Peijun Hu

List of Publications by Citations

218 papers	13,210 citations	64 h-index	109 g-index
224 ext. papers	15,119 ext. citations	8.5 avg, IF	6.73 L-index

#	Paper	IF	Citations
218	CO Oxidation on Pt(111): An Ab Initio Density Functional Theory Study. *Physical Review Letters*, **1998**, 80, 3650-3653	7.4	588
217	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
216	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
215	2D Monolayer MoS□Carbon Interoverlapped Superstructure: Engineering Ideal Atomic Interface for Lithium Ion Storage. *Advanced Materials*, **2015**, 27, 3687-95	24	441
214	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
213	Rational screening low-cost counter electrodes for dye-sensitized solar cells. *Nature Communications*, **2013**, 4, 1583	17.4	340
212	Phosphorus-Mo2C@carbon nanowires toward efficient electrochemical hydrogen evolution: composition, structural and electronic regulation. *Energy and Environmental Science*, **2017**, 10, 1262-1271	35.4	295
211	Catalytic water formation on platinum: a first-principles study. *Journal of the American Chemical Society*, **2001**, 123, 4235-42	16.4	281
210	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
209	Identifying an O2 supply pathway in CO oxidation on Au/TiO2(110): a density functional theory study on the intrinsic role of water. *Journal of the American Chemical Society*, **2006**, 128, 4017-22	16.4	225
208	Local atomic structure modulations activate metal oxide as electrocatalyst for hydrogen evolution in acidic water. *Nature Communications*, **2015**, 6, 8064	17.4	214
207	Iridium single-atom catalyst on nitrogen-doped carbon for formic acid oxidation synthesized using a general host-guest strategy. *Nature Chemistry*, **2020**, 12, 764-772	17.6	207
206	Multiple configurations of the two excess 4f electrons on defective CeO2(111): Origin and implications. *Physical Review B*, **2009**, 79,	3.3	202
205	General trends in CO dissociation on transition metal surfaces. *Journal of Chemical Physics*, **2001**, 114, 8244-8247	3.9	192
204	Understanding complete oxidation of methane on spinel oxides at a molecular level. *Nature Communications*, **2015**, 6, 7798	17.4	178
203	Activity and coke formation of nickel and nickel carbide in dry reforming: A deactivation scheme from density functional theory. *Journal of Catalysis*, **2014**, 311, 469-480	7.3	174
202	Influence of surface structures, subsurface carbon and hydrogen, and surface alloying on the activity and selectivity of acetylene hydrogenation on Pd surfaces: A density functional theory study. *Journal of Catalysis*, **2013**, 305, 264-276	7.3	169

201	Unidirectional suppression of hydrogen oxidation on oxidized platinum clusters. *Nature Communications*, **2013**, 4, 2500	17.4	162
200	Low-Temperature Methane Combustion over Pd/H-ZSM-5: Active Pd Sites with Specific Electronic Properties Modulated by Acidic Sites of H-ZSM-5. *ACS Catalysis*, **2016**, 6, 8127-8139	13.1	154
199	A quantitative determination of reaction mechanisms from density functional theory calculations: Fischer□Tropsch synthesis on flat and stepped cobalt surfaces. *Journal of Catalysis*, **2008**, 254, 285-295	7.3	153
198	Origin of extraordinarily high catalytic activity of Co3O4 and its morphological chemistry for CO oxidation at low temperature. *Journal of Catalysis*, **2012**, 296, 110-119	7.3	146
197	Br□sted□Evans□Polanyi Relation of Multistep Reactions and Volcano Curve in Heterogeneous Catalysis. *Journal of Physical Chemistry C*, **2008**, 112, 1308-1311	3.8	146
196	A robust fuel cell operated on nearly dry methane at 500 □C enabled by synergistic thermal catalysis and electrocatalysis. *Nature Energy*, **2018**, 3, 1042-1050	62.3	142
195	Density Functional Theory Study of Iron and Cobalt Carbides for Fischer□Tropsch Synthesis. *Journal of Physical Chemistry C*, **2010**, 114, 1085-1093	3.8	137
194	Origin of the Increase of Activity and Selectivity of Nickel Doped by Au, Ag, and Cu for Acetylene Hydrogenation. *ACS Catalysis*, **2012**, 2, 1027-1032	13.1	134
193	General trends in the barriers of catalytic reactions on transition metal surfaces. *Journal of Chemical Physics*, **2001**, 115, 4977-4980	3.9	133
192	A Density Functional Theory Study of the Interaction between CO and O on a Pt Surface: CO/Pt(111), O/Pt(111), and CO/O/Pt(111). *Journal of the American Chemical Society*, **1999**, 121, 7644-7652	16.4	133
191	Stable isolated metal atoms as active sites for photocatalytic hydrogen evolution. *Chemistry - A European Journal*, **2014**, 20, 2138-44	4.8	132
190	Identifying the key obstacle in photocatalytic oxygen evolution on rutile TiO2. *Nature Catalysis*, **2018**, 1, 291-299	36.5	131
189	Insight into Microscopic Reaction Pathways in Heterogeneous Catalysis. *Journal of the American Chemical Society*, **2000**, 122, 9866-9867	16.4	131
188	Synergy of Single-Atom Ni and Ru Sites on CeO for Dry Reforming of CH. *Journal of the American Chemical Society*, **2019**, 141, 7283-7293	16.4	120
187	Temperature-Controlled Selectivity of Hydrogenation and Hydrodeoxygenation in the Conversion of Biomass Molecule by the Ru/mpg-CN Catalyst. *Journal of the American Chemical Society*, **2018**, 140, 11161-11164	16.4	120
186	Ordered Porous Nitrogen-Doped Carbon Matrix with Atomically Dispersed Cobalt Sites as an Efficient Catalyst for Dehydrogenation and Transfer Hydrogenation of N-Heterocycles. *Angewandte Chemie - International Edition*, **2018**, 57, 11262-11266	16.4	119
185	Metal/oxide interfacial effects on the selective oxidation of primary alcohols. *Nature Communications*, **2017**, 8, 14039	17.4	115
184	An understanding of chemoselective hydrogenation on crotonaldehyde over Pt(111) in the free energy landscape: The microkinetics study based on first-principles calculations. *Catalysis Today*, **2011**, 165, 71-79	5.3	114

