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List of Publications by Year
in descending order

62 papers	5,765 citations	109264 35 h-index	133188 59 g-index
68 all docs	68 docs citations	68 times ranked	6870 citing authors

#	Article	IF	Citations
1	Structural Insights into Multiâ€Metal Spinel Oxide Nanoparticles for Boosting Oxygen Reduction Electrocatalysis. Advanced Materials, 2022, 34, e2107868.	11.1	30
2	Atomic Structure Modification of Feâ€'Nâ€'C Catalysts via Morphology Engineering of Graphene for Enhanced Conversion Kinetics of Lithiumâ€"Sulfur Batteries. Advanced Functional Materials, 2022, 32, .	7.8	45
3	Electrochemical Hydrogen Peroxide Synthesis from Selective Oxygen Reduction over Metal Selenide Catalysts. Nano Letters, 2022, 22, 1257-1264.	4.5	33
4	Structural Insights into Multiâ€Metal Spinel Oxide Nanoparticles for Boosting Oxygen Reduction Electrocatalysis (Adv. Mater. 8/2022). Advanced Materials, 2022, 34, .	11.1	0
5	Facet-Defined Strain-Free Spinel Oxide for Oxygen Reduction. Nano Letters, 2022, 22, 3636-3644.	4.5	3
6	Nitrogen and sulfur co-doped graphene nanoribbons with well-ordered stepped edges for high-performance potassium-ion battery anodes. Energy Storage Materials, 2022, 48, 325-334.	9.5	16
7	Pd17Se15-Pd3B nanocoral electrocatalyst for selective oxygen reduction to hydrogen peroxide in near-neutral electrolyte. Applied Catalysis B: Environmental, 2022, 309, 121265.	10.8	16
8	Promoting Oxygen Evolution Reaction Induced by Synergetic Geometric and Electronic Effects of IrCo Thin-Film Electrocatalysts. ACS Catalysis, 2022, 12, 6334-6344.	5.5	12
9	Tailoring selective pores of carbon molecular sieve membranes towards enhanced N2/CH4 separation efficiency. Journal of Membrane Science, 2021, 620, 118814.	4.1	26
10	Electrochemical Synthesis of H2O2 by Two-Electron Water Oxidation Reaction. CheM, 2021, 7, 38-63.	5.8	155
11	Local Coordination and Reactivity of a Pt Single-Atom Catalyst as Probed by Spectroelectrochemical and Computational Approaches. CCS Chemistry, 2021, 3, 241-251.	4.6	13
12	Efficient Discovery of Active, Selective, and Stable Catalysts for Electrochemical H₂O₂ Synthesis through Active Motif Screening. ACS Catalysis, 2021, 11, 2483-2491.	5.5	44
13	Three-Dimensionally Interconnected Nanoporous IrRe Thin Films Prepared by Selective Etching of Re for Oxygen Evolution Reaction. ACS Applied Energy Materials, 2021, 4, 4173-4180.	2.5	8
14	Atomic Structure-Free Representation of Active Motifs for Expedited Catalyst Discovery. Journal of Chemical Information and Modeling, 2021, 61, 4514-4520.	2.5	7
15	Defect-rich N-doped CeO₂ supported by N-doped graphene as a metal-free plasmonic hydrogen evolution photocatalyst. Journal of Materials Chemistry A, 2021, 9, 10217-10230.	5.2	32
16	Discovery of Acid-Stable Oxygen Evolution Catalysts: High-Throughput Computational Screening of Equimolar Bimetallic Oxides. ACS Applied Materials & Interfaces, 2020, 12, 38256-38265.	4.0	47
17	A Porphyrinic Zirconium Metalâ€"Organic Framework for Oxygen Reduction Reaction: Tailoring the Spacing between Active-Sites through Chain-Based Inorganic Building Units. Journal of the American Chemical Society, 2020, 142, 15386-15395.	6.6	139
18	In silico discovery of active, stable, CO-tolerant and cost-effective electrocatalysts for hydrogen evolution and oxidation. Physical Chemistry Chemical Physics, 2020, 22, 19454-19458.	1.3	12

