

Electrical and thermal transport in carbon nanostructures from first-principles simulations

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First-principles simulations have become nowadays a very powerful tool to understand, characterize, and design novel materials and devices. Their relevance becomes even more compelling at the nanoscale, where they can powerfully complement experimental characterization and screening.

I'll first show a few examples where the calculation of first-principles spectroscopic data, in combination with experimental results, allows for a detailed characterization of microscopic structural details.

Then, I'll present some of our work on electrical and thermal transport in graphene and derivatives, using density-functional perturbation theory to calculate quantum transport in the ballistic regime and in the presence of inelastic scattering channels, and semiclassically using phonon lifetimes or electron scattering times.

In particular I will focus on thermal transport and electron mobility in suspended or strained graphene, and on electrical transport in functionalized nanotubes and ribbon/tube junctions.