Jeremie Zaffran

List of Publications by Year
in descending order

21	1,051	516561 16	677027 22
papers	citations	h-index	g-index

22	22	22	1660
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical Insights into the Formation Mechanism of Methane, Ethylene and Methanol in Fischerâ€Tropsch Synthesis at Co₂C Surfaces. ChemCatChem, 2021, 13, 2674-2682.	1.8	14
2	Fast prediction of oxygen reduction reaction activity on carbon nanotubes with a localized geometric descriptor. Physical Chemistry Chemical Physics, 2020, 22, 890-895.	1.3	24
3	Dry reforming of methane over the cobalt catalyst: Theoretical insights into the reaction kinetics and mechanism for catalyst deactivation. Applied Catalysis B: Environmental, 2020, 270, 118859.	10.8	98
4	First-Principles-Based Microkinetic Simulations of CO₂ Hydrogenation to Methanol over Intermetallic GaPd₂: Method Development to Include Complex Interactions between Surface Adsorbates. Journal of Physical Chemistry C, 2020, 124, 15977-15987.	1.5	16
5	Descriptor Design in the Computational Screening of Ni-Based Catalysts with Balanced Activity and Stability for Dry Reforming of Methane Reaction. ACS Catalysis, 2020, 10, 3074-3083.	5.5	82
6	Unveiling ionic diffusion in MgNiMnO4 cathode material for Mg-ion batteries via combined computational and experimental studies. Journal of Solid State Electrochemistry, 2019, 23, 3209-3216.	1.2	10
7	Role of Surface Species Interactions in Identifying the Reaction Mechanism of Methanol Synthesis from CO₂Hydrogenation over Intermetallic PdIn(310) Steps. Journal of Physical Chemistry C, 2019, 123, 13615-13623.	1.5	32
8	Ternary Ni-Co-Fe oxyhydroxide oxygen evolution catalysts: Intrinsic activity trends, electrical conductivity, and electronic band structure. Nano Research, 2019, 12, 2288-2295.	5.8	134
9	Efficient cationic agents for exfoliating two-dimensional nickel oxide sheets. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	10
10	Hydrogen Oxidation on Ni-Based Electrocatalysts: The Effect of Metal Doping. Catalysts, 2018, 8, 454.	1.6	80
11	Influence of Electrolyte Cations on Ni(Fe)OOH Catalyzed Oxygen Evolution Reaction. Chemistry of Materials, 2017, 29, 4761-4767.	3.2	105
12	Understanding the Oxygen Evolution Reaction on a Twoâ€Dimensional NiO₂ Catalyst. ChemElectroChem, 2017, 4, 2764-2770.	1.7	29
13	Metalâ€“Oxygen Bond Ionicity as an Efficient Descriptor for Doped NiOOH Photocatalytic Activity. ChemPhysChem, 2016, 17, 1630-1636.	1.0	25
14	Designing efficient doped NiOOH catalysts for water splitting with first principles calculations. ChemistrySelect, 2016, 1, 911-916.	0.7	26
15	Benchmarking Density Functional Theory Based Methods To Model NiOOH Material Properties: Hubbard and van der Waals Corrections vs Hybrid Functionals. Journal of Chemical Theory and Computation, 2016, 12, 3807-3812.	2.3	47
16	Three fundamental questions on one of our best water oxidation catalysts: a critical perspective. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	25
17	Towards more accurate prediction of activation energies for polyalcohol dehydrogenation on transition metal catalysts in water. Catalysis Science and Technology, 2016, 6, 6615-6624.	2.1	31
18	Trade-Off between Accuracy and Universality in Linear Energy Relations for Alcohol Dehydrogenation on Transition Metals. Journal of Physical Chemistry C, 2015, 119, 12988-12998.	1.5	46

#	Article	IF	Citations
19	Linear Energy Relations As Predictive Tools for Polyalcohol Catalytic Reactivity. ACS Catalysis, 2014, 4, 464-468.	5.5	41
20	Role of water in metal catalyst performance for ketone hydrogenation: a joint experimental and theoretical study on levulinic acid conversion into gamma-valerolactone. Chemical Communications, 2014, 50, 12450-12453.	2.2	168
21	Simulation and visualization of nanodiamond and nanographite. Computer Physics Communications, 2011, 182, 2009-2012.	3.0	7