

Abstract Submitted
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Coarse-Grained Modeling of Polyelectrolyte Solutions¹ ALAN R. DENTON, SYLVIO MAY, Department of Physics, North Dakota State University — Ionic mixtures, such as electrolyte and polyelectrolyte solutions, have attracted much attention recently for their rich and challenging combination of electrostatic and non-electrostatic interparticle forces and their practical importance, from battery technologies to biological systems. Hydration of ions in aqueous solutions is known to entail ion-specific effects, including variable solubility of organic molecules, as manifested in the classic Hofmeister series for salting-in and salting-out of proteins. The physical mechanism by which the solvent (water) mediates effective interactions between ions, however, is still poorly understood. Starting from a microscopic model of a polyelectrolyte solution, we apply a perturbation theory to derive a coarse-grained model of ions interacting through both long-range electrostatic and short-range solvent-induced pair potentials. Taking these effective interactions as input to molecular dynamics simulations, we calculate structural and thermodynamic properties of aqueous ionic solutions.

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