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Heat transport in low dimensional nanostructures

Abstract

Thermal energy transport at the nanoscale is surging as an overarching problem in materials science and technology. Heat transport has a deep impact on several technological applications: for example it largely affects the performances of microelectronics devices and thermoelectric materials for renewable energy conversion.
In spite of the success of macroscopic continuum approaches, when the characteristic length of the nanostructures is of the order of 10 nm or less, atomistic simulations are necessary to provide the correct physical behavior and achieve significant understanding of thermal transport.
In this talk I will review molecular dynamics and lattice dynamics methods to compute heat transport, with examples in which the concerted application of different methods sheds light on the heat transport mechanisms in silicon and carbon based nanostructures.

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