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Abstract

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Aqueous Solvation of Charged and Hydrophobic Groups: from Simple Ions to Proteins

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Abstract: Much of biology depends on proteins interacting with each other – pairwise or in aggregates – all mediated by water and ions. Understanding the aqueous solvation of electrolytes, simple and complex, is therefore important for biology, as also for industry. But today's solvation models mostly apply to dilute solutions and, despite being supported by all-atom simulations, do not yield good results for thermodynamic properties. In recent years we applied statistical-mechanics to such systems. We used Wertheim's integral equation and thermodynamic perturbation theories, which are well suited for systems of molecules with directional forces. Such an approach is able to treat mixture of water molecules, ions and proteins, with all the species treated on equal level of approximation. We begin the presentation with the aqueous solutions of alkali halides to show the effects of ionic sizes of salt–forming ions on osmotic properties of the solution. Next, we ask ourselves how the presence of hydrophobic groups affects the solution energetics? We conclude the presentation with discussion of the protein (globular proteins as also the monoclonal antibodies) self–association. In several examples we demonstrate, that one of the crucial parameters to understand aqueous solutions is the free energy of hydration of interacting charges.

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