Zhi-Pan Liu

List of Publications by Citations

194 papers	11,312 citations	56 h-index	102 g-index
210 ext. papers	12,987 ext. citations	8.1 avg, IF	6.93 L-index

#	Paper	IF	Citations
194	Observation of an all-boron fullerene. *Nature Chemistry*, **2014**, 6, 727-31	17.6	590
193	Catalytic role of gold in gold-based catalysts: a density functional theory study on the CO oxidation on gold. *Journal of the American Chemical Society*, **2002**, 124, 14770-9	16.4	466
192	General rules for predicting where a catalytic reaction should occur on metal surfaces: a density functional theory study of C-H and C-O bond breaking/making on flat, stepped, and kinked metal surfaces. *Journal of the American Chemical Society*, **2003**, 125, 1958-67	16.4	452
191	Identification of general linear relationships between activation energies and enthalpy changes for dissociation reactions at surfaces. *Journal of the American Chemical Society*, **2003**, 125, 3704-5	16.4	452
190	Mechanism and Tafel lines of electro-oxidation of water to oxygen on RuO2(110). *Journal of the American Chemical Society*, **2010**, 132, 18214-22	16.4	406
189	Catalytic role of metal oxides in gold-based catalysts: a first principles study of CO oxidation on TiO2 supported Au. *Physical Review Letters*, **2003**, 91, 266102	7.4	358
188	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, 10996-1004	16.4	338
187	Origin and activity of oxidized gold in water-gas-shift catalysis. *Physical Review Letters*, **2005**, 94, 196102	7.4	280
186	Mechanism and activity of photocatalytic oxygen evolution on titania anatase in aqueous surroundings. *Journal of the American Chemical Society*, **2010**, 132, 13008-15	16.4	274
185	A systematic study of CO oxidation on metals and metal oxides: density functional theory calculations. *Journal of the American Chemical Society*, **2004**, 126, 8-9	16.4	238
184	Particle size, shape and activity for photocatalysis on titania anatase nanoparticles in aqueous surroundings. *Journal of the American Chemical Society*, **2011**, 133, 15743-52	16.4	237
183	Tafel Kinetics of Electrocatalytic Reactions: From Experiment to First-Principles. *ACS Catalysis*, **2014** , 4, 4364-4376	13.1	236
182	Aggregation-induced phosphorescent emission (AIPE) of iridium(III) complexes. *Chemical Communications*, **2008**, 685-7	5.8	234
181	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	3.8	210
180	General trends in CO dissociation on transition metal surfaces. *Journal of Chemical Physics*, **2001**, 114, 8244-8247	3.9	192
179	Origin and activity of gold nanoparticles as aerobic oxidation catalysts in aqueous solution. *Journal of the American Chemical Society*, **2011**, 133, 9938-47	16.4	175
178	CO2 fixation into methanol at Cu/ZrO2 interface from first principles kinetic Monte Carlo. *Journal of Catalysis*, **2009**, 263, 114-122	7.3	161

