NOMAD
NOVEL MATERIALS DISCOVERY

MAX-PLANCK-GESELLSCHAFT
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Thermal Conductivities from First Principles

The *thermal conductivity*, i.e., the ability of solid material to conduct heat at a given pressure and temperature, plays a key role in many industrial and scientific applications, e.g., in the design of semiconducting devices or in the engineering of gas- and airplane turbines. Improving, suppressing, and generally tailoring the thermal conductivity is a complex cumbersome task, since subtle details in the thermodynamic motion of the nuclei govern heat transport. Accordingly, little is yet known about the exact atomistic mechanisms that determine the thermal conductivity in real materials under realistic conditions. This is especially true at elevated temperatures, at which the dynamics of the nuclei can no longer be treated perturbatively, since strong *anharmonic* effects can become active.

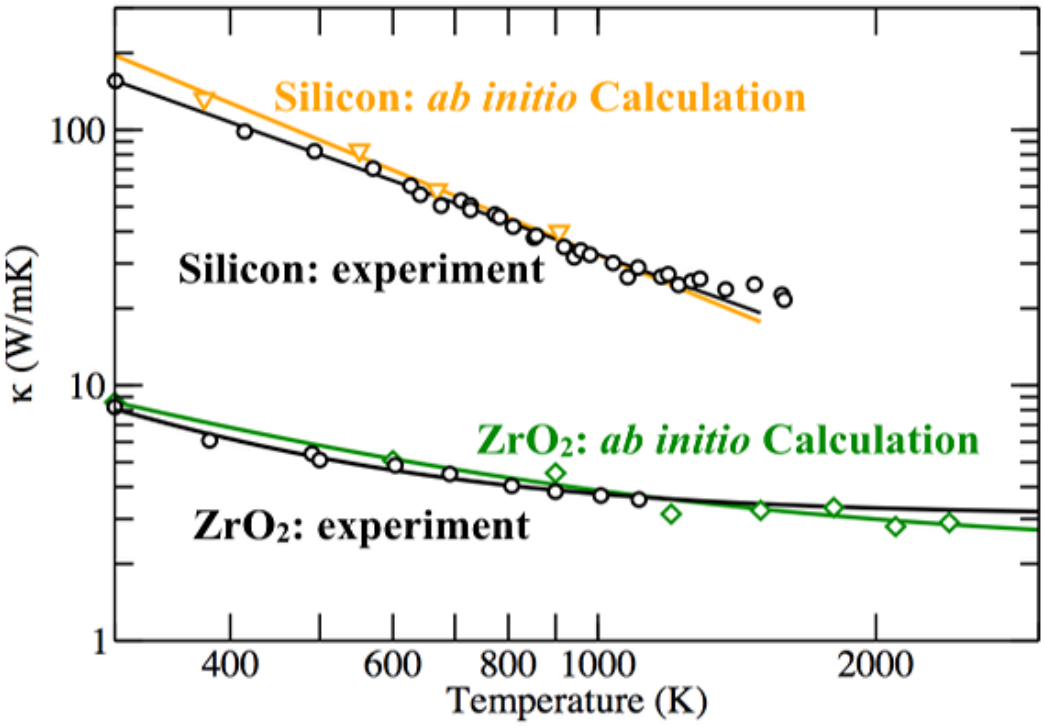

Figure 1: Thermal conductivity of silicon (heat conductor) and zirconia (ZrO_2, heat insulator) as computed from first principles. Adopted from reference **[1]**.

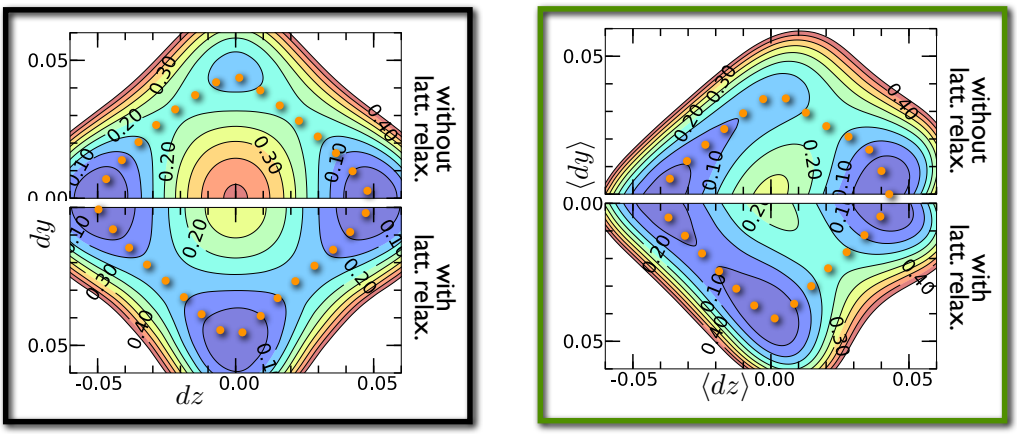

Figure 2: Potential-energy surface for pristine zirconia ZrO_2 (left) and Yttria-doped ZrO_2 (right). In the upper panels, lattice degrees of freedom are not accounted for, while in the lower panels they are. Adopted from reference **[2]**.

Recently, researchers at the *Fritz-Haber-Institute of the Max-Planck-Society* have succeeded in developing a methodology that allows computing the thermal conductivity for *all* kind of materials up to very large temperatures, i.e., up to the melting point, as shown in Fig. 1. In this technique [1], *all* anharmonic effects are accounted for, since the true dynamics of the atoms at given temperature and pressure is computed using *ab initio* molecular dynamics simulations. This allows to reliable reproduce and predict the thermal conductivity for very different materials, spanning all kind of applications. As shown in Fig. 1, the good heat conductor silicon features a thermal conductivity that is roughly one order of magnitude larger than the one of the heat insulator zirconia. Furthermore, these calculations shed light on the atomistic mechanism that results in this peculiarly low thermal conductivity: As shown in Fig. 2., the strong anharmonic effects in this material are caused by the multiple minima that the potential-energy surface of ZrO_2 exhibits for the oxygen atoms. The strength of these anharmonic effects depends of how frequently different minima are explored during the dynamics, i.e., on the height of the energetic barrier between them. As shown in Fig. 2 and discussed in Ref. [2], this barrier –and thus the thermal conductivity– can be systematically tailored via doping.

References:

[1] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).
[2] C. Carbogno *et al. Phys. Rev. B* **90**, 144109 (2014).