183	Insight into why the Langmuir–Hinshelwood mechanism is generally preferred. *Journal of Chemical Physics*, **2002**, 116, 4379-4381	3.9	106
182	Origin of low CO2 selectivity on platinum in the direct ethanol fuel cell. *Angewandte Chemie - International Edition*, **2012**, 51, 1572-5	16.4	105
181	A density functional theory study of CO and atomic oxygen chemisorption on Pt(111). *Surface Science*, **2000**, 458, 1-14	1.8	105
180	Chain Growth Mechanism in Fischer–Tropsch Synthesis: A DFT Study of C–C Coupling over Ru, Fe, Rh, and Re Surfaces. *Journal of Physical Chemistry C*, **2008**, 112, 6082-6086	3.8	101
179	Utilization of the three-dimensional volcano surface to understand the chemistry of multiphase systems in heterogeneous catalysis. *Journal of the American Chemical Society*, **2008**, 130, 10868-9	16.4	98
178	A Model to Understand the Oxygen Vacancy Formation in Zr-Doped CeO2: Electrostatic Interaction and Structural Relaxation. *Journal of Physical Chemistry C*, **2009**, 113, 10229-10232	3.8	97
177	Structural origin: water deactivates metal oxides to CO oxidation and promotes low-temperature CO oxidation with metals. *Angewandte Chemie - International Edition*, **2012**, 51, 6657-61	16.4	96
176	Origin of Efficient Catalytic Combustion of Methane over Co3O4(110): Active Low-Coordination Lattice Oxygen and Cooperation of Multiple Active Sites. *ACS Catalysis*, **2016**, 6, 5508-5519	13.1	88
175	Physical origin of the high reactivity of subsurface hydrogen in catalytic hydrogenation. *Journal of Chemical Physics*, **1999**, 111, 1343-1345	3.9	88
174	Catalytic hydrogenation of tertiary amides at low temperatures and pressures using bimetallic Pt/Re-based catalysts. *Journal of Catalysis*, **2011**, 283, 89-97	7.3	87
173	CHx hydrogenation on Co(0001): a density functional theory study. *Journal of Chemical Physics*, **2005**, 122, 024711	3.9	84
172	Evidence to challenge the universality of the Horiuti-Polanyi mechanism for hydrogenation in heterogeneous catalysis: origin and trend of the preference of a non-Horiuti-Polanyi mechanism. *Journal of the American Chemical Society*, **2013**, 135, 15244-50	16.4	83
171	Active sites on hydrogen evolution photocatalyst. *Journal of Materials Chemistry A*, **2013**, 1, 15258	13	81
170	Some Understanding of Fischer–Tropsch Synthesis from Density Functional Theory Calculations. *Topics in Catalysis*, **2010**, 53, 326-337	2.3	81
169	Why Must Oxygen Atoms Be Activated from Hollow Sites to Bridge Sites in Catalytic CO Oxidation?. *Journal of the American Chemical Society*, **2000**, 122, 2134-2135	16.4	80
168	A General Mechanism for CO Oxidation on Close-Packed Transition Metal Surfaces. *Journal of the American Chemical Society*, **1999**, 121, 7931-7932	16.4	80
167	A DFT study of the chain growth probability in Fischer–Tropsch synthesis. *Journal of Catalysis*, **2008**, 257, 221-228	7.3	79
166	Deactivation Mechanism of a Au/CeZrO4 Catalyst During a Low-Temperature Water Gas Shift Reaction. *Journal of Physical Chemistry C*, **2007**, 111, 16927-16933	3.8	79

