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Understanding the solvation structure in bulk electrolyte solutions

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Abstract

Understanding the relationship between the interaction of ions in solution with the solvation structure and its dynamics and the bulk properties like ionic conductivity, viscosity, etc is of considerable importance. Solute-solute, solute-solvent, and solvent-solvent interactions play a crucial role in determining the solvation structure and its dynamics [1-5]. The selection of suitable electrolyte can greatly impact the performace of electrical energy storage devices. In this work, we use molecular dynamics (MD) simulation to explore the solvation structure of alkali ions and halide ions in aqueous electrolyte solutions. Several structural and dynamical properties like radial distribution functions, diffusivity, velocity autocorrelation function, etc are computed to obtain a microscopic picture of solvation. In addition, we have examined the effect of counter-ion on the solvation structure of ions. We have also calculated the mean residence time (MRT) of solvent molecules in the first solvation shell (FSS) using stable states picture (SSP) approach. Results from this work can provide microscopic picture about the underlying mechanisms which play an important role in determining the macroscopic properties in electrolyte solutions.

Keywords: MD simulation, ionic conductivity, diffusivity, mean residence time, ionic solvation

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