Stephan Ehrlich

List of Publications by Year
in descending order

13 papers	54,380 citations	687363 13 h-index	1058476 14 g-index
14 all docs	14 docs citations	14 times ranked	45506 citing authors

#	Article	IF	Citations
1	A consistent and accurateab initioparametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. Journal of Chemical Physics, 2010, 132, 154104.	3.0	35,972
2	Effect of the damping function in dispersion corrected density functional theory. Journal of Computational Chemistry, 2011, 32, 1456-1465.	3.3	15,980
3	A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions. Physical Chemistry Chemical Physics, 2017, 19, 32184-32215.	2.8	1,230
4	Dispersion-Corrected Density Functional Theory for Aromatic Interactions in Complex Systems. Accounts of Chemical Research, 2013, 46, 916-926.	15.6	330
5	Systemâ€Dependent Dispersion Coefficients for the DFTâ€D3 Treatment of Adsorption Processes on Ionic Surfaces. ChemPhysChem, 2011, 12, 3414-3420.	2.1	318
6	On the Importance of the Dispersion Energy for the Thermodynamic Stability of Molecules. ChemPhysChem, 2011, 12, 1258-1261.	2.1	188
7	Automated Transition State Search and Its Application to Diverse Types of Organic Reactions. Journal of Chemical Theory and Computation, 2017, 13, 5780-5797.	5.3	125
8	A DFT-D study of structural and energetic properties of TiO₂modifications. Journal of Physics Condensed Matter, 2012, 24, 424206.	1.8	51
9	Dispersionâ€Driven Conformational Isomerism in Ïƒâ€Bonded Dimers of Larger Acenes. Angewandte Chemie - International Edition, 2013, 52, 10892-10895.	13.8	47
10	The frustrated Lewis pair pathway to methylene phosphonium systems. Chemical Science, 2014, 5, 797-803.	7.4	47
11	Towards full Quantumâ€Mechanicsâ€based Proteinâ€“Ligand Binding Affinities. ChemPhysChem, 2017, 18, 898-905.	2.1	46
12	Accurate Thermochemistry for Large Molecules with Modern Density Functionals. Topics in Current Chemistry, 2014, , 1-23.	4.0	17
13	Splitting of dihydrogen by five-membered zirconacycloallenoids: a novel pathway to conjugated diene zirconocene complexes. Chemical Communications, 2012, 48, 11085.	4.1	16