Zhi-Pan Liu

List of Publications by Year in Descending Order

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	Determination of acid structures on the surface of sulfated monoclinic and tetragonal zirconia through experimental and theoretical approaches. *Catalysis Science and Technology*, **2022**, 12, 596-605	5.5	1
193	Automated search for optimal surface phases (ASOPs) in grand canonical ensemble powered by machine learning.. *Journal of Chemical Physics*, **2022**, 156, 094104	3.9	1
192	Active Site for Fe-Catalyzed Fischer-Tropsch Synthesis: Recent Progress and Future Challenges.. *Journal of Physical Chemistry Letters*, **2022**, 3342-3352	6.4	3
191	Zeolite-confined subnanometric PtSn mimicking mortise-and-tenon joinery for catalytic propane dehydrogenation.. *Nature Communications*, **2022**, 13, 2716	17.4	4
190	Steering the Glycerol Electro-Reforming Selectivity via Cation-Intermediate Interactions.. *Angewandte Chemie - International Edition*, **2021**,	16.4	5
189	In-situ reconstructed Ru atom array on α-MnO2 with enhanced performance for acidic water oxidation. *Nature Catalysis*, **2021**, 4, 1012-1023	36.5	37
188	Innenrücktitelbild: Deciphering and Suppressing Over-Oxidized Nitrogen in Nickel-Catalyzed Urea Electrolysis (Angew. Chem. 51/2021). *Angewandte Chemie*, **2021**, 133, 27071	3.6	
187	Recent implementations in LASP 3.0: Global neural network potential with multiple elements and better long-range description. *Chinese Journal of Chemical Physics*, **2021**, 34, 583-590	0.9	2
186	Hydrogen Coupling on Platinum Using Artificial Neural Network Potentials and DFT. *Journal of Physical Chemistry Letters*, **2021**, 12, 10637-10645	6.4	6
185	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
184	Theoretical aspects on doped-zirconia for solid oxide fuel cells: From structure to conductivity. *Chinese Journal of Chemical Physics*, **2021**, 34, 125-136	0.9	2
183	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
182	Structure and Activity of Potential-Dependent Pt(110) Surface Phases Revealed from Machine-Learning Atomic Simulation. *Journal of Physical Chemistry C*, **2021**, 125, 10955-10963	3.8	1
181	Active Site of Catalytic Ethene Epoxidation: Machine-Learning Global Pathway Sampling Rules Out the Metal Sites. *ACS Catalysis*, **2021**, 11, 8317-8326	13.1	3
180	Thermodynamics and Catalytic Activity of Ruthenium Oxides Grown on Ruthenium Metal from a Machine Learning Atomic Simulation. *Journal of Physical Chemistry C*, **2021**, 125, 17088-17096	3.8	2
179	The dome of gold nanolized for catalysis. *Chemical Science*, **2021**, 12, 5664-5671	9.4	1
178	Reaction prediction via atomistic simulation: from quantum mechanics to machine learning. *IScience* , **2021**, 24, 102013	6.1	10

177	Phase junction-confined single-atom TiO2Pt1CeO2 for multiplying catalytic oxidation efficiency. *Catalysis Science and Technology*, **2021**, 11, 4650-4657	5.5	1
176	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
175	The nature of active sites for carbon dioxide electroreduction over oxide-derived copper catalysts. *Nature Communications*, **2021**, 12, 395	17.4	46
174	Active Site for CO Activation in Fe-Catalyzed Fischer-Tropsch Synthesis from Machine Learning. *Journal of the American Chemical Society*, **2021**, 143, 11109-11120	16.4	13
173	Deciphering and Suppressing Over-Oxidized Nitrogen in Nickel-Catalyzed Urea Electrolysis. *Angewandte Chemie - International Edition*, **2021**, 60, 26656-26662	16.4	17
172	Structure and Dynamics of Energy Materials from Machine Learning Simulations: A Topical Review *Chinese Journal of Chemistry*, **2021**, 39, 3144	4.9	2
171	Structure and Catalysis of NiOOH: Recent Advances on Atomic Simulation. *Journal of Physical Chemistry C*, **2021**, 125, 27033-27045	3.8	2
170	Directly Determining the Interface Structure and Band Offset of a Large-Lattice-Mismatched CdS/CdTe Heterostructure. *Chinese Physics Letters*, **2020**, 37, 096802	1.8	2
169	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
168	Characteristics of Impactful Computational Contributions to The Journal of Physical Chemistry C. *Journal of Physical Chemistry C*, **2020**, 124, 13509-13510	3.8	3
167	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
166	Stochastic Surface Walking Method and Applications to Real Materials **2020**, 2811-2834		
165	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
164	Ultrasonic Bending of Silver Nanowires. *ACS Nano*, **2020**, 14, 15286-15292	16.7	4
163	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
162	Machine Learning for Atomic Simulation and Activity Prediction in Heterogeneous Catalysis: Current Status and Future. *ACS Catalysis*, **2020**, 10, 13213-13226	13.1	39
161	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
160	Jahn-Teller Disproportionation Induced Exfoliation of Unit-Cell Scale ?-MnO. *Angewandte Chemie - International Edition*, **2020**, 59, 22659-22666	16.4	9

