Alberto Fraccarollo

List of Publications by Year
in descending order

13	231	1170033 9	1255698 13
papers	citations	h-index	g-index

13	13	13	600
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	1.5	2
2	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.	1.3	5
3	Influence of Silicodactyly in the Preparation of Hybrid Materials. Molecules, 2019, 24, 848.	1.7	5
4	Ab Initio Design of Low Band Gap 2D Tin Organohalide Perovskites. Journal of Physical Chemistry C, 2018, 122, 3677-3689.	1.5	10
5	Mesoporous silica nanoparticles incorporating squaraine-based photosensitizers: a combined experimental and computational approach. Dalton Transactions, 2018, 47, 3038-3046.	1.6	24
6	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.	2.3	12
7	An atomistic model of a disordered nanoporous solid: Interplay between Monte Carlo simulations and gas adsorption experiments. AIP Advances, 2017, 7, 045013.	0.6	3
8	First principles study of 2D layered organohalide tin perovskites. Journal of Chemical Physics, 2017, 146, 234703.	1.2	19
9	Ab initio modeling of 2D layered organohalide lead perovskites. Journal of Chemical Physics, 2016, 144, 164701.	1.2	37
10	Monte Carlo Modeling of Carbon Dioxide Adsorption in Porous Aromatic Frameworks. Langmuir, 2014, 30, 4147-4156.	1.6	19
11	Porous dipeptide crystals as selective CO₂adsorbents: experimental isotherms vs. grand canonical Monte Carlo simulations and MAS NMR spectroscopy. CrystEngComm, 2013, 15, 1503-1507.	1.3	44
12	Density Functional Theory Modeling of PbSe Nanoclusters: Effect of Surface Passivation on Shape and Composition. Journal of Physical Chemistry C, 2011, 115, 11382-11389.	1.5	37
13	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.	1.2	14