Hao Li

List of Publications by Year in descending order

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120 papers	10,619 citations	36203 51 h-index	32761 100 g-index
121 all docs	121 docs citations	121 times ranked	9800 citing authors

#	Article	IF	Citations
1	Efficient Visible Light Nitrogen Fixation with BiOBr Nanosheets of Oxygen Vacancies on the Exposed {001} Facets. Journal of the American Chemical Society, 2015, 137, 6393-6399.	6.6	1,468
2	Oxygen Vacancyâ€Mediated Photocatalysis of BiOCl: Reactivity, Selectivity, and Perspectives. Angewandte Chemie - International Edition, 2018, 57, 122-138.	7.2	871
3	Solar Water Splitting and Nitrogen Fixation with Layered Bismuth Oxyhalides. Accounts of Chemical Research, 2017, 50, 112-121.	7.6	554
4	Coupling N2 and CO2 in H2O to synthesize urea under ambient conditions. Nature Chemistry, 2020, 12, 717-724.	6.6	485
5	Dual Singleâ€Atomic Niâ€N₄ and Feâ€N₄ Sites Constructing Janus Hollow Graphene for Selective Oxygen Electrocatalysis. Advanced Materials, 2020, 32, e2003134.	11.1	376
6	Recent advances in carbon dioxide utilization. Renewable and Sustainable Energy Reviews, 2020, 125, 109799.	8.2	369
7	Progress in enhancement of CO2 absorption by nanofluids: A mini review of mechanisms and current status. Renewable Energy, 2018, 118, 527-535.	4.3	252
8	Facet-dependent solar ammonia synthesis of BiOCl nanosheets via a proton-assisted electron transfer pathway. Nanoscale, 2016, 8, 1986-1993.	2.8	242
9	Photoelectrochemical Synthesis of Ammonia on the Aerophilic-Hydrophilic Heterostructure with 37.8% Efficiency. CheM, 2019, 5, 617-633.	5.8	241
10	Sulfur Loading and Speciation Control the Hydrophobicity, Electron Transfer, Reactivity, and Selectivity of Sulfidized Nanoscale Zerovalent Iron. Advanced Materials, 2020, 32, e1906910.	11.1	204
11	Defect Engineering Strategies for Nitrogen Reduction Reactions under Ambient Conditions. Small Methods, 2019, 3, 1800331.	4.6	199
12	Effects of ensembles, ligand, and strain on adsorbate binding to alloy surfaces. Journal of Chemical Physics, 2018, 149, 174705.	1.2	193
13	Application of Artificial Neural Networks for Catalysis: A Review. Catalysts, 2017, 7, 306.	1.6	167
14	Intrinsic Activity of Metal Centers in Metalâ€“Nitrogenâ€“Carbon Single-Atom Catalysts for Hydrogen Peroxide Synthesis. Journal of the American Chemical Society, 2020, 142, 21861-21871.	6.6	163
15	Design of a Pdâ€“Au Nitrite Reduction Catalyst by Identifying and Optimizing Active Ensembles. ACS Catalysis, 2019, 9, 7957-7966.	5.5	160
16	Tuning the Catalytic Preference of Ruthenium Catalysts for Nitrogen Reduction by Atomic Dispersion. Advanced Functional Materials, 2020, 30, 1905665.	7.8	159
17	Analysis of the limitations in the oxygen reduction activity of transition metal oxide surfaces. Nature Catalysis, 2021, 4, 463-468.	16.1	156
18	Rational Design of Rhodiumâ€“Iridium Alloy Nanoparticles as Highly Active Catalysts for Acidic Oxygen Evolution. ACS Nano, 2019, 13, 13225-13234.	7.3	151

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19	Design of high-performance water-in-glass evacuated tube solar water heaters by a high-throughput screening based on machine learning: A combined modeling and experimental study. Solar Energy, 2017, 142, 61-67.	2.9	137
20	Gd-induced electronic structure engineering of a NiFe-layered double hydroxide for efficient oxygen evolution. Journal of Materials Chemistry A, 2021, 9, 2999-3006.	5.2	133
