Haijun Jiao

List of Publications by Year
in descending order

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176	13,026	43973	24179
papers	citations	48 h-index	110 g-index

181	181	181	9742
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Nucleus-Independent Chemical Shifts:â€‰A Simple and Efficient Aromaticity Probe. Journal of the American Chemical Society, 1996, 118, 6317-6318.	6.6	5,447
2	Selective Catalytic Hydrogenations of Nitriles, Ketones, and Aldehydes by Well-Defined Manganese Pincer Complexes. Journal of the American Chemical Society, 2016, 138, 8809-8814.	6.6	485
3	Hydrogenation of Esters to Alcohols with a Wellâ€Defined Iron Complex. Angewandte Chemie - International Edition, 2014, 53, 8722-8726.	7.2	269
4	Mild and selective hydrogenation of aromatic and aliphatic (di)nitriles with a well-defined iron pincer complex. Nature Communications, 2014, 5, 4111.	5.8	260
5	Hydrogenation of Esters to Alcohols Catalyzed by Defined Manganese Pincer Complexes. Angewandte Chemie - International Edition, 2016, 55, 15364-15368.	7.2	259
6	Manganese(I)â€Catalyzed Enantioselective Hydrogenation of Ketones Using a Defined Chiral PNP Pincer Ligand. Angewandte Chemie - International Edition, 2017, 56, 11237-11241.	7.2	180
7	A Stable Manganese Pincer Catalyst for the Selective Dehydrogenation of Methanol. Angewandte Chemie - International Edition, 2017, 56, 559-562.	7.2	158
8	Unravelling the Mechanism of Basic Aqueous Methanol Dehydrogenation Catalyzed by Ruâ€“PNP Pincer Complexes. Journal of the American Chemical Society, 2016, 138, 14890-14904.	6.6	155
9	The Mechanism of Potassium Promoter: Enhancing the Stability of Active Surfaces. Angewandte Chemie - International Edition, 2011, 50, 7403-7406.	7.2	141
10	Kinetic aspect of CO2 reforming of CH4 on Ni(111): A density functional theory calculation. Surface Science, 2007, 601, 1271-1284.	0.8	140
11	Control of coordinatively unsaturated Zr sites in ZrO2 for efficient Câ€“H bond activation. Nature Communications, 2018, 9, 3794.	5.8	133
12	In situ formation of ZnOx species for efficient propane dehydrogenation. Nature, 2021, 599, 234-238.	13.7	133
13	CO2Reforming of CH4on Ni(111):Â A Density Functional Theory Calculation. Journal of Physical Chemistry B, 2006, 110, 9976-9983.	1.2	124
14	Formic Acid Dehydrogenation on Ni(111) and Comparison with Pd(111) and Pt(111). Journal of Physical Chemistry C, 2012, 116, 4149-4156.	1.5	115
15	Exploring Furfural Catalytic Conversion on Cu(111) from Computation. ACS Catalysis, 2015, 5, 4020-4032.	5.5	109
16	Stability of Î²-Mo₂C Facets from ab Initio Atomistic Thermodynamics. Journal of Physical Chemistry C, 2011, 115, 22360-22368.	1.5	108
17	Accurate Calculations of Bond Dissociation Enthalpies with Density Functional Methods. Journal of Physical Chemistry A, 2003, 107, 9991-9996.	1.1	107
18	Improved Second Generation Iron Pincer Complexes for Effective Ester Hydrogenation. Advanced Synthesis and Catalysis, 2016, 358, 820-825.	2.1	104

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19	CO dissociation on clean and hydrogen precovered Fe(111) surfaces. Journal of Catalysis, 2007, 249, 174-184.	3.1	102
20	When Density Functional Approximations Meet Iron Oxides. Journal of Chemical Theory and Computation, 2016, 12, 5132-5144.	2.3	102
21	Coverage-Dependent CO Adsorption and Dissociation Mechanisms on Iron Surfaces from DFT Computations. ACS Catalysis, 2014, 4, 1991-2005.	5.5	95
22	Cooperative catalytic methoxycarbonylation of alkenes: uncovering the role of palladium complexes with hemilabile ligands. Chemical Science, 2018, 9, 2510-2516.	3.7	94
