Atomistic Studies of Thermal Transport at the Nanoscale

Rafael Gutierrez,[1] Alvaro Rodriguez Mendez,[1] Leonardo Medrano Sandonas,[2] Arezoo Dianat,[1] Vladimiro Mujica,[3,4] Gianaurelio Cuniberti[1]

[1]Institute for Materials Science, Dresden University of Technology, 01062 Dresden, Germany
[2]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg, Luxembourg
[3]School of Molecular Sciences, Arizona State University, Tempe, Arizona 85287, United States
rafael.gutierrez@tu-dresden.de

Gining control over heat flow at the nanoscale poses a major challenge to current technologies. The issue is not only the reduction of heat dissipation in nanoelectronic devices or the blocking of thermal transport to increase the thermoelectric efficiency, but also to engineer thermal devices to exploit the richness of nanoscale material properties. Thus, analogs of electronic devices, such as thermal rectifiers and thermal transistors have already been proposed. In this context, atomistic design strategies for nanodevices and nanomaterials are required, in particular the combination of computationally efficient atomistic methodologies with quantum transport based approaches. I will address two main topics: (i) Phonon filtering in nanoscale heterogeneous molecular junctions, consisting of molecular wires bridging two different nanocontacts. The obtained spectral phonon gaps are shown to strongly correlate with the properties of the vibrational spectrum of the specific molecular species in the junction. The filtering effect results from a delicate interplay between intrinsic vibrational structure of the molecular chains and the different Debye cutoffs of the thermal baths; (ii) A nanoscale phononic analog of the Ranque-Hilsch vortex tube in which heat flowing at a given temperature is split into two different streams going to the two ends of the device, inducing a temperature asymmetry. The nanoscale prototype consists of two carbon nanotubes (capped and open) connected by molecular chains. Our results show that the structural asymmetry in the contact regions is the key factor for producing the flux asymmetry and, hence, the induced temperature-bias effect.

References

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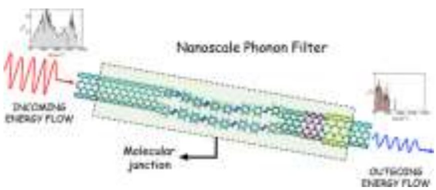

Figure 1: Schematic representation of the molecule-based nanoscale phonon filter.