TCI SEMINAR

Solvation effects in polypeptide folding

Friday, July 27, 2012
11:45 a.m. Room 8335

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Solvation plays major roles in protein folding. Small molecules and ions can have strong effects. We used both traditional and recently developed enhanced sampling molecular dynamics simulations to study polypeptide folding. These studies allowed us to quantitatively determine the folding free energy landscape of a number of polypeptides, and to investigate the effects of cosolvents, such as alcohols, and inorganic salts. The calculated results are qualitatively consistent with the experimental observations and show the usefulness of molecular dynamics simulations in understanding these multi-component and complex aqueous solutions of polypeptide. Simple theoretical models, which take into account both direct cosolute/cosolvents binding and their effects on hydration, were developed to understand the molecular mechanisms through which organic cosolvents and inorganic salts affect water structure (and dynamics), as well as protein hydration and folding. Using these models, we try to understand in a more general term how salts as well as organic cosolvents affect the protein structures. Comparisons with experiments will be discussed.