Hierarchical simulations of water-related anomalous phenomena: treating from electrons or as rigid-body molecules

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In this presentation, I will talk about our two simulation topics related to water. One is the moisture-induced weakening of the adhesive bonding, treated using the hybrid quantum-classical simulation method from the electronic level. The other is surprising dynamics of water molecules around some protein, where a water molecule is treated as a rigid body.

[1] The adhesive bonding is a key issue for advanced packaging and construction of electronic devices and systems. The bisphenol-A epoxy resin with curing agent has been used widely as the bonding glue. One of the fundamental unsolved problems in the adhesion between metal and epoxy resin is that the adhesion strength reduces significantly in a moist environment. Microscopic understanding of the mechanisms is essential to propose an innovative method to solve the problem.

The electronic-level simulation of such a system is not easy because it requires a large system size due to the inhomogeneity of the interface and largeness of the epoxy molecule. We therefore use the hybrid quantum (QM)-classical (CL) simulation method to treat such systems directly. The water molecules are placed at the interface of the partly oxidized Al and epoxy sub-systems. The QM region composed of about 1,000 atoms is set at the interface region, which is described by our original real-space grid density-functional theory (DFT) for valence electrons. Microscopic analyses find a novel adhesion reduction mechanism: a water molecule around the chemical bond between the Al and resin sub-systems acts as a catalyst to lower the energy barrier for the disruption of the chemical bond.

[2] The antifreeze proteins (AFPs) are a group of proteins found in various biological species that inhibit the growth of ice crystals at super-cooled conditions. A possible inhibition mechanisms based on the Gibbs-Thomson effect has been proposed, however, it is not yet shown that the mechanism can really cause antifreeze phenomena.

First I demonstrate the ice growth inhibition induced by type-I AFP using the hybrid atomistic-rigid body simulation at temperatures 260~268K. The ices used consist of about 1,000,000 water molecules and 12 AFPs are sitting on the $(20\bar{2}1)$ plane. In the simulation, water molecules are treated as rigid ones with the TIP4P/ice model. Improved fast time-reversible algorithm is also employed for time integrations of rigid water molecules. Second I show significantly reduced diffusion of water molecules around the protein up to the distance as far as 30 Å from the nearest neighbor atom of the protein. Its possible mechanisms will be investigated.