Zhi-Pan Liu

List of Publications by Year
in descending order

203	14,902	16411	20307
papers	citations	64 h-index	116 g-index

210	210	210	13634
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Observation of an all-boron fullerene. Nature Chemistry, 2014, 6, 727-731.	6.6	724
2	Identification of General Linear Relationships between Activation Energies and Enthalpy Changes for Dissociation Reactions at Surfaces. Journal of the American Chemical Society, 2003, 125, 3704-3705.	6.6	536
3	General Rules for Predicting Where a Catalytic Reaction Should Occur on Metal Surfaces:Â A Density Functional Theory Study of Câ^'H and Câ^'O Bond Breaking/Making on Flat, Stepped, and Kinked Metal Surfaces. Journal of the American Chemical Society, 2003, 125, 1958-1967.	6.6	534
4	Catalytic Role of Gold in Gold-Based Catalysts:Â A Density Functional Theory Study on the CO Oxidation on Gold. Journal of the American Chemical Society, 2002, 124, 14770-14779.	6.6	512
5	Mechanism and Tafel Lines of Electro-Oxidation of Water to Oxygen on RuO₂(110). Journal of the American Chemical Society, 2010, 132, 18214-18222.	6.6	492
6	Comprehensive Mechanism and Structure-Sensitivity of Ethanol Oxidation on Platinum: New Transition-State Searching Method for Resolving the Complex Reaction Network. Journal of the American Chemical Society, 2008, 130, 10996-11004.	6.6	411
7	Catalytic Role of Metal Oxides in Gold-Based Catalysts: A First Principles Study of CO Oxidation onTiO2Supported Au. Physical Review Letters, 2003, 91, 266102.	2.9	392
8	Tafel Kinetics of Electrocatalytic Reactions: From Experiment to First-Principles. ACS Catalysis, 2014, 4, 4364-4376.	5.5	365
9	In-situ reconstructed Ru atom array on Î±-MnO2 with enhanced performance for acidic water oxidation. Nature Catalysis, 2021, 4, 1012-1023.	16.1	324
10	Mechanism and Activity of Photocatalytic Oxygen Evolution on Titania Anatase in Aqueous Surroundings. Journal of the American Chemical Society, 2010, 132, 13008-13015.	6.6	311
11	Origin and Activity of Oxidized Gold in Water-Gas-Shift Catalysis. Physical Review Letters, 2005, 94, 196102.	2.9	304
12	Particle Size, Shape and Activity for Photocatalysis on Titania Anatase Nanoparticles in Aqueous Surroundings. Journal of the American Chemical Society, 2011, 133, 15743-15752.	6.6	271
13	A Systematic Study of CO Oxidation on Metals and Metal Oxides:Â Density Functional Theory Calculations. Journal of the American Chemical Society, 2004, 126, 8-9.	6.6	267
14	Aggregation-induced phosphorescent emission (AIPE) of iridium(<scp>iii</scp>) complexes. Chemical Communications, 2008, , 685-687.	2.2	258
15	Stochastic Surface Walking Method for Structure Prediction and Pathway Searching. Journal of Chemical Theory and Computation, 2013, 9, 1838-1845.	2.3	244
16	Formic Acid Oxidation at Pt/H₂O Interface from Periodic DFT Calculations Integrated with a Continuum Solvation Model. Journal of Physical Chemistry C, 2009, 113, 17502-17508.	1.5	232
17	General trends in CO dissociation on transition metal surfaces. Journal of Chemical Physics, 2001, 114, 8244-8247.	1.2	211
18	Origin and Activity of Gold Nanoparticles as Aerobic Oxidation Catalysts in Aqueous Solution. Journal of the American Chemical Society, 2011, 133, 9938-9947.	6.6	206

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19	CO2 fixation into methanol at Cu/ZrO2 interface from first principles kinetic Monte Carlo. Journal of Catalysis, 2009, 263, 114-122.	3.1	188