21	Iron and Sulfur Precursors Affect Crystalline Structure, Speciation, and Reactivity of Sulfidized Nanoscale Zerovalent Iron. Environmental Science & Technology, 2020, 54, 13294-13303.	4.6	128
22	Oxygen Reduction Reaction on Classically Immiscible Bimetallics: A Case Study of RhAu. Journal of Physical Chemistry C, 2018, 122, 2712-2716.	1.5	123
23	New insights into the solid-state hydrogen storage of nanostructured LiBH4-MgH2 system. Chemical Engineering Journal, 2020, 385, 123856.	6.6	119
24	Sea-urchin-structure g-C3N4 with narrow bandgap (Ëœ2.0â€‰eV) for efficient overall water splitting under visible light irradiation. Applied Catalysis B: Environmental, 2019, 249, 275-281.	10.8	110
25	Unveiling the Role of Sulfur in Rapid Defluorination of Florfenicol by Sulfidized Nanoscale Zero-Valent Iron in Water under Ambient Conditions. Environmental Science & Technology, 2021, 55, 2628-2638.	4.6	98
26	Tunability of the Adsorbate Binding on Bimetallic Alloy Nanoparticles for the Optimization of Catalytic Hydrogenation. Journal of the American Chemical Society, 2017, 139, 5538-5546.	6.6	96
27	Dehydrogenation Selectivity of Ethanol on Close-Packed Transition Metal Surfaces: A Computational Study of Monometallic, Pd/Au, and Rh/Au Catalysts. Journal of Physical Chemistry C, 2017, 121, 27504-27510.	1.5	96
28	Sulfidized Nanoscale Zero-Valent Iron: Tuning the Properties of This Complex Material for Efficient Groundwater Remediation. Accounts of Materials Research, 2021, 2, 420-431.	5.9	96
29	Coâ€“Feâ€“Cr (oxy)Hydroxides as Efficient Oxygen Evolution Reaction Catalysts. Advanced Energy Materials, 2021, 11, 2003412.	10.2	94
30	PdAu Alloy Nanoparticle Catalysts: Effective Candidates for Nitrite Reduction in Water. ACS Catalysis, 2017, 7, 3268-3276.	5.5	89
31	Nitrogen-doped phosphorene for electrocatalytic ammonia synthesis. Journal of Materials Chemistry A, 2020, 8, 15875-15883.	5.2	88
32	Relations between Surface Oxygen Vacancies and Activity of Methanol Formation from CO₂ Hydrogenation over In₂O₃ Surfaces. ACS Catalysis, 2021, 11, 1780-1786.	5.5	88
33	Scalable Synthesis of Tungsten Disulfide Nanosheets for Alkaliâ€Acid Electrocatalytic Sulfion Recycling and H₂ Generation. Angewandte Chemie - International Edition, 2021, 60, 21550-21557.	7.2	82
34	Selectivity for ethanol partial oxidation: the unique chemistry of single-atom alloy catalysts on Au, Ag, and Cu(111). Journal of Materials Chemistry A, 2019, 7, 23868-23877.	5.2	80
35	Correlating surface chemistry and hydrophobicity of sulfidized nanoscale zerovalent iron with its reactivity and selectivity for denitration and dechlorination. Chemical Engineering Journal, 2020, 394, 124876.	6.6	79
36	One-Dimensional van der Waals Heterostructures as Efficient Metal-Free Oxygen Electrocatalysts. ACS Nano, 2021, 15, 3309-3319.	7.3	79

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37	Exploring the potential relationship between indoor air quality and the concentration of airborne culturable fungi: a combined experimental and neural network modeling study. Environmental Science and Pollution Research, 2018, 25, 3510-3517.	2.7	77
38	Ethanol Decomposition on Pdâ€“Au Alloy Catalysts. Journal of Physical Chemistry C, 2018, 122, 22024-22032.	1.5	77
