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High Temperature Thermal Conductivity from First Principles CHRISTIAN CARBOGNO, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, RAMPI RAMPRASAD, Chemical, Materials & Biomolecular Engineering, University of Connecticut, Storrs, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — In spite of significant research efforts, a first principles determination of the thermal conductivity at high temperatures has remained elusive. Under such conditions, techniques that rely on the harmonic approximation are no longer valid, while standard non-equilibrium molecular dynamics methods require huge temperature gradients that lead to deviations from Fourier's law. The Green-Kubo method [1], which does not suffer from these shortcomings, involves the assessment of the thermal conductivity from the auto-correlation of the heat flux in equilibrium. In classical MD, the heat flux is computed from the energetic contributions of the individual atoms; we show that the Green-Kubo approach can be reformulated in terms of the energy and stress densities [2], which are directly accessible in DFT calculations. This approach leads to a unique definition of the heat flux that does not rely on any partitioning scheme for the total energy. We critically discuss the computational cost, the accuracy, and the applicability of this approach by investigating the thermal conductivity for oxides and semiconductors with low thermal conductivities.

[1] R. Kubo, M. Yokota, S. Nakajima, J. Phys. Soc. Jpn. 12, 1203 (1957).
[2] R. Ramprasad, J. Phys. Condens. Matter 14, 5497 (2002).

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