#	Article	IF	Citations
19	A Review on Challenges and Successes in Atomic-Scale Design of Catalysts for Electrochemical Synthesis of Hydrogen Peroxide. ACS Catalysis, 2020, 10, 7495-7511.	5.5	254
20	Parallelized Screening of Characterized and DFT-Modeled Bimetallic Colloidal Cocatalysts for Photocatalytic Hydrogen Evolution. ACS Catalysis, 2020, 10, 4244-4252.	5.5	41
21	Practical Deep-Learning Representation for Fast Heterogeneous Catalyst Screening. Journal of Physical Chemistry Letters, 2020, 11, 3185-3191.	2.1	63
22	Confined local oxygen gas promotes electrochemical water oxidation to hydrogen peroxide. Nature Catalysis, 2020, 3, 125-134.	16.1	252
23	Toward a Design of Active Oxygen Evolution Catalysts: Insights from Automated Density Functional Theory Calculations and Machine Learning. ACS Catalysis, 2019, 9, 7651-7659.	5.5	118
24	Precious Metal-Free Nickel Nitride Catalyst for the Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2019, 11, 26863-26871.	4.0	81
25	Convolutional Neural Network of Atomic Surface Structures To Predict Binding Energies for High-Throughput Screening of Catalysts. Journal of Physical Chemistry Letters, 2019, 10, 4401-4408.	2.1	151
26	Improved Oxygen Reduction Reaction Activity of Nanostructured CoS₂ through Electrochemical Tuning. ACS Applied Energy Materials, 2019, 2, 8605-8614.	2.5	42
27	Toward Predicting Intermetallics Surface Properties with High-Throughput DFT and Convolutional Neural Networks. Journal of Chemical Information and Modeling, 2019, 59, 4742-4749.	2.5	45
28	Highly selective oxygen reduction to hydrogen peroxide on transition metal single atom coordination. Nature Communications, 2019, 10, 3997.	5.8	528
29	Noble metal supported hexagonal boron nitride for the oxygen reduction reaction: a DFT study. Nanoscale Advances, 2019, 1, 132-139.	2.2	29
30	Mixed Transition Metal Oxide with Vacancy-Induced Lattice Distortion for Enhanced Catalytic Activity of Oxygen Evolution Reaction. ACS Catalysis, 2019, 9, 7099-7108.	5.5	85
31	ZnO As an Active and Selective Catalyst for Electrochemical Water Oxidation to Hydrogen Peroxide. ACS Catalysis, 2019, 9, 4593-4599.	5.5	176
32	Prediction of Stable and Active (Oxy-Hydro) Oxide Nanoislands on Noble-Metal Supports for Electrochemical Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2019, 11, 2006-2013.	4.0	24
33	Understanding the Effects of Au Morphology on CO₂ Electrocatalysis. Journal of Physical Chemistry C, 2018, 122, 4274-4280.	1.5	36
34	Single Metal Atoms Anchored in Twoâ€Dimensional Materials: Bifunctional Catalysts for Fuel Cell Applications. ChemCatChem, 2018, 10, 3034-3039.	1.8	50
35	Active learning with non-<i>ab initio</i> input features toward efficient CO₂ reduction catalysts. Chemical Science, 2018, 9, 5152-5159.	3.7	82
36	Ultrathin Cobalt Oxide Overlayer Promotes Catalytic Activity of Cobalt Nitride for the Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2018, 122, 4783-4791.	1.5	46

