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List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Accelerated Discovery of Singleâ€Atom Catalysts for Nitrogen Fixation via Machine Learning. Energy and Environmental Materials, 2023, 6, .	7.3	26
2	Synergistic Effect of Metal Doping and Tethered Ligand Promoted Highâ€Selectivity Conversion of CO ₂ to C ₂ Oxygenates at Ultra‣ow Potential. Energy and Environmental Materials, 2022, 5, 892-898.	7.3	14
3	Synthesis of Pd ₃ Sn and PdCuSn Nanorods with <i>L1₂</i> Phase for Highly Efficient Electrocatalytic Ethanol Oxidation. Advanced Materials, 2022, 34, e2106115.	11.1	65
4	How computations accelerate electrocatalyst discovery. CheM, 2022, 8, 1575-1610.	5.8	23
5	Preparation of Au@Pd Core–Shell Nanorods with <i>fcc</i> -2H- <i>fcc</i> Heterophase for Highly Efficient Electrocatalytic Alcohol Oxidation. Journal of the American Chemical Society, 2022, 144, 547-555.	6.6	88
6	A Universal Descriptor for Complicated Interfacial Effects on Electrochemical Reduction Reactions. Journal of the American Chemical Society, 2022, 144, 12874-12883.	6.6	49
7	Facilitating active species by decorating CeO2 on Ni3S2 nanosheets for efficient water oxidation electrocatalysis. Chinese Journal of Catalysis, 2021, 42, 482-489.	6.9	61

Screening of effective NRR electrocatalysts among the Si-based MSi₂N₄ (M =) Tj ETQq0 9.9 rgBT /34 erlock 10

9	Density Functional Theory Investigation of Structure–Activity Relationship for Efficient Electrochemical CO ₂ Reduction on Defective SnSe ₂ Nanosheets. ACS Applied Nano Materials, 2021, 4, 2760-2767.	2.4	6
10	Metastable 1T′-phase group VIB transition metal dichalcogenide crystals. Nature Materials, 2021, 20, 1113-1120.	13.3	119
11	Photocatalytic conversion of CO to fuels with water by B-doped graphene/g-C3N4 heterostructure. Science Bulletin, 2021, 66, 1186-1193.	4.3	19
12	Seeded Synthesis of Unconventional 2H-Phase Pd Alloy Nanomaterials for Highly Efficient Oxygen Reduction. Journal of the American Chemical Society, 2021, 143, 17292-17299.	6.6	59
13	Hybrid Cu ⁰ and Cu <i>^x </i> ⁺ as Atomic Interfaces Promote Highâ€Selectivity Conversion of CO ₂ to C ₂ H ₅ OH at Low Potential. Small, 2020, 16, e1901981.	5.2	92
14	Edge promotion and basal plane activation of MoS2 catalyst by isolated Co atoms for hydrodesulfurization and hydrodenitrogenation. Catalysis Today, 2020, 350, 56-63.	2.2	5
15	Phase-Selective Epitaxial Growth of Heterophase Nanostructures on Unconventional 2H-Pd Nanoparticles. Journal of the American Chemical Society, 2020, 142, 18971-18980.	6.6	111
16	Highly Efficient Photo-/Electrocatalytic Reduction of Nitrogen into Ammonia by Dual-Metal Sites. ACS Central Science, 2020, 6, 1762-1771.	5.3	135
17	Crystal phase-controlled growth of PtCu and PtCo alloys on 4H Au nanoribbons for electrocatalytic ethanol oxidation reaction. Nano Research, 2020, 13, 1970-1975.	5.8	32
18	Ethylene Selectivity in Electrocatalytic CO ₂ Reduction on Cu Nanomaterials: A Crystal Phase-Dependent Study. Journal of the American Chemical Society, 2020, 142, 12760-12766.	6.6	183

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19	A Ti ₃ C ₂ O ₂ supported single atom, trifunctional catalyst for electrochemical reactions. Journal of Materials Chemistry A, 2020, 8, 7801-7807.	5.2	69
20	Heterophase fcc-2H-fcc gold nanorods. Nature Communications, 2020, 11, 3293.	5.8	92
21	Perspective on theoretical methods and modeling relating to electro-catalysis processes. Chemical Communications, 2020, 56, 9937-9949.	2.2	52
22	Boosted electrochemical ammonia synthesis by high-percentage metallic transition metal dichalcogenide quantum dots. Nanoscale, 2020, 12, 10964-10971.	2.8	24
23	Unveiling chemical reactivity and oxidation of 1T-phased group VI disulfides. Physical Chemistry Chemical Physics, 2019, 21, 17010-17017.	1.3	7
24	New Mechanism for N ₂ Reduction: The Essential Role of Surface Hydrogenation. Journal of the American Chemical Society, 2019, 141, 18264-18270.	6.6	166
25	Photo-oxidative degradation of methylammonium lead iodide perovskite: mechanism and protection. Journal of Materials Chemistry A, 2019, 7, 2275-2282.	5.2	105
26	Metal-free electrocatalyst for reducing nitrogen to ammonia using a Lewis acid pair. Journal of Materials Chemistry A, 2019, 7, 4865-4871.	5.2	115
27	A General Two‣tep Strategy–Based Highâ€Throughput Screening of Single Atom Catalysts for Nitrogen Fixation. Small Methods, 2019, 3, 1800376.	4.6	303
28	Forming Atom–Vacancy Interface on the MoS 2 Catalyst for Efficient Hydrodeoxygenation Reactions. Small Methods, 2019, 3, 1800315.	4.6	23
29	Molybdenum sulfide clusters immobilized on defective graphene: a stable catalyst for the hydrogen evolution reaction. Journal of Materials Chemistry A, 2018, 6, 2289-2294.	5.2	44
30	Metallic MoN ultrathin nanosheets boosting high performance photocatalytic H ₂ production. Journal of Materials Chemistry A, 2018, 6, 23278-23282.	5.2	37
31	Metal-Free Single Atom Catalyst for N ₂ Fixation Driven by Visible Light. Journal of the American Chemical Society, 2018, 140, 14161-14168.	6.6	742
32	Predicting a new class of metal-organic frameworks as efficient catalyst for bi-functional oxygen evolution/reduction reactions. Journal of Catalysis, 2018, 367, 206-211.	3.1	61
33	Computation-Aided Design of Single-Atom Catalysts for One-Pot CO ₂ Capture, Activation, and Conversion. ACS Applied Materials & Interfaces, 2018, 10, 36866-36872.	4.0	70
34	Insight into the catalytic activity of MXenes for hydrogen evolution reaction. Science Bulletin, 2018, 63, 1397-1403.	4.3	61
35	Defect Engineering for Modulating the Trap States in 2D Photoconductors. Advanced Materials, 2018, 30, e1804332.	11.1	146
36	Single Molybdenum Atom Anchored on N-Doped Carbon as a Promising Electrocatalyst for Nitrogen Reduction into Ammonia at Ambient Conditions. Journal of Physical Chemistry C, 2018, 122, 16842-16847.	1.5	223

