TCI SEMINAR

The Effect of Cosolvents on Aqueous Systems and Protein Solvation

Monday, May 10, 2010
2:00 p.m. Room 9341

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Cosolvents and hydrophobic confinement both play important roles in affecting the structures, dynamics, and interfacial behavior of aqueous solutions. These effects are essential for the understanding of biological systems, for example, the folding and dynamics of proteins. Using molecular dynamics simulations, we study how cosolvents including urea, trimethylamine N-Oxide (TMAO), and alcohol affect the aqueous solution structure as well as the protein structure formation. These studies showed that cosolvents do affect the hydration of proteins. For example, urea changes the water activity and enhances water/protein and interaction. At the same time, urea can also interact directly and effectively with proteins through both hydrogen bonding and van der Waals interactions. On the other hand TMAO decreases the hydration of both hydrophilic protein backbones as well as the hydrophobic cores.

In the second part of the talk, the possible long range effects of hydrophobic confinement on the water structure will be discussed. Molecular dynamics simulations showed that a meta-stable state of water might exist in the confined environment, which is quite different, both structurally and dynamically from the bulk water. The origin of this effect will be discussed based on simple thermodynamics and statistical mechanics argument.