Peijun Hu

List of Publications by Year
in descending order

219	17,113	10979	16636
papers	citations	71 h-index	123 g-index

224	224	224	14816
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	CO Oxidation on Pt(111): AnAb InitioDensity Functional Theory Study. Physical Review Letters, 1998, 80, 3650-3653.	2.9	675
2	Identification of General Linear Relationships between Activation Energies and Enthalpy Changes for Dissociation Reactions at Surfaces. Journal of the American Chemical Society, 2003, 125, 3704-3705.	6.6	536
3	General Rules for Predicting Where a Catalytic Reaction Should Occur on Metal Surfaces:Â A Density Functional Theory Study of Câ^'H and Câ^'O Bond Breaking/Making on Flat, Stepped, and Kinked Metal Surfaces. Journal of the American Chemical Society, 2003, 125, 1958-1967.	6.6	534
4	2D Monolayer MoS₂â€“Carbon Interoverlapped Superstructure: Engineering Ideal Atomic Interface for Lithium Ion Storage. Advanced Materials, 2015, 27, 3687-3695.	11.1	504
5	Iridium single-atom catalyst on nitrogen-doped carbon for formic acid oxidation synthesized using a general hostâ€“guest strategy. Nature Chemistry, 2020, 12, 764-772.	6.6	452
6	Catalytic Role of Metal Oxides in Gold-Based Catalysts: A First Principles Study of CO Oxidation onTiO2Supported Au. Physical Review Letters, 2003, 91, 266102.	2.9	392
7	Phosphorus-Mo₂C@carbon nanowires toward efficient electrochemical hydrogen evolution: composition, structural and electronic regulation. Energy and Environmental Science, 2017, 10, 1262-1271.	15.6	379
8	Rational screening low-cost counter electrodes for dye-sensitized solar cells. Nature Communications, 2013, 4, 1583.	5.8	365
9	Catalytic Water Formation on Platinum:â€‰ A First-Principles Study. Journal of the American Chemical Society, 2001, 123, 4235-4242.	6.6	314
10	Synergy of Single-Atom Ni₁ and Ru₁ Sites on CeO₂ for Dry Reforming of CH₄. Journal of the American Chemical Society, 2019, 141, 7283-7293.	6.6	272
11	Local atomic structure modulations activate metal oxide as electrocatalyst for hydrogen evolution in acidic water. Nature Communications, 2015, 6, 8064.	5.8	270
12	A Systematic Study of CO Oxidation on Metals and Metal Oxides:Â Density Functional Theory Calculations. Journal of the American Chemical Society, 2004, 126, 8-9.	6.6	267
13	Identifying an O2Supply Pathway in CO Oxidation on Au/TiO2(110):Â A Density Functional Theory Study on the Intrinsic Role of Water. Journal of the American Chemical Society, 2006, 128, 4017-4022.	6.6	244
14	Understanding complete oxidation of methane on spinel oxides at a molecular level. Nature Communications, 2015, 6, 7798.	5.8	237
15	Multiple configurations of the two excess<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>4</mml:mn><mml:mi>f</mml:mi></mml:mrow></mml:math>electrons on defective<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CeO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms Origin and impl. Physical Review B, 2009, 79, .	1.1	233
16	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.	3.1	231
17	A robust fuel cell operated on nearly dry methane at 500 Â°C enabled by synergistic thermal catalysis and electrocatalysis. Nature Energy, 2018, 3, 1042-1050.	19.8	230
18	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.	3.1	214

