical properties. Nanoscale, 2018, 10, 18969-18979.	2.8	51
158	Hydrogen-Bonded Helices for Anion Binding and Separation. Crystal Growth and Design, 2008, 8, 1909-1915.	1.4	50
159	Insights into the PhCâ‰¡C/Au Interface. Journal of Physical Chemistry C, 2015, 119, 10804-10810.	1.5	50
160	Understanding the Impact of Surface Reconstruction of Perovskite Catalysts on CH₄ Activation and Combustion. ACS Catalysis, 2018, 8, 10306-10315.	5.5	50
161	In Situ Strong Metalâ€“Support Interaction (SMSI) Affects Catalytic Alcohol Conversion. ACS Catalysis, 2021, 11, 1938-1945.	5.5	50
162	Multiâ€Molar Absorption of CO₂ by the Activation of Carboxylate Groups in Amino Acid Ionic Liquids. Angewandte Chemie, 2016, 128, 7282-7286.	1.6	49

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