Visiting Professors

Visiting Professor
HASEGAWA, Jun-ya *(from Hokkaido University)*

Quantum Chemistry for the Excited States of Functional Molecules in Proteins and Solutions

Molecular interactions between chromophore and environment are the essential to furnish a protein with the photo-functionality. I am interested in the machinery of the photo-functions such as photo-synthesis, vision, and bioluminescence. To understand the mechanism and to develop chemical concept behind the photo-functions, we develop electronic structure theories for excited state, analytical method for excitation-energy transfer pathway, and a hybrid quantum-mechanics/molecular mechanics method. In recent studies, we have clarified color-tuning mechanism of photo-functional proteins and excitation transfer mechanism of bridge-mediated donor-acceptor systems. We are also interested in developing a configuration interaction picture for the solvatochromic response of the molecular environment.

Visiting Associate Professor
ANDO, Koji *(from Kyoto University)*

Quantum Transfer Processes in Chemical and Biological Systems

At the core of chemistry, biochemistry, and materials sciences are reduction-oxidation and acid-base reactions, in which electron and proton transfers are the key elementary processes. Our research group has been working on theoretical and computational modeling of these inherently quantum dynamical processes in condensed matters. One recent achievement is a development of new quantum Monte Carlo simulation method with an account of induced-dipole corrections obtained from fragment molecular orbital calculations. It adequately described isotope mixing effect of dielectric phase transition temperature of hydrogen-bonding organic molecular crystal. Another is a development and numerical assessment of initial-value-represented propagator for semiquantal squeezed-state wave packet propagation, which extends our previous works of nuclear wave packet molecular dynamics simulation method.

Visiting Associate Professor
MORISHITA, Tetsuya *(from AIST)*

Development of *ab initio* Mean-Force Dynamics for Free-Energy Calculations

We have been developing a method for constructing free-energy profiles in the framework of *ab initio* molecular-dynamics. It is well known that the electronic state needs to be explicitly taken into account to describe bond formation or bond breaking in. *e.g.*, conformational transformations of biomolecules, which plays an important role in constructing their free-energy profiles. Developing force-fields that can describe such bond formations is, however, considered to be extremely difficult. It is therefore of great importance to develop a method that enables us to construct free-energy profiles without empirical force-fields.

Our interest particularly focuses on the incorporation of *ab initio* interatomic interactions into logarithmic mean-force dynamics (LogMFD), which is expected to enable us to efficiently construct free-energy profiles within the accuracy of *ab initio* force-fields. A preliminary result of "*ab initio*" LogMFD calculation for glycine dipeptide molecule has been recently obtained. We found that the free-energy landscape is sensitive to the description of the hydrogen bonding, which may not be appropriately handled with an empirical force-field only.