Visiting Professors

Visiting Professor
AIDA, Misako *(from Hiroshima University)*

Topological Analysis of Water Clusters

A water cluster is relevant to a digraph and can be classified to an H-bond pattern. The NVT ensembles of water clusters are created and divided into the configurational subsets, which correspond to the topology-distinct H-bond patterns, and the relative molar Helmholtz energies of the H-bond patterns are evaluated. The method is based on the combination of the standard Monte Carlo techniques with defined H-bond patterns. The structure distributions of water clusters at different temperatures are presented based on the H-bond patterns instead of the 'inherent structures.' The thermodynamically favored structures of water clusters, which are energetically favored and readily feasible (entropy-favored for cluster formation), are presented. The aim of the present work is to demonstrate that the classification to the H-bond pattern corresponds to the division of the configurational space of water cluster structures, where the H-bond patterns can be used to distinguish water cluster structures at finite temperatures created by a simulation technique.

Visiting Associate Professor
NISHINO, Masamichi *(from National Institute for Materials Science)*

Elucidation of the Mechanism of Photoinduced Phase Transitions in Molecular Solids

The discovery of LIESST (light-induced excited spin state trapping) phenomena has accelerated studies of functional spin-crossover (SC) molecular solids. SC compounds have been studied intensively not only because of their potential applicability to novel optical devices, *e.g.*, optical data storage and optical sensors, *etc.*, but also because of the fundamental scientific interest in the mechanism of the phase transition and the accompanied nonlinear relaxation processes. Focusing on such novel phenomena, through the development of theoretical and computational methods, I am studying the properties of cooperative effects which are the key to understand the mechanism of the photoinduced phase transition.

Visiting Associate Professor
KITAO, Akio *(from The University of Tokyo)*

Theoretical Study on Dynamics and Function of Biopolymer and Biological Supramolecule

Recently, rapid progress in computational power and algorithms enable us to carry out massive molecular simulations of biomolecular systems in longer time scale than before. Proteins are essential molecules that manage various chemical reactions in biological systems. Our main targets are proteins, other biopolymers and biological supramolecules, which act as essential functional units in living organisms. We have been studying assembly process, properties and functional mechanisms of biomolecules using theoretical and computational approaches. In order to achieve this, we create new computational methodologies and programs to simulate biomolecular systems more realistically and accurately and use them to investigate atomic mechanisms of supramolecules to fold, assemble and function. We also develop methodology to extract useful information from experimental data and analyze molecular mechanisms to function. In addition, we analyze accumulated information on protein structure and function and store it as databases.