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37	High intrinsic catalytic activity of two-dimensional boron monolayers for the hydrogen evolution reaction. Nanoscale, 2017, 9, 533-537.	2.8	116
38	Template-Grown MoS ₂ Nanowires Catalyze the Hydrogen Evolution Reaction: Ultralow Kinetic Barriers with High Active Site Density. ACS Catalysis, 2017, 7, 5097-5102.	5.5	78
39	Towards a Comprehensive Understanding of the Reaction Mechanisms Between Defective MoS ₂ and Thiol Molecules. Angewandte Chemie - International Edition, 2017, 56, 10501-10505.	7.2	88
40	Nanosheet Supported Single-Metal Atom Bifunctional Catalyst for Overall Water Splitting. Nano Letters, 2017, 17, 5133-5139.	4.5	395
41	Repairing atomic vacancies in single-layer MoSe2 field-effect transistor and its defect dynamics. Npj Quantum Materials, 2017, 2, .	1.8	36
42	Towards a Comprehensive Understanding of the Reaction Mechanisms Between Defective MoS ₂ and Thiol Molecules. Angewandte Chemie, 2017, 129, 10637-10641.	1.6	4
43	Oxidation Mechanism and Protection Strategy of Ultrathin Indium Selenide: Insight from Theory. Journal of Physical Chemistry Letters, 2017, 8, 4368-4373.	2.1	62
44	Searching for Highly Active Catalysts for Hydrogen Evolution Reaction Based on O-Terminated MXenes through a Simple Descriptor. Chemistry of Materials, 2016, 28, 9026-9032.	3.2	247
45	Versatile Titanium Silicide Monolayers with Prominent Ferromagnetic, Catalytic, and Superconducting Properties: Theoretical Prediction. Journal of Physical Chemistry Letters, 2016, 7, 3723-3729.	2.1	28
46	Transition Metalâ€Promoted V ₂ CO ₂ (MXenes): A New and Highly Active Catalyst for Hydrogen Evolution Reaction. Advanced Science, 2016, 3, 1600180.	5.6	279
47	Activating Inert Basal Planes of MoS ₂ for Hydrogen Evolution Reaction through the Formation of Different Intrinsic Defects. Chemistry of Materials, 2016, 28, 4390-4396.	3.2	388
48	Hydrogen Activation on the Promoted and Unpromoted ReS2 (001) Surfaces under the Sulfidation Conditions: A First-Principles Study. Journal of Physical Chemistry C, 2015, 119, 17092-17101.	1.5	12
49	SnS ₂ nanotubes: a promising candidate for the anode material for lithium ion batteries. RSC Advances, 2015, 5, 32505-32510.	1.7	24
50	Mechanical Properties, Electronic Structures, and Potential Applications in Lithium Ion Batteries: A First-Principles Study toward SnSe ₂ Nanotubes. Journal of Physical Chemistry C, 2014, 118, 28291-28298.	1.5	37
51	Width- and edge-dependent magnetic properties, electronic structures, and stability of SnSe2 nanoribbons. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 59, 102-106.	1.3	13
52	Tuning electronic and magnetic properties of SnSe ₂ armchair nanoribbons via edge hydrogenation. Journal of Materials Chemistry C, 2014, 2, 10175-10183.	2.7	17
53	Do Ni/Cu and Cu/Ni Alloys have Different Catalytic Performances towards Waterâ€Gas Shift? A Density Functional Theory Investigation. ChemPhysChem, 2014, 15, 2490-2496.	1.0	17
54	Versatile Electronic and Magnetic Properties of SnSe ₂ Nanostructures Induced by the Strain. Journal of Physical Chemistry C, 2014, 118, 9251-9260.	1.5	68

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55	Role of Au in Graphene Growth on a Ni Surface. ACS Catalysis, 2014, 4, 892-902.	5.5	8
56	Edge-, width- and strain-dependent semiconductor–metal transition in SnSe nanoribbons. RSC Advances, 2014, 4, 6933.	1.7	23
57	Water adsorption and dissociation on Ni surface: Effects of steps, dopants, coverage and self-aggregation. Physical Chemistry Chemical Physics, 2013, 15, 17804.	1.3	28
58	Methane dehydrogenation on Au/Ni surface alloys – a first-principles study. Catalysis Science and Technology, 2013, 3, 1343.	2.1	36