Jun Li

List of Publications by Year
in descending order

479 papers	52,832 citations	2427 97 h-index	1715 213 g-index
517 all docs	517 docs citations	517 times ranked	31076 citing authors

#	Article	IF	Citations
1	Single-atom catalysis of CO oxidation using Pt1/FeOx. Nature Chemistry, 2011, 3, 634-641.	13.6	5,149
2	Single-Atom Catalysts: A New Frontier in Heterogeneous Catalysis. Accounts of Chemical Research, 2013, 46, 1740-1748.	15.6	3,405
3	Heterogeneous single-atom catalysis. Nature Reviews Chemistry, 2018, 2, 65-81.	30.2	2,728
4	Basis Set Exchange:â€‰ A Community Database for Computational Sciences. Journal of Chemical Information and Modeling, 2007, 47, 1045-1052.	5.4	2,685
5	Au20: A Tetrahedral Cluster. Science, 2003, 299, 864-867.	12.6	1,091
6	Design of Single-Atom Coâ€“N₅ Catalytic Site: A Robust Electrocatalyst for CO₂ Reduction with Nearly 100% CO Selectivity and Remarkable Stability. Journal of the American Chemical Society, 2018, 140, 4218-4221.	13.7	945
7	An efficient molybdenum disulfide/cobalt diselenide hybrid catalyst for electrochemical hydrogen generation. Nature Communications, 2015, 6, 5982.	12.8	897
8	Remarkable Performance of Ir₁/FeO_{<i>x</i>} Single-Atom Catalyst in Water Gas Shift Reaction. Journal of the American Chemical Society, 2013, 135, 15314-15317.	13.7	811
9	Direct observation of noble metal nanoparticles transforming to thermally stable single atoms. Nature Nanotechnology, 2018, 13, 856-861.	31.5	741
10	Observation of an all-boron fullerene. Nature Chemistry, 2014, 6, 727-731.	13.6	724
11	Hydrocarbon analogues of boron clusters â€” planarity, aromaticity and antiaromaticity. Nature Materials, 2003, 2, 827-833.	27.5	650
12	Planar hexagonal B36 as a potential basis for extended single-atom layer boron sheets. Nature Communications, 2014, 5, 3113.	12.8	645
13	Copper atom-pair catalyst anchored on alloy nanowires for selective and efficient electrochemical reduction of CO2. Nature Chemistry, 2019, 11, 222-228.	13.6	571
14	Fe Isolated Single Atoms on S, N Codoped Carbon by Copolymer Pyrolysis Strategy for Highly Efficient Oxygen Reduction Reaction. Advanced Materials, 2018, 30, e1800588.	21.0	511
15	Multi-site electrocatalysts for hydrogen evolution in neutral media by destabilization of water molecules. Nature Energy, 2019, 4, 107-114.	39.5	470
16	Non defect-stabilized thermally stable single-atom catalyst. Nature Communications, 2019, 10, 234.	12.8	452
17	Iridium single-atom catalyst on nitrogen-doped carbon for formic acid oxidation synthesized using a general hostâ€“guest strategy. Nature Chemistry, 2020, 12, 764-772.	13.6	452
18	Ultrahigh-Loading of Ir Single Atoms on NiO Matrix to Dramatically Enhance Oxygen Evolution Reaction. Journal of the American Chemical Society, 2020, 142, 7425-7433.	13.7	430

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19	Ultrathin rhodium nanosheets. Nature Communications, 2014, 5, 3093.	12.8	428
20	Tuning defects in oxides at roomÂtemperature by lithium reduction. Nature Communications, 2018, 9, 1302.	12.8	428
21	Ultrastable single-atom gold catalysts with strong covalent metal-support interaction (CMSI). Nano Research, 2015, 8, 2913-2924.	10.4	422
22	Heterogeneous Fe3 single-cluster catalyst for ammonia synthesis via an associative mechanism. Nature Communications, 2018, 9, 1610.	12.8	409
23	Cooperative CO2-to-ethanol conversion via enriched intermediates at moleculeâ€“metal catalyst interfaces. Nature Catalysis, 2020, 3, 75-82.	34.4	390
24	Highly Efficient Catalysis of Preferential Oxidation of CO in H₂-Rich Stream by Gold Single-Atom Catalysts. ACS Catalysis, 2015, 5, 6249-6254.	11.2	380