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19	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.	5.5	212
20	Identifying the key obstacle in photocatalytic oxygen evolution on rutile TiO2. Nature Catalysis, 2018, 1, 291-299.	16.1	212
21	General trends in CO dissociation on transition metal surfaces. Journal of Chemical Physics, 2001, 114, 8244-8247.	1.2	211
22	BrÃ¸nstedâ^'Evansâ^'Polanyi Relation of Multistep Reactions and Volcano Curve in Heterogeneous Catalysis. Journal of Physical Chemistry C, 2008, 112, 1308-1311.	1.5	201
23	Temperature-Controlled Selectivity of Hydrogenation and Hydrodeoxygenation in the Conversion of Biomass Molecule by the Ru₁/mpg-C₃N₄ Catalyst. Journal of the American Chemical Society, 2018, 140, 11161-11164.	6.6	199
24	Unidirectional suppression of hydrogen oxidation on oxidized platinum clusters. Nature Communications, 2013, 4, 2500.	5.8	197
25	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.	3.1	179
26	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, 144, 6028-6039.	6.6	179
27	Stable Isolated Metal Atoms as Active Sites for Photocatalytic Hydrogen Evolution. Chemistry - A European Journal, 2014, 20, 2138-2144.	1.7	173
28	A quantitative determination of reaction mechanisms from density functional theory calculations: Fischerâ€"Tropsch synthesis on flat and stepped cobalt surfaces. Journal of Catalysis, 2008, 254, 285-295.	3.1	168
29	Ordered Porous Nitrogenâ€Ðoped Carbon Matrix with Atomically Dispersed Cobalt Sites as an Efficient Catalyst for Dehydrogenation and Transfer Hydrogenation of Nâ€Heterocycles. Angewandte Chemie - International Edition, 2018, 57, 11262-11266.	7.2	165
30	Density Functional Theory Study of Iron and Cobalt Carbides for Fischerâ^'Tropsch Synthesis. Journal of Physical Chemistry C, 2010, 114, 1085-1093.	1.5	163
31	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.	5.5	162
32	Insight into why the Langmuirâ€"Hinshelwood mechanism is generally preferred. Journal of Chemical Physics, 2002, 116, 4379-4381.	1.2	152
33	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.	6.6	151
34	Insight into Microscopic Reaction Pathways in Heterogeneous Catalysis. Journal of the American Chemical Society, 2000, 122, 9866-9867.	6.6	146
35	General trends in the barriers of catalytic reactions on transition metal surfaces. Journal of Chemical Physics, 2001, 115, 4977-4980.	1.2	146
36	Metal/oxide interfacial effects on the selective oxidation of primary alcohols. Nature Communications, 2017, 8, 14039.	5.8	144

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37	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.	2.2	142
38	Origin of Low CO₂ Selectivity on Platinum in the Direct Ethanol Fuel Cell. Angewandte Chemie - International Edition, 2012, 51, 1572-1575.	7.2	130
39	Chain Growth Mechanism in Fischerâ˜Tropsch Synthesis:â€‰ A DFT Study of Câ˜C Coupling over Ru, Fe, Rh, and Re Surfaces. Journal of Physical Chemistry C, 2008, 112, 6082-6086.	1.5	123
40	Structural Origin: Water Deactivates Metal Oxides to CO Oxidation and Promotes Lowâ€Temperature CO Oxidation with Metals. Angewandte Chemie - International Edition, 2012, 51, 6657-6661.	7.2	119
41	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, 10868-10869.	6.6	118
42	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.	5.5	116
43	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.	1.5	113
44	A density functional theory study of CO and atomic oxygen chemisorption on Pt(111). Surface Science, 2000, 458, 1-14.	0.8	112
45	Identification of Active Area as Active Center for CO Oxidation over Single Au Atom Catalyst. ACS Catalysis, 2020, 10, 6094-6101.	5.5	106
46	Catalytic hydrogenation of tertiary amides at low temperatures and pressures using bimetallic Pt/Re-based catalysts. Journal of Catalysis, 2011, 283, 89-97.	3.1	104
47	Molecular-Level Insight into Selective Catalytic Reduction of NO_x with NH₃ to N₂ over a Highly Efficient Bifunctional V_a-MnO_x Catalyst at Low Temperature. ACS Catalysis, 2018, 8, 4937-4949.	5.5	103
48	Evidence To Challenge the Universality of the Horiutiâ€“Polanyi Mechanism for Hydrogenation in Heterogeneous Catalysis: Origin and Trend of the Preference of a Non-Horiutiâ€“Polanyi Mechanism. Journal of the American Chemical Society, 2013, 135, 15244-15250.	6.6	101
49	Understanding Catalytic Reactions over Zeolites: A Density Functional Theory Study of Selective Catalytic Reduction of NO_x by NH₃ over Cu-SAPO-34. ACS Catalysis, 2016, 6, 7882-7891.	5.5	99
50	Active sites on hydrogen evolution photocatalyst. Journal of Materials Chemistry A, 2013, 1, 15258.	5.2	96
51	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.	6.6	96
52	Physical origin of the high reactivity of subsurface hydrogen in catalytic hydrogenation. Journal of Chemical Physics, 1999, 111, 1343-1345.	1.2	94
53	CHx hydrogenation on Co(0001): A density functional theory study. Journal of Chemical Physics, 2005, 122, 024711.	1.2	94
54	Deactivation Mechanism of a Au/CeZrO₄ Catalyst During a Low-Temperature Water Gas Shift Reaction. Journal of Physical Chemistry C, 2007, 111, 16927-16933.	1.5	92

