Abstract for an Invited Paper
for the MAR06 Meeting of
The American Physical Society

Modeling water, hydrophobic interactions, and polymer collapse

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Small and large nonpolar solutes exhibit qualitatively different hydration thermodynamics. The former are naturally accommodated into bulk water via equilibrium density fluctuations, while the latter require the formation of a macroscopic solute-water interface. Although there has been significant progress on the theory of lengthscale-dependent hydration, there are still many open questions concerning how various thermodynamic parameters (e.g., pressure, additive concentration, and pH) impact the crossover between small and large solute behavior. Similarly, there is confusion over whether hydration of small, intermediate, or large lengthscales dominate in various biological self-assembly processes. In this talk, I discuss recent theoretical progress on understanding how solution conditions affect the crossover between small and large solute hydration phenomena and how simulation/theory of the collapse of hydrophobic polymers can provide new insights into the relevance of hydrophobic interactions at different lengthscales.