Philipp Pracht

List of Publications by Year
in descending order

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