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## Advances in the Implementation of Polarizable Force Fields for Molecular Simulations

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# The Electronegativity Equalization Method and the Split Charge Equilibration Applied to Organic Systems: Parameterization, Validation and Comparison

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## Abstract

An extensive benchmark of the Electronegativity Equalization Method (EEM) and the Split Charge Equilibration (SQE) model on a diverse set of organic molecules is presented. Both models efficiently compute atomic partial charges, and are used in the development of polarizable force fields. The empirical parameters in the EEM and SQE model are calibrated to reproduce results from quantum mechanical calculations. Recently, SQE has been presented as an extension of the EEM to obtain the correct size-dependence of the molecular polarizability. In this paper, 12 parameterization protocols are applied to both models and the optimal parameters are benchmarked systematically. The training data for the empirical parameters comprises MP2/Aug-CC-pVDZ calculations on 500 organic molecules containing the elements H, C, N, O, F, S, Cl and Br. These molecules have been selected from an initial set of almost 500000 small organic molecules based on an entropy maximization scheme. It is clear that the SQE model outperforms the EEM in all benchmarks. When using Hirshfeld-I charges for the calibration, the SQE model optimally reproduces the
molecular electrostatic potential from the ab initio calculations. It is remarkable that the SQE model, which does not include inducible atomic dipoles, gives a relatively accurate description of the molecular polarizability tensor. Applications on chain molecules, i.e. alkanes, alkenes and alpha alanine helices, confirm that the EEM gives rise to a divergent behavior for the polarizability, while the SQE model shows the correct trends. We conclude that the SQE model is an essential component of a polarizable force field, showing several advantages over the original EEM.

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