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55	A General Mechanism for CO Oxidation on Close-Packed Transition Metal Surfaces. Journal of the American Chemical Society, 1999, 121, 7931-7932.	6.6	90
56	A DFT study of the chain growth probability in Fischerâ€“Tropsch synthesis. Journal of Catalysis, 2008, 257, 221-228.	3.1	88
57	Quantitative Determination of Câ€“C Coupling Mechanisms and Detailed Analyses on the Activity and Selectivity for Fischerâ€“Tropsch Synthesis on Co(0001): Microkinetic Modeling with Coverage Effects. ACS Catalysis, 2019, 9, 5957-5973.	5.5	88
58	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.	6.6	87
59	Some Understanding of Fischerâ€“Tropsch Synthesis from Density Functional Theory Calculations. Topics in Catalysis, 2010, 53, 326-337.	1.3	86
60	Feedback Kinetics in Mechanochemistry: The Importance of Cohesive States. Angewandte Chemie - International Edition, 2017, 56, 15252-15256.	7.2	86
61	Maximizing the Localized Relaxation: The Origin of the Outstanding Oxygen Storage Capacity of Î³â€Ce₂Zr₂O₈. Angewandte Chemie - International Edition, 2009, 48, 8289-8292.	7.2	85
62	[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.	4.0	84
63	Understanding the Optimal Adsorption Energies for Catalyst Screening in Heterogeneous Catalysis. ACS Catalysis, 2014, 4, 182-186.	5.5	81
64	Methane transformation to carbon and hydrogen on Pd(100): Pathways and energetics from density functional theory calculations. Journal of Chemical Physics, 2002, 116, 322.	1.2	80
65	Oxygen vacancy formation in CeO2 and Ce1â^'xZrxO2 solid solutions: electron localization, electrostatic potential and structural relaxation. Physical Chemistry Chemical Physics, 2012, 14, 16521.	1.3	80
66	A first principles study of methanol decomposition on Pd(111): Mechanisms for Oâ€“H bond scission and Câ€“O bond scission. Journal of Chemical Physics, 2001, 115, 7182-7186.	1.2	77
67	A First-Principles Study of Oxygenates on Co Surfaces in Fischerâ^'Tropsch Synthesis. Journal of Physical Chemistry C, 2008, 112, 9464-9473.	1.5	76
68	Identifying the Role of Photogenerated Holes in Photocatalytic Methanol Dissociation on Rutile TiO₂(110). ACS Catalysis, 2017, 7, 2374-2380.	5.5	76
69	Perspective: Photocatalytic reduction of CO2 to solar fuels over semiconductors. Journal of Chemical Physics, 2017, 147, 030901.	1.2	76
70	Insight into the NH₃-Assisted Selective Catalytic Reduction of NO on Î²-MnO₂(110): Reaction Mechanism, Activity Descriptor, and Evolution from a Pristine State to a Steady State. ACS Catalysis, 2018, 8, 9269-9279.	5.5	76
71	Ultralow-temperature CO oxidation on an In₂O₃â€“Co₃O₄ catalyst: a strategy to tune CO adsorption strength and oxygen activation simultaneously. Chemical Communications, 2014, 50, 6835-6838.	2.2	73
72	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.	1.5	73

