

**Yongcheng Zhou**

University of California, San Diego

Title:

**Continuum modeling of macromolecular electrostatics and conformational change: mathematical analysis and simulations**

**Abstract:**

The conformational change in large spatial and temporal scale is essential for the proper functions of macromolecules such as ion channel gating, membrane transport and molecular motors; Such large deformation usually involve the electrostatic force as the major driving force. This talk will be focused on the continuum modeling and computation of the electrostatic force and its coupling with the large macromolecular deformation modeled as nonlinear elastic displacement. We will investigate the regularity and the solvability of these electro-elasticity equations, analyze a stable regularization method for solving the singular electrostatic potential from the Poisson-Boltzmann equation, discuss the numerical issues related to harmonic extension of the elastic displacement in the solvent region, and apply this model to an important biological process: the BAR domain-induced membrane curvature. I will also highlight the mathematical problems for refining this model and other ongoing projects about the electro-diffusion in molecular and cellular levels.