Center for Molecular Spectroscopy and Dynamics, IBS-Korea University

IBS Center for Molecular Spectroscopy and Dynamics

Seminar

- **SPEAKER**
  Dr. Hyun Woo Kim (KRICT)

- **TITLE**
  All-atom simulations of excitation energy transfer in the FMO complex and machine learning applications for chemical problems

- **ABSTRACT**
  In this talk, I will present two topics that I worked on during my PhD course and that I am currently working on. In the first part, I will explain one of mixed quantum-classical (MQC) approaches and how to apply this method to all-atom simulations. As we know, after the photo-excitation, chromophores in a complex environment quickly relax through various pathways including multiple electronic and vibrational states. To simulate these dynamics, we adopted mixed quantum-classical (MQC) approaches which are developed by combining concepts of both quantum and classical mechanics with reasonable approximations. Later, I will briefly present the applications of machine learning to solve chemical problems such as (1) potential energy prediction, (2) representation learning, and (3) reaction condition suggestion. In this part, I will emphasize how we can optimize the experimental results using machine learning and global optimization.

- **DATE AND VENUE**
  February 01, 2021 (Monday, 11:00 - 12:00)
  Virtual Conference