

Visiting Professors



Visiting Professor
YOSHIZAWA, Kazunari (*from Kyushu University*)

Quantum Chemical Studies on Nanostructures and Enzymatic Reactions

In my group nanostructures and enzymatic reactions are studied by using quantum chemical calculations. The first topic is concerned about functions of metal ions in the active sites of enzymes and catalysts. The direct conversion of methane to methanol under physiological conditions, the bare MO^+ complex in the gas phase, Fe-ZSM-5 zeolite, and B_{12} -dependent diol dehydratase, for example, are studied.

The second topic is chemical understanding of electron transport properties in molecular junctions, in which two electrodes have contact with a molecule, in terms of the orbital concept. We found that the phase and amplitude of the HOMO and LUMO of molecules determine essential properties of the electron transport in them. The derived rule to predict single molecules' essential transport properties was recently confirmed by collaboration with experimental groups.



Visiting Professor
SUGITA, Yuji (*from RIKEN*)

Molecular Dynamics Simulations of Large Conformational Changes in Membrane Proteins

Due to the recent advances in molecular biology and structural biology, we have more than 300 atomic coordinates of membrane proteins in protein data bank (PDB). In our research teams, we have developed simulation techniques to simulate membrane proteins with explicit solvent and lipid bilayers and carried out large-scale molecular dynamics simulations of the sarcoplasmic reticulum Ca^{2+} -ATPase (calcium ion pump), sec translocons, and so on. In the simulations of calcium ion pump, we have successfully shown the differences of the calcium-binding affinity between wild-type and two mutant ATPases, namely, Glu771Gln, and Glu908Gln. Furthermore, we have shown that the calcium affinity at the transmembrane binding sites has close relationship with the shielding of bulk water from the luminal side. This provides new insight into the mechanisms of gating of ion pathways in cation pumps.