25	Dynamic formation of single-atom catalytic active sites on ceria-supported gold nanoparticles. Nature Communications, 2015, 6, 6511.	12.8	370
26	Efficient electrically powered CO2-to-ethanol via suppression of deoxygenation. Nature Energy, 2020, 5, 478-486.	39.5	363
27	Isolated Single-Atom Pd Sites in Intermetallic Nanostructures: High Catalytic Selectivity for Semihydrogenation of Alkynes. Journal of the American Chemical Society, 2017, 139, 7294-7301.	13.7	354
28	Theoretical Understandings of Graphene-based Metal Single-Atom Catalysts: Stability and Catalytic Performance. Chemical Reviews, 2020, 120, 12315-12341.	47.7	354
29	Insight into methanol synthesis from CO2 hydrogenation on Cu(111): Complex reaction network and the effects of H2O. Journal of Catalysis, 2011, 281, 199-211.	6.2	347
30	High-Performance Rh₂P Electrocatalyst for Efficient Water Splitting. Journal of the American Chemical Society, 2017, 139, 5494-5502.	13.7	343
31	Breaking Long-Range Order in Iridium Oxide by Alkali Ion for Efficient Water Oxidation. Journal of the American Chemical Society, 2019, 141, 3014-3023.	13.7	337
32	PdZn Intermetallic Nanostructure with Pdâ€“Znâ€“Pd Ensembles for Highly Active and Chemoselective Semi-Hydrogenation of Acetylene. ACS Catalysis, 2016, 6, 1054-1061.	11.2	334
33	Toward Rational Design of Oxide-Supported Single-Atom Catalysts: Atomic Dispersion of Gold on Ceria. Journal of the American Chemical Society, 2017, 139, 6190-6199.	13.7	333
34	Regulating the coordination structure of single-atom Fe-NxCy catalytic sites for benzene oxidation. Nature Communications, 2019, 10, 4290.	12.8	326
35	Experimental Observation and Confirmation of Icosahedral W@Au12 and Mo@Au12 Molecules. Angewandte Chemie - International Edition, 2002, 41, 4786-4789.	13.8	325
36	Constructing NiCo/Fe₃O₄ Heteroparticles within MOF-74 for Efficient Oxygen Evolution Reactions. Journal of the American Chemical Society, 2018, 140, 15336-15341.	13.7	310

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37	The Role of Reducible Oxideâ€"Metal Cluster Charge Transfer in Catalytic Processes: New Insights on the Catalytic Mechanism of CO Oxidation on Au/TiO₂ from ab Initio Molecular Dynamics. Journal of the American Chemical Society, 2013, 135, 10673-10683.	13.7	308
38	The B₃₅ Cluster with a Double-Hexagonal Vacancy: A New and More Flexible Structural Motif for Borophene. Journal of the American Chemical Society, 2014, 136, 12257-12260.	13.7	298
39	Unraveling the coordination structure-performance relationship in Pt1/Fe2O3 single-atom catalyst. Nature Communications, 2019, 10, 4500.	12.8	279
40	Scalable two-step annealing method for preparing ultra-high-density single-atom catalyst libraries. Nature Nanotechnology, 2022, 17, 174-181.	31.5	279
41	Synthesis of Thermally Stable and Highly Active Bimetallic Auâ^'Ag Nanoparticles on Inert Supports. Chemistry of Materials, 2009, 21, 410-418.	6.7	262
42	Synergetic Integration of Cu_{1.94}Sâ€"Zn_{<i>x</i>}Cd_{1â€"<i>x</i>}S Heteronanorods for Enhanced Visible-Light-Driven Photocatalytic Hydrogen Production. Journal of the American Chemical Society, 2016, 138, 4286-4289.	13.7	257
43	Three-dimensional open nano-netcage electrocatalysts for efficient pH-universal overall water splitting. Nature Communications, 2019, 10, 4875.	12.8	253
44	A Durable Nickel Singleâ€Atom Catalyst for Hydrogenation Reactions and Cellulose Valorization under Harsh Conditions. Angewandte Chemie - International Edition, 2018, 57, 7071-7075.	13.8	243
45	Catalysis on singly dispersed bimetallic sites. Nature Communications, 2015, 6, 7938.	12.8	235
