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 magnet, quantum liquid crystal, and topological states of matter. In particular, our recent interest focuses on quantum phases lacking global or local space inversion symmetry. This year, we studied exotic superconductivity such as odd-parity superconductivity, odd-frequency superconductivity, noncentrosymmetric superconductivity, and ferroelectric superconductivity. Target materials include transition metal dichalcogenides such as MoS_2, heavy fermion superconductors such as UTe_2 and $CeRh_2As_2$, and perovskite oxides such as $SrTiO_3$. Interestingly, most of them are candidates of topological superconductors. We also explored new functionalities of superconductors and magnets. For instance, superconducting diode effect, giant surface Edelstein effect in d-wave superconductors, chiral photocurrent generation in parity-violating antiferromagnet, and nonlinear electric transport have been theoretically clarified, and candidate materials have been proposed.

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 reactions in condensed phases. The excited-state reaction dynamics of large systems are still one of most challenging subjects in theoretical chemistry due to the high computational cost of quantum chemical calculations for excited states and adequate statistical samplings required for molecular dynamics simulations. To overcome these difficulties, we have been developing several efficient methods combining quantum chemical calculations and molecular dynamics simulations. Recently, we analyzed the excitation energy transfer in a light-harvesting complex by using our developed methods and found that the efficient excitation energy transfer is achieved by the site-dependent fluctuations. We are now investigating the primary charge separation in photosynthetic reaction centers and the photoexcited charge separation in organic solar cells. We will reveal molecular mechanisms of environmental effects in both systems.