# MULTISCALE MODELING OF BIOMOLECULAR SYSTEMS

**Lorant Janosi**

**Dr. Ioan Kosztin, Dissertation Supervisor**

## Abstract

Studies of structure-function relationships in biomolecular systems require to follow nanometer-size 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.