Visiting Professors

Visiting Professor
TEN-NO, Seiichiro *(from Kobe University)*

New Frontier of Hybrid Stochastic and Deterministic Electronic Structure Approaches

The vast majority of ab initio electronic structure methods are on the basis of deterministic disciplines, in which a compactification of an N-factorial CI expansion is of main interest. Nevertheless, the way to calculate strongly correlated systems with quasi-degeneracy and general excited states accurately still remains open. These objectives are of significant importance for entangled electronic states involving photoinduced phenomena in biochemistry and energy conversion processes in chemistry. We have recently developed the model space quantum Monte Carlo (MSQMC) method crossing the effective Hamiltonian formalism and full configuration interaction (FCI) QMC [*ST*, *J. Chem. Phys.* **138**, 164126 (2013)]. The method sidesteps the negative sign problem in QMC arising from quasi-degeneracy transcending the storage limitation for CI vectors. Promising results are obtained for the FCI potential energy curves of various excited states for C_2, N_2, and O_2 molecules [Y. Ohtsuka and *ST*, unpublished (2014)]. The method has been also applied to the oxygen evolving center of the photo system II for low-lying spin states.

Visiting Professor
TAKADA, Shoji *(from Kyoto University)*

Computational Studies of Biomolecular Systems

I am studying in the area of computational molecular biophysics, primarily focusing on protein structure and dynamics. Even though thousands of X-ray crystal structures may provide impression that biomolecules are rigid material, in reality they are nano-scale molecules that work under thermal noise and, as such, they are dynamic. Given many crystal structures as snapshots, my ultimate goal is to understand dynamical functions of these molecules via computational analysis. Specifically, my current research includes 1) protein folding and conformational dynamics, 2) biomolecular motors, and 3) gene dynamics, together with 4) methodology development used in these topics. Protein folding and conformational dynamics is a basis to understand all the protein functions. Many proteins undergo substantial conformational change upon binding to their partner molecules, which form a molecular switch. How these molecular switch is regulated is, in my view, one of the most fundamental problems in protein science.

Visiting Associate Professor
SUGIMOTO, Manabu *(from Kumamoto University)*

Computational Molecular Science for Chemical Design and Engineering

The quantum chemical method is a powerful and insightful tool for analyzing and predicting molecular structures and chemical phenomena. Our group is interested in applying electronic-structure methods for investigating molecular functions that are of practical importance. Our on-going research is twofold: One is direct application of the quantum methods. Recently we have been studying spectral properties of supramolecular metal-ion sensors in collaboration with experimentalists. We have been successful to reveal the electronic mechanism for metal-ion sensing. We are also studying photochemical water splitting by graphitic carbon nitride. Its chemical property is expected to provide rich information for designing artificial photosynthesis. Another research is for development of chemoinformatics through which one would be able to learn, understand, investigate, predict, and design molecules and their chemistries. We are developing a system on the basis of our original electronic-structure database and new search engines. Our contribution is intended to enrich usefulness and uniqueness of Computational Molecular Science.