Effective electrolytes: Generalizing collective interactions in solution

TCI SEMINAR

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Not all interactions exist in a vacuum. The explicit environment plays a large role in the forces felt between molecules. Uncovering a true collective interaction representing the mean force between particles in solution is a cumbersome process that requires extended sampling of the available states of a given environment. Here, we present an approach for quantitative prediction of collective interactions between arbitrary particles in solution that we call interpolation Potential of Mean Force (i-PMF). i-PMF works via smooth interpolation over a regular multidimensional grid of known explicit solvent PMFs. The chief advantage of i-PMF is computational cost. Whereas it can take upwards of 100 CPU hours to compute a PMF between two ions via explicit molecular simulation, i-PMF produces an equivalently accurate PMF in seconds. We perform extensive comparisons between explicit simulation and i-PMF results for electrolyte solutions and discuss the benefits and pitfalls of this strategy. Finally, we discuss extensions of this work for rapid and accurate implicit modeling of solutions with varied and more complex solutes.

Theoretical Chemistry Institute Seminar Series