Abstract Submitted
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Intrinsic lattice thermal conductivity of diamond from first principles[1] A. WARD, D. A. BROIDO, Department of Physics, Boston College, Chestnut Hill, MA, 02467, D. A. STEWART, Cornell Nanoscale Facility, Cornell University, Ithaca, NY, 14853 — Predictive theoretical descriptions of the lattice thermal conductivity, κ_L, are essential in facilitating the design of high efficiency thermoelectric materials. In the thermal regime of interest for thermoelectrics, the κ_L of high quality crystalline semiconductors is typically limited by phonon-phonon scattering due to the anharmonicity of the interatomic potential. We have calculated κ_L for isotopically pure diamond, combining a first principles approach for the harmonic and anharmonic interatomic force constants with an iterative solution of the full phonon Boltzmann equation. Our adjustable parameter free calculation of κ_L for diamond is in excellent agreement with measurements[1-3]. This provides further validation of our *ab initio* approach previously used successfully for Si and Ge [4]. [1] D. G. Onn, et al.,Phys. Rev. Lett. 68, 2806 (1992). [2] L. Wei, et al., Phys. Rev. Lett. 70, 3764 (1993). [3] J. R. Olson, et al., Phys. Rev. B. 47, 14850 (1993). [4] D. A. Broido, et al., Appl. Phys. Lett. 91, 231922 (2007).

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