177	Stochastic Surface Walking Method for Structure Prediction and Pathway Searching. *Journal of Chemical Theory and Computation*, **2013**, 9, 1838-45	6.4	160
176	A density functional theory study on the active center of Fe-only hydrogenase: characterization and electronic structure of the redox states. *Journal of the American Chemical Society*, **2002**, 124, 5175-82	16.4	155
175	A Robust Sulfonate-Based Metal Organic Framework with Permanent Porosity for Efficient CO2 Capture and Conversion. *Chemistry of Materials*, **2016**, 28, 6276-6281	9.6	148
174	A new insight into Fischer-Tropsch synthesis. *Journal of the American Chemical Society*, **2002**, 124, 11568-8	16.4	147
173	General trends in the barriers of catalytic reactions on transition metal surfaces. *Journal of Chemical Physics*, **2001**, 115, 4977-4980	3.9	133
172	An insight into alkali promotion: a density functional theory study of CO dissociation on K/Rh(111). *Journal of the American Chemical Society*, **2001**, 123, 12596-604	16.4	125
171	Is the uniform electron gas limit important for small Ag clusters? Assessment of different density functionals for Ag(n) (n Journal of Chemical Physics, **2006**, 124, 184102	3.9	118
170	Periodic density functional theory study of propane oxidative dehydrogenation over V2O5(001) surface. *Journal of the American Chemical Society*, **2006**, 128, 11114-23	16.4	117
169	Origin of Oxide sensitivity in gold-based catalysts: a first principle study of CO oxidation over Au supported on monoclinic and tetragonal ZrO2. *Journal of the American Chemical Society*, **2007**, 129, 2642-7	16.4	96
168	Car exhaust catalysis from first principles: selective NO reduction under excess O2 conditions on Ir. *Journal of the American Chemical Society*, **2004**, 126, 10746-56	16.4	94
167	Electrocatalytic oxygen reduction kinetics on Fe-center of nitrogen-doped graphene. *Physical Chemistry Chemical Physics*, **2014**, 16, 13733-40	3.6	92
166	Revealing the Size Effect of Platinum Cocatalyst for Photocatalytic Hydrogen Evolution on TiO2 Support: A DFT Study. *ACS Catalysis*, **2018**, 8, 7270-7278	13.1	90
165	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	3.8	88
164	Stochastic surface walking method for crystal structure and phase transition pathway prediction. *Physical Chemistry Chemical Physics*, **2014**, 16, 17845-56	3.6	84
163	Material discovery by combining stochastic surface walking global optimization with a neural network. *Chemical Science*, **2017**, 8, 6327-6337	9.4	82
162	Reaction Network of Layer-to-Tunnel Transition of MnO2. *Journal of the American Chemical Society*, **2016**, 138, 5371-9	16.4	79
161	Mechanism and active site of photocatalytic water splitting on titania in aqueous surroundings. *Chemical Science*, **2014**, 5, 2256-2264	9.4	78
160	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	3.8	75

159	Nature of Rutile Nuclei in Anatase-to-Rutile Phase Transition. *Journal of the American Chemical Society*, **2015**, 137, 11532-9	16.4	74
158	Three-phase junction for modulating electron-hole migration in anatase-rutile photocatalysts. *Chemical Science*, **2015**, 6, 3483-3494	9.4	73
157	Quasi-planar aromatic B36 and B36(-) clusters: all-boron analogues of coronene. *Physical Chemistry Chemical Physics*, **2014**, 16, 18282-7	3.6	73
156	Theoretical modeling of electrode/electrolyte interface from first-principles periodic continuum solvation method. *Catalysis Today*, **2013**, 202, 98-104	5.3	72
155	Double-Ended Surface Walking Method for Pathway Building and Transition State Location of Complex Reactions. *Journal of Chemical Theory and Computation*, **2013**, 9, 5745-53	6.4	70
154	Single gold atoms in heterogeneous catalysis: selective 1,3-butadiene hydrogenation over Au/ZrO2. *Angewandte Chemie - International Edition*, **2006**, 45, 6865-8	16.4	70
153	Step-enhanced selectivity of NO reduction on platinum-group metals. *Journal of the American Chemical Society*, **2003**, 125, 14660-1	16.4	69
152	First Principles Tafel Kinetics for Resolving Key Parameters in Optimizing Oxygen Electrocatalytic Reduction Catalyst. *Journal of Physical Chemistry C*, **2012**, 116, 12696-12705	3.8	68
151	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	3.8	67
150	Active Site Revealed for Water Oxidation on Electrochemically Induced □MnO: Role of Spinel-to-Layer Phase Transition. *Journal of the American Chemical Society*, **2018**, 140, 1783-1792	16.4	66
149	CO Oxidation and NO Reduction on Metal Surfaces: Density Functional Theory Investigations. *Topics in Catalysis*, **2004**, 28, 71-78	2.3	66
148	Accelerated active phase transformation of NiO powered by Pt single atoms for enhanced oxygen evolution reaction. *Chemical Science*, **2018**, 9, 6803-6812	9.4	65
147	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	6.4	64
146	Metal boride better than Pt: HCP Pd2B as a superactive hydrogen evolution reaction catalyst. *Energy and Environmental Science*, **2019**, 12, 3099-3105	35.4	63
145	Energy Landscape of Zirconia Phase Transitions. *Journal of the American Chemical Society*, **2015**, 137, 8010-3	16.4	61
144	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	3.8	61
143	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, 7336-40	16.4	61
142	Origin of selectivity switch in Fischer-Tropsch synthesis over Ru and Rh from first-principles statistical mechanics studies. *Journal of the American Chemical Society*, **2008**, 130, 7929-37	16.4	60

