Center for Molecular Spectroscopy and Dynamics, IBS-Korea University

IBS Center for Molecular Spectroscopy and Dynamics

COLLOQUIUM

- **SPEAKER**
  Dr. Holly Freedman (IBS Center for Molecular Spectroscopy and Dynamics)

- **TITLE**
  Some Computational Studies of Molecular Structure and Dynamics Applied to Biomedical Problems

- **ABSTRACT**
  First, I will give two examples where I have applied computation to study the structure and/or dynamics of biological systems relevant to problems in virology. I will describe the prediction of a full-length model of the E1/E2 heterodimer comprising the HCV viral envelope, based on the partial crystal structures of the envelope glycoproteins E1 and E2. A better understanding of the structure and dynamics of the HCV viral envelope, which is responsible for attachment and fusion, could aid in the development of a vaccine. Next, I will discuss determining relative binding free energies of nucleotide analogues to human mitochondrial DNA-dependent RNA polymerase (POLRMT), an important source of off-target toxicity, by running molecular dynamics simulations on our Blue Gene supercomputer. I will present a comparison of relative binding affinities computed with free energy perturbation (FEP) to the experimental values. A better understanding of the dynamical process of vibrational energy transfer in proteins following ATP hydrolysis may also make it possible to design means of regulating such processes. In the second half of my talk, we will consider the coupling of amide I vibrational excitations to alpha-helical phonon modes, which was proposed by A. S. Davydov to facilitate energy storage and propagation in proteins following ATP hydrolysis. Because of the computational expense associated with fully quantum mechanical treatments of systems with many degrees of freedom, practical simulations of the Davydov-Scott model may be realized via a mixed quantum-classical approach. A surface-hopping solution of the mixed quantum-classical Liouville (MQCL) equation is implemented to study vibrational delocalization in a one-dimensional model of a protein alpha helix.

- **DATE AND VENUE**
  August 22, 2018 (Wednesday, 4:00 - 5:00 pm)
  Seminar Room A 116, KU R&D Center

- **LANGUAGE**
  English