Michael Gaus

List of Publications by Year
in descending order

17 papers	2,752 citations	516681 16 h-index	888047 17 g-index
19 all docs	19 docs citations	19 times ranked	2407 citing authors

#	Article	IF	Citations
1	DFTB3: Extension of the Self-Consistent-Charge Density-Functional Tight-Binding Method (SCC-DFTB). Journal of Chemical Theory and Computation, 2011, 7, 931-948.	5.3	828
2	Parametrization and Benchmark of DFTB3 for Organic Molecules. Journal of Chemical Theory and Computation, 2013, 9, 338-354.	5.3	743
3	Parameterization of DFTB3/3OB for Sulfur and Phosphorus for Chemical and Biological Applications. Journal of Chemical Theory and Computation, 2014, 10, 1518-1537.	5.3	275
4	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, 332-342.	5.3	227
5	Density functional tight binding: application to organic and biological molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 49-61.	14.6	157
6	Parametrization of DFTB3/3OB for Magnesium and Zinc for Chemical and Biological Applications. Journal of Physical Chemistry B, 2015, 119, 1062-1082.	2.6	138
7	Automatized Parametrization of SCC-DFTB Repulsive Potentials: Application to Hydrocarbons. Journal of Physical Chemistry A, 2009, 113, 11866-11881.	2.5	69
8	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, 14981-14997.	13.7	58
9	Parametrization of the SCC-DFTB Method for Halogens. Journal of Chemical Theory and Computation, 2013, 9, 2939-2949.	5.3	54
10	Extended Polarization in Third-Order SCC-DFTB from Chemical-Potential Equalization. Journal of Physical Chemistry A, 2012, 116, 9131-9141.	2.5	42
11	DFTB3 Parametrization for Copper: The Importance of Orbital Angular Momentum Dependence of Hubbard Parameters. Journal of Chemical Theory and Computation, 2015, 11, 4205-4219.	5.3	30
12	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.	3.1	28
13	QM/MM simulations of vibrational spectra of bacteriorhodopsin and channelrhodopsin-2. Physical Chemistry Chemical Physics, 2013, 15, 6651.	2.8	23
14	Copper Oxidation/Reduction in Water and Protein: Studies with DFTB3/MM and VALBOND Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2016, 120, 1894-1910.	2.6	22
15	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.	5.3	19
16	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, 5520-5528.	2.5	18
17	Improved Electronic Properties from Third-Order SCC-DFTB with Cost Efficient Post-SCF Extensions. Journal of Physical Chemistry A, 2012, 116, 11927-11937.	2.5	16