141	Role of nanostructured dual-oxide supports in enhanced catalytic activity: theory of CO oxidation over Au/IrO2/TiO2. *Physical Review Letters*, **2004**, 93, 156102	7.4	60
140	Mechanism of H2 metabolism on Fe-only hydrogenases. *Journal of Chemical Physics*, **2002**, 117, 8177-8180	3.9	60
139	Mechanism of CO2 hydrogenation over Cu/ZrO2(2 12) interface from first-principles kinetics Monte Carlo simulations. *Surface Science*, **2010**, 604, 1869-1876	1.8	57
138	Identification of the Active Cu Phase in the Water Gas Shift Reaction over Cu/ZrO2 from First Principles. *Journal of Physical Chemistry C*, **2010**, 114, 8423-8430	3.8	56
137	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	7.3	55
136	Atomic structure of boron resolved using machine learning and global sampling. *Chemical Science*, **2018**, 9, 8644-8655	9.4	55
135	Dynamic coordination of cations and catalytic selectivity on zinc chromium oxide alloys during syngas conversion. *Nature Catalysis*, **2019**, 2, 671-677	36.5	52
134	Selectivity of Direct Ethanol Fuel Cell Dictated by a Unique Partial Oxidation Channel. *Journal of Physical Chemistry C*, **2007**, 111, 12157-12160	3.8	51
133	LASP: Fast global potential energy surface exploration. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1415	7.9	50
132	Restructuring and Hydrogen Evolution on Pt Nanoparticle. *Chemical Science*, **2015**, 6, 1485-1490	9.4	50
131	From Atoms to Fullerene: Stochastic Surface Walking Solution for Automated Structure Prediction of Complex Material. *Journal of Chemical Theory and Computation*, **2013**, 9, 3252-60	6.4	50
130	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	3.9	50
129	Engineering Carbon Nanotube Fiber for Real-Time Quantification of Ascorbic Acid Levels in a Live Rat Model of Alzheimer's Disease. *Analytical Chemistry*, **2017**, 89, 1831-1837	7.8	49
128	Reaction sampling and reactivity prediction using the stochastic surface walking method. *Physical Chemistry Chemical Physics*, **2015**, 17, 2757-69	3.6	49
127	Chiral gold nanowires with Boerdijk-Coxeter-Bernal structure. *Journal of the American Chemical Society*, **2014**, 136, 12746-52	16.4	49
126	In Situ Generation of an N-Heterocyclic Carbene Functionalized Metal-Organic Framework by Postsynthetic Ligand Exchange: Efficient and Selective Hydrosilylation of CO. *Angewandte Chemie - International Edition*, **2019**, 58, 2844-2849	16.4	49
125	Proton-Promoted Electron Transfer in Photocatalysis: Key Step for Photocatalytic Hydrogen Evolution on Metal/Titania Composites. *ACS Catalysis*, **2017**, 7, 2744-2752	13.1	47
124	Mechanism for the high reactivity of CO oxidation on a ruthenium oxide. *Journal of Chemical Physics*, **2001**, 114, 5956-5957	3.9	47