39	Cu_xIr_{1â€“x} Nanoalloy Catalysts Achieve Near 100% Selectivity for Aqueous Nitrite Reduction to NH₃. ACS Catalysis, 2020, 10, 7915-7921.	5.5	69
40	An electro-activated bimetallic zinc-nickel hydroxide cathode for supercapacitor with super-long 140,000 cycle durability. Nano Energy, 2021, 82, 105727.	8.2	68
41	PdAg Alloy Nanocatalysts: Toward Economically Viable Nitrite Reduction in Drinking Water. ACS Catalysis, 2020, 10, 7979-7989.	5.5	64
42	Iminodiacetonitrile induce-synthesis of two-dimensional PdNi/Ni@carbon nanosheets with uniform dispersion and strong interface bonding as an effective bifunctional eletrocatalyst in air-cathode. Energy Storage Materials, 2021, 42, 118-128.	9.5	64
43	Rareâ€Earth Singleâ€Atom Catalysts: A New Frontier in Photo/Electrocatalysis. Small Methods, 2022, 6, .	4.6	63
44	Dechlorination and defluorination capability of sulfidized nanoscale zerovalent iron with suppressed water reactivity. Chemical Engineering Journal, 2020, 400, 125900.	6.6	61
45	Mechanistic insights on ethanol dehydrogenation on Pdâ€“Au model catalysts: a combined experimental and DFT study. Physical Chemistry Chemical Physics, 2017, 19, 30578-30589.	1.3	57
46	Microwave-Assisted Synthesis of Classically Immiscible Agâ€“Ir Alloy Nanoparticle Catalysts. ACS Catalysis, 2018, 8, 11386-11397.	5.5	57
47	Identify Zr Promotion Effects in Atomic Scale for Co-Based Catalysts in Fischerâ€“Tropsch Synthesis. ACS Catalysis, 2020, 10, 7894-7906.	5.5	57
48	Mining the intrinsic trends of CO2 solubility in blended solutions. Journal of CO2 Utilization, 2018, 26, 496-502.	3.3	55
49	Microwave-Assisted Synthesis of Pd_xAu_{100â€“x} Alloy Nanoparticles: A Combined Experimental and Theoretical Assessment of Synthetic and Compositional Effects upon Catalytic Reactivity. ACS Catalysis, 2016, 6, 4882-4893.	5.5	54
50	Machine learning predictive framework for CO2 thermodynamic properties in solution. Journal of CO2 Utilization, 2018, 26, 152-159.	3.3	54
51	Big to Small: Ultrafine Mo₂C Particles Derived from Giant Polyoxomolybdate Clusters for Hydrogen Evolution Reaction. Small, 2019, 15, e1900358.	5.2	53
52	Thiocyanate-Modified Silver Nanofoam for Efficient CO₂ Reduction to CO. ACS Catalysis, 2020, 10, 1444-1453.	5.5	51
53	Predictive Power of Machine Learning for Optimizing Solar Water Heater Performance: The Potential Application of High-Throughput Screening. International Journal of Photoenergy, 2017, 2017, 1-10.	1.4	49
54	Octahedral Coordinated Trivalent Cobalt Enriched Multimetal Oxygenâ€Evolution Catalysts. Advanced Energy Materials, 2020, 10, 2002593.	10.2	47

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55	Computational design of (100) alloy surfaces for the hydrogen evolution reaction. Journal of Materials Chemistry A, 2020, 8, 17987-17997.	5.2	47
56	A small change in the local atomic environment for a big improvement in single-atom catalysis. Journal of Materials Chemistry A, 2021, 9, 4184-4192.	5.2	44
57	Co₃O₄ Nanocrystals with an Oxygen Vacancy-Rich and Highly Reactive (222) Facet on Carbon Nitride Scaffolds for Efficient Photocatalytic Oxygen Evolution. ACS Applied Materials & Interfaces, 2020, 12, 44608-44616.	4.0	43
58	Catalytic activity atlas of ternary Coâ€“Feâ€“V metal oxides for the oxygen evolution reaction. Journal of Materials Chemistry A, 2020, 8, 15951-15961.	5.2	43
59	Functional Group Effects on the HOMOâ€“LUMO Gap of g-C3N4. Nanomaterials, 2018, 8, 589.	1.9	42
