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Thermal Conductivities in Solids from First Principles: Accurate Computations and Rapid Estimates CHRISTIAN CARBOGNO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
— In spite of significant research efforts, a first-principles determination of the thermal conductivity κ at high temperatures has remained elusive. Boltzmann transport techniques that account for anharmonicity perturbatively become inaccurate under such conditions. *Ab initio* molecular dynamics (MD) techniques using the *Green-Kubo* (GK) formalism capture the full anharmonicity, but can become prohibitively costly to converge in time and size. We developed a formalism that accelerates such GK simulations by several orders of magnitude and that thus enables its application within the limited time and length scales accessible in *ab initio* MD. For this purpose, we determine the *effective* harmonic potential occurring during the MD, the associated temperature-dependent phonon properties and lifetimes. Interpolation in reciprocal and frequency space then allows to extrapolate to the macroscopic scale. For both force-field and *ab initio* MD, we validate this approach by computing κ for Si and ZrO_2, two materials known for their particularly harmonic and anharmonic character. Eventually, we demonstrate how these techniques facilitate reasonable estimates of κ from existing MD calculations at virtually no additional computational cost.

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