20	A Robust Sulfonate-Based Metalâ€“Organic Framework with Permanent Porosity for Efficient CO₂ Capture and Conversion. Chemistry of Materials, 2016, 28, 6276-6281.	3.2	180
21	The nature of active sites for carbon dioxide electroreduction over oxide-derived copper catalysts. Nature Communications, 2021, 12, 395.	5.8	170
22	A Density Functional Theory Study on the Active Center of Fe-Only Hydrogenase:Â Characterization and Electronic Structure of the Redox States. Journal of the American Chemical Society, 2002, 124, 5175-5182.	6.6	168
23	A New Insight into Fischerâ€“Tropsch Synthesis. Journal of the American Chemical Society, 2002, 124, 11568-11569.	6.6	167
24	General trends in the barriers of catalytic reactions on transition metal surfaces. Journal of Chemical Physics, 2001, 115, 4977-4980.	1.2	146
25	Revealing the Size Effect of Platinum Cocatalyst for Photocatalytic Hydrogen Evolution on TiO₂ Support: A DFT Study. ACS Catalysis, 2018, 8, 7270-7278.	5.5	146
26	Material discovery by combining stochastic surface walking global optimization with a neural network. Chemical Science, 2017, 8, 6327-6337.	3.7	143
27	An Insight into Alkali Promotion:â€‰ A Density Functional Theory Study of CO Dissociation on K/Rh(111). Journal of the American Chemical Society, 2001, 123, 12596-12604.	6.6	139
28	Periodic Density Functional Theory Study of Propane Oxidative Dehydrogenation over V2O5(001) Surface. Journal of the American Chemical Society, 2006, 128, 11114-11123.	6.6	134
29	Reaction Network of Layer-to-Tunnel Transition of MnO₂. Journal of the American Chemical Society, 2016, 138, 5371-5379.	6.6	128
30	Is the uniform electron gas limit important for small Ag clusters? Assessment of different density functionals for Agn (nâ©½4). Journal of Chemical Physics, 2006, 124, 184102.	1.2	124
31	Stochastic surface walking method for crystal structure and phase transition pathway prediction. Physical Chemistry Chemical Physics, 2014, 16, 17845-17856.	1.3	123
32	LASP: Fast global potential energy surface exploration. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1415.	6.2	118
33	Recognition of Surface Oxygen Intermediates on NiFe Oxyhydroxide Oxygen-Evolving Catalysts by Homogeneous Oxidation Reactivity. Journal of the American Chemical Society, 2021, 143, 1493-1502.	6.6	111
34	Nature of Rutile Nuclei in Anatase-to-Rutile Phase Transition. Journal of the American Chemical Society, 2015, 137, 11532-11539.	6.6	106
35	Origin of Oxide Sensitivity in Gold-Based Catalysts:Â A First Principle Study of CO Oxidation over Au Supported on Monoclinic and Tetragonal ZrO2. Journal of the American Chemical Society, 2007, 129, 2642-2647.	6.6	103
36	Methanol to Olefin Conversion on HSAPO-34 Zeolite from Periodic Density Functional Theory Calculations: A Complete Cycle of Side Chain Hydrocarbon Pool Mechanism. Journal of Physical Chemistry C, 2009, 113, 4584-4591.	1.5	102

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37	Electrocatalytic oxygen reduction kinetics on Fe-center of nitrogen-doped graphene. Physical Chemistry Chemical Physics, 2014, 16, 13733-13740.	1.3	102
38	Car Exhaust Catalysis from First Principles:Â Selective NO Reduction under Excess O2Conditions on Ir. Journal of the American Chemical Society, 2004, 126, 10746-10756.	6.6	101