23	Surface morphology of HÃgg iron carbide (Ï‡-Fe5C2) from ab initio atomistic thermodynamics. Journal of Catalysis, 2012, 294, 47-53.	3.1	90
24	Hydrogenation of Esters to Alcohols Catalyzed by Defined Manganese Pincer Complexes. Angewandte Chemie, 2016, 128, 15590-15594.	1.6	88
25	Hydrogen Adsorption Structures and Energetics on Iron Surfaces at High Coverage. Journal of Physical Chemistry C, 2014, 118, 4181-4188.	1.5	84
26	The effect of phase composition and crystallite size on activity and selectivity of ZrO2 in non-oxidative propane dehydrogenation. Journal of Catalysis, 2019, 371, 313-324.	3.1	74
27	Density Function Theory Study of CO Adsorption on Fe3O4(111) Surface. Journal of Physical Chemistry B, 2006, 110, 13920-13925.	1.2	73
28	Formation of CHx Species from CO Dissociation on Double-Stepped Co(0001): Exploring Fischerâ˜Tropsch Mechanism. Journal of Physical Chemistry C, 2008, 112, 14108-14116.	1.5	71
29	Iridiumâ€Catalyzed Hydrogenation of Carboxylic Acid Esters. ChemCatChem, 2014, 6, 2810-2814.	1.8	65
30	Manganese(I)â€Catalyzed Enantioselective Hydrogenation of Ketones Using a Defined Chiral PNP Pincer Ligand. Angewandte Chemie, 2017, 129, 11389-11393.	1.6	64
31	Cobalt Pincer Complexes for Catalytic Reduction of Carboxylic Acid Esters. Chemistry - A European Journal, 2018, 24, 1046-1052.	1.7	63
32	A new strategy for the efficient synthesis of 2-methylfuran and Î³-butyrolactone. New Journal of Chemistry, 2003, 27, 208-210.	1.4	62
33	Density Functional Theory Study of CO Adsorption on Fe5C2(001), -(100), and -(110) Surfaces. Journal of Physical Chemistry B, 2004, 108, 9094-9104.	1.2	62
34	Density functional theory study of CO adsorption on the (100), (001) and (010) surfaces of Fe3C. Journal of Molecular Catalysis A, 2007, 269, 169-178.	4.8	60
35	Dissociative Hydrogen Adsorption on the Hexagonal Mo₂C Phase at High Coverage. Journal of Physical Chemistry C, 2014, 118, 8079-8089.	1.5	60
36	Coverage dependent water dissociative adsorption on Fe(110) from DFT computation. Physical Chemistry Chemical Physics, 2015, 17, 8811-8821.	1.3	60

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37	Homogeneous cobalt-catalyzed reductive amination for synthesis of functionalized primary amines. Nature Communications, 2019, 10, 5443.	5.8	57
38	Density functional theory study into the adsorption of CO2, H and CHx (x=0â€“3) as well as C2H4 on Î±-Mo2C(0001). Surface Science, 2006, 600, 2329-2337.	0.8	54
39	High Coverage CO Activation Mechanisms on Fe(100) from Computations. Journal of Physical Chemistry C, 2014, 118, 1095-1101.	1.5	54
40	Cobaltâ€Catalyzed Aqueous Dehydrogenation of Formic Acid. Chemistry - A European Journal, 2019, 25, 8459-8464.	1.7	54
41	Mechanisms and Energies of Water Gas Shift Reaction on Fe-, Co-, and Ni-Promoted MoS₂ Catalysts. Journal of Physical Chemistry C, 2012, 116, 25368-25375.	1.5	53
42	Adsorption Equilibria of CO Coverage on Î²-Mo₂C Surfaces. Journal of Physical Chemistry C, 2012, 116, 6340-6348.	1.5	53
43	Fineâ€Tuning the Reactivity and Stability by Systematic Ligand Variations in CpCo^I Complexes as Catalysts for [2+2+2] Cycloaddition Reactions. Chemistry - A European Journal, 2013, 19, 2548-2554.	1.7	52
44	High Coverage CO Adsorption and Dissociation on the Orthorhombic Mo₂C(100) Surface. Journal of Physical Chemistry C, 2014, 118, 3162-3171.	1.5	52
45	Hydrogenation of Aliphatic and Aromatic Nitriles Using a Defined Ruthenium PNP Pincer Catalyst. European Journal of Organic Chemistry, 2015, 2015, 5944-5948.	1.2	51
