Ab initio calculations of phonon-phonon and electron-phonon interactions: application to transport

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Within the last few years, it has been possible to compute phonon-phonon interactions, and therefore the lattice thermal conductivity of bulk materials, using ab initio methods. The interactions between the phonons are obtained from density functional theory and this information is incorporated into the Boltzmann equation to obtain the thermal conductivity. The good accuracy obtained from those calculations allows trying to use them to find new materials using artificial intelligence and to perform multiscale modelling. We will show a few examples of such calculations.

Along the same lines, it is also possible to compute electron-phonon interactions from ab initio calculations, and therefore to obtain electronic transport coefficients, such as electrical conductivity and thermopower. We will show a few examples of such calculations, as well as our recent implementations.

Phonon-phonon interactions, electron-phonon interactions, the Boltzmann equation and the linear response theory are the common ingredients and theoretical frameworks combined to describe the electronic and thermal transport in bulk materials. Even if the "theory" is well established from many years, it is only recently that we are able to compute such quantities from ab initio calculations. Some basic question remains however, about the model of transport that we use, or about the definition of the interactions. I will end the talk sharing our present understanding about those questions.

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