Baihai Li

List of Publications by Year
in descending order

62 papers	3,796 citations	159358 30 h-index	123241 61 g-index
63 all docs	63 docs citations	63 times ranked	4779 citing authors

#	Article	IF	Citations
1	Crystalline Carbon Nitride Supported Copper Single Atoms for Photocatalytic CO₂ Reduction with Nearly 100% CO Selectivity. ACS Nano, 2020, 14, 10552-10561.	7.3	417
2	An artificial hybrid interphase for an ultrahigh-rate and practical lithium metal anode. Energy and Environmental Science, 2021, 14, 4115-4124.	15.6	376
3	MoO₃ nanosheets for efficient electrocatalytic N₂ fixation to NH₃. Journal of Materials Chemistry A, 2018, 6, 12974-12977.	5.2	292
4	High-Performance N₂-to-NH₃ Conversion Electrocatalyzed by Mo₂C Nanorod. ACS Central Science, 2019, 5, 116-121.	5.3	292
5	Theoretical Screening of Single Transition Metal Atoms Embedded in MXene Defects as Superior Electrocatalyst of Nitrogen Reduction Reaction. Small Methods, 2019, 3, 1900337.	4.6	213
6	Highly Selective Electrochemical Reduction of CO₂ to Alcohols on an FeP Nanoarray. Angewandte Chemie - International Edition, 2020, 59, 758-762.	7.2	132
7	Enhanced selective CO₂ adsorption on polyamine/MIL-101(Cr) composites. Journal of Materials Chemistry A, 2014, 2, 14658-14665.	5.2	121
8	Electrocatalytic Hydrogenation of N₂ to NH₃ by MnO: Experimental and Theoretical Investigations. Advanced Science, 2019, 6, 1801182.	5.6	117
9	The stabilities and electronic structures of single-layer bismuth oxyhalides for photocatalytic water splitting. Physical Chemistry Chemical Physics, 2014, 16, 25854-25861.	1.3	105
10	Cr₂O₃ Nanoparticle-Reduced Graphene Oxide Hybrid: A Highly Active Electrocatalyst for N₂ Reduction at Ambient Conditions. Inorganic Chemistry, 2019, 58, 2257-2260.	1.9	97
11	Electrocatalytic N₂-to-NH₃ conversion with high faradaic efficiency enabled using a Bi nanosheet array. Chemical Communications, 2019, 55, 5263-5266.	2.2	95
12	First-Principles Study of Microporous Magnets M-MOF-74 (M = Ni, Co, Fe, Mn): the Role of Metal Centers. Inorganic Chemistry, 2013, 52, 9356-9362.	1.9	94
13	Theoretical Investigation on the Single Transition-Metal Atom-Decorated Defective MoS₂ for Electrocatalytic Ammonia Synthesis. ACS Applied Materials & Interfaces, 2019, 11, 36506-36514.	4.0	88
14	Reversible precipitation/dissolution of precious-metal clusters in perovskite-based catalyst materials: Bulk versus surface re-dispersion. Journal of Catalysis, 2012, 293, 145-148.	3.1	86
15	Alkylthiol surface engineering: an effective strategy toward enhanced electrocatalytic N₂-to-NH₃ fixation by a CoP nanoarray. Journal of Materials Chemistry A, 2021, 9, 13861-13866.	5.2	83
16	Efficient Hydrogen Evolution Electrocatalysis at Alkaline pH by Interface Engineering of Ni₂Pâ€“CeO₂. Inorganic Chemistry, 2018, 57, 548-552.	1.9	78
17	Î²-MnO2 as a cathode material for lithium ion batteries from first principles calculations. Physical Chemistry Chemical Physics, 2013, 15, 9075.	1.3	74
18	Kinetically Stabilized Pd@Pt Coreâ€“Shell Octahedral Nanoparticles with Thin Pt Layers for Enhanced Catalytic Hydrogenation Performance. ACS Catalysis, 2015, 5, 1335-1343.	5.5	72

