Visiting Professors

Visiting Associate Professor
HASEGAWA, Jun-ya *(from Kyoto 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 and biochemistry are reduction-oxidation and acid-base reactions, whose elementary processes are electron and proton transfers. Our research group has been working on theoretical and computational modeling of these inherently quantum dynamical processes. One recent achievement is a development of electron transfer (ET) pathway analysis method with use of fragment molecular orbital calculations, by which the ETs in a bacterial photosynthetic reaction center have been studied. Another is a development of nuclear wave packet molecular dynamics simulation method and its applications to hydrogen-bond exchange dynamics in water. It has been also discovered that the latter can be extended to electron wave packet simulations by exploiting the non-orthogonal valence-bond theory, which anticipates a non-Born-Oppenheimer electron–nuclear dynamical treatment.

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

First-Principles Molecular-Dynamics Simulations of Liquids and Glassy Materials

I have been interested in structural and dynamical properties of non-crystalline materials including nanoscale materials. In 2011, I have found that liquid silicon exhibits compressed exponential relaxation over a wide temperature range including the supercooled regime, in contrast to water and other glass-forming liquids, using first-principles molecular-dynamics simulations.

I have also developed a new method for free-energy calculation, Logarithmic Mean-Force Dynamics (LogMFD). This method was successfully applied to reconstruction of the free-energy profile of a dipeptide molecule, showing that LogMFD considerably outperforms conventional free-energy calculation methods such as thermodynamics integration.