

Eva Perlt

List of Publications by Year in descending order

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Version: 2024-02-01

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	TURBOMOLE: Modular program suite for <i>ab initio</i> quantum-chemical and condensed-matter simulations. <i>Journal of Chemical Physics</i> , 2020, 152, 184107.	3.0	616
2	What can clusters tell us about the bulk?. <i>Computer Physics Communications</i> , 2011, 182, 1428-1446.	7.5	46
3	Binary systems from quantum cluster equilibrium theory. <i>Journal of Chemical Physics</i> , 2011, 135, 194113.	3.0	44
4	Predicting the Ionic Product of Water. <i>Scientific Reports</i> , 2017, 7, 10244.	3.3	40
5	Coupled Cluster in Condensed Phase. Part I: Static Quantum Chemical Calculations of Hydrogen Fluoride Clusters. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 843-851.	5.3	39
6	Finding the best density functional approximation to describe interaction energies and structures of ionic liquids in molecular dynamics studies. <i>Journal of Chemical Physics</i> , 2018, 148, 193835.	3.0	38
7	Coupled Cluster in Condensed Phase. Part II: Liquid Hydrogen Fluoride from Quantum Cluster Equilibrium Theory. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 868-875.	5.3	33
8	Importance of Structural Motifs in Liquid Hydrogen Fluoride. <i>ChemPhysChem</i> , 2011, 12, 3474-3482.	2.1	31
9	Thermodynamics and proton activities of protic ionic liquids with quantum cluster equilibrium theory. <i>Journal of Chemical Physics</i> , 2018, 148, 193822.	3.0	30
10	Peacemaker 2: Making clusters talk about binary mixtures and neat liquids. <i>SoftwareX</i> , 2018, 7, 356-359.	2.6	29
11	Strong Ferromagnetic Exchange Coupling and Single-Molecule Magnetism in MoS ₄ ³⁻ -Bridged Dlanthanide Complexes. <i>Journal of the American Chemical Society</i> , 2021, 143, 8465-8475.	13.7	27
12	Predicting Mole-Fraction-Dependent Dissociation for Weak Acids. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 3212-3216.	13.8	21
13	Anharmonic effects in the quantum cluster equilibrium method. <i>Journal of Chemical Physics</i> , 2017, 146, 124114.	3.0	15
14	Molecular Orientation at the Squalene/Air Interface from Sum Frequency Generation Spectroscopy and Atomistic Modeling. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3932-3941.	2.6	13
15	A one-parameter quantum cluster equilibrium approach. <i>Journal of Chemical Physics</i> , 2012, 137, 164107.	3.0	11
16	Dissoziation schwacher Säuren über den gesamten Molenbruchbereich. <i>Angewandte Chemie</i> , 2019, 131, 3245-3249.	2.0	11
17	Benchmarking the Computational Costs and Quality of Vibrational Spectra from Ab Initio Simulations. <i>Advanced Theory and Simulations</i> , 2022, 5, 2100293.	2.8	8
18	Quantum Cluster Equilibrium. <i>Letters in Mathematical Physics</i> , 2014, , 77-96.	0.6	7

#	ARTICLE	IF	CITATIONS
19	The Ionic Product of Water in the Eye of the Quantum Cluster Equilibrium. <i>Molecules</i> , 2022, 27, 1286.	3.8	6
20	Anharmonicity of Vibrational Modes in Hydrogen Chloride–Water Mixtures. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2535-2547.	5.3	5