#	Article	IF	Citations
19	Theoretical Screening of Single-Atom-Embedded MoSSe Nanosheets for Electrocatalytic N₂ Fixation. Journal of Physical Chemistry C, 2019, 123, 14501-14507.	1.5	72
20	Electrocatalytic N₂ Fixation over Hollow VO₂ Microspheres at Ambient Conditions. ChemElectroChem, 2019, 6, 1014-1018.	1.7	59
21	CuS concave polyhedral superstructures enabled efficient N₂ electroreduction to NH₃ at ambient conditions. Inorganic Chemistry Frontiers, 2021, 8, 3105-3110.	3.0	54
22	Cu clusters immobilized on Cd-defective cadmium sulfide nano-rods towards photocatalytic CO2 reduction. Journal of Materials Science and Technology, 2022, 118, 54-63.	5.6	44
23	Investigation into the effects of sulfur on syngas reforming inside a solid oxide fuel cell. Journal of Power Sources, 2014, 258, 1-4.	4.0	43
24	Enabling Electrocatalytic N₂ Reduction to NH₃ by Y₂O₃ Nanosheet under Ambient Conditions. Industrial & Engineering Chemistry Research, 2018, 57, 16622-16627.	1.8	39
25	Vacancy-mediated diffusion of carbon in cobalt and its influence on CO activation. Physical Chemistry Chemical Physics, 2010, 12, 7848.	1.3	37
26	Mg-Doping improves the performance of Ru-based electrocatalysts for the acidic oxygen evolution reaction. Chemical Communications, 2020, 56, 1749-1752.	2.2	36
27	Promoting effects of Ce_{0.75}Zr_{0.25}O₂ on the La_{0.7}Sr_{0.3}MnO₃ electrocatalyst for the oxygen reduction reaction in metalâ€“air batteries. Journal of Materials Chemistry A, 2017, 5, 6411-6415.	5.2	35
28	La-doped TiO2 nanorods toward boosted electrocatalytic N2-to-NH3 conversion at ambient conditions. Chinese Journal of Catalysis, 2021, 42, 1755-1762.	6.9	35
29	Ceria-reduced graphene oxide nanocomposite as an efficient electrocatalyst towards artificial N₂ conversion to NH₃ under ambient conditions. Chemical Communications, 2019, 55, 10717-10720.	2.2	33
30	Catalyzed activation of CO2 by a Lewis-base site in Wâ€“Cuâ€“BTC hybrid metal organic frameworks. Chemical Science, 2012, 3, 2708.	3.7	32
31	Synergistic effects of heteroatom-decorated MXene catalysts for CO reduction reactions. Nanoscale, 2020, 12, 15880-15887.	2.8	32
32	Waterâ€Free Titaniaâ€“Bronze Thin Films with Superfast Lithiumâ€Ion Transport. Advanced Materials, 2014, 26, 7365-7370.	11.1	31
33	Thermal stress analysis of a planar anode-supported solid oxide fuel cell: Effects of anode porosity. International Journal of Hydrogen Energy, 2017, 42, 20239-20248.	3.8	30
34	Vaporâ€“Dissociationâ€“Solid Growth of Three-Dimensional Graphite-like Capsules with Delicate Morphology and Atomic-level Thickness Control. Crystal Growth and Design, 2016, 16, 5040-5048.	1.4	27
35	A Comparative Study of Hydrogen Spillover on Pd and Pt Decorated MoO₃(010) Surfaces from First Principles. Journal of Physical Chemistry C, 2010, 114, 3052-3058.	1.5	26
36	Highly Selective Electrochemical Reduction of CO₂ to Alcohols on an FeP Nanoarray. Angewandte Chemie, 2020, 132, 768-772.	1.6	26

