Weekly Seminar

Towards understanding the solution dynamics using the combination of computer simulation and spectroscopy

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Abstract

Microscopic solution dynamics is a central topic in the condense matter sciences. Optical spectroscopies play important roles in the investigations in this field. Analysis and understanding of the solution spectra are usually non-trivial due to the complex nature of the systems. We carried out series of spectral modeling based on the molecular dynamics simulation to help understanding the dynamic events in the protein aqueous solution and ionic solution systems. A technique combining the Markov State Model (MSM) and the Nonlinear Exciton Propagation (NEP) methods was developed to simulate the T-jump triggered long time peptide unfolding process and the related IR, 2DIR and fluorescence spectra. Furthermore, to overcome the convergence issue in the sampling and reduce the computational cost, implicit solvent model was introduced into the simulation, which generates converged temperature dependent peptide configuration distribution. We demonstrated that IR and 2DIR spectra simulated based on this distribution nicely reproduce the temperature dependences of experimental signals. An important, but not yet clearly addressed, issue in ionic solution research is how the microscopic dynamics in the solution is influenced by the ionic density distribution. Molecular dynamics simulations were carried out to investigate the microscopic origin of the dynamical heterogeneities in the ionic solutions, which was probed recently using the ultrafast vibrational energy exchange and anisotropy measurements. Our simulations revealed that these dynamical heterogeneities observed originate from the inhomogeneous ion density distribution in the solution, and are detectable using the combination of the ultrafast infrared, the dielectric relaxation and the optical kerr effect techniques. Simulations further suggest that, in some of the solutions, the ion pairing effect has significant contribution to the ion distribution inhomogeneity. Our studies thus provide a microscopic insight on the origin of the inhomogeneous ion density distribution and its connection with various experimentally observable dynamical phenomena in the ionic solutions.

About the Speaker

Wei Zhuang got his bachelor degree from University of Science and Technology of China in 2000 and his Ph.D degree from University of California, Irvine in 2007. His research interests are:

¹Developing a theoretical protocol, which combines molecular dynamics simulation, QM/MM Hamiltonian construction and Quasiparticle Green's function representation of the response, for the investigation of protein and RNA folding and misfolding mechanism.

¹Developing theoretical and computational techniques for the study of pathways for electron and energy transfer and self-assembly phenomena in the natural light harvesting and photosynthesis systems.

¹Developing user friendly computational software which bridges between computer simulation and ultrafast experiments and provides a unique way to investigate the spectroscopic reflection of the MD simulation observables as well as understand the physics underlying the experimental spectroscopic features.

¹Applying ultrafast correlation spectroscopies to investigate large complex biological systems and phenomena such as amyloid fibrils, membrane, chemical exchange, light harvesting systems, biosensor and polymer materials.