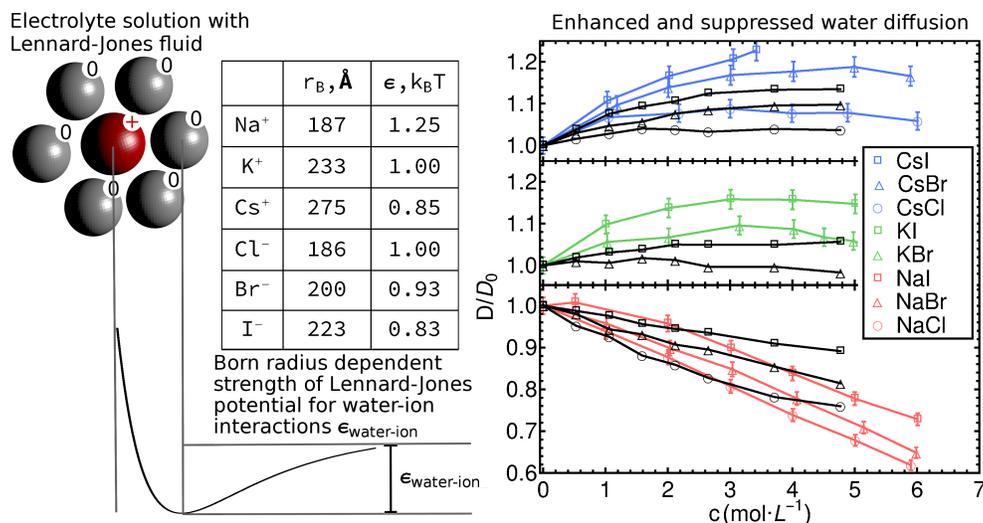


Coarse-Grained Model of the Dynamics of Electrolyte Solutions.

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Caption: Left: Outline of modeling approach. The strength of Lennard Jones interaction between ion and solvent bead is adjusted according to experimental values of Born radius. The strength for several ions are summarized in the table. Right: Comparison of calculated and experimental diffusion coefficients for several salt solutions. Both enhanced and suppressed diffusion is captured.

Scientific Achievement

A coarse-grained model of the influence of ion solvation on the dynamics of aqueous electrolyte solutions with a view to using this model later as a platform for modeling polyelectrolyte solutions was introduced. Our model for how specific ions influence the cohesive interaction strength between the ions and the solvent builds on physical arguments introduced before by Collins (Q. Rev. Biophys. 1985), that smaller ions solvate better than larger ions because of their higher charge density. We show our estimated values of water diffusion coefficient as a function of salt concentration. We find that our model indeed captures the diffusion of water in case of different types of ions and for variable salt concentration.

Significance

Ion-specific solvation has fundamental implications in biochemistry and the thermodynamics and the dynamics of aqueous salt solutions has correspondingly been investigated intensively. Nonetheless, there are fundamental unresolved issues in modeling the dynamics of aqueous salt

solutions and the related problem of polymers dissolved in these solutions. In particular, experiments show that the self-diffusion coefficient of water molecules in electrolyte solutions can be either enhanced or suppressed by particular salts having the same valence where the observed changes correlate with the Hofmeister series governing the relative solubility of proteins and water-soluble polymers in the same salt solutions.

Recent studies have demonstrated that common atomistic models of aqueous electrolyte solutions completely fail to reproduce this basic phenomenon. Drawing on similar trends observed in the field of polymer nanocomposites, we propose a coarse-grained model of aqueous electrolyte solutions that captures the observed trends and which offers physical insight into the influence of salt on the thermodynamic and dynamic properties of electrolyte/polyelectrolyte solutions.

Citation

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