165	A first principles study of methanol decomposition on Pd(111): Mechanisms for OH bond scission and CO bond scission. *Journal of Chemical Physics*, **2001**, 115, 7182-7186	3.9	74
164	Maximizing the localized relaxation: the origin of the outstanding oxygen storage capacity of kappa-Ce2Zr2O8. *Angewandte Chemie - International Edition*, **2009**, 48, 8289-92	16.4	73
163	Insights into the mechanism of nitrobenzene reduction to aniline over Pt catalyst and the significance of the adsorption of phenyl group on kinetics. *Chemical Engineering Journal*, **2016**, 293, 337-344	14.7	72
162	Oxygen vacancy formation in CeO2 and Ce(1-x)Zr(x)O2 solid solutions: electron localization, electrostatic potential and structural relaxation. *Physical Chemistry Chemical Physics*, **2012**, 14, 16521-35	3.6	71
161	Understanding Catalytic Reactions over Zeolites: A Density Functional Theory Study of Selective Catalytic Reduction of NOx by NH3 over Cu-SAPO-34. *ACS Catalysis*, **2016**, 6, 7882-7891	13.1	68
160	Methane transformation to carbon and hydrogen on Pd(100): Pathways and energetics from density functional theory calculations. *Journal of Chemical Physics*, **2002**, 116, 322	3.9	68
159	Understanding the Optimal Adsorption Energies for Catalyst Screening in Heterogeneous Catalysis. *ACS Catalysis*, **2014**, 4, 182-186	13.1	67
158	A First-Principles Study of Oxygenates on Co Surfaces in Fischer Tropsch Synthesis. *Journal of Physical Chemistry C*, **2008**, 112, 9464-9473	3.8	67
157	[1,2,4]Triazolo[1,5-a]pyridine as Building Blocks for Universal Host Materials for High-Performance Red, Green, Blue and White Phosphorescent Organic Light-Emitting Devices. *ACS Applied Materials & Interfaces*, **2018**, 10, 5714-5722	9.5	65
156	Highly electrocatalytic activity of RuO nanocrystals for triiodide reduction in dye-sensitized solar cells. *Small*, **2014**, 10, 484-92, 483	11	65
155	Feedback Kinetics in Mechanochemistry: The Importance of Cohesive States. *Angewandte Chemie - International Edition*, **2017**, 56, 15252-15256	16.4	64
154	A density functional theory study of carbon monoxide oxidation on the Cu3Pt(111) alloy surface: Comparison with the reactions on Pt(111) and Cu(111). *Journal of Chemical Physics*, **2001**, 115, 5272-5277	3.9	64
153	A density functional theory study of the olefin selectivity in Fischer Tropsch synthesis. *Journal of Catalysis*, **2008**, 255, 20-28	7.3	63
152	Role of Water and Adsorbed Hydroxyls on Ethanol Electrochemistry on Pd: New Mechanism, Active Centers, and Energetics for Direct Ethanol Fuel Cell Running in Alkaline Medium. *Journal of Physical Chemistry C*, **2014**, 118, 5762-5772	3.8	62
151	Perspective: Photocatalytic reduction of CO to solar fuels over semiconductors. *Journal of Chemical Physics*, **2017**, 147, 030901	3.9	60
150	An Energy Descriptor To Quantify Methane Selectivity in Fischer Tropsch Synthesis: A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2009**, 113, 8858-8863	3.8	60
149	Recent Advances in Understanding CO Oxidation on Gold Nanoparticles Using Density Functional Theory. *Catalysis Letters*, **2007**, 119, 21-28	2.8	60
148	Mechanism of H2 metabolism on Fe-only hydrogenases. *Journal of Chemical Physics*, **2002**, 117, 8177-8180	3.9	60

147	Molecular-Level Insight into Selective Catalytic Reduction of NOx with NH3 to N2 over a Highly Efficient Bifunctional Va-MnOx Catalyst at Low Temperature. *ACS Catalysis*, **2018**, 8, 4937-4949	13.1	59
146	Hydroprocessing of waste cooking oil over a dispersed nano catalyst: Kinetics study and temperature effect. *Applied Catalysis B: Environmental*, **2014**, 150-151, 238-248	21.8	57
145	Ultralow-temperature CO oxidation on an In2O3-Co3O4 catalyst: a strategy to tune CO adsorption strength and oxygen activation simultaneously. *Chemical Communications*, **2014**, 50, 6835-8	5.8	56
144	Softened C□H modes of adsorbed methyl and their implications for dehydrogenation: An ab initio study. *Journal of Chemical Physics*, **2001**, 114, 2523-2526	3.9	56
143	Mechanistic Study of 1,3-Butadiene Formation in Acetylene Hydrogenation over the Pd-Based Catalysts Using Density Functional Calculations. *Journal of Physical Chemistry C*, **2014**, 118, 1560-1567	3.8	54
142	Identifying the Role of Photogenerated Holes in Photocatalytic Methanol Dissociation on Rutile TiO2(110). *ACS Catalysis*, **2017**, 7, 2374-2380	13.1	52
141	Theory of the kinetics of chemical potentials in heterogeneous catalysis. *Angewandte Chemie - International Edition*, **2011**, 50, 7650-4	16.4	52
140	A density functional theory study of stepwise addition reactions in ammonia synthesis on Ru(0001). *Surface Science*, **2002**, 496, 221-230	1.8	52
139	Quantitative Determination of C□□ Coupling Mechanisms and Detailed Analyses on the Activity and Selectivity for Fischer□ropsch Synthesis on Co(0001): Microkinetic Modeling with Coverage Effects. *ACS Catalysis*, **2019**, 9, 5957-5973	13.1	51
138	A density functional theory study of hydrogen dissociation and diffusion at the perimeter sites of Au/TiO2. *Physical Chemistry Chemical Physics*, **2012**, 14, 3741-5	3.6	51
137	Identification of Active Area as Active Center for CO Oxidation over Single Au Atom Catalyst. *ACS Catalysis*, **2020**, 10, 6094-6101	13.1	50
136	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
135	Selective Hydrogenation of □Unsaturated Aldehydes and Ketones using Novel Manganese Oxide and Platinum Supported on Manganese Oxide Octahedral Molecular Sieves as Catalysts. *ChemCatChem*, **2013**, 5, 506-512	5.2	49
134	Density Functional Theory Studies of Ethanol Decomposition on Rh(211). *Journal of Physical Chemistry C*, **2011**, 115, 22429-22437	3.8	49
133	NO Oxidation on Platinum Group Metals Oxides: First Principles Calculations Combined with Microkinetic Analysis. *Journal of Physical Chemistry C*, **2009**, 113, 18746-18752	3.8	49
132	A density functional theory study of CH2 and H adsorption on Ni(111). *Journal of Chemical Physics*, **2000**, 112, 6006-6014	3.9	49
131	Exchange between sub-surface and surface oxygen vacancies on CeO2(111): a new surface diffusion mechanism. *Chemical Communications*, **2011**, 47, 6105-7	5.8	48
130	Acrolein hydrogenation on Pt(211) and Au(211) surfaces: a density functional theory study. *Physical Chemistry Chemical Physics*, **2011**, 13, 21146-52	3.6	46