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73	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.	1.2	72
74	A density functional theory study of the Î±-olefin selectivity in Fischerâ€“Tropsch synthesis. Journal of Catalysis, 2008, 255, 20-28.	3.1	72
75	An Energy Descriptor To Quantify Methane Selectivity in Fischerâ^'Tropsch Synthesis: A Density Functional Theory Study. Journal of Physical Chemistry C, 2009, 113, 8858-8863.	1.5	72
76	Theory of the Kinetics of Chemical Potentials in Heterogeneous Catalysis. Angewandte Chemie - International Edition, 2011, 50, 7650-7654.	7.2	69
77	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.	1.5	68
78	Highly Electrocatalytic Activity of RuO₂ Nanocrystals for Triiodide Reduction in Dyeâ€Sensitized Solar Cells. Small, 2014, 10, 484-492.	5.2	68
79	Insight into association reactions on metal surfaces: Density-functional theory studies of hydrogenation reactions on Rh(111). Journal of Chemical Physics, 2003, 119, 6282-6289.	1.2	66
80	Recent Advances in Understanding CO Oxidation on Gold Nanoparticles Using Density Functional Theory. Catalysis Letters, 2007, 119, 21-28.	1.4	66
81	Hydroprocessing of waste cooking oil over a dispersed nano catalyst: Kinetics study and temperature effect. Applied Catalysis B: Environmental, 2014, 150-151, 238-248.	10.8	65
82	Mechanism of H2 metabolism on Fe-only hydrogenases. Journal of Chemical Physics, 2002, 117, 8177-8180.	1.2	64
83	Reversibility Iteration Method for Understanding Reaction Networks and for Solving Microkinetics in Heterogeneous Catalysis. ACS Catalysis, 2016, 6, 7078-7087.	5.5	64
84	Selective Hydrogenation of Î±,Î²â€Unsaturated Aldehydes and Ketones using Novel Manganese Oxide and Platinum Supported on Manganese Oxide Octahedral Molecular Sieves as Catalysts. ChemCatChem, 2013, 5, 506-512.	1.8	62
85	High-Loading Single-Atomic-Site Silver Catalysts with an Ag₁â€“C₂N₁ Structure Showing Superior Performance for Epoxidation of Styrene. ACS Catalysis, 2021, 11, 4946-4954.	5.5	62
86	Softened Câ€“H modes of adsorbed methyl and their implications for dehydrogenation: An ab initio study. Journal of Chemical Physics, 2001, 114, 2523-2526.	1.2	61
87	A density functional theory study of stepwise addition reactions in ammonia synthesis on Ru(). Surface Science, 2002, 496, 221-230.	0.8	61
88	Catalyst screening: Refinement of the origin of the volcano curve and its implication in heterogeneous catalysis. Chinese Journal of Catalysis, 2015, 36, 1596-1605.	6.9	61
89	Identifying the distinct features of geometric structures for hole trapping to generate radicals on rutile TiO₂(110) in photooxidation using density functional theory calculations with hybrid functional. Physical Chemistry Chemical Physics, 2015, 17, 1549-1555.	1.3	61
90	Density Functional Theory Studies of Ethanol Decomposition on Rh(211). Journal of Physical Chemistry C, 2011, 115, 22429-22437.	1.5	60

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91	Exchange between sub-surface and surface oxygen vacancies on CeO2(111): a new surface diffusion mechanism. Chemical Communications, 2011, 47, 6105.	2.2	58
92	NO Oxidation on Platinum Group Metals Oxides: First Principles Calculations Combined with Microkinetic Analysis. Journal of Physical Chemistry C, 2009, 113, 18746-18752.	1.5	56
93	A first principles study of CH3 dehydrogenation on Ni(111). Journal of Chemical Physics, 2000, 112, 8120-8125.	1.2	53
94	A density functional theory study of CH2 and H adsorption on Ni(111). Journal of Chemical Physics, 2000, 112, 6006-6014.	1.2	52
95	A density functional theory study of hydrogen dissociation and diffusion at the perimeter sites of Au/TiO2. Physical Chemistry Chemical Physics, 2012, 14, 3741.	1.3	52
96	Dispersed Nickel Boosts Catalysis by Copper in CO₂ Hydrogenation. ACS Catalysis, 2020, 10, 9261-9270.	5.5	52
97	Selective Hydrogenation of Acetylene over Pdâ€“Boron Catalysts: A Density Functional Theory Study. Journal of Physical Chemistry C, 2014, 118, 3664-3671.	1.5	51
98	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.	5.5	50
99	Acrolein hydrogenation on Pt(211) and Au(211) surfaces: a density functional theory study. Physical Chemistry Chemical Physics, 2011, 13, 21146.	1.3	48
100	<scp>CATKINAS</scp>: A largeâ€scale catalytic microkinetic analysis software for mechanism autoâ€analysis and catalyst screening. Journal of Computational Chemistry, 2021, 42, 379-391.	1.5	48
101	Hydrogenation of S to H2S on Pt(111): A first-principles study. Journal of Chemical Physics, 2001, 115, 8570-8574.	1.2	46
102	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.	0.8	45
103	Ethanol Steam Reforming on Rh Catalysts: Theoretical and Experimental Understanding. ACS Catalysis, 2014, 4, 448-456.	5.5	44
104	Selective hydrogenation of acetylene over Cu(211), Ag(211) and Au(211): Horiutiâ€“Polanyi mechanism vs. non-Horiutiâ€“Polanyi mechanism. Catalysis Science and Technology, 2017, 7, 1508-1514.	2.1	43
105	Revealing the Volcano-Shaped Activity Trend of Triiodide Reduction Reaction: A DFT Study Coupled with Microkinetic Analysis. ACS Catalysis, 2016, 6, 733-741.	5.5	41
106	Potential Role of Methanogens in Microbial Reductive Dechlorination of Organic Chlorinated Pollutants In Situ. Environmental Science & Technology, 2021, 55, 5917-5928.	4.6	41
107	Possibility of designing catalysts beyond the traditional volcano curve: a theoretical framework for multi-phase surfaces. Chemical Science, 2015, 6, 5703-5711.	3.7	40
108	Enhancing Metalâ€“Support Interactions by Molybdenum Carbide: An Efficient Strategy toward the Chemoselective Hydrogenation of Î±,Î²â€Unsaturated Aldehydes. Chemistry - A European Journal, 2016, 22, 5698-5704.	1.7	40

