Alberto Fraccarollo

List of Publications by Year
in descending order

13	231	1040056 9	1125743 13
papers	citations	h-index	g-index

13	13	13	519
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Porous dipeptide crystals as selective CO₂adsorbents: experimental isotherms vs. grand canonical Monte Carlo simulations and MAS NMR spectroscopy. CrystEngComm, 2013, 15, 1503-1507.	2.6	44
2	Density Functional Theory Modeling of PbSe Nanoclusters: Effect of Surface Passivation on Shape and Composition. Journal of Physical Chemistry C, 2011, 115, 11382-11389.	3.1	37
3	Ab initio modeling of 2D layered organohalide lead perovskites. Journal of Chemical Physics, 2016, 144, 164701.	3.0	37
4	Mesoporous silica nanoparticles incorporating squaraine-based photosensitizers: a combined experimental and computational approach. Dalton Transactions, 2018, 47, 3038-3046.	3.3	24
5	Monte Carlo Modeling of Carbon Dioxide Adsorption in Porous Aromatic Frameworks. Langmuir, 2014, 30, 4147-4156.	3.5	19
6	First principles study of 2D layered organohalide tin perovskites. Journal of Chemical Physics, 2017, 146, 234703.	3.0	19
7	DFT simulation of Mg/Al hydrotalcite with different intercalated anions: Periodic structure and solvating effects on the iodide/triiodide redox couple. Chemical Physics Letters, 2010, 494, 274-278.	2.6	14
8	Accurate Evaluation of the Dispersion Energy in the Simulation of Gas Adsorption into Porous Zeolites. Journal of Chemical Theory and Computation, 2017, 13, 1756-1768.	5.3	12
9	Ab Initio Design of Low Band Gap 2D Tin Organohalide Perovskites. Journal of Physical Chemistry C, 2018, 122, 3677-3689.	3.1	10
10	Influence of Silicodactyly in the Preparation of Hybrid Materials. Molecules, 2019, 24, 848.	3.8	5
11	Ab initio modeling of 2D and quasi-2D lead organohalide perovskites with divalent organic cations and a tunable band gap. Physical Chemistry Chemical Physics, 2020, 22, 20573-20587.	2.8	5
12	An atomistic model of a disordered nanoporous solid: Interplay between Monte Carlo simulations and gas adsorption experiments. AIP Advances, 2017, 7, 045013.	1.3	3
13	Predicting the Conformation of Organic Catalysts Grafted on Silica Surfaces with Different Numbers of Tethering Chains: The Silicopodality Concept. Journal of Physical Chemistry C, 2021, 125, 21199-21210.	3.1	2