46	Mechanisms of Mo2C(101)-Catalyzed Furfural Selective Hydrodeoxygenation to 2-Methylfuran from Computation. ACS Catalysis, 2016, 6, 6790-6803.	5.5	51
47	Determining surface structure and stability of Îµ-Fe2C, Ï‡-Fe5C2, Î¸-Fe3C and Fe4C phases under carburization environment from combined DFT and atomistic thermodynamic studies. Journal of Lithic Studies, 2015, 1, 44-60.	0.1	50
48	High coverage adsorption and co-adsorption of CO and H₂ on Ru(0001) from DFT and thermodynamics. Physical Chemistry Chemical Physics, 2015, 17, 19446-19456.	1.3	50
49	Stability and Reactivity of Intermediates of Methanol Related Reactions and Câ€“C Bond Formation over H-ZSM-5 Acidic Catalyst: A Computational Analysis. Journal of Physical Chemistry C, 2016, 120, 6075-6087.	1.5	50
50	CO2 dissociation on Ni(211). Surface Science, 2009, 603, 2991-2998.	0.8	47
51	High Coverage Water Aggregation and Dissociation on Fe(100): A Computational Analysis. Journal of Physical Chemistry C, 2014, 118, 26139-26154.	1.5	47
52	Structureâ€“Activityâ€“Selectivity Relationships in Propane Dehydrogenation over Rh/ZrO₂ Catalysts. ACS Catalysis, 2020, 10, 6377-6388.	5.5	47
53	Structures and Energies of Coadsorbed CO and H2on Fe5C2(001), Fe5C2(110), and Fe5C2(100). Journal of Physical Chemistry B, 2005, 109, 10922-10935.	1.2	46
54	Unraveling the Origins of the Synergy Effect between ZrO₂ and CrO_x in Supported CrZrO_x for Propene Formation in Nonoxidative Propane Dehydrogenation. ACS Catalysis, 2020, 10, 1575-1590.	5.5	46

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55	Molybdenum carbide catalysed hydrogen production from formic acid â€“ A density functional theory study. Journal of Power Sources, 2014, 246, 548-555.	4.0	45
56	Density Functional Theory Study of Hydrogen Adsorption on Fe5C2(001), Fe5C2(110), and Fe5C2(100). Journal of Physical Chemistry B, 2005, 109, 833-844.	1.2	43
57	Methane formation mechanism in the initial methanol-to-olefins process catalyzed by SAPO-34. Catalysis Science and Technology, 2016, 6, 5526-5533.	2.1	43
58	Chemoselective semihydrogenation of alkynes catalyzed by manganese(<scp>i</scp>)-PNP pincer complexes. Catalysis Science and Technology, 2020, 10, 3994-4001.	2.1	43
59	On the Role of a Cobalt Promoter in a Water-Gas-Shift Reaction on Co-MoS₂. Journal of Physical Chemistry C, 2010, 114, 16669-16676.	1.5	42
60	Reactions of CO, H₂O, CO₂, and H₂ on the Clean and Precovered Fe(110) Surfaces â€“ A DFT Investigation. Journal of Physical Chemistry C, 2015, 119, 28377-28388.	1.5	40
61	The Structure and Possible Catalytic Sites of Mo3S9as a Model of Amorphous Molybdenum Trisulfide:Â A Computational Study. Journal of the American Chemical Society, 2001, 123, 7334-7339.	6.6	39
62	Activation mechanisms of H 2 , O 2 , H 2 O, CO 2 , CO, CH 4 and C 2 H x on metallic Mo 2 C(001) as well as Mo/C terminated Mo 2 C(101) from density functional theory computations. Applied Catalysis A: General, 2016, 524, 223-236.	2.2	39
63	Formation of Carbon Species on Ni(111):â€‰ Structure and Stability. Journal of Physical Chemistry C, 2007, 111, 10894-10903.	1.5	38
64	Hydrogen generation from formic acid decomposition on Ni(211), Pd(211) and Pt(211). Journal of Molecular Catalysis A, 2013, 379, 169-177.	4.8	38
65	A comparative computationally study about the defined m(II) pincer hydrogenation catalysts (mâ€‰=â€‰fe, ru,) Tj ETQq1 1 0.784314	1.5	38
66	Isomerization of Allylic Alcohols to Ketones Catalyzed by Wellâ€Defined Iron PNP Pincer Catalysts. Chemistry - A European Journal, 2018, 24, 4043-4049.	1.7	38
