Nanoscale heat transfer probed by molecular dynamics

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In this contribution, I shall illustrate how molecular dynamics (MD) simulations may shed light on nanoscale heat transfer across solid-solid and solid-liquid interfaces. I will first discuss the different routes to compute the interface thermal resistance in MD, with emphasis on the case of imperfect interfaces.
I will then briefly highlight the need to combine MD with force constants calculated using ab initio methods to correctly predict interfacial thermal transmission coefficients.
Last, I will illustrate how to tune interfacial heat transport at solid/soft interfaces. I will first characterize the effect of external pressure and discuss the physical mechanisms at the origin of the enhancement of the thermal conductance induced by pressure.
Finally, I will demonstrate how the presence of a tiny amount of nanoparticles may hinder the heat and delay ultrafast boiling.