Johannes Hoja

List of Publications by Year in descending order

15 papers	1,098 citations	758635 12 h-index	940134 16 g-index
16 all docs	16 docs citations	16 times ranked	1335 citing authors

#	Article	IF	Citations
1	QM7-X, a comprehensive dataset of quantum-mechanical properties spanning the chemical space of small organic molecules. Scientific Data, 2021, 8, 43.	2.4	46
2	Adhesion, forces and the stability of interfaces. Beilstein Journal of Organic Chemistry, 2019, 15, 106-129.	1.3	3
3	Computational polymorph screening reveals late-appearing and poorly-soluble form of rotigotine. Communications Chemistry, 2019, 2, .	2.0	39
4	Revised values for the X23 benchmark set of molecular crystals. Physical Chemistry Chemical Physics, 2019, 21, 24333-24344.	1.3	31
5	Reliable and practical computational description of molecular crystal polymorphs. Science Advances, 2019, 5, eaau3338.	4.7	127
6	Hidden Beneath the Surface: Origin of the Observed Enantioselective Adsorption on PdGa(111). Journal of the American Chemical Society, 2018, 140, 1401-1408.	6.6	16
7	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	1.6	7
8	First-principles stability ranking of molecular crystal polymorphs with the DFT+MBD approach. Faraday Discussions, 2018, 211, 253-274.	1.6	39
9	Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. Chemical Science, 2017, 8, 4926-4940.	3.7	97
10	Firstâ€principles modeling of molecular crystals: structures and stabilities, temperature and pressure. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1294.	6.2	141
11	Strong Local-Field Enhancement of the Nonlinear Soft-Mode Response in a Molecular Crystal. Physical Review Letters, 2017, 119, 097404.	2.9	19
12	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	0.5	445
13	Adsorption of Glucose, Cellobiose, and Cellotetraose onto Cellulose Model Surfaces. Journal of Physical Chemistry B, 2014, 118, 9017-9027.	1.2	13
14	Is Electrostatics Sufficient to Describe Hydrogenâ€Bonding Interactions?. Chemistry - A European Journal, 2014, 20, 2292-2300.	1.7	61
15	Variational solution of the congruently transformed Hamiltonian for many-electron systems using a full-configuration-interaction calculation. Physical Review A, 2012, 86, .	1.0	9