Jin-Xun Liu

List of Publications by Year
in descending order

50	3,986	147726 31	182361 51
papers	citations	h-index	g-index

51	51	51	4899
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Activity and Selectivity Trends in Electrocatalytic Nitrate Reduction on Transition Metals. ACS Catalysis, 2019, 9, 7052-7064.	5.5	369
2	Atomistic Theory of Ostwald Ripening and Disintegration of Supported Metal Particles under Reaction Conditions. Journal of the American Chemical Society, 2013, 135, 1760-1771.	6.6	352
3	Crystallographic Dependence of CO Activation on Cobalt Catalysts: HCP versus FCC. Journal of the American Chemical Society, 2013, 135, 16284-16287.	6.6	348
4	Machine learning for heterogeneous catalyst design and discovery. AICHE Journal, 2018, 64, 2311-2323.	1.8	258
5	High Alcohols Synthesis via Fischerâ€“Tropsch Reaction at Cobalt Metal/Carbide Interface. ACS Catalysis, 2015, 5, 3620-3624.	5.5	231
6	Surpassing the single-atom catalytic activity limit through paired Pt-O-Pt ensemble built from isolated Pt1 atoms. Nature Communications, 2019, 10, 3808.	5.8	225
7	Structure Sensitivity of Auâ€TiO₂ Strong Metalâ€“Support Interactions. Angewandte Chemie - International Edition, 2021, 60, 12074-12081.	7.2	161
8	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
9	Optimum Cu nanoparticle catalysts for CO2 hydrogenation towards methanol. Nano Energy, 2018, 43, 200-209.	8.2	133
10	A Linear Scaling Relation for CO Oxidation on CeO₂-Supported Pd. Journal of the American Chemical Society, 2018, 140, 4580-4587.	6.6	126
11	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
12	Stable Pd-Doped Ceria Structures for CH₄ Activation and CO Oxidation. ACS Catalysis, 2018, 8, 75-80.	5.5	111
13	Theoretical Approach To Predict the Stability of Supported Single-Atom Catalysts. ACS Catalysis, 2019, 9, 3289-3297.	5.5	101
14	Highly Active and Stable CH₄ Oxidation by Substitution of Ce⁴⁺ by Two Pd²⁺ Ions in CeO₂(111). ACS Catalysis, 2018, 8, 6552-6559.	5.5	90
15	Particle Size and Crystal Phase Effects in Fischer-Tropsch Catalysts. Engineering, 2017, 3, 467-476.	3.2	87
16	Structural and electronic properties of cobalt carbide Co2C and its surface stability: Density functional theory study. Surface Science, 2012, 606, 598-604.	0.8	79
17	Robust Phase Control through Hetero-Seeded Epitaxial Growth for Face-Centered Cubic Pt@Ru Nanotetrahedrons with Superior Hydrogen Electro-Oxidation Activity. Journal of Physical Chemistry C, 2015, 119, 17697-17706.	1.5	73
18	Structure sensitivity of CO methanation on Co (0001), and surfaces: Density functional theory calculations. Catalysis Today, 2013, 215, 36-42.	2.2	72

