

Baihai Li

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

62

papers

2,434

citations

26

h-index

49

g-index

63

ext. papers

3,108

ext. citations

7.8

avg, IF

5.37

L-index

#	Paper	IF	Citations
62	Cu clusters immobilized on Cd-defective cadmium sulfide nano-rods towards photocatalytic CO ₂ reduction. <i>Journal of Materials Science and Technology</i> , 2022 , 118, 54-63	9.1	1
61	Towards prediction of ordered phases in rechargeable battery chemistry via group-subgroup transformation. <i>Npj Computational Materials</i> , 2021 , 7,	10.9	2
60	An artificial hybrid interphase for an ultrahigh-rate and practical lithium metal anode. <i>Energy and Environmental Science</i> , 2021 , 14, 4115-4124	35.4	94
59	First principles study of single Fe atom supported on TiO ₂ (0 0 1) for nitrogen reduction to ammonia. <i>Applied Surface Science</i> , 2021 , 572, 151417	6.7	3
58	La-doped TiO ₂ nanorods toward boosted electrocatalytic N ₂ -to-NH ₃ conversion at ambient conditions. <i>Chinese Journal of Catalysis</i> , 2021 , 42, 1755-1762	11.3	14
57	Alkylthiol surface engineering: an effective strategy toward enhanced electrocatalytic N ₂ -to-NH ₃ fixation by a CoP nanoarray. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 13861-13866	13	45
56	Highly Selective Electrochemical Reduction of CO ₂ to Alcohols on an FeP Nanoarray. <i>Angewandte Chemie</i> , 2020 , 132, 768-772	3.6	14
55	Highly Selective Electrochemical Reduction of CO to Alcohols on an FeP Nanoarray. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 758-762	16.4	73
54	Mg-Doping improves the performance of Ru-based electrocatalysts for the acidic oxygen evolution reaction. <i>Chemical Communications</i> , 2020 , 56, 1749-1752	5.8	21
53	First-Principles Study of the Ferromagnetic Properties of CrCO and CrNO MXenes. <i>ACS Omega</i> , 2020 , 5, 25848-25853	3.9	3
52	Visible/infrared light-driven high-efficiency CO ₂ conversion into ethane based on a BiO synergistic catalyst. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 22327-22334	13	11
51	Synergistic effects of heteroatom-decorated MXene catalysts for CO reduction reactions. <i>Nanoscale</i> , 2020 , 12, 15880-15887	7.7	13
50	Crystalline Carbon Nitride Supported Copper Single Atoms for Photocatalytic CO Reduction with Nearly 100% CO Selectivity. <i>ACS Nano</i> , 2020 , 14, 10552-10561	16.7	155
49	Theoretical Investigation on the Single Transition-Metal Atom-Decorated Defective MoS ₂ for Electrocatalytic Ammonia Synthesis. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 36506-36514	9.5	49
48	CrO Nanoparticle-Reduced Graphene Oxide Hybrid: A Highly Active Electrocatalyst for N Reduction at Ambient Conditions. <i>Inorganic Chemistry</i> , 2019 , 58, 2257-2260	5.1	79
47	Tunable band gap of N V co-doped Ca:TiO ₂ B (CaTi ₅ O ₁₁) for visible-light photocatalysis. <i>International Journal of Hydrogen Energy</i> , 2019 , 44, 4716-4723	6.7	7
46	Theoretical Screening of Single-Atom-Embedded MoSSe Nanosheets for Electrocatalytic N ₂ Fixation. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 14501-14507	3.8	52

