Constructing protein nano-fiber and electronic state around metal ions

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It is interesting to investigate how to produce protein fiber while maintaining their native structures. As materials of nano-fiber, we use LARFH [1], Sulerythrin and 3-isopropylmalate dehydrogenase (IPMDH). Those proteins have two α-helices on the surface of the protein structure. Therefore we expect proteins to bind between two α-helices of one protein and two α-helices of another and to form at bonding surface a four-helix bundle structure; those structures have high thermal stability, due to the hydrophobic interaction.

We analyzed these proteins in various conditions using molecular dynamics (MD) methods and molecular orbital (MO) calculations. We carried out MD simulations with all-atom (AA) model and coarse-grained (CG) model using GROMACS. In AA model, we adopted AMBER99SB-ILDN force field [2] and calculated binding energy ΔG_{bind} using umbrella sampling method [3]. We found that in the combination of LARFH-/-LARFH, hydrophobic interaction enhanced in wild type, and electrostatic interaction is in mutant. In CG model, we used MARTINI force field [4] and calculated larger systems.

Sulerythrin includes two pairs of Zn^{2+} and Fe^{2+}. Thus we carried out MO calculation around metal ions.

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