学位申請論文公開講演会

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場所：理学館 (506)

題 目 ：Thermal energy transport and signal transduction of biomolecular machines: Molecular dynamics simulation study of proteins

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主論文の要旨

Proteins are vital macromolecules in organisms, with thermal energy transport being a key biophysical property, yet its relationship with protein structures, dynamics, and functions remains unclear. To illustrate non-uniform heat transport nature in proteins, I developed a theoretical framework for analyzing the local thermal transport properties of thermal energy based on the autocorrelation function formalism using equilibrium molecular dynamics (MD) simulations. In addition, advanced machine learning-based methods were utilized to illustrate the contributing factors of thermal transport in protein and the structural characterization of intrinsically disordered regions.

First, the local heat transport properties along peptide chains were studied using a linear-homopolymer-like model. Short-range cross-correlation corrections were introduced and employed to correct the model due to the non-neglectable independent fluctuations between residues. The local thermal transport calculation indicates that intra-residue thermal transport has a dominant contribution to the overall heat current and residue-wise thermal conductivity demonstrated distinct residue-type dependence: charged > polar > hydrophobic.

Second, the local thermal transport properties of non-bonded contacts in proteins were studied by introducing a derived physical quantity of inter-residue thermal conductivity (λ_{inter}). As a results, λ_{inter} exhibited a decreasing trend on interaction types: hydrogen bonding > π-stacking > electrostatic > hydrophobic. Furthermore, the random forest regression prediction model was used to investigate the non-linear relationship between λ_{inter} and various static and dynamical properties of the protein.

As a case study, the allosteric signaling process of the oxygen sensor domain of *Bj*FixL protein was investigated by constructing the vibrational energy exchange network (EEN) model. In addition, a hybrid approach of deep learning algorithms, MD simulation, small angle X-ray scattering (SAXS), and double electron-electron resonance electron paramagnetic resonance (DEER/EPR) spectroscopy, was developed to characterize the ensemble of a chloroplast protein, CP12, which contains intrinsically disordered regions (IDRs).