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. We further extend MSQMC to energy independent partitioning (EIP) that enable us to obtain all of the FCI solutions in the model space simultaneously.

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, using coarse-grained molecular modeling approach, we study interplay between conformational dynamics and protein function, for adenylate kinase as a model protein. Adenylate kinase exerts large-amplitude motion that couples with binding to substrates, ATP and AMP. After binding and structural change, it catalyzes chemical reaction to obtain 2ADP, which is then released coupling with conformational dynamics. Modeling the entire process of this enzyme can be an ideal computational model for complete cycles of molecular machines.

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. For example, we have recently carried out the calculations to characterize electronic excitations in supramolecular systems, and developed a computational scheme to study elastic deformation of a molecule by external force. We are also studying materials related to energy conversion such as hydrogen-production catalysts and those in photovoltaics. 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 computer 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.