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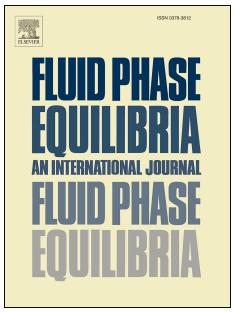

Recent progress in the molecular simulation of thermodynamic properties of aqueous electrolyte solutions

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Recent progress in the molecular simulation of thermodynamic properties of aqueous electrolyte solutions

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Abstract

We review progress in the development and application of molecular simulation methodology to predict the thermodynamic properties of aqueous electrolytes, focussing on work published since our previous review along similar lines [I. Nezbeda, et al., Mol. Phys. 114 (2016) 1665]. We consider such developments in the context of the use of Monte Carlo (MC) or Molecular Dynamics (MD) simulation methodologies using classical force fields. Special attention is paid to the incorporation of charge scaling approaches in the force fields, as well as to the simulation methodology used to compute solubility and osmotic pressure, and the use of the latter quantity to calculate the water activity and osmotic coefficient, and the electrolyte activity coefficient. We emphasize the importance of the statistical analysis of thermodynamic properties obtained from simulation data, and illustrate it with an example analyzing simulation osmotic pressure and electrolyte chemical potential data.

Keywords: molecular simulation, aqueous electrolytes, force fields, polarizable force fields, charge scaling, coarse grained models, osmotic ensemble, solubility, statistical analysis

1. Introduction

Electrolyte solutions are ubiquitous, in both natural and industrial systems. Examples range from biological, medical, oceanographic and geological to industrial applications, and the systems and properties of interest are similarly diverse. The same applies also to the computational tools used, the goals pursued, and the thermodynamic conditions of interest. This paper reviews progress in the development

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