Ziyun Wang

List of Publications by Year
in descending order

60	8,607	87888 38	138484 58
papers	citations	h-index	g-index

64	64	64	6735
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Accelerated discovery of CO2 electrocatalysts using active machine learning. Nature, 2020, 581, 178-183.	27.8	807
2	Molecular tuning of CO2-to-ethylene conversion. Nature, 2020, 577, 509-513.	27.8	682
3	Enhanced Nitrate-to-Ammonia Activity on Copperâ€“Nickel Alloys via Tuning of Intermediate Adsorption. Journal of the American Chemical Society, 2020, 142, 5702-5708.	13.7	638
4	High-valence metals improve oxygen evolution reaction performance by modulating 3d metal oxidation cycle energetics. Nature Catalysis, 2020, 3, 985-992.	34.4	390
5	Cooperative CO2-to-ethanol conversion via enriched intermediates at moleculeâ€“metal catalyst interfaces. Nature Catalysis, 2020, 3, 75-82.	34.4	390
6	Efficient electrically powered CO2-to-ethanol via suppression of deoxygenation. Nature Energy, 2020, 5, 478-486.	39.5	363
7	Copper nanocavities confine intermediates for efficient electrosynthesis of C3 alcohol fuels from carbon monoxide. Nature Catalysis, 2018, 1, 946-951.	34.4	354
8	Binding Site Diversity Promotes CO₂ Electroreduction to Ethanol. Journal of the American Chemical Society, 2019, 141, 8584-8591.	13.7	338
9	Catalyst synthesis under CO2 electroreduction favours faceting and promotes renewable fuels electrosynthesis. Nature Catalysis, 2020, 3, 98-106.	34.4	325
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.	13.7	272
11	Understanding complete oxidation of methane on spinel oxides at a molecular level. Nature Communications, 2015, 6, 7798.	12.8	237
12	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.	6.2	231
13	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.	39.5	230
14	Constraining CO coverage on copper promotes high-efficiency ethylene electroproduction. Nature Catalysis, 2019, 2, 1124-1131.	34.4	214
15	Stabilizing Highly Active Ru Sites by Suppressing Lattice Oxygen Participation in Acidic Water Oxidation. Journal of the American Chemical Society, 2021, 143, 6482-6490.	13.7	204
16	Hydroxide promotes carbon dioxide electroreduction to ethanol on copper via tuning of adsorbed hydrogen. Nature Communications, 2019, 10, 5814.	12.8	201
17	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.	13.7	199
18	High carbon utilization in CO2 reduction to multi-carbon products in acidic media. Nature Catalysis, 2022, 5, 564-570.	34.4	197

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19	Efficient electrocatalytic conversion of carbon monoxide to propanol using fragmented copper. Nature Catalysis, 2019, 2, 251-258.	34.4	188
20	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 - International Edition, 2018, 57, 11262-11266.	13.8	165
21	Efficient Methane Electrosynthesis Enabled by Tuning Local CO₂ Availability. Journal of the American Chemical Society, 2020, 142, 3525-3531.	13.7	154
22	Copper adparticle enabled selective electrosynthesis of n-propanol. Nature Communications, 2018, 9, 4614.	12.8	153
23	CO₂ Electroreduction from Carbonate Electrolyte. ACS Energy Letters, 2019, 4, 1427-1431.	17.4	141
24	Efficient upgrading of CO to C3 fuel using asymmetric C-C coupling active sites. Nature Communications, 2019, 10, 5186.	12.8	127
25	Tuning OH binding energy enables selective electrochemical oxidation of ethylene to ethylene glycol. Nature Catalysis, 2020, 3, 14-22.	34.4	120
26	High-Rate and Efficient Ethylene Electrosynthesis Using a Catalyst/Promoter/Transport Layer. ACS Energy Letters, 2020, 5, 2811-2818.	17.4	106
27	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.	11.2	99
28	Efficient electrosynthesis of n-propanol from carbon monoxide using a Agâ€“Ruâ€“Cu catalyst. Nature Energy, 2022, 7, 170-176.	39.5	96
29	Promoting CO2 methanation via ligand-stabilized metal oxide clusters as hydrogen-donating motifs. Nature Communications, 2020, 11, 6190.	12.8	93
30	Silica-copper catalyst interfaces enable carbon-carbon coupling towards ethylene electrosynthesis. Nature Communications, 2021, 12, 2808.	12.8	91
31	Nonâ€Thermal Plasma Activation of Goldâ€Based Catalysts for Lowâ€Temperature Waterâ€“Gas Shift Catalysis. Angewandte Chemie - International Edition, 2017, 56, 5579-5583.	13.8	77
32	Enhanced multi-carbon alcohol electroproduction from CO via modulated hydrogen adsorption. Nature Communications, 2020, 11, 3685.	12.8	72
33	Gold-in-copper at low *CO coverage enables efficient electromethanation of CO2. Nature Communications, 2021, 12, 3387.	12.8	70
34	Deep Separation of Benzene from Cyclohexane by Liquid Extraction Using Ionic Liquids as the Solvent. Industrial & Engineering Chemistry Research, 2012, 51, 5559-5564.	3.7	66
35	Boride-derived oxygen-evolution catalysts. Nature Communications, 2021, 12, 6089.	12.8	51
36	Evaluation of the ionic liquids 1-alkyl-3-methylimidazolium hexafluorophosphate as a solvent for the extraction of benzene from cyclohexane: (Liquid+liquid) equilibria. Journal of Chemical Thermodynamics, 2012, 48, 145-149.	2.0	49