159	Jahn□Teller Disproportionation Induced Exfoliation of Unit-Cell Scale ?-MnO2. *Angewandte Chemie*, **2020**, 132, 22848-22855	3.6	1
158	Thermodynamic rules for zeolite formation from machine learning based global optimization. *Chemical Science*, **2020**, 11, 10113-10118	9.4	10
157	Improving the performance of phase-change memory by grain refinement. *Journal of Applied Physics*, **2020**, 128, 075101	2.5	14
156	Dynamic coordination of cations and catalytic selectivity on zinc□hromium oxide alloys during syngas conversion. *Nature Catalysis*, **2019**, 2, 671-677	36.5	52
155	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
154	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
153	LASP: Fast global potential energy surface exploration. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1415	7.9	50
152	A New Type of Capping Agent in Nanoscience: Metal Cations. *Small*, **2019**, 15, e1900444	11	4
151	Stochastic Surface Walking Method and Applications to Real Materials **2019**, 1-24		
150	Heterogeneous catalysis from structure to activity via SSW-NN method. *Journal of Chemical Physics*, **2019**, 151, 050901	3.9	25
149	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
148	The Periodic Table. *Journal of Physical Chemistry A*, **2019**, 123, 5837-5848	2.8	1
147	The JPC Periodic Table. *Journal of Physical Chemistry C*, **2019**, 123, 17063-17074	3.8	1
146	The JPC Periodic Table. *Journal of Physical Chemistry Letters*, **2019**, 10, 4051-4062	6.4	1
145	3-D Tunnel TiO2 Crystal Phase as a Fast Charging Lithium Battery Anode from Stochastic Surface Walking-Based Material Screening. *Journal of Physical Chemistry C*, **2019**, 123, 19347-19353	3.8	3
144	Ultrasmall Au clusters supported on pristine and defected CeO: Structure and stability. *Journal of Chemical Physics*, **2019**, 151, 174702	3.9	6
143	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
142	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

141	Massively parallelization strategy for material simulation using high-dimensional neural network potential. *Journal of Computational Chemistry*, **2019**, 40, 1091-1096	3.5	9
140	In Situ Generation of an N-Heterocyclic Carbene Functionalized Metal□Organic Framework by Postsynthetic Ligand Exchange: Efficient and Selective Hydrosilylation of CO2. *Angewandte Chemie*, **2019**, 131, 2870-2875	3.6	19
139	Investigation of Non-covalent Interactions of 18-Crown-6 with Amino Acids in Gas Phase by Mass Spectrometry. *Chinese Journal of Analytical Chemistry*, **2018**, 46, 273-279	1.6	3
138	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
137	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
136	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
135	Microporous Titania Crystals with Penta-oxygen Coordination. *ACS Applied Energy Materials*, **2018**, 1, 22-26	6.1	11
134	Two-Stage Solid-Phase Transition of Cubic Ice to Hexagonal Ice: Structural Origin and Kinetics. *Journal of Physical Chemistry C*, **2018**, 122, 29009-29016	3.8	10
133	Group-VIII transition metal boride as promising hydrogen evolution reaction catalysts. *Physical Chemistry Chemical Physics*, **2018**, 20, 27752-27757	3.6	11
132	TiH Hydride Formed on Amorphous Black Titania: Unprecedented Active Species for Photocatalytic Hydrogen Evolution. *ACS Catalysis*, **2018**, 8, 9711-9721	13.1	26
131	Atomic structure of boron resolved using machine learning and global sampling. *Chemical Science*, **2018**, 9, 8644-8655	9.4	55
130	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
129	Pressure-induced silica quartz amorphization studied by iterative stochastic surface walking reaction sampling. *Physical Chemistry Chemical Physics*, **2017**, 19, 4725-4733	3.6	16
128	Graphite to Diamond: Origin for Kinetics Selectivity. *Journal of the American Chemical Society*, **2017**, 139, 2545-2548	16.4	33
127	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
126	Inherent Simple Cubic Lattice Being Responsible for Ultrafast Solid-Phase Change of GeSbTe. *Journal of Physical Chemistry Letters*, **2017**, 8, 2560-2564	6.4	10
125	Intrinsic Features of an Ideal Glass. *Chinese Physics Letters*, **2017**, 34, 026402	1.8	7
124	Glassy nature and glass-to-crystal transition in the binary metallic glass CuZr. *Physical Review B*, **2017**, 95,	3.3	5

