Visiting Professors

Visiting Professor
MORI, Hirotoshi *(from Chuo University)*

Electronic Structure Informatics for Designing Functional Liquid Materials

Mixed liquids exhibit various chemical functions depending on their composition and mixing ratio. Contrary to its fundamental scientific importance, however, the chemistry of mixing is an area where molecular level knowledge is not still enough. With the backgrounds, we have been challenging the predictive chemistry of functional liquid materials by developing a novel *ab initio* molecular simulation method with conventional computational cost (Effective fragment potential molecular dynamics; EFP-MD) and a data science approach. In fiscal 2020, we worked on the prediction of Henry's constant values related to the absorption of various industrial exhaust gases for non-aqueous mixed solutions (mixed ionic liquids, ionic liquids/organic solvent mixtures) which supports environmental chemical engineers shortly. We will proceed with our research aiming at the construction of statistical thermodynamic theory for real systems that predict mixed thermodynamics.

Visiting Professor
YANASE, Youichi *(from Kyoto University)*

Theoretical Study of Exotic Quantum Phases

We are working on theoretical studies of exotic quantum phases such as unconventional superconductivity, parity-violating antiferromagnet, quantum liquid crystal, and topological state of matter. In particular, my recent interest focuses on quantum phases lacking global or local space inversion symmetry. For instance, we classified such quantum phases in terms of multipole moment with the use of group theory, and explored emergent electromagnetic responses, such as magnetopiezoelectric effect and chiral photocurrent. Furthermore, a rigorous and gauge-invariant formulation of multipole moment was given by the thermodynamic definition, which is directly related to the magnetoelectric effect. Superconductivity induced by multipole fluctuations was clarified. To develop the functionality of superconductors, we showed a giant superconducting Edelstein effect in topological superconductors. By considering a light-matter interaction, we proposed laser-induced topological superconductivity in TMD.

Visiting Associate Professor
HIGASHI, Masahiro *(from Kyoto University)*

Theoretical Study on the Excited-State Reactions in Condensed Phases

We are theoretically investigating chemical reactions and physical properties in condensed phases such as solutions and proteins. In particular, we are focusing on the excited-state reaction dynamics in condensed phases. Theoretical studies on the excited-state reaction dynamics of large systems is still one of most challenging tasks due to the high computational cost of electronic structure calculations for excited states and adequate statistical samplings required for molecular dynamics simulations. To overcome this difficulty, we have been developing several efficient methods combining electronic structure calculations and molecular dynamics simulations. Recently, we analyzed the excitation energy transfer in a light-harvesting complex by using our developed methods. The calculated excitation energies of pigments and their fluctuations are in quantitative agreement with the experimental ones. It is found that the fluctuations of pigments are largely affected by the individual protein environments and that the efficient excitation energy transfer is achieved by the site-dependent fluctuations.