129	A first principles study of CH3 dehydrogenation on Ni(111). *Journal of Chemical Physics*, **2000**, 112, 8120-8125	3.9	46
128	Identifying the distinct features of geometric structures for hole trapping to generate radicals on rutile TiO(110) in photooxidation using density functional theory calculations with hybrid functional. *Physical Chemistry Chemical Physics*, **2015**, 17, 1549-55	3.6	45
127	Insight into the NH3-Assisted Selective Catalytic Reduction of NO on MnO2(110): Reaction Mechanism, Activity Descriptor, and Evolution from a Pristine State to a Steady State. *ACS Catalysis*, **2018**, 8, 9269-9279	13.1	45
126	Hydrogenation of S to H2S on Pt(111): A first-principles study. *Journal of Chemical Physics*, **2001**, 115, 8570-8574	3.9	45
125	Selective Hydrogenation of Acetylene over PdBoron Catalysts: A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2014**, 118, 3664-3671	3.8	41
124	Importance of surface carbide formation on the activity and selectivity of Pd surfaces in the selective hydrogenation of acetylene. *Surface Science*, **2016**, 646, 45-49	1.8	40
123	Ethanol Steam Reforming on Rh Catalysts: Theoretical and Experimental Understanding. *ACS Catalysis*, **2014**, 4, 448-456	13.1	38
122	Revealing the Volcano-Shaped Activity Trend of Triiodide Reduction Reaction: A DFT Study Coupled with Microkinetic Analysis. *ACS Catalysis*, **2016**, 6, 733-741	13.1	37
121	Understanding the Dual Active Sites of the FeO/Pt(111) Interface and Reaction Kinetics: Density Functional Theory Study on Methanol Oxidation to Formaldehyde. *ACS Catalysis*, **2017**, 7, 4281-4290	13.1	36
120	Possibility of designing catalysts beyond the traditional volcano curve: a theoretical framework for multi-phase surfaces. *Chemical Science*, **2015**, 6, 5703-5711	9.4	36
119	Catalyst screening: Refinement of the origin of the volcano curve and its implication in heterogeneous catalysis. *Chinese Journal of Catalysis*, **2015**, 36, 1596-1605	11.3	36
118	Reversibility Iteration Method for Understanding Reaction Networks and for Solving Microkinetics in Heterogeneous Catalysis. *ACS Catalysis*, **2016**, 6, 7078-7087	13.1	36
117	Reaction Mechanisms of Crotonaldehyde Hydrogenation on Pt(111): Density Functional Theory and Microkinetic Modeling. *Journal of Physical Chemistry C*, **2011**, 115, 19819-19827	3.8	35
116	Selective hydrogenation of acetylene over Cu(211), Ag(211) and Au(211): HoriutiPolanyi mechanism vs. non-HoriutiPolanyi mechanism. *Catalysis Science and Technology*, **2017**, 7, 1508-1514	5.5	34
115	C-H bond activation over metal oxides: a new insight into the dissociation kinetics from density functional theory. *Journal of Chemical Physics*, **2008**, 128, 051101	3.9	34
114	Elucidating the mechanism and active site of the cyclohexanol dehydrogenation on copper-based catalysts: A density functional theory study. *Surface Science*, **2015**, 640, 181-189	1.8	32
113	Enhancing Metal-Support Interactions by Molybdenum Carbide: An Efficient Strategy toward the Chemoselective Hydrogenation of Unsaturated Aldehydes. *Chemistry - A European Journal*, **2016**, 22, 5698-704	4.8	31
112	Structure and Catalytic Activity of Gold in Low-Temperature CO Oxidation. *Journal of Physical Chemistry C*, **2009**, 113, 6124-6131	3.8	31

