Eva Perlt

List of Publications by Year in descending order

20 papers	1,070 citations	687363 13 h-index	752698 20 g-index
20 all docs	20 docs citations	20 times ranked	1111 citing authors

#	Article	IF	Citations
1	Benchmarking the Computational Costs and Quality of Vibrational Spectra from Ab Initio Simulations. Advanced Theory and Simulations, 2022, 5, 2100293.	2.8	8
2	The Ionic Product of Water in the Eye of the Quantum Cluster Equilibrium. Molecules, 2022, 27, 1286.	3.8	6
3	Molecular Orientation at the Squalene/Air Interface from Sum Frequency Generation Spectroscopy and Atomistic Modeling. Journal of Physical Chemistry B, 2021, 125, 3932-3941.	2.6	13
4	Strong Ferromagnetic Exchange Coupling and Single-Molecule Magnetism in MoS₄³^{â€“}-Bridged Dilanthanide Complexes. Journal of the American Chemical Society, 2021, 143, 8465-8475.	13.7	27
5	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	3.0	616
6	Anharmonicity of Vibrational Modes in Hydrogen Chlorideâ€“Water Mixtures. Journal of Chemical Theory and Computation, 2019, 15, 2535-2547.	5.3	5
7	Predicting Moleâ€Fractionâ€Dependent Dissociation for Weak Acids. Angewandte Chemie - International Edition, 2019, 58, 3212-3216.	13.8	21
8	Dissoziation schwacher SÃuren Ã¼ber den gesamten Molenbruchbereich. Angewandte Chemie, 2019, 131, 3245-3249.	2.0	11
9	Finding the best density functional approximation to describe interaction energies and structures of ionic liquids in molecular dynamics studies. Journal of Chemical Physics, 2018, 148, 193835.	3.0	38
10	Thermodynamics and proton activities of protic ionic liquids with quantum cluster equilibrium theory. Journal of Chemical Physics, 2018, 148, 193822.	3.0	30
11	Peacemaker 2: Making clusters talk about binary mixtures and neat liquids. SoftwareX, 2018, 7, 356-359.	2.6	29
12	Anharmonic effects in the quantum cluster equilibrium method. Journal of Chemical Physics, 2017, 146, 124114.	3.0	15
13	Predicting the Ionic Product of Water. Scientific Reports, 2017, 7, 10244.	3.3	40
14	Quantum Cluster Equilibrium. Letters in Mathematical Physics, 2014, , 77-96.	0.6	7
15	A one-parameter quantum cluster equilibrium approach. Journal of Chemical Physics, 2012, 137, 164107.	3.0	11
16	Coupled Cluster in Condensed Phase. Part II: Liquid Hydrogen Fluoride from Quantum Cluster Equilibrium Theory. Journal of Chemical Theory and Computation, 2011, 7, 868-875.	5.3	33
17	Coupled Cluster in Condensed Phase. Part I: Static Quantum Chemical Calculations of Hydrogen Fluoride Clusters. Journal of Chemical Theory and Computation, 2011, 7, 843-851.	5.3	39
18	Binary systems from quantum cluster equilibrium theory. Journal of Chemical Physics, 2011, 135, 194113.	3.0	44

#	Article	IF	Citations
19	What can clusters tell us about the bulk?. Computer Physics Communications, 2011, 182, 1428-1446.	7.5	46
20	Importance of Structural Motifs in Liquid Hydrogen Fluoride. ChemPhysChem, 2011, 12, 3474-3482.	2.1	31