Visiting Professors

Visiting Professor
NAKAI, Hiromi *(from Waseda University)*

Linear-Scaling Divide-and-Conquer Correlation Theory for Treating Large Systems

"Divide each of the difficulties under examination into as many parts as possible, and as might be necessary for its adequate solution." This quote is from René Descartes, the famous French philosopher regarded as a founder of modern philosophy, in his "Discourse on Method." This phrase is none other than the first statement of the divide-and-conquer (DC) approach. The importance of this philosophy has been universal among almost all sciences, especially computer science. The conventional correlation calculation posed difficulties with large systems due to its unfavorable scaling of computational costs. Nakai *et al.* have presented a breakthrough in correlation calculations by combining the DC method with energy density analysis (EDA). The DC-correlation method is capable of achieving linear scaling of CPU times with respect to system size. This success will open new vistas for computational chemistry across a wide range of scientific and technological fields, nanomaterials and biosystems among them.

Visiting Professor
TANIMURA, Yoshitaka *(from Kyoto University)*

Modeling, Calculating, and Analyzing Multidimensional Spectroscopies

Spectral line shapes in a condensed phase contain information from various dynamic processes that modulate the transition energy, such as microscopic dynamics, inter- and intra-molecular couplings, and solvent dynamics. In multidimensional spectroscopy, the nonlinear response functions of a molecular dipole or polarizability are measured using ultra-short pulses to monitor inter- and intra-molecular vibrational motions. Because complex profile of such signal depends on the many dynamic and structural aspects of molecular system, researchers would like to have a theoretical understanding of these phenomena. We explore and describe the roles of different physical phenomena that arise from the peculiarities of the system-bath coupling in multidimensional spectra. Using the hierarchy formalism, we precisely calculate multi-dimensional spectra for a single and multi-mode anharmonic system for inter- and intra-molecular vibrational modes.

Visiting Associate Professor
NISHIYAMA, Katsura *(from Shimane University)*

Elucidation of Primary Photochemical Processes of Nanoscaled Luminescent Devices

We have synthesized nanoscaled structures likewise nanorods, nanotubes, and nanowires with a skeleton of rare earth elements. To drive luminescent functions form nanostructures produced in our group, we introduce "light-harvesting antennas" having organic/rare earth hybridized structures into the nano skeleton. Along with the experimental projects, our group has also carried out theoretical studies for the elucidation of primary photochemical processes in the condensed phase. For instance, the RISM framework incorporated with theories describing time evolution of the system has been employed to obtain molecular view of solvation dynamics. Recently we undertake to describe initial luminescent processes using the RISM theory together with quantum chemical approaches.