46	Surface Single-Cluster Catalyst for N₂-to-NH₃ Thermal Conversion. Journal of the American Chemical Society, 2018, 140, 46-49.	13.7	233
47	Identification of the Electronic and Structural Dynamics of Catalytic Centers in Single-Fe-Atom Material. CheM, 2020, 6, 3440-3454.	11.7	231
48	Experimental and Theoretical Evidence of an Axially Chiral Borospherene. ACS Nano, 2015, 9, 754-760.	14.6	228
49	Noble Gas-Actinide Compounds: Complexation of the CUO Molecule by Ar, Kr, and Xe Atoms in Noble Gas Matrices. Science, 2002, 295, 2242-2245.	12.6	224
50	Coordination engineering of iridium nanocluster bifunctional electrocatalyst for highly efficient and pH-universal overall water splitting. Nature Communications, 2020, 11, 4246.	12.8	221
51	Design of Efficient Catalysts with Double Transition Metal Atoms on C₂N Layer. Journal of Physical Chemistry Letters, 2016, 7, 1750-1755.	4.6	196
52	Theoretical understanding of the stability of single-atom catalysts. National Science Review, 2018, 5, 638-641.	9.5	194
53	Rh single atoms on TiO2 dynamically respond to reaction conditions by adapting their site. Nature Communications, 2019, 10, 4488.	12.8	191
54	Selective photoelectrochemical oxidation of glycerol to high value-added dihydroxyacetone. Nature Communications, 2019, 10, 1779.	12.8	185

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55	Size-dependent dynamic structures of supported gold nanoparticles in CO oxidation reaction condition. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 7700-7705.	7.1	183
56	Isolated Ni Atoms Dispersed on Ru Nanosheets: High-Performance Electrocatalysts toward Hydrogen Oxidation Reaction. Nano Letters, 2020, 20, 3442-3448.	9.1	172
57	Identification of an iridium-containing compound with a formal oxidation state of IX. Nature, 2014, 514, 475-477.	27.8	171
58	From planar boron clusters to borophenes and metalloborophenes. Nature Reviews Chemistry, 2017, 1, .	30.2	169
59	Probing the structures and bonding of size-selected boron and doped-boron clusters. Chemical Society Reviews, 2019, 48, 3550-3591.	38.1	169
60	Shape Control of CdSe Nanocrystals with Zinc Blende Structure. Journal of the American Chemical Society, 2009, 131, 16423-16429.	13.7	168
61	A Supramolecular Radical Dimer: Highâ€Efficiency NIRâ€II Photothermal Conversion and Therapy. Angewandte Chemie - International Edition, 2019, 58, 15526-15531.	13.8	168
62	Atomically Dispersed Ruthenium Species Inside Metalâ€"Organic Frameworks: Combining the High Activity of Atomic Sites and the Molecular Sieving Effect of MOFs. Angewandte Chemie - International Edition, 2019, 58, 4271-4275.	13.8	162
63	Single Iridium Atom Doped Ni₂P Catalyst for Optimal Oxygen Evolution. Journal of the American Chemical Society, 2021, 143, 13605-13615.	13.7	162
64	Evidence of Significant Covalent Bonding in Au(CN)₂^{â^’}. Journal of the American Chemical Society, 2009, 131, 16368-16370.	13.7	161
65	CO Oxidation on Au/TiO₂: Condition-Dependent Active Sites and Mechanistic Pathways. Journal of the American Chemical Society, 2016, 138, 10467-10476.	13.7	159
66	Sn122-:Â Stannaspherene. Journal of the American Chemical Society, 2006, 128, 8390-8391.	13.7	157
67	Maximizing the Number of Interfacial Sites in Singleâ€Atom Catalysts for the Highly Selective, Solventâ€Free Oxidation of Primary Alcohols. Angewandte Chemie - International Edition, 2018, 57, 7795-7799.	13.8	151
68	Constructing High-Loading Single-Atom/Cluster Catalysts via an Electrochemical Potential Window Strategy. Journal of the American Chemical Society, 2020, 142, 3375-3383.	13.7	147