39	Machine Learning for Atomic Simulation and Activity Prediction in Heterogeneous Catalysis: Current Status and Future. ACS Catalysis, 2020, 10, 13213-13226.	5.5	99
40	Double-Ended Surface Walking Method for Pathway Building and Transition State Location of Complex Reactions. Journal of Chemical Theory and Computation, 2013, 9, 5745-5753.	2.3	98
41	Dynamic coordination of cations and catalytic selectivity on zincâ€“chromium oxide alloys during syngas conversion. Nature Catalysis, 2019, 2, 671-677.	16.1	97
42	Accelerated active phase transformation of NiO powered by Pt single atoms for enhanced oxygen evolution reaction. Chemical Science, 2018, 9, 6803-6812.	3.7	96
43	Active Site Revealed for Water Oxidation on Electrochemically Induced Î´-MnO₂: Role of Spinel-to-Layer Phase Transition. Journal of the American Chemical Society, 2018, 140, 1783-1792.	6.6	95
44	Atomic structure of boron resolved using machine learning and global sampling. Chemical Science, 2018, 9, 8644-8655.	3.7	95
45	Metal boride better than Pt: HCP Pd₂B as a superactive hydrogen evolution reaction catalyst. Energy and Environmental Science, 2019, 12, 3099-3105.	15.6	93
46	Quasi-planar aromatic B₃₆and B₃₆^{â^'}clusters: all-boron analogues of coronene. Physical Chemistry Chemical Physics, 2014, 16, 18282.	1.3	91
47	Mechanism and active site of photocatalytic water splitting on titania in aqueous surroundings. Chemical Science, 2014, 5, 2256-2264.	3.7	91
48	Three-phase junction for modulating electronâ€“hole migration in anataseâ€“rutile photocatalysts. Chemical Science, 2015, 6, 3483-3494.	3.7	86
49	Constrained Broyden Minimization Combined with the Dimer Method for Locating Transition State of Complex Reactions. Journal of Chemical Theory and Computation, 2010, 6, 1136-1144.	2.3	85
50	Single Gold Atoms in Heterogeneous Catalysis: Selective 1,3-Butadiene Hydrogenation over Au/ZrO2. Angewandte Chemie - International Edition, 2006, 45, 6865-6868.	7.2	84
51	Combined Surface-Enhanced Infrared Spectroscopy and First-Principles Study on Electro-Oxidation of Formic Acid at Sb-Modified Pt Electrodes. Journal of Physical Chemistry C, 2010, 114, 3102-3107.	1.5	82
52	First Principles Tafel Kinetics for Resolving Key Parameters in Optimizing Oxygen Electrocatalytic Reduction Catalyst. Journal of Physical Chemistry C, 2012, 116, 12696-12705.	1.5	81
53	Deciphering and Suppressing Overâ€Oxidized Nitrogen in Nickelâ€Catalyzed Urea Electrolysis. Angewandte Chemie - International Edition, 2021, 60, 26656-26662.	7.2	81
54	Step-Enhanced Selectivity of NO Reduction on Platinum-Group Metals. Journal of the American Chemical Society, 2003, 125, 14660-14661.	6.6	79

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55	Catalytic Role of Minority Species and Minority Sites for Electrochemical Hydrogen Evolution on Metals: Surface Charging, Coverage, and Tafel Kinetics. Journal of Physical Chemistry C, 2013, 117, 7669-7680.	1.5	79
56	Theoretical modeling of electrode/electrolyte interface from first-principles periodic continuum solvation method. Catalysis Today, 2013, 202, 98-104.	2.2	76
57	Energy Landscape of Zirconia Phase Transitions. Journal of the American Chemical Society, 2015, 137, 8010-8013.	6.6	75
58	CO Oxidation and NO Reduction on Metal Surfaces: Density Functional Theory Investigations. Topics in Catalysis, 2004, 28, 71-78.	1.3	73