123	The nature of active sites for carbon dioxide electroreduction over oxide-derived copper catalysts. *Nature Communications*, **2021**, 12, 395	17.4	46
122	Constrained Broyden Dimer Method with Bias Potential for Exploring Potential Energy Surface of Multistep Reaction Process. *Journal of Chemical Theory and Computation*, **2012**, 8, 2215-22	6.4	45
121	Oxidative Dehydrogenation of Ethane over V2O5(001): A Periodic Density Functional Theory Study. *Journal of Physical Chemistry C*, **2008**, 112, 3719-3725	3.8	43
120	Optimum nanoparticles for electrocatalytic oxygen reduction: the size, shape and new design. *Physical Chemistry Chemical Physics*, **2013**, 15, 18555-61	3.6	42
119	Layered niobic acid with self-exfoliatable nanosheets and adjustable acidity for catalytic hydration of ethylene oxide. *Journal of Catalysis*, **2011**, 280, 247-254	7.3	42
118	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	5.3	41
117	Catalytic hydrogenation of benzene to cyclohexene on Ru(0 0 0 1) from density functional theory investigations. *Catalysis Today*, **2011**, 160, 234-241	5.3	40
116	Small molecule-mediated control of hydroxyapatite growth: free energy calculations benchmarked to density functional theory. *Journal of Computational Chemistry*, **2014**, 35, 70-81	3.5	39
115	Variable-cell double-ended surface walking method for fast transition state location of solid phase transitions. *Journal of Chemical Theory and Computation*, **2015**, 11, 4885-94	6.4	39
114	Machine Learning for Atomic Simulation and Activity Prediction in Heterogeneous Catalysis: Current Status and Future. *ACS Catalysis*, **2020**, 10, 13213-13226	13.1	39
113	In-situ reconstructed Ru atom array on □MnO2 with enhanced performance for acidic water oxidation. *Nature Catalysis*, **2021**, 4, 1012-1023	36.5	37
112	Oxygen Evolution Activity on NiOOH Catalysts: Four-Coordinated Ni Cation as the Active Site and the Hydroperoxide Mechanism. *ACS Catalysis*, **2020**, 10, 2581-2590	13.1	35
111	Stabilizing CO on Au with NO2: electronegative species as promoters on coinage metals?. *Physical Review Letters*, **2005**, 95, 266102	7.4	35
110	Graphite to Diamond: Origin for Kinetics Selectivity. *Journal of the American Chemical Society*, **2017**, 139, 2545-2548	16.4	33
109	Carbonyl bonding on oxophilic metal centers: infrared photodissociation spectroscopy of mononuclear and dinuclear titanium carbonyl cation complexes. *Journal of Physical Chemistry A*, **2013**, 117, 1514-21	2.8	33
108	Towards active and stable oxygen reduction cathodes: a density functional theory survey on Pt2M skin alloys. *Energy and Environmental Science*, **2011**, 4, 1268	35.4	33
107	Real-time observation of nonadiabatic surface dynamics: the first picosecond in the dissociation of NO on iridium. *Physical Review Letters*, **2006**, 97, 186105	7.4	33
106	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	16.4	32

105	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	16.4	32
104	Must an N-Heterocyclic Carbene Be a Terminal Ligand?. *Organometallics*, **2010**, 29, 2403-2405	3.8	31
103	Stepwise addition reactions in ammonia synthesis: A first principles study. *Journal of Chemical Physics*, **2001**, 115, 609-611	3.9	30
102	Large-Scale Atomic Simulation via Machine Learning Potentials Constructed by Global Potential Energy Surface Exploration. *Accounts of Chemical Research*, **2020**, 53, 2119-2129	24.3	30
101	Design and Observation of Biphase TiO2 Crystal with Perfect Junction. *Journal of Physical Chemistry Letters*, **2014**, 5, 3162-8	6.4	29
100	Infrared photodissociation spectroscopy of trigonal bipyramidal 19-electron . *Chemical Physics Letters*, **2012**, 542, 33-36	2.5	27
99	Density functional study of small neutral and charged silver cluster hydrides. *Journal of Physical Chemistry A*, **2006**, 110, 11537-42	2.8	27
98	First principles Tafel kinetics of methanol oxidation on Pt(111). *Surface Science*, **2015**, 631, 42-47	1.8	26
97	TiH Hydride Formed on Amorphous Black Titania: Unprecedented Active Species for Photocatalytic Hydrogen Evolution. *ACS Catalysis*, **2018**, 8, 9711-9721	13.1	26
96	Heterogeneous catalysis from structure to activity via SSW-NN method. *Journal of Chemical Physics*, **2019**, 151, 050901	3.9	25
95	Facile formation and redox of benzoxazole-2-thiolate-bridged dinuclear Pt(II/III) complexes. *Dalton Transactions*, **2012**, 41, 12568-76	4.3	25
94	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	3.8	25
93	A Strange Nickel(I)Nickel(0) Binuclear Complex and Its Unexpected Ethylene Oligomerization. *Organometallics*, **2007**, 26, 2950-2952	3.8	25
92	The Temperature Dependence of the Adsorption of NO on Pt{211}: A RAIRS and DFT Investigation. *Journal of Physical Chemistry B*, **2004**, 108, 289-296	3.4	24
91	Insight into the Synergetic Effect in Ternary Gold-Based Catalysts: Ultrastability and High Activity of Au on Alumina Modified Titania. *Journal of Physical Chemistry C*, **2007**, 111, 13539-13546	3.8	23
90	Infrared photodissociation spectra of mass selected homoleptic nickel carbonyl cluster cations in the gas phase. *Physical Chemistry Chemical Physics*, **2013**, 15, 10224-32	3.6	22
89	Multiscale Study of Hydrogen Adsorption, Diffusion, and Desorption on Li-Doped Phthalocyanine Covalent Organic Frameworks. *Journal of Physical Chemistry C*, **2012**, 116, 15908-15917	3.8	22
88	Enhanced Emission and Analyte Sensing by Cinchonine Iridium(III) Cyclometalated Complexes Bearing Bent Diphosphine Chelators. *Organometallics*, **2013**, 32, 2908-2917	3.8	22