#	Article	IF	Citations
37	Visible/infrared light-driven high-efficiency CO₂ conversion into ethane based on a Bâ€“Co synergistic catalyst. Journal of Materials Chemistry A, 2020, 8, 22327-22334.	5.2	24
38	Asymmetric MXene/monolayer transition metal dichalcogenide heterostructures for functional applications. Npj Computational Materials, 2019, 5, .	3.5	23
39	Origin of Rh and Pd agglomeration on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CeO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2010, 82, .	1.1	18
40	Density functional study of hydrogen spillover on direct Pd-doped metal-organic frameworks IRMOF-1. International Journal of Hydrogen Energy, 2012, 37, 5081-5089.	3.8	18
41	Fabrication of nickel-YSZ cermet nanofibers via electrospinning. Journal of Alloys and Compounds, 2017, 693, 1214-1219.	2.8	18
42	Creating high quality Ca:TiO₂-B (CaTi₅O₁₁) and TiO₂-B epitaxial thin films by pulsed laser deposition. Chemical Communications, 2015, 51, 8584-8587.	2.2	15
43	Co-fabrication of nickel-YSZ cermet nanofibers via an electrospinning technique. Materials Research Bulletin, 2017, 86, 38-43.	2.7	15
44	First principles study of single Fe atom supported on TiO2(0 0 1) for nitrogen reduction to ammonia. Applied Surface Science, 2022, 572, 151417.	3.1	15
45	Prompted hydrogenation of carbon nanotubes by doping light metals. Applied Physics Letters, 2008, 93, .	1.5	13
46	A Joint Theoretical and Experimental Study of Phase Equilibria and Evolution in Pt-Doped Calcium Titanate under Redox Conditions. Chemistry of Materials, 2015, 27, 18-28.	3.2	13
47	Spin-flip phenomena at the Co|graphene|Co interfaces. Applied Physics Letters, 2011, 98, .	1.5	12
48	Mechanism of Phosphorus and Chlorine Passivating a Nickel Catalyst: A Density Functional Theory Study. Electrochimica Acta, 2015, 167, 147-150.	2.6	12
49	Tunable band gap of N V co-doped Ca:TiO2B (CaTi5O11) for visible-light photocatalysis. International Journal of Hydrogen Energy, 2019, 44, 4716-4723.	3.8	12
50	First principles study of oxygen adsorption and dissociation on the Pd/Au surface alloys. Physical Chemistry Chemical Physics, 2011, 13, 7112.	1.3	11
51	Surface-termination-dependent Pd bonding and aggregation of nanoparticles on LaFeO3 (001). Journal of Chemical Physics, 2013, 138, 144705.	1.2	10
52	First-Principles Study of the Ferromagnetic Properties of Cr₂CO₂ and Cr₂NO₂ MXenes. ACS Omega, 2020, 5, 25848-25853.	1.6	9
53	Towards prediction of ordered phases in rechargeable battery chemistry via groupâ€“subgroup transformation. Npj Computational Materials, 2021, 7, .	3.5	8
54	Atomic structure of defects and interfaces in TiO₂-B and Ca:TiO₂-B (CaTi₅O₁₁) films grown on SrTiO₃. CrystEngComm, 2015, 17, 4309-4315.	1.3	6

#	Article	IF	Citations
55	A first-principles study of CO oxidation by surface oxygen on Pt-incorporated perovskite catalyst (CaPt_xTi_{1â”x}O₃). RSC Advances, 2014, 4, 30530-30535.	1.7	5
56	Monopolar Magnetic MOF-74 with Hybrid Node Niâ€“Fe. Journal of Physical Chemistry C, 2016, 120, 26908-26914.	1.5	5
57	A Dominant Dissociation Mode of cis-Dichloroethylene on Si(100)2 Ã— 1: Adjacent Si Dimer Double Dechlorination. Journal of Physical Chemistry C, 2009, 113, 21797-21804.	1.5	3
58	A first-principles study on the adhesion of Pt layers to NiO(100) and IrO₂(110) surfaces. Journal of Physics Condensed Matter, 2010, 22, 015003.	0.7	3
59	The isomeric effect on the adjacent Si dimer didechlorination of trans and iso-dichloroethylene on Si(100)-2Ã—1. Physical Chemistry Chemical Physics, 2011, 13, 7121.	1.3	2
60	Formation of New Phases to Improve the Visible-Light Photocatalytic Activity of Tio₂ (B) Via Introducing Alien Elements. Journal of Physical Chemistry C, 2017, 121, 52-59.	1.5	1
61	Theoretical study of the rutile based semiconductor with visible-light responsive photocatalytic activity for water splitting. International Journal of Hydrogen Energy, 2018, 43, 6131-6137.	3.8	1
62	3-Fold-Periodic Size-Dependence in Electronic Properties of Monolayer-TMDC Nanotriangles. Journal of Physical Chemistry Letters, 2018, 9, 1346-1352.	2.1	1