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List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Suppression of Hydrogen Evolution Reaction in Electrochemical N ₂ Reduction Using Single-Atom Catalysts: A Computational Guideline. ACS Catalysis, 2018, 8, 7517-7525.	5.5	545
2	Highly selective oxygen reduction to hydrogen peroxide on transition metal single atom coordination. Nature Communications, 2019, 10, 3997.	5.8	528
3	Active Sites of Au and Ag Nanoparticle Catalysts for CO ₂ Electroreduction to CO. ACS Catalysis, 2015, 5, 5089-5096.	5.5	434
4	Single-atom catalysts for CO ₂ electroreduction with significant activity and selectivity improvements. Chemical Science, 2017, 8, 1090-1096.	3.7	430
5	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
6	Confined local oxygen gas promotes electrochemical water oxidation to hydrogen peroxide. Nature Catalysis, 2020, 3, 125-134.	16.1	252
7	Balancing activity, stability and conductivity of nanoporous core-shell iridium/iridium oxide oxygen evolution catalysts. Nature Communications, 2017, 8, 1449.	5.8	250
8	TiC- and TiN-Supported Single-Atom Catalysts for Dramatic Improvements in CO ₂ Electrochemical Reduction to CH ₄ . ACS Energy Letters, 2017, 2, 969-975.	8.8	186
9	ZnO As an Active and Selective Catalyst for Electrochemical Water Oxidation to Hydrogen Peroxide. ACS Catalysis, 2019, 9, 4593-4599.	5.5	176
10	Selective Heterogeneous CO ₂ Electroreduction to Methanol. ACS Catalysis, 2015, 5, 965-971.	5.5	167
11	On the mechanism of electrochemical ammonia synthesis on the Ru catalyst. Physical Chemistry Chemical Physics, 2016, 18, 9161-9166.	1.3	155
12	Electrochemical Synthesis of H ₂ O ₂ by Two-Electron Water Oxidation Reaction. Chem, 2021, 7, 38-63.	5.8	155
13	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
14	A Porphyrinic Zirconium Metal-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
15	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
16	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
17	The Role of Adsorbed CN and Cl on an Au Electrode for Electrochemical CO ₂ Reduction. ACS Catalysis, 2018, 8, 1178-1185.	5.5	98
18	Bifunctional Interface of Au and Cu for Improved CO ₂ Electroreduction. ACS Applied Materials & Interfaces, 2016, 8, 23022-23027.	4.0	93

#	ARTICLE	IF	CITATIONS
19	Doping palladium with tellurium for the highly selective electrocatalytic reduction of aqueous CO ₂ to CO. <i>Chemical Science</i> , 2018, 9, 483-487.	3.7	93
20	Mixed Transition Metal Oxide with Vacancy-Induced Lattice Distortion for Enhanced Catalytic Activity of Oxygen Evolution Reaction. <i>ACS Catalysis</i> , 2019, 9, 7099-7108.	5.5	85
21	Active learning with non- <i>ab initio</i> input features toward efficient CO ₂ reduction catalysts. <i>Chemical Science</i> , 2018, 9, 5152-5159.	3.7	82
22	Precious Metal-Free Nickel Nitride Catalyst for the Oxygen Reduction Reaction. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 26863-26871.	4.0	81
23	Practical Deep-Learning Representation for Fast Heterogeneous Catalyst Screening. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3185-3191.	2.1	63
24	On the mechanism of high product selectivity for HCOOH using Pb in CO ₂ electroreduction. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 9652-9657.	1.3	60
25	Computational exploration of borophane-supported single transition metal atoms as potential oxygen reduction and evolution electrocatalysts. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21095-21104.	1.3	54
26	Highly active and selective Au thin layer on Cu polycrystalline surface prepared by galvanic displacement for the electrochemical reduction of CO ₂ to CO. <i>Applied Catalysis B: Environmental</i> , 2017, 213, 211-215.	10.8	53
27	Single Metal Atoms Anchored in Two-Dimensional Materials: Bifunctional Catalysts for Fuel Cell Applications. <i>ChemCatChem</i> , 2018, 10, 3034-3039.	1.8	50
28	Discovery of Acid-Stable Oxygen Evolution Catalysts: High-Throughput Computational Screening of Equimolar Bimetallic Oxides. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 38256-38265.	4.0	47
29	Ultrathin Cobalt Oxide Overlayer Promotes Catalytic Activity of Cobalt Nitride for the Oxygen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4783-4791.	1.5	46
30	Toward Predicting Intermetallics Surface Properties with High-Throughput DFT and Convolutional Neural Networks. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4742-4749.	2.5	45
31	Atomic Structure Modification of Fe-N-C Catalysts via Morphology Engineering of Graphene for Enhanced Conversion Kinetics of Lithium-Sulfur Batteries. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	45
32	Efficient Discovery of Active, Selective, and Stable Catalysts for Electrochemical H ₂ O ₂ Synthesis through Active Motif Screening. <i>ACS Catalysis</i> , 2021, 11, 2483-2491.	5.5	44
33	Improved Oxygen Reduction Reaction Activity of Nanostructured CoS ₂ through Electrochemical Tuning. <i>ACS Applied Energy Materials</i> , 2019, 2, 8605-8614.	2.5	42
34	Parallelized Screening of Characterized and DFT-Modeled Bimetallic Colloidal Cocatalysts for Photocatalytic Hydrogen Evolution. <i>ACS Catalysis</i> , 2020, 10, 4244-4252.	5.5	41
35	Dynamic Workflows for Routine Materials Discovery in Surface Science. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 2392-2400.	2.5	39
36	Understanding the Effects of Au Morphology on CO ₂ Electrocatalysis. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4274-4280.	1.5	36