69	Theoretical and Experimental Investigations on Single-Atom Catalysis: Ir₁/FeO_{<i>x</i>} for CO Oxidation. Journal of Physical Chemistry C, 2014, 118, 21945-21951.	3.1	145
70	[B₃₀]^{â^’}: A Quasiplanar Chiral Boron Cluster. Angewandte Chemie - International Edition, 2014, 53, 5540-5545.	13.8	144
71	A highly efficient Fenton-like catalyst based on isolated diatomic Fe-Co anchored on N-doped porous carbon. Chemical Engineering Journal, 2021, 404, 126376.	12.7	143
72	Observation and characterization of the smallest borospherene, B28â^’ and B28. Journal of Chemical Physics, 2016, 144, 064307.	3.0	141

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73	Theoretical Investigations of Pt₁@CeO₂ Single-Atom Catalyst for CO Oxidation. Journal of Physical Chemistry C, 2017, 121, 11281-11289.	3.1	138
74	Icosahedral gold cage clusters: M@Au[sub 12][sup âˆ’] (M=V, Nb, and Ta). Journal of Chemical Physics, 2004, 121, 8369.	3.0	137
75	MOFâ€Confined Subâ€2 nm Atomically Ordered Intermetallic PdZn Nanoparticles as Highâ€Performance Catalysts for Selective Hydrogenation of Acetylene. Advanced Materials, 2018, 30, e1801878.	21.0	133
76	Experimental and Theoretical Investigation of the Electronic and Geometrical Structures of the Au32 Cluster. Angewandte Chemie - International Edition, 2005, 44, 7119-7123.	13.8	129
77	Bimetallic Auâ€“Pd Alloy Catalysts for N₂O Decomposition: Effects of Surface Structures on Catalytic Activity. Journal of Physical Chemistry C, 2012, 116, 6222-6232.	3.1	128
78	Reaction of Laser-Ablated Uranium Atoms with CO:â€‰ Infrared Spectra of the CUO, CUO-, OUCCO, (Î·2-C2)UO2, and U(CO)x (x = 1âˆ’6) Molecules in Solid Neon. Journal of the American Chemical Society, 1999, 121, 9712-9721.	13.7	125
79	Noble Gasâˆ’Actinide Complexes of the CUO Molecule with Multiple Ar, Kr, and Xe Atoms in Noble-Gas Matrices. Journal of the American Chemical Society, 2003, 125, 3126-3139.	13.7	124
80	Conversion of PtNi alloy from disordered to ordered for enhanced activity and durability in methanol-tolerant oxygen reduction reactions. Nano Research, 2015, 8, 2777-2788.	10.4	124
81	Pb122-:Â Plumbaspherene. Journal of Physical Chemistry A, 2006, 110, 10169-10172.	2.5	122
82	Theoretical Inspection of M₁/PMA Single-Atom Electrocatalyst: Ultra-High Performance for Water Splitting (HER/OER) and Oxygen Reduction Reactions (OER). ACS Catalysis, 2021, 11, 8929-8941.	11.2	121
83	On the Nature of Support Effects of Metal Dioxides MO₂ (M = Ti, Zr, Hf, Ce, Th) in Single-Atom Gold Catalysts: Importance of Quantum Primogenic Effect. Journal of Physical Chemistry C, 2016, 120, 17514-17526.	3.1	120
84	A Water-Promoted Mechanism of Alcohol Oxidation on a Au(111) Surface: Understanding the Catalytic Behavior of Bulk Gold. ACS Catalysis, 2013, 3, 1693-1699.	11.2	118
85	Recent advances in computational modeling and simulations on the An(III)/Ln(III) separation process. Coordination Chemistry Reviews, 2012, 256, 1406-1417.	18.8	117
86	Pd₂@Sn₁₈⁴⁻:â€‰ Fusion of Two Endohedral Stannaspherenes. Journal of the American Chemical Society, 2007, 129, 9560-9561.	13.7	116
87	Highly active enzymeâ€“metal nanohybrids synthesized in proteinâ€“polymer conjugates. Nature Catalysis, 2019, 2, 718-725.	34.4	115
88	Electronic Structure Differences in ZrO2vs HfO2â€. Journal of Physical Chemistry A, 2005, 109, 11521-11525.	2.5	114
89	Observation of a metal-centered B₂-Ta@B₁₈^{âˆ’}tubular molecular rotor and a perfect Ta@B₂₀^{âˆ’}boron drum with the record coordination number of twenty. Chemical Communications, 2017, 53, 1587-1590.	4.1	114