111	A density functional theory study of the reaction of C+O, C+N, and C+H on close packed metal surfaces. *Journal of Chemical Physics*, **2001**, 114, 5792-5795	3.9	31
110	Feedback Kinetics in Mechanochemistry: The Importance of Cohesive States. *Angewandte Chemie*, **2017**, 129, 15454-15458	3.6	30
109	Theoretical insight into the selectivities of copper-catalyzing heterogeneous reduction of carbon dioxide. *Science China Chemistry*, **2015**, 58, 553-564	7.9	30
108	Stepwise addition reactions in ammonia synthesis: A first principles study. *Journal of Chemical Physics*, **2001**, 115, 609-611	3.9	30
107	The possibility of single CH bond activation in CH4 on a MoO3-supported Pt catalyst: A density functional theory study. *Journal of Chemical Physics*, **2002**, 116, 4281-4285	3.9	28
106	Turning indium oxide into a superior electrocatalyst: deterministic heteroatoms. *Scientific Reports*, **2013**, 3, 3109	4.9	27
105	Insights into Different Products of Nitrosobenzene and Nitrobenzene Hydrogenation on Pd(111) under Realistic Reaction Conditions. *Journal of Physical Chemistry C*, **2018**, 122, 20337-20350	3.8	25
104	A density functional theory study of CO oxidation on Ru(0001) at low coverage. *Journal of Chemical Physics*, **2000**, 112, 10564-10570	3.9	25
103	Methane activation over a boron nitride catalyst driven by in situ formed molecular water. *Catalysis Science and Technology*, **2018**, 8, 2051-2055	5.5	24
102	Identifying the trend of reactivity for sp2 materials: an electron delocalization model from first principles calculations. *Physical Chemistry Chemical Physics*, **2013**, 15, 9498-502	3.6	24
101	First-Principles Determination of CO Adsorption and Desorption on Pt(111) in the Free Energy Landscape. *Journal of Physical Chemistry C*, **2018**, 122, 21478-21483	3.8	24
100	Theory and applications of surface micro-kinetics in the rational design of catalysts using density functional theory calculations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, 7, e1321	7.9	24
99	Hydrogen Spillover-Bridged Volmer/Tafel Processes Enabling Ampere-Level Current Density Alkaline Hydrogen Evolution Reaction under Low Overpotential.. *Journal of the American Chemical Society*, **2022**,	16.4	24
98	Dispersed Nickel Boosts Catalysis by Copper in CO2 Hydrogenation. *ACS Catalysis*, **2020**, 10, 9261-9270	13.1	23
97	Ordered Porous Nitrogen-Doped Carbon Matrix with Atomically Dispersed Cobalt Sites as an Efficient Catalyst for Dehydrogenation and Transfer Hydrogenation of N-Heterocycles. *Angewandte Chemie*, **2018**, 130, 11432-11436	3.6	23
96	Amorphous Surface PdOX and Its Activity toward Methane Combustion. *ACS Catalysis*, **2019**, 9, 10317-10323	13.1	22
95	Theoretical Study of Heteroatom Doping in Tuning the Catalytic Activity of Graphene for Triiodide Reduction. *ACS Catalysis*, **2016**, 6, 6804-6813	13.1	22
94	Amorphous Catalysis: Machine Learning Driven High-Throughput Screening of Superior Active Site for Hydrogen Evolution Reaction. *Journal of Physical Chemistry C*, **2020**, 124, 10483-10494	3.8	21

93	Insight into Room-Temperature Catalytic Oxidation of Nitric oxide by Cr2O3: A DFT Study. *ACS Catalysis*, **2018**, 8, 5415-5424	13.1	21
92	Significant enhancement of the selectivity of propylene epoxidation for propylene oxide: a molecular oxygen mechanism. *Physical Chemistry Chemical Physics*, **2017**, 19, 25129-25139	3.6	21
91	High energy resolution fluorescence detection XANES an in situ method to study the interaction of adsorbed molecules with metal catalysts in the liquid phase. *Catalysis Science and Technology*, **2013**, 3, 1497	5.5	21
90	A density functional theory study on the water formation at high coverages and the water effect in the Fischer ropsch synthesis. *Molecular Physics*, **2004**, 102, 993-1000	1.7	21
89	CATKINAS: A large-scale catalytic microkinetic analysis software for mechanism auto-analysis and catalyst screening. *Journal of Computational Chemistry*, **2021**, 42, 379-391	3.5	21
88	Activity Trend for Low-Concentration NO Oxidation at Room Temperature on Rutile-Type Metal Oxides. *ACS Catalysis*, **2018**, 8, 10864-10870	13.1	21
87	An understanding and implications of the coverage of surface free sites in heterogeneous catalysis. *Journal of Chemical Physics*, **2009**, 130, 224701	3.9	20
86	Interconversion of hydrated protons at the interface between liquid water and platinum. *Physical Chemistry Chemical Physics*, **2019**, 21, 5932-5940	3.6	20
85	A first-principles microkinetic study on the hydrogenation of carbon dioxide over Cu(211) in the presence of water. *Science China Chemistry*, **2019**, 62, 1686-1697	7.9	19
84	Insight into the solvent effect: a density functional theory study of cisplatin hydrolysis. *Journal of Chemical Physics*, **2006**, 125, 091101	3.9	19
83	Organic horganic-Hybrid-Derived Molybdenum Carbide Nanoladders: Impacts of Surface Oxidation for Hydrogen Evolution Reaction. *ChemNanoMat*, **2018**, 4, 194-202	3.5	19
82	Examination of the key issues in microkinetics: CO oxidation on Rh(1 1 1). *Journal of Catalysis*, **2019**, 379, 52-59	7.3	18
81	Theoretical insight into methanol steam reforming on indium oxide with different coordination environments. *Science China Chemistry*, **2018**, 61, 336-343	7.9	18
80	Ceria foam with atomically thin single-crystal walls. *Angewandte Chemie - International Edition*, **2012** , 51, 3611-5	16.4	18
79	Quantitative Studies of the Key Aspects in Selective Acetylene Hydrogenation on Pd(111) by Microkinetic Modeling with Coverage Effects and Molecular Dynamics. *ACS Catalysis*, **2021**, 11, 4094-4106	13.1	18
78	Unexpected C Bond Cleavage Mechanism in Ethylene Combustion at Low Temperature: Origin and Implications. *ACS Catalysis*, **2016**, 6, 5393-5398	13.1	18
77	Theoretical insights into how the first C-C bond forms in the methanol-to-olefin process catalysed by HSAPO-34. *Physical Chemistry Chemical Physics*, **2016**, 18, 14495-502	3.6	18
76	First-Principles Insight into the Degradation Mechanism of CH3NH3PbI3 Perovskite: Light-Induced Defect Formation and Water Dissociation. *Journal of Physical Chemistry C*, **2018**, 122, 27340-27349	3.8	18