60	Prediction of CO2 absorption by physicalÂsolvents using a chemoinformatics-based machine learning model. Environmental Chemistry Letters, 2019, 17, 1397-1404.	8.3	42
61	Investigation of dust loading and culturable microorganisms of HVAC systems in 24 office buildings in Beijing. Energy and Buildings, 2015, 103, 166-174.	3.1	40
62	Origin of the hydrophobicity of sulfur-containing iron surfaces. Physical Chemistry Chemical Physics, 2021, 23, 13971-13976.	1.3	38
63	Quick Estimation Model for the Concentration of Indoor Airborne Culturable Bacteria: An Application of Machine Learning. International Journal of Environmental Research and Public Health, 2017, 14, 857.	1.2	37
64	Higher photocatalytic removal of organic pollutants using pangolin-like composites made of 3â€“4 atomic layers of MoS2 nanosheets deposited on tourmaline. Environmental Chemistry Letters, 2021, 19, 3573-3582.	8.3	37
65	Data-Mining for Processes in Chemistry, Materials, and Engineering. Processes, 2019, 7, 151.	1.3	36
66	User-friendly optimization approach of fed-batch fermentation conditions for the production of iturin A using artificial neural networks and support vector machine. Electronic Journal of Biotechnology, 2015, 18, 273-280.	1.2	35
67	3d Transitionâ€Metalâ€Mediated Columbite Nanocatalysts for Decentralized Electrosynthesis of Hydrogen Peroxide. Small, 2021, 17, e2007249.	5.2	35
68	Integrating Covalent Organic Framework with Transition Metal Phosphide for Nobleâ€Metalâ€Free Visibleâ€Lightâ€Driven Photocatalytic H₂ Evolution. Small, 2022, 18, .	5.2	33
69	Novel Method for Measuring the Heat Collection Rate and Heat Loss Coefficient of Water-in-Glass Evacuated Tube Solar Water Heaters Based on Artificial Neural Networks and Support Vector Machine. Energies, 2015, 8, 8814-8834.	1.6	32
70	New insights on CO and CO2 hydrogenation for methanol synthesis: The key role of adsorbate-adsorbate interactions on Cu and the highly active MgO-Cu interface. Journal of Catalysis, 2021, 400, 325-331.	3.1	32
71	Design of 3d transition metal anchored B₅N₃ catalysts for electrochemical CO₂ reduction to methane. Journal of Materials Chemistry A, 2022, 10, 9737-9745.	5.2	31
72	Gold boosts nitrate reduction and deactivation resistance to indium-promoted palladium catalysts. Applied Catalysis B: Environmental, 2022, 305, 121048.	10.8	29

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73	Oxidative Cross-Esterification and Related Pathways of Co-Adsorbed Oxygen and Ethanol on Pdâ€“Au. ACS Catalysis, 2019, 9, 4516-4525.	5.5	28
74	Electrochemical behavior of a Ni₃N OER precatalyst in Fe-purified alkaline media: the impact of self-oxidation and Fe incorporation. Materials Advances, 2021, 2, 2299-2309.	2.6	28
75	Layer structured materials for ambient nitrogen fixation. Coordination Chemistry Reviews, 2022, 460, 214468.	9.5	28
76	Evaluation Models for Soil Nutrient Based on Support Vector Machine and Artificial Neural Networks. Scientific World Journal, The, 2014, 2014, 1-7.	0.8	25
77	Comparative Study on Theoretical and Machine Learning Methods for Acquiring Compressed Liquid Densities of 1,1,1,2,3,3,3-Heptafluoropropane (R227ea) via Song and Mason Equation, Support Vector Machine, and Artificial Neural Networks. Applied Sciences (Switzerland), 2016, 6, 25.	1.3	25
78	Electrical and Structural Dual Function of Oxygen Vacancies for Promoting Electrochemical Capacitance in Tungsten Oxide. Small, 2020, 16, e2004709.	5.2	24
