Public Abstract

First Name:Jiong

Middle Name:

Last Name:Zhang

Adviser's First Name:Ioan

Adviser's Last Name:Kosztin

Co-Adviser's First Name:

Co-Adviser's Last Name:

Graduation Term:SP 2016

Department:Physics

Degree:PhD

Title:THEORETICAL AND COMPUTATIONAL
STUDIES OF BIO-MOLECULAR SYSTEMS:
STRUCTURE AND DYNAMICS

This dissertation describes a series of studies of complex bio-molecular systems and processes that cover aspects from structures to dynamics. Protein structures are crucial to understand the processes of living activities. Experimental methods, such as X-ray crystallography and NMR, are generally used to determine the 3D structures of proteins. However, these methods are expensive and time-consuming. Therefore, the gap between known sequences and structures is getting bigger and bigger. Scientists are trying to develop computational methods for predicting the 3D structures from amino acid sequences. It has reached a level that numerous server could generate a large pool of near-native protein structure models, but the refinement and selection of the best model remain problematic. I developed a selective refinement method and a selective molecular dynamics simulation based selection method. Using these two methods, I developed a protein structure prediction server, which performs well in the world wide competition for estimating protein structure prediction methods. Besides structures, we also need to understand the dynamics to relate structures and functions. I developed a method to simultaneously determine the potential of mean force and dynamics model of biomolecular systems. With the potential of mean force and dynamics model, the system can be fully characterized.