45	Theoretical Screening of Single Transition Metal Atoms Embedded in MXene Defects as Superior Electrocatalyst of Nitrogen Reduction Reaction. <i>Small Methods</i> , 2019 , 3, 1900337	12.8	124
44	Electrocatalytic N-to-NH conversion with high faradaic efficiency enabled using a Bi nanosheet array. <i>Chemical Communications</i> , 2019 , 55, 5263-5266	5.8	84
43	Asymmetric MXene/monolayer transition metal dichalcogenide heterostructures for functional applications. <i>Npj Computational Materials</i> , 2019 , 5,	10.9	13
42	Ceria-reduced graphene oxide nanocomposite as an efficient electrocatalyst towards artificial N conversion to NH under ambient conditions. <i>Chemical Communications</i> , 2019 , 55, 10717-10720	5.8	24
41	High-Performance N-to-NH Conversion Electrocatalyzed by MoC Nanorod. <i>ACS Central Science</i> , 2019 , 5, 116-121	16.8	223
40	Electrocatalytic Hydrogenation of N to NH by MnO: Experimental and Theoretical Investigations. <i>Advanced Science</i> , 2019 , 6, 1801182	13.6	92
39	Electrocatalytic N ₂ Fixation over Hollow VO ₂ Microspheres at Ambient Conditions. <i>ChemElectroChem</i> , 2019 , 6, 1014-1018	4.3	43
38	Theoretical study of the rutile based semiconductor with visible-light responsive photocatalytic activity for water splitting. <i>International Journal of Hydrogen Energy</i> , 2018 , 43, 6131-6137	6.7	0
37	3-Fold-Periodic Size-Dependence in Electronic Properties of Monolayer-TMDC Nanotriangles. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 1346-1352	6.4	
36	Efficient Hydrogen Evolution Electrocatalysis at Alkaline pH by Interface Engineering of NiP-CeO. <i>Inorganic Chemistry</i> , 2018 , 57, 548-552	5.1	63
35	MoO ₃ nanosheets for efficient electrocatalytic N ₂ fixation to NH ₃ . <i>Journal of Materials Chemistry A</i> , 2018 , 6, 12974-12977	13	227
34	Enabling Electrocatalytic N ₂ Reduction to NH ₃ by Y ₂ O ₃ Nanosheet under Ambient Conditions. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 16622-16627	3.9	28
33	Promoting effects of Ce _{0.75} Zr _{0.25} O ₂ on the La _{0.7} Sr _{0.3} MnO ₃ electrocatalyst for the oxygen reduction reaction in metal-air batteries. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 6411-6415	13	30
32	Formation of New Phases to Improve the Visible-Light Photocatalytic Activity of TiO ₂ (B) Via Introducing Alien Elements. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 52-59	3.8	1
31	Thermal stress analysis of a planar anode-supported solid oxide fuel cell: Effects of anode porosity. <i>International Journal of Hydrogen Energy</i> , 2017 , 42, 20239-20248	6.7	21
30	Co-fabrication of nickel-YSZ cermet nanofibers via an electrospinning technique. <i>Materials Research Bulletin</i> , 2017 , 86, 38-43	5.1	12
29	Fabrication of nickel-YSZ cermet nanofibers via electrospinning. <i>Journal of Alloys and Compounds</i> , 2017 , 693, 1214-1219	5.7	11
28	Monopolar Magnetic MOF-74 with Hybrid Node NiFe. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 26908-26914	5.14	5

