Visiting Professors

Visiting Professor
SATO, Hirofumi *(from Kyoto University)*

Theoretical Study of Electronic Structure and Statistical Mechanics for Molecular Systems

Our research focuses on developing new quantum chemistry and statistical mechanics theories and analysing chemical phenomena in condensed matter systems consisting of polyatomic molecules.

(1) Based on biorthogonal second quantisation, we proposed a method to extract the resonance structures embedded in molecular orbital and the local spin structures. A geminal theory for a molecule's electronic structure is also proposed based on generalised electron pairing. (2) The statistical mechanics of molecular liquids is an analytical and systematic approach to understanding liquids' structure and thermodynamic properties. In addition to hybrid methods with quantum chemistry, we have developed many novel methods, including density functional theory and diffusion equations for polyatomic molecular systems. Recently, we proposed an ab initio theory for NMR chemical shifts based on the RISM-SCF-SEDD method. (3) The mechanisms of various chemical reactions and phenomena have been clarified at the molecular level. For example, the self-assembly process of the transition metal complex system was clarified.

Visiting Professor
YOSHIDA, Norio *(from Nagoya University)*

Theoretical Study of Chemical and Biological Processes in Solution

We are interested in the chemical and biological processes in solution with a particular focus on the role of solvents in these processes. Our group is studying the role of solvents in these processes based on the integral equation theory of molecular liquids. Recently, based on a multiscale hybrid method of integral equation theory and quantum chemical methods, we have elucidated the mechanism of pKa shift due to molecular recognition in solution. In addition, using a hybrid Monte Carlo framework, we developed a method for structural sampling of biomolecules in solution that satisfies the Hamiltonian based on integral equation theory.

Visiting Associate Professor
NOGUCHI, Hiroshi *(from University of Tokyo)*

Theoretical Study on Soft Matter and Biophysics

We study soft-matter physics and biophysics using theory and simulations. Our main targets are the structure formation of biomembrane and the dynamics of complex fluids under various conditions. This year, we investigated the shape transformation of membrane induced by curvature-inducing proteins. We estimated the anisotropic bending rigidity and spontaneous curvature of crescent curvature-inducing proteins from tethered-vesicle experimental data using a mean-field theory. Our coarse-grained simulations revealed that reaction waves of curvature-inducing proteins can induce large shape transformations, such as membrane budding and necking, that erase or divide the wave. Moreover, we demonstrated that the occasional disappearance of the waves can alter the pathway of wave propagation on a membrane network.