

Modeling Biomolecular Association and Structure

Monday, September 24, 2012
3:00 p.m. Room 8335



Professor Pengyu Ren
Department of Biomedical Engineering
The University of Texas at Austin

Electrostatic forces play important roles in specific recognition between biomolecules. I will present a classical model for intermolecular forces based on polarizable atomic multipoles, and its applications to ions and protein-ligand interactions. The importance and treatment of short-range electrostatic interactions and polarization effect will be discussed. In the second part of the talk, I will present our work on modeling RNA structure with a statistical/physics-based low-resolution model, and its potential for high-throughput structure determination.

Theoretical Chemistry Institute Seminar Series