Visiting Professors

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

Theoretical Study of Electronic Structure and Statistical Mechanics for Molecular Systems

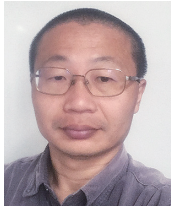
Our research focuses on developing new theories in quantum chemistry and statistical mechanics and on analysing chemical phenomena in condensed matter systems consisting of polyatomic molecules.

(1) Based on biorthogonal second quantisation, we proposed a method to extract the resonance structures embedded in molecular orbital computations and the local spin structures. (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. The phenomena at the electrode interface were systematised based on molecular dynamics simulation.

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, we have developed an accurate pKa prediction method for molecules in solution based on a hybrid method of integral equation theory and quantum chemical methods. Related to the method, in collaboration with the Institute for Molecular Science, we are developing an efficient structural sampling method for the pH-dependent protonation state of dissociative amino acid residues in proteins. We are also developing a novel integral equation theory that takes into account the electronic polarization of the solvent and applies it to electron-transfer reactions in solution.



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 using mean-field theory and coarse-grained membrane simulations. We clarified the difference between laterally anisotropic and isotropic proteins in the curvature sensing and generation. In particular, the sensing curvature of the anisotropic proteins depends on the protein density, whereas that of the isotropic proteins is constant. Traveling waves of chemical reactions containing curvature-inducing proteins change the membrane shapes and vice versa. Moreover, we investigated cavitation and bubble oscillation in sound-wave propagation using massively parallel simulations.