59	In Situ Generation of an Nâ€Heterocyclic Carbene Functionalized Metalâ€“Organic Framework by Postsynthetic Ligand Exchange: Efficient and Selective Hydrosilylation of CO₂. Angewandte Chemie - International Edition, 2019, 58, 2844-2849.	7.2	73
60	Engineering Carbon Nanotube Fiber for Real-Time Quantification of Ascorbic Acid Levels in a Live Rat Model of Alzheimerâ€™s Disease. Analytical Chemistry, 2017, 89, 1831-1837.	3.2	71
61	Oxygen Evolution Activity on NiOOH Catalysts: Four-Coordinated Ni Cation as the Active Site and the Hydroperoxide Mechanism. ACS Catalysis, 2020, 10, 2581-2590.	5.5	71
62	Why Is Silver Catalytically Active for NO Reduction? A Unique Pathway via an Inverted (NO)2 Dimer. Journal of the American Chemical Society, 2004, 126, 7336-7340.	6.6	68
63	Large-Scale Atomic Simulation via Machine Learning Potentials Constructed by Global Potential Energy Surface Exploration. Accounts of Chemical Research, 2020, 53, 2119-2129.	7.6	67
64	Insight into association reactions on metal surfaces: Density-functional theory studies of hydrogenation reactions on Rh(111). Journal of Chemical Physics, 2003, 119, 6282-6289.	1.2	66
65	Role of Nanostructured Dual-Oxide Supports in Enhanced Catalytic Activity: Theory of CO Oxidation OverAu/IrO2/TiO2. Physical Review Letters, 2004, 93, 156102.	2.9	66
66	From Atoms to Fullerene: Stochastic Surface Walking Solution for Automated Structure Prediction of Complex Material. Journal of Chemical Theory and Computation, 2013, 9, 3252-3260.	2.3	66
67	Reaction sampling and reactivity prediction using the stochastic surface walking method. Physical Chemistry Chemical Physics, 2015, 17, 2757-2769.	1.3	66
68	Proton-Promoted Electron Transfer in Photocatalysis: Key Step for Photocatalytic Hydrogen Evolution on Metal/Titania Composites. ACS Catalysis, 2017, 7, 2744-2752.	5.5	65
69	Mechanism of H2 metabolism on Fe-only hydrogenases. Journal of Chemical Physics, 2002, 117, 8177-8180.	1.2	64
70	Origin of Selectivity Switch in Fischerâ€“Tropsch Synthesis over Ru and Rh from First-Principles Statistical Mechanics Studies. Journal of the American Chemical Society, 2008, 130, 7929-7937.	6.6	64
71	Chiral Gold Nanowires with Boerdijkâ€“Coxeterâ€“Bernal Structure. Journal of the American Chemical Society, 2014, 136, 12746-12752.	6.6	64
72	Surface Phase Diagram and Oxygen Coupling Kinetics on Flat and Stepped Pt Surfaces under Electrochemical Potentials. Journal of Physical Chemistry C, 2009, 113, 9765-9772.	1.5	62

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73	Catalytic activity and selectivity of methylbenzenes in HSAPO-34 catalyst for the methanol-to-olefins conversion from first principles. Journal of Catalysis, 2010, 271, 386-391.	3.1	62
74	Mechanism of CO2 hydrogenation over Cu/ZrO2(2Ì...12) interface from first-principles kinetics Monte Carlo simulations. Surface Science, 2010, 604, 1869-1876.	0.8	62
75	Selectivity of Direct Ethanol Fuel Cell Dictated by a Unique Partial Oxidation Channel. Journal of Physical Chemistry C, 2007, 111, 12157-12160.	1.5	61
76	Identification of the Active Cu Phase in the Waterâ^'Gas Shift Reaction over Cu/ZrO₂ from First Principles. Journal of Physical Chemistry C, 2010, 114, 8423-8430.	1.5	61
77	Restructuring and Hydrogen Evolution on Pt Nanoparticle. Chemical Science, 2015, 6, 1485-1490.	3.7	61
78	Glucose to 5-Hydroxymethylfurfural: Origin of Site-Selectivity Resolved by Machine Learning Based Reaction Sampling. Journal of the American Chemical Society, 2019, 141, 20525-20536.	6.6	59
