Hai-Yan Su

List of Publications by Year
in descending order

48 papers	7,175 citations	212478 28 h-index	232693 48 g-index
50 all docs	50 docs citations	50 times ranked	10775 citing authors

#	Article	IF	Citations
1	Finding Key Factors for Efficient Water and Methanol Activation at Metals, Oxides, MXenes, and Metal/Oxide Interfaces. ACS Catalysis, 2022, 12, 1237-1246.	5.5	5
2	Single-atom metal tuned sulfur vacancy for efficient H2 activation and hydrogen evolution reaction on MoS2 basal plane. Applied Surface Science, 2022, 597, 153614.	3.1	9
3	Photochemical construction of the ZnCdS/PO/FeCoNiPiâ€“MnO composite for efficient tandem application of photocatalytic partial water splitting and overall water splitting. Journal of Materials Chemistry A, 2022, 10, 16029-16036.	5.2	5
4	A synergetic effect between a single Cu site and S vacancy on an MoS₂ basal plane for methanol synthesis from syngas. Catalysis Science and Technology, 2021, 11, 3261-3269.	2.1	7
5	Bridge sulfur vacancies in MoS2 catalyst for reverse water gas shift: A first-principles study. Applied Surface Science, 2021, 561, 149925.	3.1	12
6	Synthesis of Iron-Carbide Nanoparticles: Identification of the Active Phase and Mechanism of Fe-Based Fischerâ€“Tropsch Synthesis. CCS Chemistry, 2021, 3, 2712-2724.	4.6	41
7	Mechanistic Insights into Direct Methane Oxidation to Methanol on Single-Atom Transition-Metal-Modified Graphyne. ACS Applied Nano Materials, 2021, 4, 12006-12016.	2.4	17
8	Highly Selective Production of Ethylene by the Electroreduction of Carbon Monoxide. Angewandte Chemie, 2020, 132, 160-166.	1.6	13
9	Highly Selective Production of Ethylene by the Electroreduction of Carbon Monoxide. Angewandte Chemie - International Edition, 2020, 59, 154-160.	7.2	68
10	Frontispiece: Highly Selective Production of Ethylene by the Electroreduction of Carbon Monoxide. Angewandte Chemie - International Edition, 2020, 59, .	7.2	0
11	Frontispiz: Highly Selective Production of Ethylene by the Electroreduction of Carbon Monoxide. Angewandte Chemie, 2020, 132, .	1.6	0
12	Application of coverage-dependent micro-kinetic study to investigate direct H2O2 synthesis mechanism on Pd(111) surface. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	4
13	Trends in Câ€“O and Nâ€“O bond scission on rutile oxides described using oxygen vacancy formation energies. Chemical Science, 2020, 11, 4119-4124.	3.7	16
14	Intermediate Adsorption States Switch to Selectively Catalyze Electrochemical CO₂ Reduction. ACS Catalysis, 2020, 10, 3871-3880.	5.5	89
15	CO activation and methanation mechanism on hexagonal close-packed Co catalysts: effect of functionals, carbon deposition and surface structure. Catalysis Science and Technology, 2020, 10, 3387-3398.	2.1	5
16	Facet-Dependent of Catalytic Selectivity: The Case of H₂O₂ Direct Synthesis on Pd Surfaces. Journal of Physical Chemistry C, 2019, 123, 26324-26337.	1.5	34
17	Single Ru Sites-Embedded Rutile TiO2 Catalyst for Non-Oxidative Direct Conversion of Methane: A First-Principles Study. Journal of Physical Chemistry C, 2019, 123, 14391-14397.	1.5	13
18	Influence of Cobalt Crystal Structures on Activation of Nitrogen Molecule: A First-Principles Study. Journal of Physical Chemistry C, 2019, 123, 10956-10966.	1.5	19

