Arnim Hellweg

List of Publications by Year
in descending order

15	2,185	840776 11	996975 15
papers	citations	h-index	g-index

15	15	15	3000
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	3.0	616
2	Optimized accurate auxiliary basis sets for RI-MP2 and RI-CC2 calculations for the atoms Rb to Rn. Theoretical Chemistry Accounts, 2007, 117, 587-597.	1.4	577
3	Benchmarking the performance of spin-component scaled CC2 in ground and electronically excited states. Physical Chemistry Chemical Physics, 2008, 10, 4119.	2.8	276
4	TmoleXâ€"A graphical user interface for TURBOMOLE. Journal of Computational Chemistry, 2010, 31, 2967-2970.	3.3	257
5	Distributed memory parallel implementation of energies and gradients for second-order MÃ¸llerâ€"Plesset perturbation theory with the resolution-of-the-identity approximation. Physical Chemistry Chemical Physics, 2006, 8, 1159.	2.8	223
6	Development of new auxiliary basis functions of the Karlsruhe segmented contracted basis sets including diffuse basis functions (def2-SVPD, def2-TZVPPD, and def2-QVPPD) for RI-MP2 and RI-CC calculations. Physical Chemistry Chemical Physics, 2015, 17, 1010-1017.	2.8	102
7	Brick by brick computation of the gibbs free energy of reaction in solution using quantum chemistry and COSMOâ€RS. AICHE Journal, 2017, 63, 3944-3954.	3.6	56
8	On the internal rotations in p-cresol in its ground and first electronically excited states. Journal of Chemical Physics, 2007, 127, 024307.	3.0	24
9	The accuracy of dipole moments from spin-component scaled CC2 in ground and electronically excited states. Journal of Chemical Physics, 2011, 134, 064103.	3.0	18
10	Inversion, internal rotation, and nitrogen nuclear quadrupole coupling of p-toluidine as obtained from microwave spectroscopy and ab initio calculations. Chemical Physics, 2008, 344, 281-290.	1.9	15
11	Heuristic control of kinetic energy in dynamic reaction coordinate calculations. Journal of Computational Chemistry, 2013, 34, 1835-1841.	3.3	11
12	Determining the internal rotations of p-thiocresol. Chemical Physics Letters, 2009, 475, 198-201.	2.6	4
13	Prediction of acid pK_a values in the solvent acetone based on COSMOâ€RS. Journal of Computational Chemistry, 2022, 43, 1011-1022.	3.3	4
14	thermocalc â€" A poor man's approach to computational thermochemistry. Journal of Computational Chemistry, 2012, 33, 881-886.	3.3	1
15	On the formation of the formate anion: Insights from population analyses. Computational and Theoretical Chemistry, 2013, 1012, 8-13.	2.5	1