79	Constrained Broyden Dimer Method with Bias Potential for Exploring Potential Energy Surface of Multistep Reaction Process. Journal of Chemical Theory and Computation, 2012, 8, 2215-2222.	2.3	58
80	Variable-Cell Double-Ended Surface Walking Method for Fast Transition State Location of Solid Phase Transitions. Journal of Chemical Theory and Computation, 2015, 11, 4885-4894.	2.3	58
81	In Situ Surface Structures of PdAg Catalyst and Their Influence on Acetylene Semihydrogenation Revealed by Machine Learning and Experiment. Journal of the American Chemical Society, 2021, 143, 6281-6292.	6.6	58
82	In Situ Active Site for CO Activation in Fe-Catalyzed Fischerâ€“Tropsch Synthesis from Machine Learning. Journal of the American Chemical Society, 2021, 143, 11109-11120.	6.6	52
83	Mechanism for the high reactivity of CO oxidation on a rutheniumâ€“oxide. Journal of Chemical Physics, 2001, 114, 5956-5957.	1.2	51
84	Layered niobic acid with self-exfoliatable nanosheets and adjustable acidity for catalytic hydration of ethylene oxide. Journal of Catalysis, 2011, 280, 247-254.	3.1	51
85	Graphite to Diamond: Origin for Kinetics Selectivity. Journal of the American Chemical Society, 2017, 139, 2545-2548.	6.6	51
86	Oxidative Dehydrogenation of Ethane over V₂O₅(001):â€‰ A Periodic Density Functional Theory Study. Journal of Physical Chemistry C, 2008, 112, 3719-3725.	1.5	48
87	Theoretical insight into the minor role of paring mechanism in the methanol-to-olefins conversion within HSAPO-34 catalyst. Microporous and Mesoporous Materials, 2012, 158, 264-271.	2.2	47
88	Catalytic hydrogenation of benzene to cyclohexene on Ru(0001) from density functional theory investigationsâ˜†. Catalysis Today, 2011, 160, 234-241.	2.2	46
89	Optimum nanoparticles for electrocatalytic oxygen reduction: the size, shape and new design. Physical Chemistry Chemical Physics, 2013, 15, 18555.	1.3	45
90	Carbonyl Bonding on Oxophilic Metal Centers: Infrared Photodissociation Spectroscopy of Mononuclear and Dinuclear Titanium Carbonyl Cation Complexes. Journal of Physical Chemistry A, 2013, 117, 1514-1521.	1.1	42

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91	Small moleculeâ€mediated control of hydroxyapatite growth: Free energy calculations benchmarked to density functional theory. Journal of Computational Chemistry, 2014, 35, 70-81.	1.5	42
92	Heterogeneous catalysis from structure to activity via SSW-NN method. Journal of Chemical Physics, 2019, 151, 050901.	1.2	39
93	Real-Time Observation of Nonadiabatic Surface Dynamics: The First Picosecond in the Dissociation of NO on Iridium. Physical Review Letters, 2006, 97, 186105.	2.9	38
94	First principles Tafel kinetics of methanol oxidation on Pt(111). Surface Science, 2015, 631, 42-47.	0.8	38
95	Steering the Glycerol Electroâ€Reforming Selectivity via Cationâ€“Intermediate Interactions. Angewandte Chemie - International Edition, 2022, 61, .	7.2	37
96	Towards active and stable oxygen reduction cathodes: a density functional theory survey on Pt2M skin alloys. Energy and Environmental Science, 2011, 4, 1268.	15.6	36
97	TiH Hydride Formed on Amorphous Black Titania: Unprecedented Active Species for Photocatalytic Hydrogen Evolution. ACS Catalysis, 2018, 8, 9711-9721.	5.5	36
