

Nicolas G Härmann

List of Publications by Year in descending order

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Version: 2024-02-01

12
papers

713
citations

933447

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1199594

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14
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14
docs citations

14
times ranked

1021
citing authors

#	ARTICLE	IF	CITATIONS
1	Potential-induced nanoclustering of metallic catalysts during electrochemical CO ₂ reduction. <i>Nature Communications</i> , 2018, 9, 3117.	12.8	253
2	Grand canonical simulations of electrochemical interfaces in implicit solvation models. <i>Journal of Chemical Physics</i> , 2019, 150, 041730.	3.0	122
3	Implicit Solvation Methods for Catalysis at Electrified Interfaces. <i>Chemical Reviews</i> , 2022, 122, 10777-10820.	47.7	82
4	Self-activation of copper electrodes during CO electro-oxidation in alkaline electrolyte. <i>Nature Catalysis</i> , 2020, 3, 797-803.	34.4	60
5	Some challenges in the first-principles modeling of structures and processes in electrochemical energy storage and transfer. <i>Journal of Power Sources</i> , 2015, 275, 531-538.	7.8	49
6	Electrosorption at metal surfaces from first principles. <i>Npj Computational Materials</i> , 2020, 6, .	8.7	49
7	Absolute band alignment at semiconductor-water interfaces using explicit and implicit descriptions for liquid water. <i>Npj Computational Materials</i> , 2019, 5, .	8.7	48
8	Thermodynamic Cyclic Voltammograms Based on <i>Ab Initio</i> Calculations: Ag(111) in Halide-Containing Solutions. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1782-1794.	5.3	15
9	Field Effects at Protruding Defect Sites in Electrocatalysis at Metal Electrodes?. <i>ACS Catalysis</i> , 2022, 12, 6143-6148.	11.2	14
10	Thermodynamic cyclic voltammograms: peak positions and shapes. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 264004.	1.8	10
11	Phase field parameters for battery compounds from first-principles calculations. <i>Physical Review Materials</i> , 2019, 3, .	2.4	8
12	Static and dynamic water structures at interfaces: A case study with focus on Pt(111). <i>Journal of Chemical Physics</i> , 2021, 155, 194702.	3.0	3