Hongliang Xin

List of Publications by Year
in descending order

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46 papers	7,326 citations	136950 32 h-index	233421 45 g-index
47 all docs	47 docs citations	47 times ranked	9625 citing authors

#	Article	IF	Citations
1	CO oxidation on MgAl₂O₄ supported Ir_n: activation of lattice oxygen in the subnanometer regime and emergence of nuclearity-activity volcano. Journal of Materials Chemistry A, 2022, 10, 4266-4278.	10.3	4
2	Heterostructured Biâ€“Cu₂S nanocrystals for efficient CO₂ electroreduction to formate. Nanoscale Horizons, 2022, 7, 508-514.	8.0	16
3	Breaking adsorption-energy scaling limitations of electrocatalytic nitrate reduction on intermetallic CuPd nanocubes by machine-learned insights. Nature Communications, 2022, 13, 2338.	12.8	119
4	Machine learning of lateral adsorbate interactions in surface reaction kinetics. Current Opinion in Chemical Engineering, 2022, 36, 100825.	7.8	11
5	Catalytic CO Oxidation on MgAl₂O₄-Supported Iridium Single Atoms: Ligand Configuration and Site Geometry. Journal of Physical Chemistry C, 2021, 125, 11380-11390.	3.1	13
6	Infusing theory into deep learning for interpretable reactivity prediction. Nature Communications, 2021, 12, 5288.	12.8	38
7	High-performance ammonia oxidation catalysts for anion-exchange membrane direct ammonia fuel cells. Energy and Environmental Science, 2021, 14, 1449-1460.	30.8	100
8	Algorithm-derived feature representations for explainable AI in catalysis. Trends in Chemistry, 2021, 3, 990-992.	8.5	1
9	Interpretable Machine Learning of Chemical Bonding at Solid Surfaces. Journal of Physical Chemistry Letters, 2021, 12, 11476-11487.	4.6	30
10	Monodisperse PdSn/SnO_xcore/shell nanoparticles with superior electrocatalytic ethanol oxidation performance. Journal of Materials Chemistry A, 2020, 8, 20931-20938.	10.3	33
11	Bayesian learning of chemisorption for bridging the complexity of electronic descriptors. Nature Communications, 2020, 11, 6132.	12.8	42
12	Nanoporous V-Doped Ni₅P₄ Microsphere: A Highly Efficient Electrocatalyst for Hydrogen Evolution Reaction at All pH. ACS Applied Materials & Interfaces, 2020, 12, 37092-37099.	8.0	40
13	An Adaptive Machine Learning Strategy for Accelerating Discovery of Perovskite Electrocatalysts. ACS Catalysis, 2020, 10, 4377-4384.	11.2	75
14	Ternary PtIrNi Catalysts for Efficient Electrochemical Ammonia Oxidation. ACS Catalysis, 2020, 10, 3945-3957.	11.2	104
15	In Situ Formed Pt₃Ti Nanoparticles on a Two-Dimensional Transition Metal Carbide (MXene) Used as Efficient Catalysts for Hydrogen Evolution Reactions. Nano Letters, 2019, 19, 5102-5108.	9.1	133
16	New Insights into Electrochemical Ammonia Oxidation on Pt(100) from First Principles. Industrial & Engineering Chemistry Research, 2019, 58, 10819-10828.	3.7	71
17	Predicting Catalytic Activity of High-Entropy Alloys for Electrocatalysis. CheM, 2019, 5, 502-504.	11.7	37
18	Reactive Metalâ€“Biopolymer Interactions for Semihydrogenation of Acetylene. ACS Catalysis, 2019, 9, 11146-11152.	11.2	22