75	Insights into the selective catalytic reduction of NO by NH3 over Mn3O4(110): a DFT study coupled with microkinetic analysis. *Science China Chemistry*, **2018**, 61, 457-467	7.9	18
74	Towards rational catalyst design: a general optimization framework. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2016**, 374,	3	17
73	Insight into CO Activation over Cu(100) under Electrochemical Conditions. *Electrochimica Acta*, **2016**, 190, 446-454	6.7	17
72	Orange Zinc Germanate with Metallic Ge-Ge Bonds as a Chromophore-Like Center for Visible-Light-Driven Water Splitting. *Angewandte Chemie - International Edition*, **2015**, 54, 11467-71	16.4	17
71	Theoretical investigation of NH3-SCR processes over zeolites: A review. *International Journal of Quantum Chemistry*, **2015**, 115, 618-630	2.1	17
70	A DFT study of the transition metal promotion effect on ethylene chemisorption on Co(0 0 0 1). *Surface Science*, **2009**, 603, 2752-2758	1.8	17
69	Insight into the Superior Catalytic Activity of MnO2 for Low-Content NO Oxidation at Room Temperature. *Journal of Physical Chemistry C*, **2018**, 122, 25365-25373	3.8	17
68	Quantitative Studies of the Coverage Effects on Microkinetic Simulations for NO Oxidation on Pt(111). *Journal of Physical Chemistry C*, **2019**, 123, 27594-27602	3.8	16
67	A Simple Method To Locate the Optimal Adsorption Energy for the Best Catalysts Directly. *ACS Catalysis*, **2019**, 9, 2633-2638	13.1	16
66	The mechanism and ligand effects of single atom rhodium supported on ZSM-5 for the selective oxidation of methane to methanol. *Physical Chemistry Chemical Physics*, **2020**, 22, 11686-11694	3.6	15
65	Formulating the bonding contribution equation in heterogeneous catalysis: a quantitative description between the surface structure and adsorption energy. *Physical Chemistry Chemical Physics*, **2017**, 19, 5063-5069	3.6	14
64	A DFT study of direct furfural conversion to 2-methylfuran on the Ru/CoO surface. *Physical Chemistry Chemical Physics*, **2019**, 21, 1597-1605	3.6	14
63	Unique Trapped Dimer State of the Photogenerated Hole in Hybrid Orthorhombic CHNHPbI Perovskite: Identification, Origin, and Implications. *Nano Letters*, **2017**, 17, 7724-7730	11.5	14
62	Insight into chemoselectivity of nitroarene hydrogenation: A DFT-D3 study of nitroarene adsorption on metal surfaces under the realistic reaction conditions. *Applied Surface Science*, **2017**, 392, 456-471	6.7	14
61	Insight into room-temperature catalytic oxidation of NO by CrO2(110): A DFT study. *Chinese Chemical Letters*, **2019**, 30, 618-623	8.1	14
60	Perspective on computational reaction prediction using machine learning methods in heterogeneous catalysis. *Physical Chemistry Chemical Physics*, **2021**, 23, 11155-11179	3.6	14
59	The Effect of H2 and the Presence of hot-O(ads) During the Decomposition of N2O on Platinum. *Catalysis Letters*, **2004**, 94, 103-108	2.8	13
58	High-Loading Single-Atomic-Site Silver Catalysts with an Ag1O2N1 Structure Showing Superior Performance for Epoxidation of Styrene. *ACS Catalysis*, **2021**, 11, 4946-4954	13.1	13

