

Public Abstract

First Name:Lorant

Middle Name:

Last Name:Janosi

Adviser's First Name:Ioan

Adviser's Last Name:Kosztin

Co-Adviser's First Name:

Co-Adviser's Last Name:

Graduation Term:FS 2007

Department:Physics

Degree:PhD

Title:Multiscale Modeling of Biomolecular Systems

Studies of structure-function relationships in biomolecular systems require to follow nanometersize systems on time scales spanning from pico- to micro-seconds, while maintaining atomic scale spatial resolution in all-atom molecular dynamics (MD) simulations. In this work we propose new methods to investigate the following, intrinsically multiscale problems: (i) theoretical prediction of optical and spectral properties of pigment-protein complexes, (ii) reconstruction of potential of mean force and its corresponding diffusion coefficient from non-equilibrium molecular dynamics simulations, (iii) transport of potassium ion through the Gramicidin A channel and of glycerol through the GlpF channel, and (iv) prediction of the species-dependent oligomerization state of the light harvesting antenna complexes. The main novelty of these methods is that they rely only on the high resolution atomic structure of the biomolecular system. Therefore, they have not only explanatory, but predictive power as well.