98	Methanol Synthesis from CO₂/CO Mixture on Cuâ€“Zn Catalysts from Microkinetics-Guided Machine Learning Pathway Search. Journal of the American Chemical Society, 2022, 144, 13401-13414.	6.6	36
99	Stabilizing CO on Au withNO2: Electronegative Species as Promoters on Coinage Metals?. Physical Review Letters, 2005, 95, 266102.	2.9	35
100	Stability and Phase Transition of Cobalt Oxide Phases by Machine Learning Global Potential Energy Surface. Journal of Physical Chemistry C, 2019, 123, 17539-17547.	1.5	35
101	Stepwise addition reactions in ammonia synthesis: A first principles study. Journal of Chemical Physics, 2001, 115, 609-611.	1.2	34
102	Must an N-Heterocyclic Carbene Be a Terminal Ligand?. Organometallics, 2010, 29, 2403-2405.	1.1	34
103	Density Functional Study of Small Neutral and Charged Silver Cluster Hydrides. Journal of Physical Chemistry A, 2006, 110, 11537-11542.	1.1	33
104	Design and Observation of Biphase TiO₂ Crystal with Perfect Junction. Journal of Physical Chemistry Letters, 2014, 5, 3162-3168.	2.1	33
105	Zeolite-confined subnanometric PtSn mimicking mortise-and-tenon joinery for catalytic propane dehydrogenation. Nature Communications, 2022, 13, 2716.	5.8	33
106	Pressure-induced silica quartz amorphization studied by iterative stochastic surface walking reaction sampling. Physical Chemistry Chemical Physics, 2017, 19, 4725-4733.	1.3	32
107	Stable All-Solid-State Lithium Metal Batteries Enabled by Machine Learning Simulation Designed Halide Electrolytes. Nano Letters, 2022, 22, 2461-2469.	4.5	32
108	Infrared photodissociation spectroscopy of trigonal bipyramidal 19-electron <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mtext>Ni</mml:mtext><mml:mo stretchy="false">(</mml:mo><mml:mtext>CO</mml:mtext><mml:msubsup><mml:mrow><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf cation. Chemical Physics Letters, 2012, 542, 33-36.	1.2	30

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109	Sharp Increase in Catalytic Selectivity in Acetylene Semihydrogenation on Pd Achieved by a Machine Learning Simulation-Guided Experiment. ACS Catalysis, 2020, 10, 9694-9705.	5.5	30
110	The Temperature Dependence of the Adsorption of NO on Pt{211}:Â A RAIRS and DFT Investigation. Journal of Physical Chemistry B, 2004, 108, 289-296.	1.2	29
111	Facile formation and redox of benzoxazole-2-thiolate-bridged dinuclear Pt(ii/iii) complexes. Dalton Transactions, 2012, 41, 12568.	1.6	29
112	Resolving the Temperature and Composition Dependence of Ion Conductivity for Yttria-Stabilized Zirconia from Machine Learning Simulation. Journal of Physical Chemistry C, 2020, 124, 15085-15093.	1.5	29
113	Multiscale Study of Hydrogen Adsorption, Diffusion, and Desorption on Li-Doped Phthalocyanine Covalent Organic Frameworks. Journal of Physical Chemistry C, 2012, 116, 15908-15917.	1.5	28
114	A Strange Nickel(I)â^'Nickel(0) Binuclear Complex and Its Unexpected Ethylene Oligomerization. Organometallics, 2007, 26, 2950-2952.	1.1	26
115	Infrared photodissociation spectra of mass selected homoleptic nickel carbonyl cluster cations in the gas phase. Physical Chemistry Chemical Physics, 2013, 15, 10224.	1.3	26
116	Constant-Charge Reaction Theory for Potential-Dependent Reaction Kinetics at the Solidâ€“Liquid Interface. Journal of Physical Chemistry C, 2014, 118, 3629-3635.	1.5	26
117	Jahnâ€“Teller Disproportionation Induced Exfoliation of Unitâ€Cell Scale Ïµâ€MnO₂. Angewandte Chemie - International Edition, 2020, 59, 22659-22666.	7.2	26
