

Computational Studies of the Thermophysical Properties of Biomolecule-Water Interfaces

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Biological molecules have developed mechanisms and structures that enable the efficient and rapid dissipation of excess energy, either through the biomolecule structure and through biomolecule-solution interfaces. The relaxation timescale can influence the kinetics of biomolecular reactions. Finding the microscopic mechanisms controlling energy transport in biomolecules represents a considerable challenge, which can provide a route to rationalize complex biological processes. Recent experiments have shown how molecular motors such as Ca²⁺-ATPase dissipate heat under working conditions. The thermal gradients inferred from the analysis of the experiments indicate significant heat dissipation. These observations make necessary the development of tools to quantify the heat resistivity of the biomolecule-water interface to heat transfer. We will discuss recent approaches we have developed to achieve this objective. Our approach provides a route to estimate the thermal conductivity of the biomolecule as well as the thermal conductance of the biomolecule-solution interfaces. The latter is shown to be larger than the thermal conductance of the hydrophilic interfaces measured in experiments. We suggest that interface curvature and chemical composition both contribute to this enhancement in the thermal conductance. Overall we conclude that the thermophysical properties of protein-water interfaces should play a major role in determining the thermal relaxation of biomolecules.

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[2] A. Lervik, F. Bresme and S. Kjelstrup, Heat transfer in soft nanoscale interfaces: the influence of interface curvature, *Soft Matter*, 5, 2407(2009).