67	Zirconiumâ€Catalyzed Atomâ€Economical Synthesis of 1,1â€Diborylalkanes from Terminal and Internal Alkenes. Angewandte Chemie - International Edition, 2020, 59, 13608-13612.	7.2	38
68	Stable surface terminations of orthorhombic Mo2C catalysts and their CO activation mechanisms. Applied Catalysis A: General, 2014, 478, 146-156.	2.2	37
69	A Stable Manganese Pincer Catalyst for the Selective Dehydrogenation of Methanol. Angewandte Chemie, 2017, 129, 574-577.	1.6	37
70	Enantioselective Hydrogenation of Ketones using Different Metal Complexes with a Chiral PNP Pincer Ligand. Advanced Synthesis and Catalysis, 2019, 361, 1913-1920.	2.1	37
71	Adsorption and Dissociation of CO as Well as CH_x Coupling and Hydrogenation on the Clean and Oxygen Pre-covered Co(0001) Surfaces. Journal of Physical Chemistry C, 2008, 112, 3840-3848.	1.5	36
72	Aerobic Oxidative Homo- and Cross-Coupling of Amines Catalyzed by Phenazine Radical Cations. Journal of Organic Chemistry, 2018, 83, 13481-13490.	1.7	36

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73	Morphology and Reactivity Evolution of HCP and FCC Ru Nanoparticles under CO Atmosphere. ACS Catalysis, 2019, 9, 2768-2776.	5.5	36
74	Morphology control of K2O promoter on HÃgg carbide (Ï‡-Fe5C2) under Fischerâ€“Tropsch synthesis condition. Catalysis Today, 2016, 261, 93-100.	2.2	35
75	Selective Baseâ€free Transfer Hydrogenation of Î±,Î²â€Unsaturated Carbonyl Compounds using iPrOH or EtOH as Hydrogen Source. Chemistry - A European Journal, 2018, 24, 2725-2734.	1.7	34
76	A selective route to aryl-triphosphiranes and their titanocene-induced fragmentation. Chemical Science, 2019, 10, 7859-7867.	3.7	34
77	Density functional theory study of CO adsorption on the Fe(111) surface. Chemical Physics Letters, 2004, 400, 35-41.	1.2	33
78	Density Functional Theory Study of Triangular Molybdenum Sulfide Nanocluster and CO Adsorption on It. Journal of Physical Chemistry B, 2005, 109, 13704-13710.	1.2	33
79	Ligandâ€•and Solventâ€Tuned Chemoselective Carbonylation of Bromoaryl Triflates. Chemistry - A European Journal, 2017, 23, 13369-13378.	1.7	32
80	Exploring the mechanisms of aqueous methanol dehydrogenation catalyzed by defined PNP Mn and Re pincer complexes under base-free as well as strong base conditions. Catalysis Science and Technology, 2018, 8, 3649-3665.	2.1	32
81	Tuning the Selectivity of Palladium Catalysts for Hydroformylation and Semihydrogenation of Alkynes: Experimental and Mechanistic Studies. ACS Catalysis, 2020, 10, 12167-12181.	5.5	31
82	Synthesis of Group 9 Metalâ€Olefin Complexes with Identical Ligand Frameworks and Comparison of their Catalytic Activity in [2+2+2]â€‰Cycloaddition and other Addition Reactions. Advanced Synthesis and Catalysis, 2011, 353, 3423-3433.	2.1	30
83	Energetics of Carbon deposition on Fe(100) and Fe(110) surfaces and subsurfaces. Surface Science, 2012, 606, 733-739.	0.8	30
84	Copper Promotion in CO Adsorption and Dissociation on the Fe(100) Surface. Journal of Physical Chemistry C, 2014, 118, 20472-20480.	1.5	30
85	Theoretical study about Mo₂C(101)-catalyzed hydrodeoxygenation of butyric acid to butane for biomass conversion. Catalysis Science and Technology, 2016, 6, 4923-4936.	2.1	30
86	Location, distribution and acidity of Al substitution in ZSM-5 with different Si/Al ratios â€“ a periodic DFT computation. Catalysis Science and Technology, 2017, 7, 5694-5708.	2.1	30
87	General and selective synthesis of primary amines using Ni-based homogeneous catalysts. Chemical Science, 2020, 11, 4332-4339.	3.7	29
88	Coverage Dependent Water Dissociative Adsorption on the Clean and O-Precovered Fe(111) Surfaces. Journal of Physical Chemistry C, 2015, 119, 11714-11724.	1.5	27