#	Article	IF	Citations
19	Theoretical Study of Ripening Mechanisms of Pd Clusters on Ceria. Chemistry of Materials, 2017, 29, 9456-9462.	3.2	67
20	Charge Transport over the Defective CeO₂(111) Surface. Chemistry of Materials, 2016, 28, 5652-5658.	3.2	52
21	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
22	Carbon Monoxide Activation on Cobalt Carbide for Fischerâ€“Tropsch Synthesis from First-Principles Theory. ACS Catalysis, 2019, 9, 8093-8103.	5.5	47
23	Optimum Particle Size for Gold-Catalyzed CO Oxidation. Journal of Physical Chemistry C, 2018, 122, 8327-8340.	1.5	45
24	Stability of heterogeneous single-atom catalysts: a scaling law mapping thermodynamics to kinetics. Npj Computational Materials, 2020, 6, .	3.5	44
25	Coâ€“Co₂C and Coâ€“Co₂C/AC Catalysts for Hydroformylation of 1-Hexene under Low Pressure: Experimental and Theoretical Studies. Journal of Physical Chemistry C, 2014, 118, 19114-19122.	1.5	41
26	Atomically dispersed Ir/Î±-MoC catalyst with high metal loading and thermal stability for water-promoted hydrogenation reaction. National Science Review, 2022, 9, nwab026.	4.6	41
27	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
28	Two-to-three dimensional transition in neutral gold clusters: The crucial role of van der Waals interactions and temperature. Physical Review Materials, 2019, 3, .	0.9	40
29	Compensation between Surface Energy and hcp/fcc Phase Energy of Late Transition Metals from First-Principles Calculations. Journal of Physical Chemistry C, 2020, 124, 11005-11014.	1.5	37
30	Theoretical study of crystal phase effect in heterogeneous catalysis. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 571-583.	6.2	36
31	Understanding the Impact of Defects on Catalytic CO Oxidation of LaFeO₃-Supported Rh, Pd, and Pt Single-Atom Catalysts. Journal of Physical Chemistry C, 2019, 123, 7290-7298.	1.5	36
32	Transition metal doping of Pd(1 1 1) for the NOâ€¯+â€¯CO reaction. Journal of Catalysis, 2018, 363, 154-163.	3.1	34
33	First-principles microkinetics simulations of electrochemical reduction of CO2 over Cu catalysts. Electrochimica Acta, 2020, 335, 135665.	2.6	32
34	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
35	Reconstruction of the Wet Chemical Synthesis Process: The Case of Fe₅C₂ Nanoparticles. Journal of Physical Chemistry C, 2017, 121, 5154-5160.	1.5	24
36	Amine-ligand modulated ruthenium nanoclusters as a superior bi-functional hydrogen electrocatalyst in alkaline media. Journal of Materials Chemistry A, 2021, 9, 22934-22942.	5.2	24

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37	Interplay Between Site Activity and Density of BCC Iron for Ammonia Synthesis Based on Firstâ€Principles Theory. ChemCatChem, 2019, 11, 1928-1934.	1.8	20
38	Nitrogen-doped graphene layers for electrochemical oxygen reduction reaction boosted by lattice strain. Journal of Catalysis, 2019, 378, 113-120.	3.1	19
39	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
40	Carbon induced selective regulation of cobalt-based Fischerâ€“Tropsch catalysts by ethylene treatment. Faraday Discussions, 2017, 197, 207-224.	1.6	17
41	CO oxidation on Rh-doped hexadecagold clusters. Catalysis Science and Technology, 2017, 7, 75-83.	2.1	15
42	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
43	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
44	Hydroxyl improving the activity, selectivity and stability of supported Ni single atoms for selective semi-hydrogenation. Chemical Science, 2021, 12, 10290-10298.	3.7	13
45	H₂ Activation on Pristine and Substitutional ZnO(101Ì…0) and Cr₂O₃(001) Surfaces by Density Functional Theory Calculations. Journal of Physical Chemistry C, 2022, 126, 9059-9068.	1.5	13
46	Structure Sensitivity of Auâ€TiO 2 Strong Metalâ€“Support Interactions. Angewandte Chemie, 2021, 133, 12181-12188.	1.6	11
47	Morphology Evolution of FCC and HCP Cobalt Induced by a CO Atmosphere from Ab Initio Thermodynamics. Journal of Physical Chemistry C, 2020, 124, 23200-23209.	1.5	10
48	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
49	Crystallographic and morphological sensitivity of N2 activation over ruthenium. Chinese Journal of Chemical Physics, 2021, 34, 263-272.	0.6	4
50	Achieving anti-sintering of supported platinum nanoparticles using a thermal management strategy. Science China Materials, 2021, 64, 1930-1938.	3.5	1