57	DFT study of furfural conversion on a Re/Pt bimetallic surface: synergetic effect on the promotion of hydrodeoxygenation. *Physical Chemistry Chemical Physics*, **2019**, 21, 8384-8393	3.6	12
56	Some Attempts in the Rational Design of Heterogeneous Catalysts Using Density Functional Theory Calculations. *Topics in Catalysis*, **2015**, 58, 633-643	2.3	12
55	Improved Prediction for the Methane Activation Mechanism on Rutile Metal Oxides by a Machine Learning Model with Geometrical Descriptors. *Journal of Physical Chemistry C*, **2019**, 123, 28802-28810	3.8	12
54	Insights into the Staggered Nature of Hydrogenation Reactivity over the 4d Transition Metals. *Journal of Physical Chemistry C*, **2009**, 113, 5222-5227	3.8	12
53	A rational catalyst design of CO oxidation using the bonding contribution equation. *Chemical Communications*, **2017**, 53, 8106-8109	5.8	11
52	Enhanced Interfacial H2 Activation for Nitrostyrene Catalytic Hydrogenation over Rutile Titania-Supported Gold by Coadsorption: A First-Principles Microkinetic Simulation Study. *ACS Catalysis*, **2019**, 9, 11288-11301	13.1	11
51	The dissociation of molecularly adsorbed CO and CN over the 4d transition metals: A universal relationship between the reaction barriers and the reaction enthalpies. *Surface Science*, **2007**, 601, 341-345	1.8	11
50	Identifying the general trend of activity of non-stoichiometric metal oxide phases for CO oxidation on Pd(111). *Science China Chemistry*, **2019**, 62, 784-789	7.9	10
49	Multi sites vs single site for catalytic combustion of methane over Co3O4(110): A first-principles kinetic Monte Carlo study. *Chinese Journal of Catalysis*, **2020**, 41, 1369-1377	11.3	10
48	Density Functional Theory Study on the Cleavage Mechanism of the Carbonyl Bond in Amides on Flat and Stepped Ru Surfaces: Hydrogen-Induced or Direct C□O Bond Breaking?. *Journal of Physical Chemistry C*, **2012**, 116, 18713-18721	3.8	10
47	Achieving rational design of alloy catalysts using a descriptor based on a quantitative structure-energy equation. *Chemical Communications*, **2020**, 56, 3214-3217	5.8	9
46	DFT+U Study on Catalysis by Co3O4: Influence of U Value and a Surface□Bulk Bi-U Strategy. *Journal of Physical Chemistry C*, **2018**, 122, 19593-19602	3.8	9
45	An approach to calculate the free energy changes of surface reactions using free energy decomposition on brute-force molecular dynamics trajectories. *Physical Chemistry Chemical Physics*, **2020**, 22, 21340-21349	3.6	9
44	Quantitative Insights into the Reaction Mechanism for the Direct Synthesis of H2O2 over Transition Metals: Coverage-Dependent Microkinetic Modeling. *ACS Catalysis*, **2021**, 11, 1202-1221	13.1	9
43	A fast species redistribution approach to accelerate the kinetic Monte Carlo simulation for heterogeneous catalysis. *Physical Chemistry Chemical Physics*, **2020**, 22, 7348-7364	3.6	8
42	Identification of the active sites and mechanism for partial methane oxidation to methanol over copper-exchanged CHA zeolites. *Science China Chemistry*, **2020**, 63, 850-859	7.9	8
41	Origin of Low CO2 Selectivity on Platinum in the Direct Ethanol Fuel Cell. *Angewandte Chemie*, **2012** , 124, 1604-1607	3.6	7
40	Understanding supported noble metal catalysts using first-principles calculations. *Journal of Chemical Physics*, **2019**, 151, 180902	3.9	7

39	SSIA: A sensitivity-supervised interlock algorithm for high-performance microkinetic solving. *Journal of Chemical Physics*, **2021**, 154, 024108	3.9	7
38	Interface-tuned selective reductive coupling of nitroarenes to aromatic azo and azoxy: a first-principles-based microkinetics study. *Physical Chemistry Chemical Physics*, **2019**, 21, 12555-12565	3.6	6
37	Hydrogen Coupling on Platinum Using Artificial Neural Network Potentials and DFT. *Journal of Physical Chemistry Letters*, **2021**, 12, 10637-10645	6.4	6
36	An effective structural descriptor to quantify the reactivity of lattice oxygen in CeO subnano-clusters. *Physical Chemistry Chemical Physics*, **2020**, 22, 1721-1726	3.6	6
35	Potential Role of Methanogens in Microbial Reductive Dechlorination of Organic Chlorinated Pollutants. *Environmental Science & Technology*, **2021**, 55, 5917-5928	10.3	6
34	Investigating the innate selectivity issues of methane to methanol: consideration of an aqueous environment. *Chemical Science*, **2021**, 12, 4443-4449	9.4	6
33	Evidence of the O-Pd-O and Pd-O structure units as oxide seeds and their origin on Pd(211): revealing the mechanism of surface oxide formation. *Physical Chemistry Chemical Physics*, **2019**, 21, 6499-6505	3.6	5
32	Accelerating Metadynamics-Based Free-Energy Calculations with Adaptive Machine Learning Potentials. *Journal of Chemical Theory and Computation*, **2021**, 17, 4465-4476	6.4	5
31	Batteries: 2D Monolayer MoS2Carbon Interoverlapped Superstructure: Engineering Ideal Atomic Interface for Lithium Ion Storage (Adv. Mater. 24/2015). *Advanced Materials*, **2015**, 27, 3582-3582	24	4
30	Resolving the Intricate Mechanism and Selectivity of Syngas Conversion on Reduced ZnCr2Ox: A Quantitative Study from DFT and Microkinetic Simulations. *ACS Catalysis*,12977-12988	13.1	4
29	A general doping rule: rational design of Ir-doped catalysts for the oxygen evolution reaction. *Chemical Communications*, **2020**, 56, 15201-15204	5.8	4
28	Unraveling the Photogenerated Electron Localization on the Defect-Free CHNHPbI(001) Surfaces: Understanding and Implications from a First-Principles Study. *Journal of Physical Chemistry Letters*, **2020**, 11, 8041-8047	6.4	4
27	Influence of surface defects on activity and selectivity: a quantitative study of structure sensitivity of Pd catalysts for acetylene hydrogenation. *Catalysis Science and Technology*,	5.5	4
26	Boosting Photocatalytic Water Oxidation Over Bifunctional Rh -Rh Sites. *Angewandte Chemie - International Edition*, **2021**, 60, 22761-22768	16.4	4
25	Understanding the Dynamic Potential Distribution at the Electrode Interface by Stochastic Collision Electrochemistry. *Journal of the American Chemical Society*, **2021**, 143, 12428-12432	16.4	4
24	Gold Segregation Improves Electrocatalytic Activity of Icosahedron Au@Pt Nanocluster: Insights from Machine Learning*Chinese Journal of Chemistry*,	4.9	4
23	Towards the object-oriented design of active hydrogen evolution catalysts on single-atom alloys. *Chemical Science*, **2021**, 12, 10634-10642	9.4	4
22	Solar Cells: Highly Electrocatalytic Activity of RuO2 Nanocrystals for Triiodide Reduction in Dye-Sensitized Solar Cells (Small 3/2014). *Small*, **2014**, 10, 483-483	11	3

