Visiting Professors

Visiting Professor
NAKANO, Masayoshi *(from Osaka University)*

Theoretical Study on Photofunctionalities of Open-Shell Molecular Systems

Through close collaboration between theoretical and experimental research groups, we have clarified a new structure-property correlation between diradical character and singlet–triplet energy gap for indenoindenodibenzothiophene diradicals: Inclusion of thiophenes within a quinoidal polycyclic hydrocarbon imparts appreciable diradical character yet retains the large singlet–triplet energy gap, a phenomenon that has no precedent in the literature. Theoretical investigation has revealed that the low aromatic character of thiophene and its electron-rich nature are the key properties leading to these unique findings. This new structure–property relationship is not only extremely important in the field of diradical chemistry and organic electronics, but also provides new insights into the versatility of π-electron chemical bonding. We have also developed a computational method for analyzing the singlet fission dynamics for molecular aggregates beyond dimer models. Using this method, we have clarified unique size and architecture dependences of SF dynamics, which will be useful for constructing novel design guidelines for highly-efficient SF materials.

Visiting Professor
NAKAYAMA, Akira *(from The University of Tokyo)*

First-Principles Simulations of the Molecular Process at the Interface of Liquid/Metal-Oxide

A detailed understanding of the interface between liquid and metal-oxide is fundamental due to its relevance to the broad range of physicochemical phenomena and technological applications. To provide microscopic insight into the structures and dynamics at the liquid/metal-oxide interface, we perform the first-principles molecular dynamics simulations and unveil the intricate molecular process occurring at the interface. In this year, we have focused on the catalytic reactions at the water/CeO_2 and methanol/CeO_2 interfaces and investigated the role of acid-base and redox sites over CeO_2. In particular, we have worked on the following topics: (1) Substrate-specific adsorption of 2-cyanopyridine and hydration reaction over CeO_2. (2) The reaction mechanism for the direct synthesis of dimethyl carbonate from methanol and CO_2 over CeO_2 and ZrO_2. (3) Enhanced sampling employing the temperature-accelerated sliced sampling scheme for constructing multi-dimensional free energy landscape.

Visiting Associate Professor
KIM, Kang *(from Osaka University)*

Theoretical and Computational Research for Complex Fluids and Soft Matters

We are working on theoretical and simulation approaches to reveal various dynamical processes in complex fluids and soft matters. Recent topics in my research are related to slow dynamics in supercooled water. In particular, we have developed the cage jump model for the dynamics of supercooled water. The caged and jumping states of a water molecule are introduced with respect to the hydrogen-bond rearrangement process and describe the motion in supercooled states. It is then demonstrated from the molecular dynamics simulation that the characteristic length and time scales of cage jump motions provide a good description of the self-diffusion constant. Furthermore, using molecular dynamics simulations we have assessed the violations of the Stokes–Einstein and Stokes–Einstein–Debye relationships in supercooled water by the identification of timescales that appropriately characterize transport coefficients, such as translational diffusion constant, rotational relaxation time, and shear viscosity.