118	Thermodynamic rules for zeolite formation from machine learning based global optimization. Chemical Science, 2020, 11, 10113-10118.	3.7	26
119	Mechanism of Oxygen Electro-Reduction on Au-Modified Pt: Minimizing O Coverage and Pt Site Exposure toward Highly Stable and Active Cathode. Journal of Physical Chemistry C, 2011, 115, 17508-17515.	1.5	25
120	In Situ Generation of an Nâ€Heterocyclic Carbene Functionalized Metalâ€“Organic Framework by Postsynthetic Ligand Exchange: Efficient and Selective Hydrosilylation of CO 2. Angewandte Chemie, 2019, 131, 2870-2875.	1.6	25
121	Improving the performance of phase-change memory by grain refinement. Journal of Applied Physics, 2020, 128, 075101.	1.1	25
122	Reaction prediction via atomistic simulation: from quantum mechanics to machine learning. IScience, 2021, 24, 102013.	1.9	25
123	Oxide-supported single gold catalyst for selective hydrogenation of acrolein predicted from first principles. Journal of Catalysis, 2009, 266, 343-350.	3.1	24
124	Subnano Pt Particles from a First-Principles Stochastic Surface Walking Global Search. Journal of Chemical Theory and Computation, 2016, 12, 4698-4706.	2.3	24
125	NaOH alone can be a homogeneous catalyst for selective aerobic oxidation of alcohols in water. Journal of Catalysis, 2017, 353, 37-43.	3.1	24
126	Insight into the Synergetic Effect in Ternary Gold-Based Catalysts:â€‰ Ultrastability and High Activity of Au on Alumina Modified Titania. Journal of Physical Chemistry C, 2007, 111, 13539-13546.	1.5	23

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127	Enhanced Emission and Analyte Sensing by Cinchonine Iridium(III) Cyclometalated Complexes Bearing Bent Diphosphine Chelators. Organometallics, 2013, 32, 2908-2917.	1.1	23
128	Structure and Catalysis of NiOOH: Recent Advances on Atomic Simulation. Journal of Physical Chemistry C, 2021, 125, 27033-27045.	1.5	23
129	Is Transition Metal Oxide a Must? Moisture-Assisted Oxygen Activation in CO Oxidation on Gold/Î³-Alumina. Journal of Physical Chemistry C, 2010, 114, 16989-16995.	1.5	22
130	Dehydrogenation inhibition on nano-Au/ZSM-5 catalyst: a novel route for anti-coking in methanol to propylene reaction. Chemical Communications, 2012, 48, 5787.	2.2	22
131	Searching for active binary rutile oxide catalyst for water splitting from first principles. Physical Chemistry Chemical Physics, 2012, 14, 16612.	1.3	22
132	Infrared Photodissociation Spectroscopy of Mass Selected Homoleptic Copper Carbonyl Cluster Cations in the Gas Phase. Journal of Physical Chemistry A, 2013, 117, 7810-7817.	1.1	22
133	Searching for new TiO2crystal phases with better photoactivity. Journal of Physics Condensed Matter, 2015, 27, 134203.	0.7	22
134	Stochastic surface walking reaction sampling for resolving heterogeneous catalytic reaction network: A revisit to the mechanism of water-gas shift reaction on Cu. Journal of Chemical Physics, 2017, 147, 152706.	1.2	22
135	CO₂ Photoreduction via Quantum Tunneling: Thin TiO₂-Coated GaP with Coherent Interface To Achieve Electron Tunneling. ACS Catalysis, 2019, 9, 5668-5678.	5.5	22
136	Hydrogen Coupling on Platinum Using Artificial Neural Network Potentials and DFT. Journal of Physical Chemistry Letters, 2021, 12, 10637-10645.	2.1	22
137	Infrared Photodissociation Spectra of Massâ€Selected Homoleptic Dinuclear Palladium Carbonyl Cluster Cations in the Gas Phase. Chinese Journal of Chemistry, 2012, 30, 2131-2137.	2.6	21
