Visiting Professors

Visiting Professor
TAKETSUGU, Tetsuya *(from Hokkaido University)*

Ab Initio Dynamics Study of Excited-State Chemical Reactions

We have developed an ab initio molecular dynamics (AIMD) program code for excited-state reaction dynamics, combined with the quantum chemistry program packages, MOLPRO and GAMESS, and applied it to several significant photoreactions at the state-averaged CASSCF level. In the current code, non-adiabatic transitions are treated by the Tully's surface hopping algorithm, while the solvent effects are treated by QM/MM approach. The applications include the excited-state dynamics of 7-azaindole-H_2O cluster (excited-state proton transfer), coumarin 151 in water solution (large solvent effects), cytosine (examination of photostability), photo-isomerization of azobenzene (examination of reaction pathways), dissociative recombination reactions of small molecules (surface hopping dynamics), and photodissociation of CH_3I (spin-orbit coupling effects). Through these applications, the code has been extended for general use to examine excited-state dynamics of real molecular system.

Visiting Associate Professor
NAKAJIMA, Takahito *(from The University of Tokyo)*

Development of Large-Scale Molecular Theory

With the emergence of peta-scale computing platforms we are entering a new period of the molecular simulation. The computer simulations can be carried out for larger, more complex, and more realistic molecular systems such as nano- and bio-materials than ever before. To make the most of the computer resource, we should achieve some breakthroughs of conventional theoretical approaches. We have proposed several efficient molecular theories to treat large molecular systems accurately via relativistic and non-relativistic treatments. These approaches include several types of auxiliary basis approaches, such as the pseudospectral method, the resolution of the identity method, the augmented plane-waves method, and the augmented finite-elements method. We expect that these approaches will be capable of the clarification of chemical phenomena in nano- and bio-materials with the help of the next generation supercomputer.

Visiting Associate Professor
HAYASHI, Shigehiko *(from Kyoto University)*

Molecular Simulation Studies of Protein Functions

Protein functional activities involve dynamic molecular conformational changes of complex protein systems. Hence molecular dynamics underlying functional activities are necessary to be revealed for understanding of molecular nature of protein functions. We performed molecular dynamics (MD) simulations on photochemical dynamics of rhodopsins (Rh) and ligand migration dynamics in myoglobin (Mb). We carried out an ab initio quantum mechanical/molecular mechanical MD simulation for the retinal photoisomerization processes in Rh, and revealed a dynamic regulation mechanism for the fast photoisomerization. We also examined the ligand migration dynamics in Mb by a meta-dynamics simulation and a linear response theory, and identified remarkable collective protein motions coupled to the transient ligand migrations through the migration channels.