Michael Diedenhofen

List of Publications by Year
in descending order

11	4,543	933447 10	1281871 11
papers	citations	h-index	g-index

11	11	11	5463
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
2	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	3.0	616
3	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
4	COSMO-RS as a tool for property prediction of IL mixturesâ€"A review. Fluid Phase Equilibria, 2010, 294, 31-38.	2.5	368
5	Prediction of Infinite Dilution Activity Coefficients of Organic Compounds in Ionic Liquids Using COSMO-RS. Journal of Chemical & Engineering Data, 2003, 48, 475-479.	1.9	215
6	Prediction of the vapor pressure and vaporization enthalpy of 1-n-alkyl-3-methylimidazolium-bis-(trifluoromethanesulfonyl) amide ionic liquids. Physical Chemistry Chemical Physics, 2007, 9, 4653.	2.8	79
7	Calculation of Solvation Free Energies with DCOSMO-RS. Journal of Physical Chemistry A, 2015, 119, 5439-5445.	2.5	65
8	Polarization charge densities provide a predictive quantification of hydrogen bond energies. Physical Chemistry Chemical Physics, 2012, 14, 955-963.	2.8	54
9	A refined cavity construction algorithm for the conductorâ€like screening model. Journal of Computational Chemistry, 2018, 39, 1648-1655.	3.3	41
10	Benchmarking Different QM Levels for Usage with COSMO-RS. Journal of Chemical Information and Modeling, 2019, 59, 4806-4813.	5.4	20
11	Mobility and adsorption of liquid organic hydrogen carriers (LOHCs) in soils â€“ environmental hazard perspective. Green Chemistry, 2020, 22, 6519-6530.	9.0	6