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109	Reaction Mechanisms of Crotonaldehyde Hydrogenation on Pt(111): Density Functional Theory and Microkinetic Modeling. Journal of Physical Chemistry C, 2011, 115, 19819-19827.	1.5	39
110	Perspective on computational reaction prediction using machine learning methods in heterogeneous catalysis. Physical Chemistry Chemical Physics, 2021, 23, 11155-11179.	1.3	39
111	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.	0.8	38
112	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.	1.5	38
113	Câ€“H bond activation over metal oxides: A new insight into the dissociation kinetics from density functional theory. Journal of Chemical Physics, 2008, 128, 051101.	1.2	37
114	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.	1.5	37
115	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.	5.5	37
116	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.	1.2	35
117	Theoretical Study of Heteroatom Doping in Tuning the Catalytic Activity of Graphene for Triiodide Reduction. ACS Catalysis, 2016, 6, 6804-6813.	5.5	35
118	Theory and applications of surface microâ€kinetics in the rational design of catalysts using density functional theory calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1321.	6.2	35
119	Stepwise addition reactions in ammonia synthesis: A first principles study. Journal of Chemical Physics, 2001, 115, 609-611.	1.2	34
120	Theoretical insight into the selectivities of copper-catalyzing heterogeneous reduction of carbon dioxide. Science China Chemistry, 2015, 58, 553-564.	4.2	34
121	Feedback Kinetics in Mechanochemistry: The Importance of Cohesive States. Angewandte Chemie, 2017, 129, 15454-15458.	1.6	34
122	Methane activation over a boron nitride catalyst driven by in situ formed molecular water. Catalysis Science and Technology, 2018, 8, 2051-2055.	2.1	34
123	Amorphous Surface PdO_X and Its Activity toward Methane Combustion. ACS Catalysis, 2019, 9, 10317-10323.	5.5	34
124	The possibility of single Câ€“H bond activation in CH4 on a MoO3-supported Pt catalyst: A density functional theory study. Journal of Chemical Physics, 2002, 116, 4281-4285.	1.2	33
125	Achieving Theoryâ€“Experiment Parity for Activity and Selectivity in Heterogeneous Catalysis Using Microkinetic Modeling. Accounts of Chemical Research, 2022, 55, 1237-1248.	7.6	33
126	Structure and Catalytic Activity of Gold in Low-Temperature CO Oxidation. Journal of Physical Chemistry C, 2009, 113, 6124-6131.	1.5	32

