Nico Holmberg

List of Publications by Year
in descending order

12	1,981	840119 11	1199166 12
papers	citations	h-index	g-index

12	12	12	2785
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194103.	1.2	1,371
2	Diabatic model for electrochemical hydrogen evolution based on constrained DFT configuration interaction. Journal of Chemical Physics, 2018, 149, 104702.	1.2	10
3	Hydrogen adsorption on MoS₂-surfaces: a DFT study on preferential sites and the effect of sulfur and hydrogen coverage. Physical Chemistry Chemical Physics, 2017, 19, 16231-16241.	1.3	64
4	Electrochemical Activation of Single-Walled Carbon Nanotubes with Pseudo-Atomic-Scale Platinum for the Hydrogen Evolution Reaction. ACS Catalysis, 2017, 7, 3121-3130.	5.5	279
5	Efficient Constrained Density Functional Theory Implementation for Simulation of Condensed Phase Electron Transfer Reactions. Journal of Chemical Theory and Computation, 2017, 13, 587-601.	2.3	40
6	Molecular Resolution of the Water Interface at an Alkali Halide with Terraces and Steps. Journal of Physical Chemistry C, 2016, 120, 19714-19722.	1.5	21
7	Charge distribution and Fermi level in bimetallic nanoparticles. Physical Chemistry Chemical Physics, 2016, 18, 2924-2931.	1.3	47
8	Ab Initio Electrochemistry: Exploring the Hydrogen Evolution Reaction on Carbon Nanotubes. Journal of Physical Chemistry C, 2015, 119, 16166-16178.	1.5	45
9	Theoretical Insight into the Hydrogen Evolution Activity of Open-Ended Carbon Nanotubes. Journal of Physical Chemistry Letters, 2015, 6, 3956-3960.	2.1	31
10	Ion Transport through a Waterâ€“Organic Solvent Liquidâ€“Liquid Interface: A Simulation Study. Journal of Physical Chemistry B, 2014, 118, 5957-5970.	1.2	14
11	Dissolution of NaCl nanocrystals: an ab initio molecular dynamics study. Physical Chemistry Chemical Physics, 2014, 16, 17437-17446.	1.3	29
12	Ab initio Kinetic Monte Carlo simulations of dissolution at the NaClâ€“water interface. Physical Chemistry Chemical Physics, 2014, 16, 22545-22554.	1.3	30