87	Oxide-supported single gold catalyst for selective hydrogenation of acrolein predicted from first principles. *Journal of Catalysis*, **2009**, 266, 343-350	7.3	22
86	Constant-Charge Reaction Theory for Potential-Dependent Reaction Kinetics at the Solid□liquid Interface. *Journal of Physical Chemistry C*, **2014**, 118, 3629-3635	3.8	21
85	Is Transition Metal Oxide a Must? Moisture-Assisted Oxygen Activation in CO Oxidation on Gold/□Alumina□*Journal of Physical Chemistry C*, **2010**, 114, 16989-16995	3.8	21
84	Infrared Photodissociation Spectra of Mass-Selected Homoleptic Dinuclear Palladium Carbonyl Cluster Cations in the Gas Phase. *Chinese Journal of Chemistry*, **2012**, 30, 2131-2137	4.9	20
83	Dehydrogenation inhibition on nano-Au/ZSM-5 catalyst: a novel route for anti-coking in methanol to propylene reaction. *Chemical Communications*, **2012**, 48, 5787-9	5.8	20
82	Stability and Phase Transition of Cobalt Oxide Phases by Machine Learning Global Potential Energy Surface. *Journal of Physical Chemistry C*, **2019**, 123, 17539-17547	3.8	19
81	Infrared photodissociation spectroscopy of mass selected homoleptic copper carbonyl cluster cations in the gas phase. *Journal of Physical Chemistry A*, **2013**, 117, 7810-7	2.8	19
80	In Situ Generation of an N-Heterocyclic Carbene Functionalized Metal□rganic Framework by Postsynthetic Ligand Exchange: Efficient and Selective Hydrosilylation of CO2. *Angewandte Chemie*, **2019**, 131, 2870-2875	3.6	19
79	Searching for new TiO□rystal phases with better photoactivity. *Journal of Physics Condensed Matter*, **2015**, 27, 134203	1.8	18
78	Searching for active binary rutile oxide catalyst for water splitting from first principles. *Physical Chemistry Chemical Physics*, **2012**, 14, 16612-7	3.6	18
77	Toward Anticorrosion Electrodes: Site-Selectivity and Self-Acceleration in the Electrochemical Corrosion of Platinum. *Journal of Physical Chemistry C*, **2010**, 114, 4057-4062	3.8	18
76	Sharp Increase in Catalytic Selectivity in Acetylene Semihydrogenation on Pd Achieved by a Machine Learning Simulation-Guided Experiment. *ACS Catalysis*, **2020**, 10, 9694-9705	13.1	18
75	Subnano Pt Particles from a First-Principles Stochastic Surface Walking Global Search. *Journal of Chemical Theory and Computation*, **2016**, 12, 4698-706	6.4	17
74	Structure and water oxidation activity of 3d metal oxides. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 47-64	7.9	17
73	Deciphering and Suppressing Over-Oxidized Nitrogen in Nickel-Catalyzed Urea Electrolysis. *Angewandte Chemie - International Edition*, **2021**, 60, 26656-26662	16.4	17
72	Pressure-induced silica quartz amorphization studied by iterative stochastic surface walking reaction sampling. *Physical Chemistry Chemical Physics*, **2017**, 19, 4725-4733	3.6	16
71	Atomic Structure of Heterophase Junction from Theoretical Prediction. *Topics in Catalysis*, **2015**, 58, 644-654	2.3	15
70	Confined platinum nanoparticle in carbon nanotube: structure and oxidation. *Physical Chemistry Chemical Physics*, **2015**, 17, 2078-87	3.6	15

