

Hydration Properties with Polarizable Multipole Force Fields

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During the last decades, deficiencies of classic biomolecular force fields (fixed point charge, no polarization) have become increasingly evident. Therefore, new types of next-generation force fields that include terms for polarizability and anisotropic charge distribution such as AMOEBA (Atomic Multipole Optimized Energetics for Biomolecular Applications) have become increasingly more important. In order to enhance the performance of classical (fixed point charge) force fields, a new treatment of the electrostatics is crucial. Fixed multipoles as a higher basis set for the description of the electron density on each atom provide access to a better representation of the electrostatic properties of a molecule. In this work, we use the AMOEBA force field, which covers polarization effects through an induced dipole on every atom [1]. Polarization effects, which are not covered by conventional force fields, are of major interests as atoms are able to react upon their environment [2] resulting in a force field which can in an ideal case be used to describe molecules in both gas- and condensed phase.

In this work the differences between polarizable multipole force fields and conventional force fields regarding the description of ions in water were investigated. Ions and charged residues play a significant role in biomolecular interaction. The ion in water problem has a spherical symmetry and due to this symmetry properties like radial distribution functions (RDF) can easily be calculated and compared to reference methods. As a first test case for validating the improvement of the physical model we compared the RDF distributions for ions in solution obtained with AMOEBA and conventional force field calculations to those from QM/MM simulations.

Our initial results show that this new generation force field is describing the first hydration shell of ions better than conventional ones. Especially for negatively charged ions and divalent cations, polarizable force fields yield coordination numbers and RDFs which are closer to reference values than the standard AMBER water models tip3p, tip4p or tip5p.

[1] J. W. Ponder et al., *J. Phys. Chem. B*, **2010**, *114*, 2549-2564.

[2] A. Warshel, M. Kato, A. V. Pisliakov, *J. Chem. Theory. Comput.*, **2007**, *3*, 2034-2045.