27	Vapor Dissociation Solid Growth of Three-Dimensional Graphite-like Capsules with Delicate Morphology and Atomic-level Thickness Control. <i>Crystal Growth and Design</i> , 2016 , 16, 5040-5048	3.5	22
26	Kinetically Stabilized Pd@Pt Core Shell Octahedral Nanoparticles with Thin Pt Layers for Enhanced Catalytic Hydrogenation Performance. <i>ACS Catalysis</i> , 2015 , 5, 1335-1343	13.1	62
25	Mechanism of Phosphorus and Chlorine Passivating a Nickel Catalyst: A Density Functional Theory Study. <i>Electrochimica Acta</i> , 2015 , 167, 147-150	6.7	12
24	Atomic structure of defects and interfaces in TiO ₂ -B and Ca:TiO ₂ -B (CaTi ₅ O ₁₁) films grown on SrTiO ₃ . <i>CrystEngComm</i> , 2015 , 17, 4309-4315	3.3	6
23	Creating high quality Ca:TiO ₂ -B (CaTi ₅ O ₁₁) and TiO ₂ -B epitaxial thin films by pulsed laser deposition. <i>Chemical Communications</i> , 2015 , 51, 8584-7	5.8	13
22	A Joint Theoretical and Experimental Study of Phase Equilibria and Evolution in Pt-Doped Calcium Titanate under Redox Conditions. <i>Chemistry of Materials</i> , 2015 , 27, 18-28	9.6	10
21	Investigation into the effects of sulfur on syngas reforming inside a solid oxide fuel cell. <i>Journal of Power Sources</i> , 2014 , 258, 1-4	8.9	38
20	Water-free titania-bronze thin films with superfast lithium-ion transport. <i>Advanced Materials</i> , 2014 , 26, 7365-70	24	30
19	The stabilities and electronic structures of single-layer bismuth oxyhalides for photocatalytic water splitting. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 25854-61	3.6	90
18	Enhanced selective CO ₂ adsorption on polyamine/MIL-101(Cr) composites. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 14658-14665	13	98
17	A first-principles study of CO oxidation by surface oxygen on Pt-incorporated perovskite catalyst (CaPt _x Ti _{1-x} O ₃). <i>RSC Advances</i> , 2014 , 4, 30530-30535	3.7	4
16	First-principles study of microporous magnets M-MOF-74 (M = Ni, Co, Fe, Mn): the role of metal centers. <i>Inorganic Chemistry</i> , 2013 , 52, 9356-62	5.1	79
15	LiMnO ₂ as a cathode material for lithium ion batteries from first principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 9075-83	3.6	62
14	Surface-termination-dependent Pd bonding and aggregation of nanoparticles on LaFeO ₃ (001). <i>Journal of Chemical Physics</i> , 2013 , 138, 144705	3.9	9
13	Reversible precipitation/dissolution of precious-metal clusters in perovskite-based catalyst materials: Bulk versus surface re-dispersion. <i>Journal of Catalysis</i> , 2012 , 293, 145-148	7.3	74
12	Catalyzed activation of CO ₂ by a Lewis-base site in W ^{VI} /BTC hybrid metal organic frameworks. <i>Chemical Science</i> , 2012 , 3, 2708	9.4	26
11	Density functional study of hydrogen spillover on direct Pd-doped metal-organic frameworks IRMOF-1. <i>International Journal of Hydrogen Energy</i> , 2012 , 37, 5081-5089	6.7	17
10	Spin-flip phenomena at the Co graphene Co interfaces. <i>Applied Physics Letters</i> , 2011 , 98, 133111	3.4	11

9	First principles study of oxygen adsorption and dissociation on the Pd/Au surface alloys. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 7112-20	3.6	8
8	The isomeric effect on the adjacent Si dimer didechlorination of trans and iso-dichloroethylene on Si(100)-2 \times 1. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 7121-8	3.6	2
7	A first-principles study on the adhesion of Pt layers to NiO(100) and IrO ₂ (110) surfaces. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 015003	1.8	2
6	Origin of Rh and Pd agglomeration on the CeO ₂ (111) surface. <i>Physical Review B</i> , 2010 , 82,	3.3	17
5	Vacancy-mediated diffusion of carbon in cobalt and its influence on CO activation. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 7848-55	3.6	34
4	A Comparative Study of Hydrogen Spillover on Pd and Pt Decorated MoO ₃ (010) Surfaces from First Principles. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 3052-3058	3.8	23
3	A Dominant Dissociation Mode of cis-Dichloroethylene on Si(100)2 \times 1: Adjacent Si Dimer Double Dechlorination. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 21797-21804	3.8	3
2	Prompted hydrogenation of carbon nanotubes by doping light metals. <i>Applied Physics Letters</i> , 2008 , 93, 043104	3.4	13
1	CuS concave polyhedral superstructures enabled efficient N ₂ electroreduction to NH ₃ at ambient conditions. <i>Inorganic Chemistry Frontiers</i> ,	6.8	32