69	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	3.9	15
68	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	16.4	15
67	CO2 Photoreduction via Quantum Tunneling: Thin TiO2-Coated GaP with Coherent Interface To Achieve Electron Tunneling. *ACS Catalysis*, **2019**, 9, 5668-5678	13.1	14
66	CO oxidation on Au□TiOx□Mo{112}: Structure characterization and catalytic activity studied using ab initio calculations. *Physical Review B*, **2006**, 73,	3.3	14
65	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	3.8	14
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63	NaOH alone can be a homogeneous catalyst for selective aerobic oxidation of alcohols in water. *Journal of Catalysis*, **2017**, 353, 37-43	7.3	13
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60	Ultrafast Vibrational Dynamics of NO and CO Adsorbed on an Iridium Surface. *Journal of Physical Chemistry C*, **2007**, 111, 14198-14206	3.8	11
59	Microporous Titania Crystals with Penta-oxygen Coordination. *ACS Applied Energy Materials*, **2018**, 1, 22-26	6.1	11
58	Group-VIII transition metal boride as promising hydrogen evolution reaction catalysts. *Physical Chemistry Chemical Physics*, **2018**, 20, 27752-27757	3.6	11
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55	Single Gold Atoms in Heterogeneous Catalysis: Selective 1,3-Butadiene Hydrogenation over Au/ZrO2. *Angewandte Chemie*, **2006**, 118, 7019-7022	3.6	10
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49	Electrochemical reactions at the electrode/solution interface: Theory and applications to water electrolysis and oxygen reduction. *Science China Chemistry*, **2010**, 53, 543-552	7.9	9
48	Jahn-Teller Disproportionation Induced Exfoliation of Unit-Cell Scale ?-MnO. *Angewandte Chemie - International Edition*, **2020**, 59, 22659-22666	16.4	9
47	Massively parallelization strategy for material simulation using high-dimensional neural network potential. *Journal of Computational Chemistry*, **2019**, 40, 1091-1096	3.5	9
46	Ultrasonic Electrochemical Reaction on Boron-Doped Diamond Electrodes: Reaction Pathway and Mechanism. *ChemElectroChem*, **2015**, 2, 366-373	4.3	8
45	Origin of the type-II band offset between rutile and anatase titanium dioxide: Classical and quantum-mechanical interactions between O ions. *Physical Review B*, **2017**, 95,	3.3	8
44	Intrinsic Features of an Ideal Glass. *Chinese Physics Letters*, **2017**, 34, 026402	1.8	7
43	Ultrasmall Au clusters supported on pristine and defected CeO: Structure and stability. *Journal of Chemical Physics*, **2019**, 151, 174702	3.9	6
42	Crystal phase transition of urea: what governs the reaction kinetics in molecular crystal phase transitions. *Physical Chemistry Chemical Physics*, **2017**, 19, 32125-32131	3.6	6
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40	Hydrogen Coupling on Platinum Using Artificial Neural Network Potentials and DFT. *Journal of Physical Chemistry Letters*, **2021**, 12, 10637-10645	6.4	6
39	Zirconia-Supported ZnO Single Layer for Syngas Conversion Revealed from Machine-Learning Atomic Simulation. *Journal of Physical Chemistry Letters*, **2021**, 12, 3328-3334	6.4	6
38	Energy Landscape and Crystal-to-Crystal Transition of Ternary Silicate Mg2SiO4. *Journal of Physical Chemistry C*, **2016**, 120, 25110-25116	3.8	6
37	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	3.9	5
36	Glassy nature and glass-to-crystal transition in the binary metallic glass CuZr. *Physical Review B*, **2017**, 95,	3.3	5
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34	Coaxial alkaline-earth dimetal units sandwiched between hydrosilver compounds: A DFT Study. *Computational and Theoretical Chemistry*, **2007**, 808, 163-166		5

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