138	Confined platinum nanoparticle in carbon nanotube: structure and oxidation. Physical Chemistry Chemical Physics, 2015, 17, 2078-2087.	1.3	21
139	Structure and water oxidation activity of 3d metal oxides. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 47-64.	6.2	20
140	Toward Anticorrosion Electrodes: Site-Selectivity and Self-Acceleration in the Electrochemical Corrosion of Platinum. Journal of Physical Chemistry C, 2010, 114, 4057-4062.	1.5	18
141	Atomic Structure of Heterophase Junction from Theoretical Prediction. Topics in Catalysis, 2015, 58, 644-654.	1.3	18
142	Deciphering and Suppressing Overâ€Oxidized Nitrogen in Nickelâ€Catalyzed Urea Electrolysis. Angewandte Chemie, 2021, 133, 26860-26866.	1.6	18
143	Smallest Stable <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Si</mml:mi><mml:mo>/</mml:mo><mml:msub><mml:mi>SiO</mml:mi><mml:mn>2</mml:mn> Interface that Suppresses Quantum Tunneling from Machine-Learning-Based Global Search. Physical Review Letters, 2022, 128, .	2.9	18
144	Group-VIII transition metal boride as promising hydrogen evolution reaction catalysts. Physical Chemistry Chemical Physics, 2018, 20, 27752-27757.	1.3	17

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145	Ultrafast Vibrational Dynamics of NO and CO Adsorbed on an Iridium Surface. Journal of Physical Chemistry C, 2007, 111, 14198-14206.	1.5	16
146	Microporous Titania Crystals with Penta-oxygen Coordination. ACS Applied Energy Materials, 2018, 1, 22-26.	2.5	16
147	Inherent Simple Cubic Lattice Being Responsible for Ultrafast Solid-Phase Change of Ge₂Sb₂Te₅. Journal of Physical Chemistry Letters, 2017, 8, 2560-2564.	2.1	15
148	Two-Stage Solid-Phase Transition of Cubic Ice to Hexagonal Ice: Structural Origin and Kinetics. Journal of Physical Chemistry C, 2018, 122, 29009-29016.	1.5	15
149	Stability and anion diffusion kinetics of Yttria-stabilized zirconia resolved from machine learning global potential energy surface exploration. Journal of Chemical Physics, 2020, 152, 094703.	1.2	15
150	Zirconia-Supported ZnO Single Layer for Syngas Conversion Revealed from Machine-Learning Atomic Simulation. Journal of Physical Chemistry Letters, 2021, 12, 3328-3334.	2.1	15
151	Active Site of Catalytic Ethene Epoxidation: Machine-Learning Global Pathway Sampling Rules Out the Metal Sites. ACS Catalysis, 2021, 11, 8317-8326.	5.5	15
152	Machine learning potential era of zeolite simulation. Chemical Science, 2022, 13, 5055-5068.	3.7	15
153	CO oxidation onAuâˆ•TiOxâˆ•Mo{112}: Structure characterization and catalytic activity studied usingab initiocalculations. Physical Review B, 2006, 73, .	1.1	14
154	NO restructuring of surface Ir and bond formation to preadsorbed O on Ir{100} at 95K. Surface Science, 2005, 584, 214-224.	0.8	13
155	Massively parallelization strategy for material simulation using highâ€dimensional neural network potential. Journal of Computational Chemistry, 2019, 40, 1091-1096.	1.5	13
156	In Situ Active Site for Fe-Catalyzed Fischerâ€“Tropsch Synthesis: Recent Progress and Future Challenges. Journal of Physical Chemistry Letters, 2022, 13, 3342-3352.	2.1	13
157	Mechanism and microstructures in Ga₂O₃ pseudomartensitic solid phase transition. Physical Chemistry Chemical Physics, 2016, 18, 18563-18574.	1.3	12
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