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THERMAL TRANSPORT ACROSS NANOPARTICLE-FLUID INTERFACES

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The potential uses of nanoparticles in several biomedical applications, such as drug delivery, hyperthermia treatment, magnetic resonance imaging and tissue repair, have been recognized in previous works. Many of these applications involve transport of heat from the nanoparticles to the surrounding media and exploit the resulting increase in local temperature to, for example, destroy target cancer cells or to induce ion flux through biological membranes and nanoscale pores (1,2,3).

A full description of the mechanism of heat flow across the interface of solid nanoparticles and surrounding fluid requires an understanding of the complex interplay between various interfacial properties, such as surface free energies, interfacial curvature and microscopic structure. Specifically, at the nanoscale, the heat transport between two different phases is characterised by a temperature drop at the interface, quantified by a thermal boundary resistance, known as the Kapitza resistance, which offers a measure of the efficiency of heat transport.

Using non-equilibrium molecular dynamics computations, we have found that the thermal resistance of the interface depends strongly both on the wetting characteristics of the nanoparticle–fluid interface and on the nanoparticle size (4). Strong nanoparticle–fluid interactions, leading to full wetting states in the host fluid, result in high thermal conductances and efficient interfacial transport of heat. Moreover, the strength of the fluid-nanoparticle interactions has been found to influence the variation of the thermal conductance with particle size, with strongly hydrophilic particle showing the strongest curvature dependence. A general and effective equation has, therefore, been derived to describes the thermal conductance of nanoparticles in terms of curvature and interaction strength, with the aim to rationalize available computations and experimental data and motivate new investigations.

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