Visiting Professors

Visiting Professor
SHIGETA, Yasuteru *(from University of Tsukuba)*

Theoretical Analyses on Functions of Biomolecules

Several biological functions, such as molecular recognition, enzyme catalysis, signal transduction, allosteric regulation, and protein folding, are strongly related to conformational transitions of biomolecules. In order to understand these biologically relevant phenomena, we have developed new algorithms for conformational search, a fragment molecular orbital method, first-principles molecular dynamics simulations and applied them to protein folding problems, energy transfer in proteins, and enzymatic reaction analyses. In particular, we have investigated conformational changes of a GDP binding form of FtsZ from Staphylococcus aureus, which are related to shrink of Z-ring during a cell fission processes by using a newly developed conformational search method. We also suggest a few amino acid residues that are important for recognition of GDP and thus the conformational changes.

Visiting Associate Professor
NAGATA, Yuki *(from Max Planck Institute for Polymer Research)*

Combined Simulation and Experiment Reveals Physics of Ice Interface

Our group aims at obtaining molecular level understanding of the structure and dynamics of aqueous liquid interfaces, with particular emphasis on water, thought 'theoretical sum-frequency generation (SFG) spectroscopy.' The main highlight in our group in 2016 and 2017 is the SFG probe of the ice interface. We worked on the water conformation near the ice nucleation protein, where we found that the hydrophobic and hydrophilic patterns would be crucial for ice nucleation (*Sci. Adv.* 2016). Further focus has been made on the anomaly of the ice surface melting, where we found the presence of the excess hydrogen bond at the top most ice layer at 200 K, through the formation of non-hexagonal ice (*PRL* 2017). The details of the peak assignment of the SFG spectra were also made (*JPCL* 2017). In addition, we have contributed to several review papers for vibrational spectroscopy of water (*Chem. Rev.* 2016), modeling of interface (*JPCB* 2016) and TMAO molecule (*PCCP* 2017). Through this, it was also very fruitful to start a new collaboration, in particular, with Prof. Wataru Mizukami (Kyusyu Univ.) who used to be a graduate student in IMS.

Visiting Associate Professor
KATO, Tsuyoshi *(from The University of Tokyo)*

Development of Effective Potential Theory for Quantal Dynamics

I am studying in the area of quantal molecular dynamics focusing on the developments of new methods to calculate the electronic and nuclear dynamics in molecules. I am constructing a time-dependent effective potential theory that could be used to calculate the exact time-dependent wave function of a many-electron system. During the development of the effective potential theory, I found a solution algorithm for the time-independent/dependent inverse Kohn-Sham problem in terms of the effective potential calculated for an exact time-dependent/stationary wave function. Given the exact time-dependent wave function describing quantal many-particle dynamics, my final goal is to establish a method to derive an exact effective single- and two-particle potentials out of the many-particle wave function in order to deepen the understanding of quantal dynamics in atoms and molecules.