89	1-Titanacyclobuta-2,3-diene â€“ an elusive four-membered cyclic allene. Chemical Science, 2019, 10, 5319-5325.	3.7	26
90	A General and Highly Selective Palladiumâ€Catalyzed Hydroamidation of 1,3â€Diynes. Angewandte Chemie - International Edition, 2021, 60, 371-379.	7.2	26

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91	Efficient Palladiumâ€Catalyzed Carbonylation of 1,3â€Dienes: Selective Synthesis of Adipates and Other Aliphatic Diesters. Angewandte Chemie - International Edition, 2021, 60, 9527-9533.	7.2	26
92	CO Adsorption on Fe₄C (100), (110), and (111) Surfaces in Fischerâ€'Tropsch Synthesis. Journal of Physical Chemistry C, 2008, 112, 19018-19029.	1.5	25
93	Density functional theory study into H2O dissociative adsorption on the Fe5C2(010) surface. Applied Catalysis A: General, 2013, 468, 370-383.	2.2	25
94	Mechanisms of H₂O and CO₂ Formation from Surface Oxygen Reduction on Co(0001). Journal of Physical Chemistry C, 2016, 120, 19265-19270.	1.5	25
95	Mechanism of Graphene Formation via Detonation Synthesis: AÂDFTB Nanoreactor Approach. Journal of Chemical Theory and Computation, 2019, 15, 3654-3665.	2.3	25
96	Surface morphology of orthorhombic Mo2C catalyst and high coverage hydrogen adsorption. Surface Science, 2016, 651, 195-202.	0.8	23
97	Structures of seven molybdenum surfaces and their coverage dependent hydrogen adsorption. Physical Chemistry Chemical Physics, 2016, 18, 6005-6012.	1.3	23
98	Reaction of CO, H₂O, H₂ and CO₂ on the clean as well as O, OH and H precovered Fe(100) and Fe(111) surfaces. Catalysis Science and Technology, 2017, 7, 427-440.	2.1	22
99	Toward Green Acylation of (Hetero)arenes: Palladium-Catalyzed Carbonylation of Olefins to Ketones. ACS Central Science, 2018, 4, 30-38.	5.3	22
100	Kinetics and thermodynamics of polymethylbenzene formation over zeolites with different pore sizes for understanding the mechanisms of methanol to olefin conversion â€“ a computational study. Catalysis Science and Technology, 2016, 6, 5326-5335.	2.1	21
101	Mechanistic Aspects of CO Activation and Câ€“C Bond Formation on the Fe/C- and Fe-Terminated Fe₃C(010) Surfaces. ACS Catalysis, 2020, 10, 877-890.	5.5	21
102	Density functional theory study of H2 adsorption on the (100), (001) and (010) surfaces of Fe3C. Journal of Molecular Catalysis A, 2008, 292, 14-20.	4.8	20
103	Visiting the Limits between a Highly Strained 1â€Zirconacyclobutaâ€2,3â€diene and Chemically Robust Dizirconacyclooctatetraene. Chemistry - A European Journal, 2018, 24, 5667-5674.	1.7	20
104	Visiting CH4 formation and C1â€¯+â€¯C1 couplings to tune CH4 selectivity on Fe surfaces. Journal of Catalysis, 2019, 372, 217-225.	3.1	19
105	Mechanisms of H- and OH-assisted CO activation as well as Câ€“C coupling on the flat Co(0001) surface â€“ revisited. Catalysis Science and Technology, 2016, 6, 8336-8343.	2.1	18
106	Determining the structures, acidity and adsorption properties of Al substituted HZSM-5. Physical Chemistry Chemical Physics, 2019, 21, 18758-18768.	1.3	18
107	Coverage dependent adsorption and co-adsorption of CO and H₂ on the CdI₂-antitype metallic Mo₂C(001) surface. Physical Chemistry Chemical Physics, 2015, 17, 1907-1917.	1.3	17
108	The Facile Dissociation of Carbonâ€“Oxygen Bonds in CO₂and CO on the Surface of LaCoSiH_xIntermetallic Compound. Angewandte Chemie - International Edition, 2021, 60, 25538-25545.	7.2	17

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109	Regiodivergent Reductive Opening of Epoxides by Catalytic Hydrogenation Promoted by a (Cyclopentadienone)iron Complex. ACS Catalysis, 2022, 12, 235-246.	5.5	17
