Visiting Professors

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

Computational Analyses on Biological Functions at the Atomic Scale

Life is a system that converts a variety of energy (mechanical, electrostatic, thermal, chemical, information, and so forth) into each other to maintain itself. For the understanding and controlling phenomena in the life, elucidation of the relationship between the three-dimensional conformational changes and biological functions of proteins at the atomic scale has become one of the most important issues. However, these conformational changes are induced as slow dynamics upon collective motions, including biologically relevant large-amplitude fluctuations of proteins. Our group develops an efficient conformational search method using molecular dynamics simulations and investigates dynamics of proteins that drive specific biological functions on the basis of quantum mechanical and statistical physics-based methods.

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

Combined Simulation and Experiment Reveals Physics of Aqueous Interface

Our group aims at obtaining molecular-level understanding of the structure and dynamics of aqueous liquid interfaces, with particular emphasis on water. To this end, by using molecular dynamics (MD) simulations, we have made a direct connection to experiments using 'theoretical sum-frequency generation (SFG) spectroscopy'—both in aiding the interpretation of experimental results, as well as designing novel experiments and experimental schemes. We have interrogated the molecular conformation of water at the water-air and water-lipid interface as well as the effects of surface-active molecules on the conformation of the interfacial water molecules. One research highlights that the water's O–H group near zwitterionic lipids orients *up* toward lipid uniformly, although zwitterionic lipids can be, in principle, electronegative/positive. Having established an excellent agreement between SFG simulation and experiment, we also predicted the molecular mechanism of water evaporation from MD simulation. It turned out that the evaporation is not stochastic process, but has certain pathway for transferring the momentum of water.

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

Development of Quantal Dynamical Theory and Its Application to Molecular Dynamics

I am studying in the area of quantal molecular dynamics mainly focusing on the developments of new methods to calculate the electronic and nuclear dynamics in molecules interacting with strong laser field. Currently, 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 Kohn-Sham problem, and presently I am analyzing the relations among some exact wave function theories and density functional theory. 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. Consequently, we are able to use the notions, that are deduced from the analysis of the properties of the exact effective potentials, within the quantum optimal control theory as well as to analyze the chemical reactions.