236c Improved Polarizable Potential Model and Simulation Study of Aqueous Systems of Polyethylene Oxide and Inorganic Salts

zhi Tao and Peter T. Cummings

Polymer electrolytes, consisting of inorganic salts dissolved in a polymer matrix exhibiting high ionic conductivities, are the basic components of polymer batteries. These materials are becoming the subjects of intense study [1, 2]. One of the most promising polymer hosts for these polymer/salt systems is polyethylene oxide (PEO), - $(CH_2 - CH_2 - O)_n$-, which has demonstrated capability to solvate inorganic salts [1]. Previous experiments and computer simulations have focused mainly on the properties of PEO and salt mixtures forming the basis of the PEO/salt batteries. To achieve improved performance of this type of batteries, detailed information on the microscopic properties of the PEO and its mixtures is needed, for which an accurate atomic-level model is essential. Here is a hint about how to improve current models. Recent reports [3, 4] suggest that the polarizability of the solvent has an important effect on the structure, conformations, and dynamics of PEO, especially in its aqueous solutions. The ultimate goal of our study is to develop a reliable and accurate force field for the calculation of the structural, electrostatic, and dynamic properties of PEO in water and aqueous solutions of electrolytes, usable over a wide range of operating conditions. Here, we report our recent efforts in using molecular simulation to develop and optimize the force field and then to obtain detailed information about the polymer systems. In the first step, we simulate PEO dissolved in pure water. Initially, we use the simple SPC model for water and a potential model of PEO obtained from ab initio calculations [5]. Since polar interactions contribute significantly to the overall intermolecular forces, in the next step we extend the water, ions, and polymer potentials to explicitly account for the polarizability. To assess the reliability and accuracy of the developed force field, the resulting structural information from simulations is compared to data from neutron scattering experiments.

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