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19	Room-temperature electrochemical waterâ€“gas shift reaction for high purity hydrogen production. Nature Communications, 2019, 10, 86.	5.8	62
20	First-Principles and Microkinetic Simulation Studies of the Structure Sensitivity of Cu Catalyst for Methanol Steam Reforming. Journal of Physical Chemistry C, 2018, 122, 10811-10819.	1.5	20
21	First-Principles microkinetic study of methanol synthesis on Cu(221) and ZnCu(221) surfaces. Chinese Journal of Chemical Physics, 2018, 31, 284-290.	0.6	13
22	Structures and stability of adsorbed methanol on TiO2(110) surface studied by ab initio thermodynamics and kinetic Monte Carlo simulation. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	4
23	Chemical Insights into the Design and Development of Face-Centered Cubic Ruthenium Catalysts for Fischerâ€“Tropsch Synthesis. Journal of the American Chemical Society, 2017, 139, 2267-2276.	6.6	147
24	First-principles study of structure sensitivity of chain growth and selectivity in Fischerâ€“Tropsch synthesis using HCP cobalt catalysts. Catalysis Science and Technology, 2017, 7, 2967-2977.	2.1	30
25	Theoretical Insights and the Corresponding Construction of Supported Metal Catalysts for Highly Selective CO₂ to CO Conversion. ACS Catalysis, 2017, 7, 4613-4620.	5.5	104
26	Differentiating Intrinsic Reactivity of Copper, Copperâ€“Zinc Alloy, and Copper/Zinc Oxide Interface for Methanol Steam Reforming by First-Principles Theory. Journal of Physical Chemistry C, 2017, 121, 21553-21559.	1.5	37
27	Establishing and Understanding Adsorptionâ€“Energy Scaling Relations with Negative Slopes. Journal of Physical Chemistry Letters, 2016, 7, 5302-5306.	2.1	43
28	CO Dissociation on Face-Centered Cubic and Hexagonal Close-Packed Nickel Catalysts: A First-Principles Study. Journal of Physical Chemistry C, 2016, 120, 24895-24903.	1.5	52
29	High Alcohols Synthesis via Fischerâ€“Tropsch Reaction at Cobalt Metal/Carbide Interface. ACS Catalysis, 2015, 5, 3620-3624.	5.5	231
30	DFT study of the stability of oxygen vacancy in cubic ABO3 perovskites. Journal of Materials Science, 2015, 50, 1701-1709.	1.7	45
31	A Firstâ€Principles Study of Carbonâ€“Oxygen Bond Scission in Multiatomic Molecules on Flat and Stepped Metal Surfaces. ChemCatChem, 2014, 6, 1755-1762.	1.8	13
32	Stability of polar ZnO surfaces studied by pair potential method and local energy density method. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	10
33	Single Pd Atom Embedded in CeO₂(111) for NO Reduction with CO: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 12216-12223.	1.5	98
34	Structure sensitivity of CO methanation on Co (0001), and surfaces: Density functional theory calculations. Catalysis Today, 2013, 215, 36-42.	2.2	72
35	Crystallographic Dependence of CO Activation on Cobalt Catalysts: HCP versus FCC. Journal of the American Chemical Society, 2013, 135, 16284-16287.	6.6	348
36	Number of outer electrons as descriptor for adsorption processes on transition metals and their oxides. Chemical Science, 2013, 4, 1245.	3.7	273

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37	Platinum-Modulated Cobalt Nanocatalysts for Low-Temperature Aqueous-Phase Fischerâ€“Tropsch Synthesis. Journal of the American Chemical Society, 2013, 135, 4149-4158.	6.6	116
38	Identifying active surface phases for metal oxide electrocatalysts: a study of manganese oxide bi-functional catalysts for oxygen reduction and water oxidation catalysis. Physical Chemistry Chemical Physics, 2012, 14, 14010.	1.3	332
39	CO Oxidation at the Perimeters of an FeO/Pt(111) Interface and how Water Promotes the Activity: A Firstâ€Principles Study. ChemSusChem, 2012, 5, 871-878.	3.6	37
40	Force reversed method for locating transition states. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	63
41	Rh-Decorated Cu Alloy Catalyst for Improved C₂Oxygenate Formation from Syngas. Journal of Physical Chemistry C, 2011, 115, 18247-18256.	1.5	62
42	Universality in Oxygen Evolution Electrocatalysis on Oxide Surfaces. ChemCatChem, 2011, 3, 1159-1165.	1.8	3,208
43	Tailoring the Activity for Oxygen Evolution Electrocatalysis on Rutile TiO₂(110) by Transitionâ€Metal Substitution. ChemCatChem, 2011, 3, 1607-1611.	1.8	169
44	Carbon Chain Growth by Formyl Insertion on Rhodium and Cobalt Catalysts in Syngas Conversion. Angewandte Chemie - International Edition, 2011, 50, 5335-5338.	7.2	105
45	Carbon monoxide adsorption and dissociation on Mn-decorated Rh(111) and Rh(553) surfaces: A first-principles study. Catalysis Today, 2011, 160, 228-233.	2.2	26
46	Interface-Confined Ferrous Centers for Catalytic Oxidation. Science, 2010, 328, 1141-1144.	6.0	866
47	The Effect of Water on the CO Oxidation on Ag(111) and Au(111) Surfaces: A First-Principle Study. Journal of Physical Chemistry C, 2008, 112, 17303-17310.	1.5	160
48	Modulating the reactivity of Ni-containing Pt(111)-skin catalysts by density functional theory calculations. Journal of Chemical Physics, 2008, 128, 194707.	1.2	46