90	Atomically-precise dopant-controlled single cluster catalysis for electrochemical nitrogen reduction. Nature Communications, 2020, 11, 4389.	12.8	110

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91	High Uptake of ReO₄^{â^'} and CO₂ Conversion by a Radiationâ€Resistant Thoriumâ€"Nickle [Th₄₈Ni₆] Nanocageâ€Based Metalâ€"Organic Framework. Angewandte Chemie - International Edition, 2019, 58, 6022-6027.	13.8	109
92	Formation and Characterization of the Boron Dicarbonyl Complex [B(CO)₂]^{â^'}. Angewandte Chemie - International Edition, 2015, 54, 11078-11083.	13.8	107
93	Manganese-centered tubular boron cluster â€" MnB16â^': A new class of transition-metal molecules. Journal of Chemical Physics, 2016, 144, 154310.	3.0	107
94	Toward the Solution Synthesis of the Tetrahedral Au20Cluster. Journal of Physical Chemistry B, 2004, 108, 12259-12263.	2.6	106
95	Endohedral Stannaspherenes M@Sn12â^': A Rich Class of Stable Molecular Cage Clusters. Angewandte Chemie - International Edition, 2007, 46, 742-745.	13.8	106
96	Au34-:â€‰ A Fluxional Coreâ^'Shell Cluster. Journal of Physical Chemistry C, 2007, 111, 8228-8232.	3.1	103
97	Unique CO Chemisorption Properties of Gold Hexamer:â€‰ Au6(CO)n- (n = 0â^'3). Journal of the American Chemical Society, 2005, 127, 12098-12106.	13.7	102
98	Dual Metal Active Sites in an Ir₁/FeO_{<i>x</i>}Singleâ€Atom Catalyst: A Redox Mechanism for the Waterâ€Gas Shift Reaction. Angewandte Chemie - International Edition, 2020, 59, 12868-12875.	13.8	102
99	High-Valent Nickel Promoted by Atomically Embedded Copper for Efficient Water Oxidation. ACS Catalysis, 2020, 10, 9725-9734.	11.2	100
100	Introduction: Heterogeneous Single-Atom Catalysis. Chemical Reviews, 2020, 120, 11699-11702.	47.7	99
101	Theoretical investigations of the catalytic role of water in propene epoxidation on gold nanoclusters: A hydroperoxyl-mediated pathway. Nano Research, 2011, 4, 131-142.	10.4	98
102	Competition between drum and quasi-planar structures in RhB₁₈^{â^'}: motifs for metallo-boronanotubes and metallo-borophenes. Chemical Science, 2016, 7, 7020-7027.	7.4	97
103	TGMin: A global-minimum structure search program based on a constrained basin-hopping algorithm. Nano Research, 2017, 10, 3407-3420.	10.4	97
104	Trivalent Actinide and Lanthanide Separations by Tetradentate Nitrogen Ligands: A Quantum Chemistry Study. Inorganic Chemistry, 2011, 50, 9230-9237.	4.0	96
105	Remarkable active-site dependent H2O promoting effect in CO oxidation. Nature Communications, 2019, 10, 3824.	12.8	96
106	A multicentre-bonded [ZnI]8 cluster with cubic aromaticity. Nature Communications, 2015, 6, 6331.	12.8	94
107	Electronic Structure of Cycloheptatrienyl Sandwich Compounds of Actinides:Â An(Î·7-C7H7)2(An = Th, Pa,) Tj ETQq1 1 0.784314 rgBT	13.7	93
108	Thermodynamic Studies and Hydride Transfer Reactions from a Rhodium Complex to BX₃ Compounds. Journal of the American Chemical Society, 2009, 131, 14454-14465.	13.7	93

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109	The Planar CoB₁₈^{â^’} Cluster as a Motif for Metalloâ€Borophenes. Angewandte Chemie - International Edition, 2016, 55, 7358-7363.	13.8	90
110	Synergy of the catalytic activation on Ni and the CeO₂â€“TiO₂/Ce₂Ti₂O₇ stoichiometric redox cycle for dramatically enhanced solar fuel production. Energy and Environmental Science, 2019, 12, 767-779.	30.8	90
111	Density functional theory investigations on the catalytic mechanisms of hydrazine decompositions on Ir(111). Catalysis Today, 2011, 165, 80-88.	4.4	87
