Predicting the Chemical Potential of Solutes in Aqueous Solutions Using Infinite Dilution Properties

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The ability to predict the chemical potential of solutes at finite concentrations in aqueous solutions is of great importance. Such information is central to the design of aqueous based extraction processes and to understanding the phase behavior of biological compounds and environmental pollutants in solutions.

While it would be best to directly model the desired system at the finite concentrations of interest, this may not always be practical. For example, the equilibrium composition is likely unknown a priori, and great computation effort may be needed to locate it. If the equilibrium concentration is unknown, calculations may unknowingly be performed on a metastable system beyond the equilibrium composition. Additionally, for complex biological systems, the difficulty (and time) to adequately explore configurational phase space likely increases with concentration. For a solute at infinite dilution, we can be sure that the simulation is both stable and that the burden to sample phase space is reduced.

In this talk we will show a simple, analytical expression that may be used to accurately extrapolate the residual chemical potential of solutes at infinite dilution in aqueous solutions to finite concentrations. The method will be applied to binary systems containing water and the following co-solvents: methanol, ethanol, 2-propanol, acetone, and 1,4-dioxane. In all cases, the infinite dilution residual chemical potential was computed using conventional free energy methodologies, and the results compared to simulations at finite concentrations.