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37	Electrochemical Hydrogen Peroxide Synthesis from Selective Oxygen Reduction over Metal Selenide Catalysts. <i>Nano Letters</i> , 2022, 22, 1257-1264.	4.5	33
38	Defect-rich N-doped CeO ₂ supported by N-doped graphene as a metal-free plasmonic hydrogen evolution photocatalyst. <i>Journal of Materials Chemistry A</i> , 2021, 9, 10217-10230.	5.2	32
39	Structural Insights into Multi-Metal Spinel Oxide Nanoparticles for Boosting Oxygen Reduction Electrocatalysis. <i>Advanced Materials</i> , 2022, 34, e2107868.	11.1	30
40	Noble metal supported hexagonal boron nitride for the oxygen reduction reaction: a DFT study. <i>Nanoscale Advances</i> , 2019, 1, 132-139.	2.2	29
41	Importance of Ligand Effects Breaking the Scaling Relation for Core-Shell Oxygen Reduction Catalysts. <i>ChemCatChem</i> , 2017, 9, 3173-3179.	1.8	28
42	Activating Transition Metal Dichalcogenides by Substitutional Nitrogen-Doping for Potential ORR Electrocatalysts. <i>ChemElectroChem</i> , 2018, 5, 4029-4035.	1.7	27
43	Probing surface oxide formations on SiO ₂ -supported platinum nanocatalysts under CO oxidation. <i>RSC Advances</i> , 2017, 7, 45003-45009.	1.7	26
44	Tailoring selective pores of carbon molecular sieve membranes towards enhanced N ₂ /CH ₄ separation efficiency. <i>Journal of Membrane Science</i> , 2021, 620, 118814.	4.1	26
45	Ordered Supramolecular Gels Based on Graphene Oxide and Tetracationic Cyclophanes. <i>Advanced Materials</i> , 2014, 26, 2725-2729.	11.1	25
46	Prediction of Stable and Active (Oxy-Hydro) Oxide Nanoislands on Noble-Metal Supports for Electrochemical Oxygen Reduction Reaction. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 2006-2013.	4.0	24
47	Ultralow Overpotential of Hydrogen Evolution Reaction using Fe-Doped Defective Graphene: A Density Functional Study. <i>ChemCatChem</i> , 2018, 10, 4450-4455.	1.8	22
48	Nitrogen and sulfur co-doped graphene nanoribbons with well-ordered stepped edges for high-performance potassium-ion battery anodes. <i>Energy Storage Materials</i> , 2022, 48, 325-334.	9.5	16
49	Pd ₁₇ Se ₁₅ -Pd ₃ B nanocoral electrocatalyst for selective oxygen reduction to hydrogen peroxide in near-neutral electrolyte. <i>Applied Catalysis B: Environmental</i> , 2022, 309, 121265.	10.8	16
50	Local Coordination and Reactivity of a Pt Single-Atom Catalyst as Probed by Spectroelectrochemical and Computational Approaches. <i>CCS Chemistry</i> , 2021, 3, 241-251.	4.6	13
51	In silico discovery of active, stable, CO-tolerant and cost-effective electrocatalysts for hydrogen evolution and oxidation. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19454-19458.	1.3	12
52	Promoting Oxygen Evolution Reaction Induced by Synergetic Geometric and Electronic Effects of IrCo Thin-Film Electrocatalysts. <i>ACS Catalysis</i> , 2022, 12, 6334-6344.	5.5	12
53	Three-Dimensionally Interconnected Nanoporous IrRe Thin Films Prepared by Selective Etching of Re for Oxygen Evolution Reaction. <i>ACS Applied Energy Materials</i> , 2021, 4, 4173-4180.	2.5	8
54	Atomic Structure-Free Representation of Active Motifs for Expedited Catalyst Discovery. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4514-4520.	2.5	7

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55	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
56	Unexpected solution phase formation of hollow PtSn alloy nanoparticles from Sn deposition on Pt dendritic structures. CrystEngComm, 2016, 18, 6019-6023.	1.3	5
57	Facet-Defined Strain-Free Spinel Oxide for Oxygen Reduction. Nano Letters, 2022, 22, 3636-3644.	4.5	3
58	(Invited) Single Metal Atom Embedded in Two Dimensional Supports for Active Oxygen Reduction Reaction. ECS Meeting Abstracts, 2018, , .	0.0	1
59	Enhancing Oxygen Reduction Reaction Activity Using Single Atom Catalyst Supported on Tantalum Pentoxide. ChemCatChem, 0, , .	1.8	1
60	(Invited) Active and Stable Metal Supported Thin Film Metal (Hydroxy-) Oxides for Oxygen Reduction/Evolution Reactions. ECS Meeting Abstracts, 2018, , .	0.0	0
61	Active Non-Precious Metal Based Nitride Catalysts for the Oxygen Reduction Reaction. ECS Meeting Abstracts, 2018, , .	0.0	0
62	Structural Insights into Multi-Metal Spinel Oxide Nanoparticles for Boosting Oxygen Reduction Electrocatalysis (Adv. Mater. 8/2022). Advanced Materials, 2022, 34, .	11.1	0