Physics > Chemical Physics

Atomistic simulations of electrolyte solutions and hydrogels with explicit solvent models

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Two of the most challenging tasks in molecular simulation consist in capturing the properties of systems with long-range interactions (e.g. electrolyte solutions) as well as systems containing large molecules such as hydrogels. For the development and optimization of molecular force fields and models, a large number of simulation runs have to be evaluated to obtain the sensitivity of the target properties with respect to the model parameters. The present work discusses force field development for electrolytes regarding thermodynamic properties of their aqueous solutions. Furthermore, simulations are conducted for the volume transition of hydrogels in the presence of electrolytes. It is shown that the properties of these complex systems can be captured by molecular simulation.

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