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127	Insight into Room-Temperature Catalytic Oxidation of Nitric oxide by Cr₂O₃: A DFT Study. ACS Catalysis, 2018, 8, 5415-5424.	5.5	32
128	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.	5.5	32
129	Significant enhancement of the selectivity of propylene epoxidation for propylene oxide: a molecular oxygen mechanism. Physical Chemistry Chemical Physics, 2017, 19, 25129-25139.	1.3	31
130	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.	4.2	31
131	Examination of the key issues in microkinetics: CO oxidation on Rh(1â€¯1â€¯1). Journal of Catalysis, 2019, 379, 52-59.	3.1	31
132	Identifying the trend of reactivity for sp2 materials: an electron delocalization model from first principles calculations. Physical Chemistry Chemical Physics, 2013, 15, 9498.	1.3	30
133	Quantitative Studies of the Coverage Effects on Microkinetic Simulations for NO Oxidation on Pt(111). Journal of Physical Chemistry C, 2019, 123, 27594-27602.	1.5	30
134	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.	1.5	29
135	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.	1.5	29
136	Turning Indium Oxide into a Superior Electrocatalyst: Deterministic Heteroatoms. Scientific Reports, 2013, 3, 3109.	1.6	28
137	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.	1.5	28
138	A density functional theory study of CO oxidation on Ru(0001) at low coverage. Journal of Chemical Physics, 2000, 112, 10564-10570.	1.2	27
139	Unexpected Câ€“C Bond Cleavage Mechanism in Ethylene Combustion at Low Temperature: Origin and Implications. ACS Catalysis, 2016, 6, 5393-5398.	5.5	27
140	Theoretical investigation of NH₃â€SCR processes over zeolites: A review. International Journal of Quantum Chemistry, 2015, 115, 618-630.	1.0	26
141	Activity Trend for Low-Concentration NO Oxidation at Room Temperature on Rutile-Type Metal Oxides. ACS Catalysis, 2018, 8, 10864-10870.	5.5	26
142	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.	4.2	26
143	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.	3.1	25
144	Interconversion of hydrated protons at the interface between liquid water and platinum. Physical Chemistry Chemical Physics, 2019, 21, 5932-5940.	1.3	25

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145	In Operando Identification of In Situ Formed Metalloid Zinc^{Î´+} Active Sites for Highly Efficient Electrocatalyzed Carbon Dioxide Reduction. Angewandte Chemie - International Edition, 2022, 61, .	7.2	25
146	High energy resolution fluorescence detection XANES â€“ 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.	2.1	24
147	Ordered Porous Nitrogenâ€Doped Carbon Matrix with Atomically Dispersed Cobalt Sites as an Efficient Catalyst for Dehydrogenation and Transfer Hydrogenation of Nâ€Heterocycles. Angewandte Chemie, 2018, 130, 11432-11436.	1.6	24
148	A Simple Method To Locate the Optimal Adsorption Energy for the Best Catalysts Directly. ACS Catalysis, 2019, 9, 2633-2638.	5.5	24
149	Understanding the Dynamic Potential Distribution at the Electrode Interface by Stochastic Collision Electrochemistry. Journal of the American Chemical Society, 2021, 143, 12428-12432.	6.6	24
150	Resolving the Intricate Mechanism and Selectivity of Syngas Conversion on Reduced ZnCr₂O_x: A Quantitative Study from DFT and Microkinetic Simulations. ACS Catalysis, 2021, 11, 12977-12988.	5.5	24
151	Organicâ"Inorganicâ€Hybridâ€Derived Molybdenum Carbide Nanoladders: Impacts of Surface Oxidation for Hydrogen Evolution Reaction. ChemNanoMat, 2018, 4, 194-202.	1.5	23
152	Accelerating Metadynamics-Based Free-Energy Calculations with Adaptive Machine Learning Potentials. Journal of Chemical Theory and Computation, 2021, 17, 4465-4476.	2.3	23
153	Towards rational catalyst design: a general optimization framework. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20150078.	1.6	22
154	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.	1.5	22
155	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.	1.3	22
156	Hydrogen Coupling on Platinum Using Artificial Neural Network Potentials and DFT. Journal of Physical Chemistry Letters, 2021, 12, 10637-10645.	2.1	22
157	A density functional theory study on the water formation at high coverages and the water effect in the Fischerâ€"Tropsch synthesis. Molecular Physics, 2004, 102, 993-1000.	0.8	21
158	Insight into the solvent effect: A density functional theory study of cisplatin hydrolysis. Journal of Chemical Physics, 2006, 125, 091101.	1.2	21
159	An understanding and implications of the coverage of surface free sites in heterogeneous catalysis. Journal of Chemical Physics, 2009, 130, 224701.	1.2	21
160	Theoretical insights into how the first Câ€"C bond forms in the methanol-to-olefin process catalysed by HSAPO-34. Physical Chemistry Chemical Physics, 2016, 18, 14495-14502.	1.3	21
161	Theoretical insight into methanol steam reforming on indium oxide with different coordination environments. Science China Chemistry, 2018, 61, 336-343.	4.2	20
162	Insight into room-temperature catalytic oxidation of NO by CrO2(110): A DFT study. Chinese Chemical Letters, 2019, 30, 618-623.	4.8	20