21	CO2 Reforming of Ethanol: Density Functional Theory Calculations, Microkinetic Modeling, and Experimental Studies. *ACS Catalysis*, **2020**, 10, 9624-9633	13.1	3
20	Molecular Adsorption Kinetics: Nonlinear Entropy–Enthalpy Loss Quantified by Constrained AIMD and Insights into the Adsorption-Site Determination on Metal Oxides. *Journal of Physical Chemistry C*, **2021**, 125, 10974-10982	3.8	3
19	Rational catalyst design for CO oxidation: a gradient-based optimization strategy. *Catalysis Science and Technology*, **2021**, 11, 2604-2615	5.5	3
18	Breaking through the Peak Height Limit of the Volcano-Shaped Activity Curve for Metal Catalysts: Role of Distinct Surface Structures on Transition Metal Oxides. *Journal of Physical Chemistry C*, **2022** , 126, 183-191	3.8	2
17	General trends in Horiuti-Polanyi mechanism vs non-Horiuti-Polanyi mechanism for water formation on transition metal surfaces. *Chinese Journal of Catalysis*, **2020**, 41, 294-301	11.3	2
16	Screening performance of methane activation over atomically dispersed metal catalysts on defective boron nitride monolayers: A density functional theory study. *Chinese Chemical Letters*, **2021**, 32, 1972-1976	8.1	2
15	Electrochemical CO2 reduction: water/catalyst interface versus polymer/catalyst interface. *Journal of Materials Chemistry A*, **2021**, 9, 17474-17480	13	2
14	Ceria Foam with Atomically Thin Single-Crystal Walls. *Angewandte Chemie*, **2012**, 124, 3671-3675	3.6	1
13	Investigation of inhibition phenomenon on Cu (0 0 1) surface by computer simulation. *Materials Research Innovations*, **2013**, 17, 392-395	1.9	1
12	Discovery of a New Solvent Co-Catalyzed Mechanism in Heterogeneous Catalysis: A First-Principles Study with Molecular Dynamics on Acetaldehyde Hydrogenation on Birnessite.. *Jacs Au*, **2022**, 2, 328-334		1
11	Origin of Water-Induced Deactivation of MnO2-Based Catalyst for Room-Temperature NO Oxidation: A First-Principles Microkinetic Study. *ACS Catalysis*, **2021**, 11, 6835-6845	13.1	1
10	Computational Simulation of Trapped Charge Carriers in TiO2 and Their Impacts on Photocatalytic Water Splitting. *ACS Symposium Series*, **2019**, 67-100	0.4	1
9	Universal Skeleton Feature of the Three-Dimensional Volcano Surface and the Thermodynamic Rule in Locating the Catalyst in Heterogeneous Catalysis. *ACS Catalysis*, **2022**, 12, 247-258	13.1	1
8	A Simple and Ligand-Free Synthesis of Light and Durable Metal-TiO 2 Polymer Films with Enhanced Photocatalytic Properties. *Advanced Materials Interfaces*,2101241	4.6	0
7	Resolving the Two-Track Scaling Trend for Adsorbates on Rutile-Type Metal Oxides: New Descriptors for Adsorption Energies. *Journal of Physical Chemistry C*, **2021**, 125, 23162-23168	3.8	0
6	Boosting Photocatalytic Water Oxidation Over Bifunctional Rh0-Rh3+ Sites. *Angewandte Chemie*, **2021**, 133, 22943	3.6	0
5	Coordination Number-Dependent Complete Oxidation of Methane on NiO Catalysts. *ACS Catalysis*, **2021**, 11, 9837-9849	13.1	0
4	Robust stability analysis for delayed Cohen-Grossberg-type bidirectional associative memory neural networks with norm-bounded uncertainties. *Proceedings of the Institution of Mechanical Engineers Part I: Journal of Systems and Control Engineering*, **2009**, 223, 693-707	1	

3	Molecular Heterogeneous Catalysis. A Conceptual and Computational Approach. Herausgegeben von Rutger A. van Santen und Matthew Neurock.. *Angewandte Chemie*, **2007**, 119, 329-331	3.6
2	Innenr□ktitelbild: Boosting Photocatalytic Water Oxidation Over Bifunctional Rh0-Rh3+ Sites (Angew. Chem. 42/2021). *Angewandte Chemie*, **2021**, 133, 23211	3.6
1	Achieving accuracy and efficiency at the same time: a new kinetic Monte Carlo approach for complicated catalytic systems. *Science China Chemistry*, **2018**, 61, 1479-1480	7.9