110	Potassium promotion on CO hydrogenation on the Ï‡-Fe 5 C 2 (111) surface with carbon vacancy. Applied Catalysis A: General, 2017, 534, 22-29.	2.2	16
111	About copper promotion in CH 4 formation from CO hydrogenation on Fe(100): A density functional theory study. Applied Catalysis A: General, 2017, 530, 83-92.	2.2	16
112	Benyzl Alcohol Dehydrogenative Coupling Catalyzed by Defined Mn and Re PNP Pincer Complexes â€“ A Computational Mechanistic Study. European Journal of Inorganic Chemistry, 2018, 2018, 4643-4657.	1.0	16
113	About the Inversion Barriers of Pâ€Chirogenic Triarylâ€Substituted Phosphanes. European Journal of Organic Chemistry, 2018, 2018, 2984-2994.	1.2	16
114	Molybdenum carbide supported metal catalysts (M_n/Mo_xC; M = Co, Ni, Cu, Pd,) Tj ETQq0 0 0 rgBT /Overlock 1 3029-3046.	2.1	15
115	Pyrimidopteridine-Catalyzed Hydroamination of Stilbenes with Primary Amines: A Dual Photoredox and Hydrogen Atom Transfer Catalyst. ACS Catalysis, 2021, 11, 4862-4869.	5.5	15
116	Acetylene Hydroformylation with HCo(CO)3 as Catalyst. A Density Functional Study. Organometallics, 2004, 23, 765-773.	1.1	14
117	Adsorption and energetics of H2O molecules and O atoms on the Ï‡-Fe5C2 (111), (â^'411) and (001) surfaces from DFT. Applied Catalysis A: General, 2014, 475, 186-194.	2.2	14
118	Adsorption Structures and Energies of Cun Clusters on the Fe(110) and Fe3C(001) Surfaces. Journal of Physical Chemistry C, 2014, 118, 21963-21974.	1.5	14
119	Surface Morphology of Cu Adsorption on Different Terminations of the HÃgg Iron Carbide (Ï‡-Fe₅C₂) Phase. Journal of Physical Chemistry C, 2015, 119, 7371-7385.	1.5	14
120	Redoxâ€Disproportionation of a Decamethyltitanocene(III) Isonitrile Alkynyl Complex. Chemistry - A European Journal, 2017, 23, 7891-7895.	1.7	14
121	Ironâ€“PNPâ€Pincerâ€Catalyzed Transfer Dehydrogenation of Secondary Alcohols. ChemSusChem, 2019, 12, 2988-2993.	3.6	14
122	Manganese PNP-pincer catalyzed isomerization of allylic/homo-allylic alcohols to ketones â€“ activity, selectivity, efficiency. Catalysis Science and Technology, 2019, 9, 6327-6334.	2.1	14
123	Hydrocracking of Fused Aromatic Hydrocarbons Catalyzed by Al-Substituted HZSM-5â€”A Case Study of 9,10-Dihydroanthracene. ACS Catalysis, 2020, 10, 9215-9226.	5.5	13
124	Zirconium-hydride-catalyzed site-selective hydroboration of amides for the synthesis of amines: Mechanism, scope, and application. Chinese Journal of Catalysis, 2021, 42, 2059-2067.	6.9	13
125	Bifunctional aliphatic PNP pincer catalysts for hydrogenation: Mechanisms and scope. Advances in Inorganic Chemistry, 2019, 73, 323-384.	0.4	13
126	How far away are iron carbide clusters from the bulk?. Physical Chemistry Chemical Physics, 2016, 18, 32944-32951.	1.3	12

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127	Mechanisms of CO Activation, Surface Oxygen Removal, Surface Carbon Hydrogenation, and Câ€“C Coupling on the Stepped Fe(710) Surface from Computation. Journal of Physical Chemistry C, 2018, 122, 15505-15519.	1.5	12
128	Nitridation of the metallic Mo2C(001) surface from NH3 dissociative adsorptionâ€”A DFT study. Surface Science, 2019, 689, 121466.	0.8	12
129	Fe(II) Hydride Complexes for the Homogeneous Dehydrocoupling of Hydrazine Borane: Catalytic Mechanism via DFT Calculations and Detailed Spectroscopic Characterization. Organometallics, 2019, 38, 2714-2723.	1.1	12
130	High-Coverage CO Adsorption and Dissociation on Ir(111), Ir(100), and Ir(110) from Computations. Journal of Physical Chemistry C, 2019, 123, 6487-6495.	1.5	12
