# HEAT TRANSFER AND DISSIPATION IN BIOMLECULES: COMPUTATIONAL STUDIES

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## EXTENDED ABSTRACT

Non-equilibrium phenomena play an essential role in many processes of relevance in biology, physics and material science. One of such non-equilibrium processes is thermoelectricity, in which a temperature gradient applied to a circuit made from different metals induces an electric current. Temperature measuring devices, and some refrigerators rely on these thermoelectric effects. One major application of this principle in material sciences is the synthesis of materials that can efficiently convert waste heat into electricity. It has been suggested that thermoelectricity can represent a physical mechanism used by some fish to sense temperature gradients.

Recent work indicates the possibility of generating large thermal gradients in nanoscale assemblies. Such large thermal gradients have been inferred from theoretical analyses of systems involving metal nanoparticles heated with electromagnetic radiation, a notion that is being used in cancer therapy treatments. Similarly experimental studies of molecular motors, such as $Ca^{2+}$-ATPase, indicate that significant thermal gradients can develop during the ion transport process. Quantifying thermal relaxation as well as the microscopic mechanisms operating at thermolecular scales characteristic of these nanomotors is therefore a very important objective. The environment, namely, the bilayer structure supporting these proteins, is expected to play a role in determining the relaxation. In fact, recent work has shown that the thermodynamic efficiency associated to ion transport reaches a maximum value at specific bilayer compositions, showing the relevance of the environment in regulating biological activity.

Recent developments on fluorescent thermometry have revealed the existence of thermal gradients inside the cell too. These results indicate important correlations between local temperature and organelle function and raise interesting questions on how the resulting thermal gradients can influence biochemical reactions or transport of solutes inside biological structures. We are interested in developing computational approaches to quantify thermal transport in biological structures, including the transport of proteins and other biomolecules driven by thermak gradients. Also, for small systems, nanomaterials, e.g., nanofluids, and in particular biomolecules, interfacial effects become relevant as compared with bulk effects. In order to understand processes of relevance in biophysics, it is necessary to quantify the resistivity of the interfaces to heat transfer. The relevant structures in biological system involve aqueous interfaces. We are currently investigating the response of aqueous solutions and interfacial water to thermal perturbations. Our work suggests that water does not behave as a passive medium that transports heat only. We have recently described a novel phenomenon whereby water molecules reorient as a response to the thermal gradient, and polarize along the direction of the gradient. This polarization can result in electrostatic fields for thermal gradients that are achievable in biological processes. Thermoelectric effects are well known in semiconductors, but we find that related mechanisms can arise in polar fluids.

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