123	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
122	Material discovery by combining stochastic surface walking global optimization with a neural network. *Chemical Science*, **2017**, 8, 6327-6337	9.4	82
121	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
120	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
119	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
118	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
117	Mechanism and microstructures in Ga2O3 pseudomartensitic solid phase transition. *Physical Chemistry Chemical Physics*, **2016**, 18, 18563-74	3.6	4
116	Anisotropic kinetics of solid phase transition from first principles: alpha-omega phase transformation of Zr. *Physical Chemistry Chemical Physics*, **2016**, 18, 4527-34	3.6	9
115	Energy Landscape and Crystal-to-Crystal Transition of Ternary Silicate Mg2SiO4. *Journal of Physical Chemistry C*, **2016**, 120, 25110-25116	3.8	6
114	Reaction Network of Layer-to-Tunnel Transition of MnO2. *Journal of the American Chemical Society*, **2016**, 138, 5371-9	16.4	79
113	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
112	Structure and water oxidation activity of 3d metal oxides. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 47-64	7.9	17
111	Atomic Structure of Heterophase Junction from Theoretical Prediction. *Topics in Catalysis*, **2015**, 58, 644-654	2.3	15
110	Energy Landscape of Zirconia Phase Transitions. *Journal of the American Chemical Society*, **2015**, 137, 8010-3	16.4	61
109	Three-phase junction for modulating electron-hole migration in anatase-rutile photocatalysts. *Chemical Science*, **2015**, 6, 3483-3494	9.4	73
108	Nature of Rutile Nuclei in Anatase-to-Rutile Phase Transition. *Journal of the American Chemical Society*, **2015**, 137, 11532-9	16.4	74
107	Restructuring and Hydrogen Evolution on Pt Nanoparticle. *Chemical Science*, **2015**, 6, 1485-1490	9.4	50
106	Ultrasonic Electrochemical Reaction on Boron-Doped Diamond Electrodes: Reaction Pathway and Mechanism. *ChemElectroChem*, **2015**, 2, 366-373	4.3	8

105	Reaction sampling and reactivity prediction using the stochastic surface walking method. *Physical Chemistry Chemical Physics*, **2015**, 17, 2757-69	3.6	49
104	First principles Tafel kinetics of methanol oxidation on Pt(111). *Surface Science*, **2015**, 631, 42-47	1.8	26
103	Confined platinum nanoparticle in carbon nanotube: structure and oxidation. *Physical Chemistry Chemical Physics*, **2015**, 17, 2078-87	3.6	15
102	Searching for new TiO₂ crystal phases with better photoactivity. *Journal of Physics Condensed Matter*, **2015**, 27, 134203	1.8	18
101	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
100	Tafel Kinetics of Electrocatalytic Reactions: From Experiment to First-Principles. *ACS Catalysis*, **2014**, 4, 4364-4376	13.1	236
99	Quasi-planar aromatic B36 and B36(-) clusters: all-boron analogues of coronene. *Physical Chemistry Chemical Physics*, **2014**, 16, 18282-7	3.6	73
98	Stochastic surface walking method for crystal structure and phase transition pathway prediction. *Physical Chemistry Chemical Physics*, **2014**, 16, 17845-56	3.6	84
97	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
96	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
95	Design and Observation of Biphase TiO2 Crystal with Perfect Junction. *Journal of Physical Chemistry Letters*, **2014**, 5, 3162-8	6.4	29
94	Chiral gold nanowires with Boerdijk-Coxeter-Bernal structure. *Journal of the American Chemical Society*, **2014**, 136, 12746-52	16.4	49
93	Mechanism and active site of photocatalytic water splitting on titania in aqueous surroundings. *Chemical Science*, **2014**, 5, 2256-2264	9.4	78
92	Observation of an all-boron fullerene. *Nature Chemistry*, **2014**, 6, 727-31	17.6	590
91	Experimental Evidence of Chiral Gold Nanowires with Boerdijk-Coxeter-Bernal Structure by Atomic-Resolution Imaging. *Microscopy and Microanalysis*, **2014**, 20, 1060-1061	0.5	1
90	Electrocatalytic oxygen reduction kinetics on Fe-center of nitrogen-doped graphene. *Physical Chemistry Chemical Physics*, **2014**, 16, 13733-40	3.6	92
89	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
88	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