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19	Identification of the active complex for CO oxidation over single-atom Ir-on-MgAl2O4 catalysts. Nature Catalysis, 2019, 2, 149-156.	34.4	222
20	Machine-Learning Energy Gaps of Porphyrins with Molecular Graph Representations. Journal of Physical Chemistry A, 2018, 122, 4571-4578.	2.5	40
21	Coordination numbers for unraveling intrinsic size effects in gold-catalyzed CO oxidation. Physical Chemistry Chemical Physics, 2018, 20, 6055-6059.	2.8	24
22	Two-dimensional transition metal carbides as supports for tuning the chemistry of catalytic nanoparticles. Nature Communications, 2018, 9, 5258.	12.8	188
23	Overcoming Site Heterogeneity In Search of Metal Nanocatalysts. ACS Combinatorial Science, 2018, 20, 567-572.	3.8	15
24	Toward artificial intelligence in catalysis. Nature Catalysis, 2018, 1, 641-642.	34.4	70
25	Ambient ammonia synthesis via palladium-catalyzed electrohydrogenation of dinitrogen at low overpotential. Nature Communications, 2018, 9, 1795.	12.8	620
26	Feature engineering of machine-learning chemisorption models for catalyst design. Catalysis Today, 2017, 280, 232-238.	4.4	165
27	Agâ€“Sn Bimetallic Catalyst with a Coreâ€“Shell Structure for CO₂ Reduction. Journal of the American Chemical Society, 2017, 139, 1885-1893.	13.7	455
28	Orbitalwise Coordination Number for Predicting Adsorption Properties of Metal Nanocatalysts. Physical Review Letters, 2017, 118, 036101.	7.8	131
29	Insights into electrochemical CO2 reduction on tin oxides from first-principles calculations. Green Energy and Environment, 2017, 2, 168-171.	8.7	34
30	High-throughput screening of bimetallic catalysts enabled by machine learning. Journal of Materials Chemistry A, 2017, 5, 24131-24138.	10.3	246
31	Analyzing relationships between surface perturbations and local chemical reactivity of metal sites: Alkali promotion of O2 dissociation on Ag(111). Journal of Chemical Physics, 2016, 144, 234704.	3.0	13
32	Chemical Bond Activation Observed with an X-ray Laser. Journal of Physical Chemistry Letters, 2016, 7, 3647-3651.	4.6	21
33	Engineering Complex, Layered Metal Oxides: High-Performance Nickelate Oxide Nanostructures for Oxygen Exchange and Reduction. ACS Catalysis, 2015, 5, 4013-4019.	11.2	30
34	Machine-Learning-Augmented Chemisorption Model for CO₂ Electroreduction Catalyst Screening. Journal of Physical Chemistry Letters, 2015, 6, 3528-3533.	4.6	314
35	Effects of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>d</mml:mi></mml:math>-band shape on the surface reactivity of transition-metal alloys. Physical Review B, 2014, 89, .	3.2	387
36	Controlling Catalytic Selectivity on Metal Nanoparticles by Direct Photoexcitation of Adsorbateâ€“Metal Bonds. Nano Letters, 2014, 14, 5405-5412.	9.1	217

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37	Identifying optimal active sites for heterogeneous catalysis by metal alloys based on molecular descriptors and electronic structure engineering. Current Opinion in Chemical Engineering, 2013, 2, 312-319.	7.8	54
38	Catalytic and Photocatalytic Transformations on Metal Nanoparticles with Targeted Geometric and Plasmonic Properties. Accounts of Chemical Research, 2013, 46, 1890-1899.	15.6	245
39	Predictive Structureâ€“Reactivity Models for Rapid Screening of Pt-Based Multimetallic Electrocatalysts for the Oxygen Reduction Reaction. ACS Catalysis, 2012, 2, 12-16.	11.2	127
40	Singular characteristics and unique chemical bond activation mechanisms of photocatalytic reactions on plasmonic nanostructures. Nature Materials, 2012, 11, 1044-1050.	27.5	720
41	Electronic Structure Engineering in Heterogeneous Catalysis: Identifying Novel Alloy Catalysts Based on Rapid Screening for Materials with Desired Electronic Properties. Topics in Catalysis, 2012, 55, 376-390.	2.8	80
42	Visible-light-enhanced catalytic oxidation reactions on plasmonic silver nanostructures. Nature Chemistry, 2011, 3, 467-472.	13.6	1,662
43	Establishing Relationships Between the Geometric Structure and Chemical Reactivity of Alloy Catalysts Based on Their Measured Electronic Structure. Topics in Catalysis, 2010, 53, 348-356.	2.8	60
44	Communications: Exceptions to the d-band model of chemisorption on metal surfaces: The dominant role of repulsion between adsorbate states and metal d-states. Journal of Chemical Physics, 2010, 132, 221101.	3.0	201
45	Communications: Developing relationships between the local chemical reactivity of alloy catalysts and physical characteristics of constituent metal elements. Journal of Chemical Physics, 2010, 132, 111101.	3.0	13
46	Alkylation of benzene with 1-dodecene in ionic liquids [Rmim]+Al2Cl6Xâ¯ (R=butyl, octyl and dodecyl;) Tj ETQq0 0 0 rgBT /Overlock 10 T	4.3	83