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37	Ternary Alloys Enable Efficient Production of Methoxylated Chemicals via Selective Electrocatalytic Hydrogenation of Lignin Monomers. Journal of the American Chemical Society, 2021, 143, 17226-17235.	13.7	43
38	Possibility of designing catalysts beyond the traditional volcano curve: a theoretical framework for multi-phase surfaces. Chemical Science, 2015, 6, 5703-5711.	7.4	40
39	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.	1.9	38
40	Identifying the trend of reactivity for sp2 materials: an electron delocalization model from first principles calculations. Physical Chemistry Chemical Physics, 2013, 15, 9498.	2.8	30
41	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.	3.1	29
42	Dopant-tuned stabilization of intermediates promotes electrosynthesis of valuable C3 products. Nature Communications, 2019, 10, 4807.	12.8	26
43	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.	2.0	24
44	Towards rational catalyst design: a general optimization framework. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20150078.	3.4	22
45	Ionic-Liquid-Controlled Two-Dimensional Monolayer Bi₂MoO₆ and Its Adsorption of Azo Molecules. ACS Applied Nano Materials, 2018, 1, 5083-5091.	5.0	19
46	Insights into the mechanism of electrochemical ozone production via water splitting on the Ni and Sb doped SnO₂ catalyst. Physical Chemistry Chemical Physics, 2017, 19, 3800-3806.	2.8	18
47	Some Attempts in the Rational Design of Heterogeneous Catalysts Using Density Functional Theory Calculations. Topics in Catalysis, 2015, 58, 633-643.	2.8	15
48	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.	2.8	15
49	Hydrogenation of benzoic acid to benzyl alcohol over Pt/SnO2. Applied Catalysis A: General, 2020, 593, 117420.	4.3	15
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.	8.2	13
51	Achieving rational design of alloy catalysts using a descriptor based on a quantitative structureâ€“energy equation. Chemical Communications, 2020, 56, 3214-3217.	4.1	13
52	Nonâ€Thermal Plasma Activation of Goldâ€Based Catalysts for Lowâ€Temperature Waterâ€“Gas Shift Catalysis. Angewandte Chemie, 2017, 129, 5671-5675.	2.0	11
53	A rational catalyst design of CO oxidation using the bonding contribution equation. Chemical Communications, 2017, 53, 8106-8109.	4.1	11
54	Coordination Number-Dependent Complete Oxidation of Methane on NiO Catalysts. ACS Catalysis, 2021, 11, 9837-9849.	11.2	9

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55	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.	2.8	7
56	Rational catalyst design for CO oxidation: a gradient-based optimization strategy. Catalysis Science and Technology, 2021, 11, 2604-2615.	4.1	5
57	Seeing is believing: In-situ visualising dynamic evolution in CO2 electrolysis. Current Opinion in Electrochemistry, 2022, 31, 100846.	4.8	5
58	Accurate and Affordable Explicit Solvent Quantum Mechanics for Electrocatalysis Investigations. Matter, 2021, 4, 12-14.	10.0	4
59	Extraordinary mechanical properties of monatomic C3N2chain. Molecular Simulation, 2015, 41, 256-261.	2.0	0
60	Gas Surface Interaction and Surface Reactions. Springer Handbooks, 2020, , 905-928.	0.6	0