87	Optimum nanoparticles for electrocatalytic oxygen reduction: the size, shape and new design. *Physical Chemistry Chemical Physics*, **2013**, 15, 18555-61	3.6	42
86	Dual reaction channels for photocatalytic oxidation of phenylmethanol on anatase. *Physical Chemistry Chemical Physics*, **2013**, 15, 1082-7	3.6	10
85	Theoretical modeling of electrode/electrolyte interface from first-principles periodic continuum solvation method. *Catalysis Today*, **2013**, 202, 98-104	5.3	72
84	Enhanced Emission and Analyte Sensing by Cinchonine Iridium(III) Cyclometalated Complexes Bearing Bent Diphosphine Chelators. *Organometallics*, **2013**, 32, 2908-2917	3.8	22
83	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
82	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
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	Stochastic Surface Walking Method for Structure Prediction and Pathway Searching. *Journal of Chemical Theory and Computation*, **2013**, 9, 1838-45	6.4	160
79	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
78	Efficient softest mode finding in transition states calculations. *Journal of Chemical Physics*, **2013**, 138, 094110	3.9	5
77	Investigation on Non-covalent Complexes of Cyclodextrins with Li+ in Gas Phase by Mass Spectrometry. *Chinese Journal of Chemical Physics*, **2013**, 26, 287-294	0.9	4
76	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
75	Searching for active binary rutile oxide catalyst for water splitting from first principles. *Physical Chemistry Chemical Physics*, **2012**, 14, 16612-7	3.6	18
74	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
73	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
72	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
71	Infrared photodissociation spectroscopy of trigonal bipyramidal 19-electron . *Chemical Physics Letters*, **2012**, 542, 33-36	2.5	27
70	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

69	Facile formation and redox of benzoxazole-2-thiolate-bridged dinuclear Pt(II/III) complexes. *Dalton Transactions*, **2012**, 41, 12568-76	4.3	25
68	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
67	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
66	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
65	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
64	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
63	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
62	Mechanism and kinetics for methanol synthesis from CO2/H2 over Cu and Cu/oxide surfaces: Recent investigations by first-principles-based simulation. *Frontiers of Chemistry in China: Selected Publications From Chinese Universities*, **2011**, 6, 164-172		9
61	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
60	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
59	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
58	Must an N-Heterocyclic Carbene Be a Terminal Ligand?. *Organometallics*, **2010**, 29, 2403-2405	3.8	31
57	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
56	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
55	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
54	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
53	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
52	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

51	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
50	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
49	CO2 fixation into methanol at Cu/ZrO2 interface from first principles kinetic Monte Carlo. *Journal of Catalysis*, **2009**, 263, 114-122	7.3	161
48	Oxide-supported single gold catalyst for selective hydrogenation of acrolein predicted from first principles. *Journal of Catalysis*, **2009**, 266, 343-350	7.3	22
47	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
46	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
45	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
44	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
43	Aggregation-induced phosphorescent emission (AIPE) of iridium(III) complexes. *Chemical Communications*, **2008**, 685-7	5.8	234
42	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
41	Local Hybrid Divide-and-Conquer Method for the Computation of Medium and Large Molecules. *Journal of Chemical Theory and Computation*, **2008**, 4, 2049-56	6.4	6
40	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
39	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
38	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
37	Ultrafast Vibrational Dynamics of NO and CO Adsorbed on an Iridium Surface. *Journal of Physical Chemistry C*, **2007**, 111, 14198-14206	3.8	11
36	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
35	A Strange Nickel(I)Nickel(0) Binuclear Complex and Its Unexpected Ethylene Oligomerization. *Organometallics*, **2007**, 26, 2950-2952	3.8	25
34	Coaxial alkaline-earth dimetal units sandwiched between hydrosilver compounds: A DFT Study. *Computational and Theoretical Chemistry*, **2007**, 808, 163-166		5

33	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
32	Single Gold Atoms in Heterogeneous Catalysis: Selective 1,3-Butadiene Hydrogenation over Au/ZrO2. *Angewandte Chemie*, **2006**, 118, 7019-7022	3.6	10
31	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
30	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
29	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
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