Charge Transfer Potential Models for Ions.

Marielle Soniat and Steve W. Rick

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1 Abstract

Charge transfer contributes significantly to the interactions involving ions, resulting in ionic charges which deviate from integer values. Charge transfer affects both short range interactions directly through the transfer of charge and affects long range interactions by reducing the Coulomb energy. These interactions are typically neglected in atomistic simulations. This poster will present a first look at a new model of polarizable ions which include charge transfer, extending previous work on water potentials. This will allow the application of charge transfer models to dilute electrolyte solutions containing Na+, K+, and Cl-. This model also provides a computationally cheap method to study the effects of charge transfer on the structure and dynamics dilute salt solutions. The model allows discrete charge transfer between ions and water as well as between counter-ion pairs. The ion-water interactions are parameterized to reproduce the dimer energy and distance at the energy minimum, as well as the radial distribution function of a single ion in water. The ion-ion interactions are parameterized using the Lorentz-Berthelot combining rules for Lennard-Jones parameters and adjusting the charge transfer and damping parameters to reproduce the energy and electrostatic properties of the dimer. The ions performance is assessed by calculating their free energy of hydration, diffusion constants, and the structure of the water around the ions. The ions correctly reproduce the whole salt hydration free energy. The models result in an average charge of about 0.9 e for the cations and -0.8 e for the chloride ion, in good agreement with electronic structure results.