112	Significant Interactions between Uranium and Noble-Gas Atoms: Coordination of the UO2+ Cation by Ne, Ar, Kr, and Xe Atoms. Angewandte Chemie - International Edition, 2004, 43, 2554-2557.	13.8	86
113	DFT+U Study on the Localized Electronic States and Their Potential Role During H₂O Dissociation and CO Oxidation Processes on CeO₂(111) Surface. Journal of Physical Chemistry C, 2013, 117, 23082-23089.	3.1	85
114	On the Structure and Chemical Bonding of Tri-Tungsten Oxide Clusters W3On- and W3On (n = 7â^’10):â€‰ W3O8 As A Potential Molecular Model for O-Deficient Defect Sites in Tungsten Oxides. Journal of Physical Chemistry A, 2006, 110, 85-92.	2.5	83
115	3D hierarchical heterostructure assembled by NiFe LDH/(NiFe)Sx on biomass-derived hollow carbon microtubes as bifunctional electrocatalysts for overall water splitting. Electrochimica Acta, 2020, 348, 136339.	5.2	83
116	Low-lying isomers of the B9â^’ boron cluster: The planar molecular wheel versus three-dimensional structures. Journal of Chemical Physics, 2008, 129, 024302.	3.0	82
117	A Ligandâ€Protected Golden Fullerene: The Dipyridylamido Au₃₂⁸⁺ Nanocluster. Angewandte Chemie - International Edition, 2019, 58, 5906-5909.	13.8	82
118	Catalysis on Singly Dispersed Rh Atoms Anchored on an Inert Support. ACS Catalysis, 2018, 8, 110-121.	11.2	81
119	A general strategy for preparing pyrrolic-N4 type single-atom catalysts via pre-located isolated atoms. Nature Communications, 2021, 12, 6806.	12.8	81
120	Formation of unprecedented actinidecarbon triple bonds in uranium methylidyne molecules. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 18919-18924.	7.1	80
121	Recent progresses of global minimum searches of nanoclusters with a constrained Basin-Hopping algorithm in the TGMin program. Computational and Theoretical Chemistry, 2017, 1107, 57-65.	2.5	80
122	Theoretical investigations of non-noble metal single-atom catalysis: Ni₁/FeO_x for CO oxidation. Catalysis Science and Technology, 2016, 6, 6886-6892.	4.1	79
123	Implanting Mo Atoms into Surface Lattice of Pt₃Mn Alloys Enclosed by High-Indexed Facets: Promoting Highly Active Sites for Ethylene Glycol Oxidation. ACS Catalysis, 2019, 9, 442-455.	11.2	79
124	On the Electronic Structure of Molecular UO2in the Presence of Ar Atoms:Â Evidence for Direct Uâ^’Ar Bonding. Journal of the American Chemical Society, 2004, 126, 3424-3425.	13.7	76
125	Shape control of CoO and LiCoO2 nanocrystals. Nano Research, 2010, 3, 1-7.	10.4	76
126	Synergistic effect between undercoordinated platinum atoms and defective nickel hydroxide on enhanced hydrogen evolution reaction in alkaline solution. Nano Energy, 2018, 48, 590-599.	16.0	76

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127	Single-Atom Au^Iâ€“N₃ Site for Acetylene Hydrochlorination Reaction. ACS Catalysis, 2020, 10, 1865-1870.	11.2	76
128	A systematic theoretical study on FeOx-supported single-atom catalysts: M1/FeOx for CO oxidation. Nano Research, 2018, 11, 1599-1611.	10.4	75
129	3-Fold-Interpenetrated Uraniumâ€“Organic Frameworks: New Strategy for Rationally Constructing Three-Dimensional Uranyl Organic Materials. Inorganic Chemistry, 2012, 51, 3103-3107.	4.0	74
130	Observation of highly stable and symmetric lanthanide octa-boron inverse sandwich complexes. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E6972-E6977.	7.1	72
131	Few-Atom Pt Ensembles Enable Efficient Catalytic Cyclohexane Dehydrogenation for Hydrogen Production. Journal of the American Chemical Society, 2022, 144, 3535-3542.	13.7	72
132	Symmetrical clusters of carbon and boron. Chemical Physics Letters, 1993, 201, 465-469.	2.6	70
