## Heat transport from first principles in FHI-aims

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Materials with suitable thermal conductivities are crucial for a variety of applications, e.g., for the advancement of thermoelectric elements [1] or for the design of novel thermal barrier coatings for gas and airplane turbines [2]. The development and the optimization of such materials – a notoriously tedious task requiring extended and costly test series – can be considerably accelerated when aided and guided by *ab initio* calculations.

In this talk, we will cover the different *first-principles* techniques that are available to date for the assessment of thermal conductivities. We will first discuss perturbative [3] and/or non-equilibrium methods [4] that are suitable for the simulation of thermal transport at low temperatures, i.e., well below the Debye temperature. In particular, we will discuss the *laser-flash method* [5] that involves the preparation of supercells in non-equilibrium by means of the harmonic approximation. The thermal conductivity is then determined by monitoring the re-equilibration of such supercells in *ab initio MD*.

At elevated temperatures, e.g., at 70% of the melting temperature or higher, simulation techniques that rely on the harmonic approximation and/or on supercells that are unphysically far from equilibrium become questionable. These short-comings are overcome in the Green-Kubo method, which involves the assessment of the thermal conductivity from the auto-correlation of the heat flux in equilibrium *ab initio MD* [6]. We will discuss our *first-principles* formulation of the heat flux that is based on the *energy-* and *stress-densities* [7], two quantities that we have recently implemented in FHI-aims and that now allow to perform *ab initio Green-Kubo simulations*.

Eventually, we will critically discuss the computational cost, the accuracy, the convergence behavior, the limits, and the applicability of these techniques by presenting thermal conductivity data computed with the aforementioned methods for doped semiconductors and oxides.

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