79	Emulsion-template synthesis of mesoporous nickel oxide nanoflowers composed of crossed nanosheets for effective nitrogen reduction. Dalton Transactions, 2021, 50, 5835-5844.	1.6	24
80	Properties and reactivity of sulfidized nanoscale zero-valent iron prepared with different borohydride amounts. Environmental Science: Nano, 2021, 8, 2607-2617.	2.2	24
81	MgH₂/single-atom heterojunctions: effective hydrogen storage materials with facile dehydrogenation. Journal of Materials Chemistry A, 2022, 10, 19839-19851.	5.2	23
82	Stability and Activity of Cobalt Antimonate for Oxygen Reduction in Strong Acid. ACS Energy Letters, 2022, 7, 993-1000.	8.8	21
83	Rapid Synthesis of Rhodiumâ€“Palladium Alloy Nanocatalysts. ChemCatChem, 2018, 10, 329-333.	1.8	19
84	Non-Monotonic Trends of Hydrogen Adsorption on Single Atom Doped g-C3N4. Catalysts, 2019, 9, 84.	1.6	19
85	Liâ€“Zn Overlayer to Facilitate Uniform Lithium Deposition for Lithium Metal Batteries. ACS Applied Materials & Interfaces, 2021, 13, 9985-9993.	4.0	19
86	Understanding Trends in Ethylene Epoxidation on Group IB Metals. ACS Catalysis, 2021, 11, 12052-12057.	5.5	19
87	Threeâ€inâ€One Alkylamineâ€Tuned MoO_x for Labâ€Scale to Realâ€Life Aqueous Supercapacitors. Advanced Functional Materials, 2022, 32, .	7.8	18
88	Electrocatalytic ammonia synthesis catalyzed by mesoporous nickel oxide nanosheets loaded with Pt nanoparticles. Chinese Journal of Catalysis, 2022, 43, 1371-1378.	6.9	18
89	A computational study of supported Cu-based bimetallic nanoclusters for CO oxidation. Physical Chemistry Chemical Physics, 2018, 20, 7508-7513.	1.3	17
90	Stabilizer-Free CuIr Alloy Nanoparticle Catalysts. Chemistry of Materials, 2019, 31, 10225-10235.	3.2	16

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91	Opportunities and Challenges in Electrolytic Propylene Epoxidation. Journal of Physical Chemistry Letters, 2022, 13, 2057-2063.	2.1	15
92	Artificial Neural Networks-Based Software for Measuring Heat Collection Rate and Heat Loss Coefficient of Water-in-Glass Evacuated Tube Solar Water Heaters. PLoS ONE, 2015, 10, e0143624.	1.1	13
93	Probing the reactivity of microhydrated Î±â€nucleophile in the anionic gasâ€phase S_N2 reaction. Journal of Computational Chemistry, 2015, 36, 844-852.	1.5	13
94	Mechanism of hydrogen storage on Fe₃B. Chemical Communications, 2020, 56, 14235-14238.	2.2	13
95	Direct In Situ Vertical Growth of Interlaced Mesoporous NiO Nanosheets on Carbon Felt for Electrocatalytic Ammonia Synthesis. Chemistry - A European Journal, 2022, 28, .	1.7	13
96	Understanding trends in the mercury oxidation activity of single-atom catalysts. Environmental Science: Nano, 2022, 9, 2041-2050.	2.2	13
97	The adsorption and activation of oxygen molecule on nickel clusters doped graphene-based support by DFT. Molecular Catalysis, 2019, 477, 110547.	1.0	12
98	Hydrogen generation during the purification of metallurgical-grade silicon. International Journal of Hydrogen Energy, 2021, 46, 23406-23416.	3.8	12
99	Calculations of Hydrogen Associative Desorption on Mono- and Bimetallic Catalysts. Journal of Physical Chemistry C, 2021, 125, 12028-12037.	1.5	12
100	Computationally Assisted STEM and EXAFS Characterization of Tunable Rh/Au and Rh/Ag Bimetallic Nanoparticle Catalysts. Microscopy and Microanalysis, 2017, 23, 2030-2031.	0.2	10
