Accurate charges for transition metals in Molecular Mechanics

Peter Comba, Bodo Martin and Avik Sanyal

Anorganisch-Chemisches Institüt, Universität Heidelberg

The concept of partial atomic charges is fundamental for the accurate description of molecules with Molecular Mechanics (MM). This is because, a significant part of non-bonded interactions between polar species (atoms or atom groups) is electrostatic. Traditionally, force fields assign fixed partial charges to specific sites within a molecule and allow them to interact via a Coulomb-type interaction.This method fails for systems where polarization effects are important. One method of treating polarization that has found widespread application in various chemical and biological systems is the geometry-dependent fluctuating charge model. While fixed and variable charge schemes are available for organic and biological force fields (eg., AMBER, CHARMM, OPLS) our aim is to develop a method that can be used with comparable accuracy for transition metals as well. A new scheme for the fast calculation of geometry-dependent charges is presented here, which is based on the Charge Equilibration (QEq) method of Rappe and Goddard [1]. The model parameters can be parametrized by fitting to ab-initio/DFT based partial charges of a suitable reference set of molecules. We employ an automatic parametrization procedure developed in our group to obtain the optimal model parameters. This fast as well as accurate geometry-dependent charge model has the potential to be extended to both Molecular Dynamics (MD) simulations and hybrid QM/MM approaches.

[1] A.K. Rappe, W.A. Goddard III, *J. Phys. Chem.*, **1991**, *95*, 3358-3363