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37	The Role of Adsorbed CN and Cl on an Au Electrode for Electrochemical CO₂ Reduction. ACS Catalysis, 2018, 8, 1178-1185.	5.5	98
38	Doping palladium with tellurium for the highly selective electrocatalytic reduction of aqueous CO₂ to CO. Chemical Science, 2018, 9, 483-487.	3.7	93
39	Dynamic Workflows for Routine Materials Discovery in Surface Science. Journal of Chemical Information and Modeling, 2018, 58, 2392-2400.	2.5	39
40	Suppression of Hydrogen Evolution Reaction in Electrochemical N₂ Reduction Using Single-Atom Catalysts: A Computational Guideline. ACS Catalysis, 2018, 8, 7517-7525.	5.5	545
41	Computational exploration of borophane-supported single transition metal atoms as potential oxygen reduction and evolution electrocatalysts. Physical Chemistry Chemical Physics, 2018, 20, 21095-21104.	1.3	54
42	Ultralow Overpotential of Hydrogen Evolution Reaction using Feâ€Doped Defective Graphene: A Density Functional Study. ChemCatChem, 2018, 10, 4450-4455.	1.8	22
43	Activating Transition Metal Dichalcogenides by Substitutional Nitrogenâ€Doping for Potential ORR Electrocatalysts. ChemElectroChem, 2018, 5, 4029-4035.	1.7	27
44	(Invited) Active and Stable Metal Supported Thin Film Metal (Hydroxy-) Oxides for Oxygen Reduction/Evolution Reactions. ECS Meeting Abstracts, 2018, , .	0.0	0
45	(Invited) Single Metal Atom Embedded in Two Dimensional Supports for Active Oxygen Reduction Reaction. ECS Meeting Abstracts, 2018, , .	0.0	1
46	Active Non-Precious Metal Based Nitride Catalysts for the Oxygen Reduction Reaction. ECS Meeting Abstracts, 2018, , .	0.0	0
47	Importance of Ligand Effects Breaking the Scaling Relation for Coreâ€“Shell Oxygen Reduction Catalysts. ChemCatChem, 2017, 9, 3173-3179.	1.8	28
48	Highly active and selective Au thin layer on Cu polycrystalline surface prepared by galvanic displacement for the electrochemical reduction of CO2 to CO. Applied Catalysis B: Environmental, 2017, 213, 211-215.	10.8	53
49	TiC- and TiN-Supported Single-Atom Catalysts for Dramatic Improvements in CO₂ Electrochemical Reduction to CH₄. ACS Energy Letters, 2017, 2, 969-975.	8.8	186
50	Probing surface oxide formations on SiO₂-supported platinum nanocatalysts under CO oxidation. RSC Advances, 2017, 7, 45003-45009.	1.7	26
51	Balancing activity, stability and conductivity of nanoporous core-shell iridium/iridium oxide oxygen evolution catalysts. Nature Communications, 2017, 8, 1449.	5.8	250
52	Single-atom catalysts for CO₂ electroreduction with significant activity and selectivity improvements. Chemical Science, 2017, 8, 1090-1096.	3.7	430
53	Unexpected solution phase formation of hollow PtSn alloy nanoparticles from Sn deposition on Pt dendritic structures. CrystEngComm, 2016, 18, 6019-6023.	1.3	5
54	Bifunctional Interface of Au and Cu for Improved CO₂ Electroreduction. ACS Applied Materials & Interfaces, 2016, 8, 23022-23027.	4.0	93

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55	On the mechanism of high product selectivity for HCOOH using Pb in CO₂ electroreduction. Physical Chemistry Chemical Physics, 2016, 18, 9652-9657.	1.3	60
56	On the mechanism of electrochemical ammonia synthesis on the Ru catalyst. Physical Chemistry Chemical Physics, 2016, 18, 9161-9166.	1.3	155
57	Active Sites of Au and Ag Nanoparticle Catalysts for CO₂ Electroreduction to CO. ACS Catalysis, 2015, 5, 5089-5096.	5.5	434
58	Selective Heterogeneous CO₂ Electroreduction to Methanol. ACS Catalysis, 2015, 5, 965-971.	5.5	167
59	Ordered Supramolecular Gels Based on Graphene Oxide and Tetracationic Cyclophanes. Advanced Materials, 2014, 26, 2725-2729.	11.1	25
60	Improved reversibility in lithium-oxygen battery: Understanding elementary reactions and surface charge engineering of metal alloy catalyst. Scientific Reports, 2014, 4, 4225.	1.6	133
61	On the structure of Si(100) surface: Importance of higher order correlations for buckled dimer. Journal of Chemical Physics, 2013, 138, 204709.	1.2	6
62	Enhancing Oxygen Reduction Reaction Activity Using Single Atom Catalyst Supported on Tantalum Pentoxide. ChemCatChem, 0, , .	1.8	1