Michael Gaus

List of Publications by Year in Descending Order

18 papers	2,057 citations	15 h-index	19 g-index
19 ext. papers	2,447 ext. citations	5.4 avg, IF	5.16 L-index

#	Paper	IF	Citations
18	Copper Oxidation/Reduction in Water and Protein: Studies with DFTB3/MM and VALBOND Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2016**, 120, 1894-910	3.4	19
17	DFTB3 Parametrization for Copper: The Importance of Orbital Angular Momentum Dependence of Hubbard Parameters. *Journal of Chemical Theory and Computation*, **2015**, 11, 4205-19	6.4	27
16	Parameterization of the DFTB3 method for Br, Ca, Cl, F, I, K, and Na in organic and biological systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 332-42	6.4	164
15	Parametrization of DFTB3/3OB for magnesium and zinc for chemical and biological applications. *Journal of Physical Chemistry B*, **2015**, 119, 1062-82	3.4	90
14	Parameterization of DFTB3/3OB for Sulfur and Phosphorus for Chemical and Biological Applications. *Journal of Chemical Theory and Computation*, **2014**, 10, 1518-1537	6.4	195
13	A density functional tight binding model with an extended basis set and three-body repulsion for hydrogen under extreme thermodynamic conditions. *Journal of Physical Chemistry A*, **2014**, 118, 5520-8	2.8	17
12	Density functional tight binding: application to organic and biological molecules. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 49-61	7.9	127
11	QM/MM simulations of vibrational spectra of bacteriorhodopsin and channelrhodopsin-2. *Physical Chemistry Chemical Physics*, **2013**, 15, 6651-9	3.6	21
10	Parametrization and Benchmark of DFTB3 for Organic Molecules. *Journal of Chemical Theory and Computation*, **2013**, 9, 338-54	6.4	524
9	Parametrization of the SCC-DFTB Method for Halogens. *Journal of Chemical Theory and Computation*, **2013**, 9, 2939-49	6.4	45
8	Determination of a Density Functional Tight Binding Model with an Extended Basis Set and Three-Body Repulsion for Carbon Under Extreme Pressures and Temperatures. *Journal of Physical Chemistry C*, **2013**, 117, 7885-7894	3.8	24
7	Extended polarization in third-order SCC-DFTB from chemical-potential equalization. *Journal of Physical Chemistry A*, **2012**, 116, 9131-41	2.8	38
6	Improved electronic properties from third-order SCC-DFTB with cost efficient post-SCF extensions. *Journal of Physical Chemistry A*, **2012**, 116, 11927-37	2.8	15
5	DFTB3: Extension of the self-consistent-charge density-functional tight-binding method (SCC-DFTB). *Journal of Chemical Theory and Computation*, **2012**, 7, 931-948	6.4	620
4	Self-Consistent-Charge Density Functional Tight-Binding Method: An Efficient Approximation of Density Functional Theory **2011**, 287-307		5
3	Proton storage site in bacteriorhodopsin: new insights from quantum mechanics/molecular mechanics simulations of microscopic pK(a) and infrared spectra. *Journal of the American Chemical Society*, **2011**, 133, 14981-97	16.4	48
2	Vibrational Raman Spectra from the Self-Consistent Charge Density Functional Tight Binding Method via Classical Time-Correlation Functions. *Journal of Chemical Theory and Computation*, **2010**, 6, 1240-1255	6.4	15

List of Publications

1	Automatized parametrization of SCC-DFTB repulsive potentials: application to hydrocarbons. *Journal of Physical Chemistry A*, **2009**, 113, 11866-81	2.8	63