#	Article	IF	Citations
163	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.	4.2	20
164	A DFT study of the transition metal promotion effect on ethylene chemisorption on Co(0001). Surface Science, 2009, 603, 2752-2758.	0.8	19
165	Insight into CO Activation over Cu(100) under Electrochemical Conditions. Electrochimica Acta, 2016, 190, 446-454.	2.6	19
166	Unique Trapped Dimer State of the Photogenerated Hole in Hybrid Orthorhombic CH₃NH₃PbI₃ Perovskite: Identification, Origin, and Implications. Nano Letters, 2017, 17, 7724-7730.	4.5	19
167	Boosting Photocatalytic Water Oxidation Over Bifunctional Rh⁰â€Rh³⁺ Sites. Angewandte Chemie - International Edition, 2021, 60, 22761-22768.	7.2	19
168	Ceria Foam with Atomically Thin Singleâ€Crystal Walls. Angewandte Chemie - International Edition, 2012, 51, 3611-3615.	7.2	18
169	Orange Zinc Germanate with Metallic Geï£¿Ge Bonds as a Chromophoreâ€Like Center for Visibleâ€Lightâ€Driven Water Splitting. Angewandte Chemie - International Edition, 2015, 54, 11467-11471.	7.2	18
170	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.	1.3	18
171	A DFT study of direct furfural conversion to 2-methylfuran on the Ru/Co₃O₄ surface. Physical Chemistry Chemical Physics, 2019, 21, 1597-1605.	1.3	17
172	Influence of surface defects on activity and selectivity: a quantitative study of structure sensitivity of Pd catalysts for acetylene hydrogenation. Catalysis Science and Technology, 0, , .	2.1	17
173	Investigating the innate selectivity issues of methane to methanol: consideration of an aqueous environment. Chemical Science, 2021, 12, 4443-4449.	3.7	17
174	SSIA: A sensitivity-supervised interlock algorithm for high-performance microkinetic solving. Journal of Chemical Physics, 2021, 154, 024108.	1.2	17
175	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.	6.9	16
176	Some Attempts in the Rational Design of Heterogeneous Catalysts Using Density Functional Theory Calculations. Topics in Catalysis, 2015, 58, 633-643.	1.3	15
177	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.	1.3	15
178	The Effect of H2and the Presence of hot-O(ads)During the Decomposition of N2O on Platinum. Catalysis Letters, 2004, 94, 103-108.	1.4	14
179	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.	5.5	14
180	Understanding supported noble metal catalysts using first-principles calculations. Journal of Chemical Physics, 2019, 151, 180902.	1.2	14

#	Article	IF	Citations
181	Insights into the Staggered Nature of Hydrogenation Reactivity over the 4d Transition Metals. Journal of Physical Chemistry C, 2009, 113, 5222-5227.	1.5	13
182	DFT+U Study on Catalysis by Co₃O₄: Influence of U Value and a Surfaceâ€“Bulk Bi-U Strategy. Journal of Physical Chemistry C, 2018, 122, 19593-19602.	1.5	13
183	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.	4.2	13
184	Achieving rational design of alloy catalysts using a descriptor based on a quantitative structureâ€“energy equation. Chemical Communications, 2020, 56, 3214-3217.	2.2	13
185	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.	0.8	12
186	An effective structural descriptor to quantify the reactivity of lattice oxygen in CeO2 subnano-clusters. Physical Chemistry Chemical Physics, 2020, 22, 1721-1726.	1.3	12
187	CO₂ Reforming of Ethanol: Density Functional Theory Calculations, Microkinetic Modeling, and Experimental Studies. ACS Catalysis, 2020, 10, 9624-9633.	5.5	12
188	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.	4.8	12
189	Density Functional Theory Study on the Cleavage Mechanism of the Carbonyl Bond in Amides on Flat and Stepped Ru Surfaces: Hydrogen-Induced or Direct Câ€“O Bond Breaking?. Journal of Physical Chemistry C, 2012, 116, 18713-18721.	1.5	11
190	A rational catalyst design of CO oxidation using the bonding contribution equation. Chemical Communications, 2017, 53, 8106-8109.	2.2	11
191	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.	1.3	10
192	An approach to calculate the free energy changes of surface reactions using free energy decomposition on ab initio brute-force molecular dynamics trajectories. Physical Chemistry Chemical Physics, 2020, 22, 21340-21349.	1.3	10
193	Gold Segregation Improves Electrocatalytic Activity of Icosahedron Au@Pt Nanocluster: Insights from Machine Learning â€. Chinese Journal of Chemistry, 0, , .	2.6	10
194	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.	3.6	10
195	A general doping rule: rational design of Ir-doped catalysts for the oxygen evolution reaction. Chemical Communications, 2020, 56, 15201-15204.	2.2	9
196	A fast species redistribution approach to accelerate the kinetic Monte Carlo simulation for heterogeneous catalysis. Physical Chemistry Chemical Physics, 2020, 22, 7348-7364.	1.3	9
197	Coordination Number-Dependent Complete Oxidation of Methane on NiO Catalysts. ACS Catalysis, 2021, 11, 9837-9849.	5.5	9
198	Towards the object-oriented design of active hydrogen evolution catalysts on single-atom alloys. Chemical Science, 2021, 12, 10634-10642.	3.7	9