101	Design strategy of bifunctional catalysts for CO oxidation. Fuel, 2022, 320, 123909.	3.4	10
102	Analysis of the Oil Content of Rapeseed Using Artificial Neural Networks Based on Near Infrared Spectral Data. Journal of Spectroscopy, 2014, 2014, 1-5.	0.6	9
103	Prediction of the physicochemical properties of woody biomass using linear prediction and artificial neural networks. Energy Sources, Part A: Recovery, Utilization and Environmental Effects, 2016, 38, 1569-1573.	1.2	9
104	Testing the predictive power of theory for Pd_xIr_(100â^'x) alloy nanoparticles for the oxygen reduction reaction. Journal of Materials Chemistry A, 2020, 8, 8421-8429.	5.2	9
105	Extreme learning machine: a new alternative for measuring heat collection rate and heat loss coefficient of water-in-glass evacuated tube solar water heaters. SpringerPlus, 2016, 5, 626.	1.2	8
106	Pair-distribution-function guided optimization of fingerprints for atom-centered neural network potentials. Journal of Chemical Physics, 2020, 152, 224102.	1.2	8
107	Exploring the Effects of Ionic Defects on the Stability of CsPbI₃ with a Deep Learning Potential. ChemPhysChem, 2022, 23, e202100841.	1.0	8
108	Effects of a conductive support on the bonding of oxygen containing molecules to transition metal oxide surfaces. Physical Chemistry Chemical Physics, 2020, 22, 26216-26222.	1.3	7

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109	Factors that influence hydrogen binding at metal-atop sites. Journal of Chemical Physics, 2021, 155, 024703.	1.2	7
110	A WS2/sepiolite composite with highly dispersed WS2 nanosheets for photocatalytic wastewater treatment. Applied Clay Science, 2022, 228, 106576.	2.6	7
111	Evaluation of a V₈C₇ Anode for Oxygen Evolution in Alkaline Media: Unusual Morphological Behavior. ACS Sustainable Chemistry and Engineering, 2020, 8, 14101-14108.	3.2	6
112	Methane activation on dual-atom catalysts supported on graphene. Chemical Communications, 2021, 57, 12127-12130.	2.2	6
113	Infrared Spectroscopic Study on the Modified Mechanism of Aluminum-Impregnated Bone Charcoal. Journal of Spectroscopy, 2014, 2014, 1-7.	0.6	5
114	Artificial Neural Network Analysis of Xinhui Pericarpium <i>Citri Reticulatae</i> Using Gas Chromatography - Mass Spectrometer - Automated Mass Spectral Deconvolution and Identification System. Tropical Journal of Pharmaceutical Research, 2015, 14, 2071.	0.2	5
115	Scalable Synthesis of Tungsten Disulfide Nanosheets for Alkaliâ€Acid Electrocatalytic Sulfion Recycling and H₂ Generation. Angewandte Chemie, 2021, 133, 21720-21727.	1.6	4
116	Performance Prediction and Optimization of Solar Water Heater via a Knowledge-Based Machine Learning Method. Advances in Computer and Electrical Engineering Book Series, 2018, , 55-74.	0.2	4
117	Application of Artificial Neural Networks in predicting abrasion resistance of solution polymerized styrene-butadiene rubber based composites. , 2014, , .		3
118	Hydrogen coverage dependent C C hydrogenation activity on Rh(1Â1Â1). Chemical Physics Letters, 2020, 746, 137287.	1.2	3
119	Tracking the redox reaction-induced reconstruction of NiAu nanoparticles via environmental scanning transmission electron microscopy. Nanoscale, 2022, 14, 4089-4097.	2.8	2
120	Performance Prediction and Optimization of Solar Water Heater via a Knowledge-Based Machine Learning Method. , 2022, , 714-733.		0