Photodimerizer (Pd) is a blue light-regulated dimerizing module consisting of a basic leucine zipper (bZip) and a light-oxygen-voltage-sensing (LOV) domains. To understand the molecular mechanism for dimerization, we investigated the concentration dependencies of Pd and N-terminally-truncated Pds, composed of Zip-LOV, linker-LOV and only LOV domain. The dynamic light scattering and size exclusion chromatography measurements indicated that blue light induces the dimerization of all Pds. In the dark state, monomeric forms of bZip-LOV and Zip-LOV are more stable than those of linker-LOV and LOV, probably due to the synergistic interactions between Zip and LOV domains. Consequently, blue light drives configurational switching of monomeric Pd into the dimeric form.

The solvent-accessible surface area of proteins is a key factor for hydration structure and dynamics in crowded environment. An efficient implementation of the three-dimensional reference interaction site model (3D-RISM) theory to the fragment model orbital (FMO) method was proposed. The method allows us to treat an electronic structure of whole part of macromolecules, such as protein, as well as a solvent distribution around the solute macromolecules. In this study, we propose a procedure to save the computational cost for calculating the electrostatic potential in the framework of FMO method. The results are compared with those from the other methods.

Hydration water behavior classified by mixture model: Simulation data-mining approach

Taka Mizukami1, Hieu Chi Dam2, Tu Bao Ho3, Viet Cuong Nguyen3 (1JAIST, Materials Science, 2JAIST, Knowledge Science, 3HPC Systems, Inc)

Water plays important roles in bio-molecular dynamics. The identification of the hydration water has been a difficult task, because the physicochemical parameters disperse widely. We employed “the simulation data mining approach” to overcome these difficulties. In this study, under the motivation to investigate the water dynamics surrounding protein, we focused the water behavior in the vicinity of soluble proteins. The MD trajectory of the individual water molecule was mapped into the feature-space by means of mixture model. The classification on the feature-space of new categories of hydration water was succeeded. One of the classes of water behavior is consistent with the first hydration water. A long-range water structure originated by protein was detected.