NYU-ECNU Institute of Mathematical Sciences at NYU Shanghai

WEEKLY SEMINAR

Topic: **Protein Structure and Dynamics, Polarization and MD Simulation**

Speaker: **John Z.H. Zhang, NYU-ECNU Center for Computational Chemistry at New York University Shanghai**

Time: 14:30-16:30, 23 October 2013

Venue: Room 153, Geography Building, 3663 Zhongshan Road North, Shanghai (华东师范大学中山北路校区，地理楼 153 室)

ABSTRACT OF THE TALK

Electrostatic interaction is perhaps the most important interaction in biomolecules, but so far the molecular force fields widely used to describe protein systems lack the polarization effect. In order to correctly describe the structure and interaction dynamics of biomolecules, important effects such as polarization, charge transfer, hydrogen bonding and metal coordination, etc., need to be properly represented and included in the form of force field for dynamics simulation and sampling. Based on the recently developed fragment quantum method for proteins, we developed polarized protein-specific force field which takes into account polarization effect of specific protein structures. In this talk, we focus on the effect of polarization on structure and dynamics of proteins, protein-ligand interaction, protein-protein interaction, protein folding. These studies demonstrated that proper inclusion of these important quantum-based effects in biomolecular simulations are important and even critical in our understanding of structure and interaction dynamics of biomolecular systems.

BIOGRAPHY

John Zhang received his BS degree from the Physics Department of East China Normal University in 1982 and Ph. D from University of Houston in 1987. His current research focus is the development of novel computational methods for accurate and efficient study of biological systems; quantum mechanical methods and their applications to accurately predict protein structure; protein folding; free energy in protein-drug and protein-protein bindings; development of new polarized force field for biomolecular simulation; molecular dynamics simulation and rational drug design.