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List of Publications by Year in descending order

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23 papers	3,030 citations	430442 18 h-index	642321 23 g-index
23 all docs	23 docs citations	23 times ranked	3727 citing authors

#	Article	IF	Citations
1	Establishing a Theoretical Landscape for Identifying Basal Plane Active 2D Metal Borides (MBenes) toward Nitrogen Electroreduction. Advanced Functional Materials, 2021, 31, 2008056.	7.8	97
2	Doubleâ€sided surface functionalization: An effective approach to stabilize and modulate the electronic structure of grapheneâ€like borophene. InformaÄnÃ-MateriÃ¡ly, 2021, 3, 327-336.	8.5	18
3	MX Anti-MXenes from Non-van der Waals Bulks for Electrochemical Applications: The Merit of Metallicity and Active Basal Plane. ACS Nano, 2021, 15, 6233-6242.	7.3	26
4	Single-atom catalysts with anionic metal centers: Promising electrocatalysts for the oxygen reduction reaction and beyond. Journal of Energy Chemistry, 2021, 63, 285-293.	7.1	15
5	Molecular Crowding Effect in Aqueous Electrolytes to Suppress Hydrogen Reduction Reaction and Enhance Electrochemical Nitrogen Reduction. Advanced Energy Materials, 2021, 11, 2101699.	10.2	73
6	Coordination tailoring towards efficient single-atom catalysts for N2 fixation: A case study of iron-nitrogen-carbon (Fe@N-C) systems. Catalysis Today, 2020, 350, 91-99.	2.2	45
7	Semiconducting SN₂ monolayer with three-dimensional auxetic properties: a global minimum with tetracoordinated sulfurs. Nanoscale, 2020, 12, 85-92.	2.8	21
8	Scalable synthesis of 2D hydrogen-substituted graphdiyne on Zn substrate for high-yield N2 fixation. Nano Energy, 2020, 78, 105283.	8.2	38
9	A super stable assembled P nanowire with variant structural and magnetic/electronic properties via transition metal adsorption. Nanoscale, 2020, 12, 12454-12461.	2.8	8
10	Polymorphism of low dimensional boron nanomaterials driven by electrostatic gating: a computational discovery. Nanoscale, 2020, 12, 10543-10549.	2.8	5
11	Metallic FeSe monolayer as an anode material for Li and non-Li ion batteries: a DFT study. Physical Chemistry Chemical Physics, 2020, 22, 8902-8912.	1.3	79
12	Tackling the Activity and Selectivity Challenges of Electrocatalysts toward the Nitrogen Reduction Reaction via Atomically Dispersed Biatom Catalysts. Journal of the American Chemical Society, 2020, 142, 5709-5721.	6.6	664
13	Highly porous, low band-gap Ni_xMn_{3â^'x}O₄(0.55 â‰¤xâ‰¤ 1.2) spinel nanoparticles within situcoated carbon as advanced cathode materials for zinc-ion batteries. Journal of Materials Chemistry A, 2019, 7, 17854-17866.	5.2	65
14	Oxygen Evolution Reaction on 2D Ferromagnetic Fe₃GeTe₂: Boosting the Reactivity by the Selfâ€Reduction of Surface Hydroxyl. Advanced Functional Materials, 2019, 29, 1904782.	7.8	42
15	Simultaneously Achieving High Activity and Selectivity toward Two-Electron O₂ Electroreduction: The Power of Single-Atom Catalysts. ACS Catalysis, 2019, 9, 11042-11054.	5.5	314
16	Defect-rich and ultrathin N doped carbon nanosheets as advanced trifunctional metal-free electrocatalysts for the ORR, OER and HER. Energy and Environmental Science, 2019, 12, 322-333.	15.6	1,078
17	Prediction of novel SiX2(Xâ€¯=â€¯S, Se) monolayer semiconductors by density functional theory. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 114, 113581.	1.3	25
18	Boosting ORR/OER Activity of Graphdiyne by Simple Heteroatom Doping. Small Methods, 2019, 3, 1800550.	4.6	149

#	Article	IF	Citations
19	Porous silaphosphorene, silaarsenene and silaantimonene: a sweet marriage of Si and P/As/Sb. Journal of Materials Chemistry A, 2018, 6, 3738-3746.	5.2	14
20	Penta-P2X (X=C, Si) monolayers as wide-bandgap semiconductors: A first principles prediction. Frontiers of Physics, 2018, 13, 1.	2.4	60
21	Porous hexagonal boron oxide monolayer with robust wide band gap: A computational study. FlatChem, 2018, 9, 27-32.	2.8	29
22	Spindle nodal chain in three-dimensional Î±â€² boron. Physical Chemistry Chemical Physics, 2018, 20, 23500-23506.	1.3	21
23	Component Matters: Paving the Roadmap toward Enhanced Electrocatalytic Performance of Graphitic C₃N₄-Based Catalysts via Atomic Tuning. ACS Nano, 2017, 11, 6004-6014.	7.3	144