

Philipp Pracht

List of Publications by Year in descending order

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Version: 2024-02-01

14
papers

2,289
citations

686830

13
h-index

1058022

14
g-index

16
all docs

16
docs citations

16
times ranked

1762
citing authors

#	ARTICLE	IF	CITATIONS
1	Automated exploration of the low-energy chemical space with fast quantum chemical methods. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 7169-7192.	1.3	966
2	Extended tight-binding quantum chemistry methods. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1493.	6.2	596
3	Fully Automated Quantum-Chemistry-Based Computation of Spin-Coupled Nuclear Magnetic Resonance Spectra. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 14763-14769.	7.2	158
4	Efficient Quantum Chemical Calculation of Structure Ensembles and Free Energies for Nonrigid Molecules. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4039-4054.	1.1	105
5	Calculation of absolute molecular entropies and heat capacities made simple. <i>Chemical Science</i> , 2021, 12, 6551-6568.	3.7	83
6	Theoretical study on conformational energies of transition metal complexes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 287-299.	1.3	52
7	High accuracy quantum-chemistry-based calculation and blind prediction of macroscopic pKa values in the context of the SAMPL6 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 1139-1149.	1.3	50
8	Automated and efficient quantum chemical determination and energetic ranking of molecular protonation sites. <i>Journal of Computational Chemistry</i> , 2017, 38, 2618-2631.	1.5	49
9	Automated Molecular Cluster Growing for Explicit Solvation by Efficient Force Field and Tight Binding Methods. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3174-3189.	2.3	45
10	Vollautomatisierte quantenchemische Berechnung von Spin-gekoppelten magnetischen Kernspinresonanzspektren. <i>Angewandte Chemie</i> , 2017, 129, 14958-14964.	1.6	32
11	Comprehensive Assessment of GFN Tight-Binding and Composite Density Functional Theory Methods for Calculating Gas-Phase Infrared Spectra. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7044-7060.	2.3	32
12	Efficient Quantum-Chemical Calculations of Acid Dissociation Constants from Free-Energy Relationships. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5681-5692.	1.1	18
13	Towards understanding solvation effects on the conformational entropy of non-rigid molecules. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 12249-12259.	1.3	15
14	High-Throughput Non-targeted Chemical Structure Identification Using Gas-Phase Infrared Spectra. <i>Analytical Chemistry</i> , 2021, 93, 10688-10696.	3.2	4