#	Article	IF	Citations
199	Subtle Structure Matters: The Vicinity of Surface Ti_{5c} Cations Alters the Photooxidation Behaviors of Anatase and Rutile TiO₂ under Aqueous Environments. ACS Catalysis, 2022, 12, 8242-8251.	5.5	9
200	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.	5.5	8
201	Evidence of the Oâ€“Pdâ€“O and Pdâ€“O₄ 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.	1.3	7
202	Batteries: 2D Monolayer MoS₂â€“Carbon Interoverlapped Superstructure: Engineering Ideal Atomic Interface for Lithium Ion Storage (Adv. Mater. 24/2015). Advanced Materials, 2015, 27, 3582-3582.	11.1	6
203	Unraveling the Photogenerated Electron Localization on the Defect-Free CH3NH3PbI3(001) Surfaces: Understanding and Implications from a First-Principles Study. Journal of Physical Chemistry Letters, 2020, 11, 8041-8047.	2.1	6
204	Molecular Adsorption Kinetics: Nonlinear Entropyâ€“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.	1.5	6
205	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.	5.5	6
206	Rational catalyst design for CO oxidation: a gradient-based optimization strategy. Catalysis Science and Technology, 2021, 11, 2604-2615.	2.1	5
207	Electrochemical CO2 reduction: water/catalyst interface versus polymer/catalyst interface. Journal of Materials Chemistry A, 2021, 9, 17474-17480.	5.2	5
208	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.	6.9	4
209	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.	1.5	4
210	A Simple and Ligandâ€Free Synthesis of Light and Durable Metalâ€TiO₂ Polymer Films with Enhanced Photocatalytic Properties. Advanced Materials Interfaces, 2021, 8, .	1.9	4
211	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.	1.5	4
212	Solar Cells: Highly Electrocatalytic Activity of RuO2Nanocrystals for Triiodide Reduction in Dye-Sensitized Solar Cells (Small 3/2014). Small, 2014, 10, 483-483.	5.2	3
213	Boosting Photocatalytic Water Oxidation Over Bifunctional Rh 0 â€Rh 3+ Sites. Angewandte Chemie, 2021, 133, 22943.	1.6	2
214	Investigation of inhibition phenomenon on Cu (0 0 1) surface by computer simulation. Materials Research Innovations, 2013, 17, 392-395.	1.0	1
215	Computational Simulation of Trapped Charge Carriers in TiO₂ and Their Impacts on Photocatalytic Water Splitting. ACS Symposium Series, 2019, , 67-100.	0.5	1
216	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.	0.7	0

#	Article	IF	Citations
217	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.	4.2	0
218	InnenrÃ¼cktitelbild: Boosting Photocatalytic Water Oxidation Over Bifunctional Rh‹sup›0‹/sup›â€Rh‹sup›3+‹/sup› Sites (Angew. Chem. 42/2021). Angewandte Chemie, 2021, 133, 23211-23211.	1.6	0
219	Operando Metalloid ZnÎ´+ Active Sites for Highly Efficient Carbon Dioxide Reduction Electrocatalysis. Angewandte Chemie, 0, , .	1.6	0