131	Structures and energies of Cu clusters on Fe and Fe₃C surfaces from density functional theory computation. Physical Chemistry Chemical Physics, 2014, 16, 26997-27011.	1.3	11
132	Hydrogenation of phenyl-substituted Cî€,N, Cî€N,Cî€,C, Cî€C and Cî€O functional groups by Cr, Mo and W PNP pincer complexes â€“ a DFT study. Catalysis Science and Technology, 2017, 7, 2298-2307.	2.1	11
133	Mechanism of coverage dependent CO adsorption and dissociation on the Mo(100) surface. Physical Chemistry Chemical Physics, 2017, 19, 2186-2192.	1.3	11
134	Successive Dissociation of CO, CH₄, C₂H₆, and CH₃CHO on Fe(110): Retrosynthetic Understanding of FTS Mechanism. Journal of Physical Chemistry C, 2018, 122, 28846-28855.	1.5	11
135	A recyclable CoGa intermetallic compound catalyst for the hydroformylation reaction. Journal of Catalysis, 2021, 404, 244-249.	3.1	11
136	Mechanistic insight into CO activation, methanation and C-C bond formation from coverage dependent CO hydrogenation on Fe(110). Surface Science, 2019, 689, 121456.	0.8	10
137	Synthesis of Phosphinines from Co^{II}-Catalyzed [2+2+2] Cycloaddition Reactions. ACS Catalysis, 2021, 11, 13434-13444.	5.5	10
138	Titanocene Silylpropyne Complexes: Promising Intermediates en route to a Fourâ€Membered 1â€Metallacyclobutaâ€2,3â€diene?. Chemistry - A European Journal, 2017, 23, 14158-14162.	1.7	9
139	Molecular or dissociative adsorption of water on clean and oxygen pre-covered Ni(111) surfaces. Catalysis Science and Technology, 2019, 9, 199-212.	2.1	9
140	CO Self-Promoting Hydrogenation on CO-Saturated Ru(0001): A New Theoretical Insight into How H₂ Participates in CO Activation. Journal of Physical Chemistry C, 2019, 123, 6508-6515.	1.5	9
141	Mechanisms of Co^{II} and Acid Jointly Catalyzed Domino Conversion of CO₂, H₂, and CH₃OH to Dialkoxymethane: A DFT Study. ACS Catalysis, 2021, 11, 6908-6919.	5.5	9
142	Adsorption and dissociation of H 2 O and CO 2 on the clean and O-pre-covered Ru(0001) surface. Applied Catalysis A: General, 2017, 540, 31-36.	2.2	8
143	Exploring the activities of vanadium, niobium, and tantalumÂPNP pincer complexes in the hydrogenation of phenyl-substituted CN, CN, CC, CC, and CO functional groups. Comptes Rendus Chimie, 2018, 21, 303-309.	0.2	8
144	Coverage dependent structure and energy of water dissociative adsorption on clean and O-pre-covered Ni (100) and Ni(110). Catalysis Science and Technology, 2019, 9, 4725-4743.	2.1	8

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145	Hydrogen Adsorption on Ir(111), Ir(100) and Ir(110)â€"Surface and Coverage Dependence. Surface Science, 2020, 692, 121514.	0.8	8
146	Versatile Fluorinated Building Blocks by Stereoselective (Per)fluoroalkenylation of Ketones. European Journal of Organic Chemistry, 2020, 2020, 70-81.	1.2	8
147	Dehydropolymerisation of methylamine borane using highly active rhodium(<scp>iii</scp>) bis(thiophosphinite) pincer complexes: catalytic and mechanistic insights. Catalysis Science and Technology, 2021, 11, 3514-3526.	2.1	8
148	Cycloaddition mechanisms of CO₂ and epoxide catalyzed by salophen â€" an organocatalyst free from metals and halides. Catalysis Science and Technology, 2021, 11, 2529-2539.	2.1	8
149	Zirconiumâ€Catalyzed Atomâ€Economical Synthesis of 1,1â€Diborylalkanes from Terminal and Internal Alkenes. Angewandte Chemie, 2020, 132, 13710-13714.	1.6	7
150	A General and Highly Selective Palladiumâ€Catalyzed Hydroamidation of 1,3â€Diynes. Angewandte Chemie, 2021, 133, 375-383.	1.6	7
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