**Computational studies of thermal transport in molecular fluids and biomolecules:**

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Non-equilibrium phenomena play an essential role in many processes of relevance in biology, physics and materials science. One of such non-equilibrium phenomena 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. This principle s being used to manufacture materials that can efficiently convert waste heat into electricity.

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 Ca2+-ATPase, indicate that significant thermal gradients can develop during the ion transport process. Many of these processes, particularly those in bio-molecules occur in aqueous solutions. We are currently investigating the response of aqueous solutions and interfacial water to thermal perturbations. 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 significant electrostatic fields for thermal gradients that are achievable in biological processes and nanomaterial applications. Thermoelectric effects are well known in semiconductors, but we find that related mechanisms can arise in molecular fluids.

For small systems, nanomaterials, e.g., nanofluids, and biomolecules, interfacial effects become relevant as compared with bulk effects. In order to enhance the properties of materials relevant to thermoelectric energy conversion and understand processes of relevance in biophysics, it is necessary to quantify the resistivity of the interfaces to heat transfer. I will discuss computational approaches to quantify thermal transport in models of nanoparticles and proteins. We find that the high curvature associated to these nanometre size interfaces has a strong impact on the interfacial resistivity, which is much lower than in a planar interface.