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Ab initio lattice thermal conductivity in pure and doped half-Heusler thermoelectric materials.

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Half-Heusler phases are promising intermetallics for applications in thermoelectric generators. Optimization of their thermal transport properties is essential to improve their overall conversion efficiency [1]. Our goal is to perform a theoretical evaluation of thermal transport properties directly from first-principles calculations for various pure and doped half-Heusler compounds. The electronic structures are modeled in the framework of the density functional theory (DFT) [2]. The ab initio thermal properties are deduced from harmonic and anharmonic interatomic force constants calculations using finite size displacements method. Many-body perturbation theory is used for calculating the phonon-phonon interactions which yields the lifetime of phonons as function of momentum and band index [3]. Finally, thanks to a direct solution to the phonons Boltzmann transport equation [4] we computed the ab initio thermal conductivities, which are found in good agreement with the experimental data. The figure 1 and 2 show an example of the results for the thermal conductivity and inverse phonon lifetimes for one half-Heusler compound.

Figure 1: Lattice thermal conductivity of ZrCoSb half-Heusler structure.
As a second step, we study specific localized impurities and size-controlled nanoparticles as they can lead to better thermal transport properties enhancing the thermoelectric efficiency [5-8]. In order to calculate the thermal conductivity in presence of localized defects, we developed a model to account for substitution defects and disorder in half-Heusler phases using perturbation theory and configurational analysis. Our results provide good insights for understanding the behavior of the thermal conductivity, which will be useful to guide experimental work to find pathways to improve the thermoelectric efficiency of these materials.