133	Mechanistic Insights into Propene Epoxidation with O₂â€“H₂O Mixture on Au₇/Î±-Al₂O₃: A Hydroproxyl Pathway from ab Initio Molecular Dynamics Simulations. ACS Catalysis, 2016, 6, 2525-2535.	11.2	70
134	A Supramolecularly Activated Radical Cation for Accelerated Catalytic Oxidation. Angewandte Chemie - International Edition, 2016, 55, 8933-8937.	13.8	69
135	Identification of activity trends for CO oxidation on supported transition-metal single-atom catalysts. Catalysis Science and Technology, 2017, 7, 5860-5871.	4.1	69
136	Structural basis of ubiquitin modification by the Legionella effector SdeA. Nature, 2018, 557, 674-678.	27.8	69
137	Uranyl-Glycine-Water Complexes in Solution: Comprehensive Computational Modeling of Coordination Geometries, Stabilization Energies, and Luminescence Properties. Inorganic Chemistry, 2011, 50, 2082-2093.	4.0	68
138	New mechanistic pathways for CO oxidation catalyzed by single-atom catalysts: Supported and doped Au1/ThO2. Nano Research, 2016, 9, 3868-3880.	10.4	68
139	Electronic and Structural Evolution and Chemical Bonding in Ditungsten Oxide Clusters:Â W2On-and W2On(n= 1âˆ’6). Journal of Physical Chemistry A, 2005, 109, 6019-6030.	2.5	67
140	The OH radical-H2O molecular interaction potential. Journal of Chemical Physics, 2006, 124, 224318.	3.0	67
141	Experimental and Theoretical Characterization of Superoxide Complexes [W2O6(O2âˆ’)] and [W3O9(O2âˆ’)]: Models for the Interaction of O2 with Reduced W Sites on Tungsten Oxide Surfaces. Angewandte Chemie - International Edition, 2006, 45, 657-660.	13.8	66
142	Pentavalent Lanthanide Compounds: Formation and Characterization of Praseodymium(V) Oxides. Angewandte Chemie - International Edition, 2016, 55, 6896-6900.	13.8	66
143	Remarkable Dinitrogen Activation and Cleavage by the Gd Dimer: From Dinitrogen Complexes to Ring and Cage Nitrides. Angewandte Chemie - International Edition, 2007, 46, 2911-2914.	13.8	65
144	Unusual Selectivity of Gold Catalysts for Hydrogenation of 1,3-Butadiene toward <i>cis</i>-2-Butene: A Joint Experimental and Theoretical Investigation. Journal of Physical Chemistry C, 2010, 114, 3131-3139.	3.1	65

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145	The Key Role of Support Surface Hydrogenation in the CH₄ to CH₃OH Selective Oxidation by a ZrO₂-Supported Single-Atom Catalyst. ACS Catalysis, 2019, 9, 8903-8909.	11.2	65
146	[La(Î·^x-B_x)La]^{âˆ’} (<i>x</i> = 7â€“9): a new class of inverse sandwich complexes. Chemical Science, 2019, 10, 2534-2542.	7.4	65
147	A Durable Nickel Singleâ€Atom Catalyst for Hydrogenation Reactions and Cellulose Valorization under Harsh Conditions. Angewandte Chemie, 2018, 130, 7189-7193.	2.0	64
148	Reactions of Laser-Ablated U and Th with CO2:Â Neon Matrix Infrared Spectra and Density Functional Calculations of OUCO, OThCO, and Other Products. Journal of the American Chemical Society, 2000, 122, 11440-11449.	13.7	63
149	PrB₇^{âˆ’}: A Praseodymiumâ€Doped Boron Cluster with a Pr^{II} Center Coordinated by a Doubly Aromatic Planar Î·⁷â€B₇^{3âˆ’} Ligand. Angewandte Chemie - International Edition, 2017, 56, 6916-6920.	13.8	63
150	A diuranium carbide cluster stabilized inside a C80 fullerene cage. Nature Communications, 2018, 9, 2753.	12.8	63
151	Understanding Heterolytic H₂ Cleavage and Water-Assisted Hydrogen Spillover on Fe₃O₄(001)-Supported Single Palladium Atoms. ACS Catalysis, 2019, 9, 7876-7887.	11.2	63
152	Self-Selective Catalyst Synthesis for CO2 Reduction. Joule, 2019, 3, 1927-1936.	24.0	63
153	Molecular nitrogen promotes catalytic hydrodeoxygenation. Nature Catalysis, 2019, 2, 1078-1087.	34.4	63
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