Abstract Submitted
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Ab-initio thermal properties of semiconductors with higher order anharmonicities NAVANEETHA K RAVICHANDRAN, DAVID BROIDO, Boston College — The thermal properties of semiconductor materials are intimately connected to the anharmonicity of the crystal potential. In many such materials, calculations including only the third-order anharmonic processes involving three phonons are sufficient to accurately reproduce the measured thermal properties such as specific heat, thermal expansion and thermal conductivity. However, in highly anharmonic materials such as those used for thermoelectric applications, higher order anharmonicities in the crystal potential can become important [1, 2, 3]. In this talk, we describe an approach to calculate the ab-initio thermal properties of highly anharmonic thermoelectric semiconductor materials, by including up to fourth order anharmonicity in the crystal potential. By evaluating higher order anharmonic contributions to the free energy, phonon line shifts and line widths, our work will inform accurate prediction of crystal stability, neutron scattering cross-sections and thermal conductivity of several challenging anharmonic semiconductor crystals. [1] D. J. Ecsedy and P. G. Klemens, Phys. Rev. B 15, 5957 (1977) [2] Olle Hellman, Peter Steneteg, I. A. Abrikosov, and S. I. Simak, Phys. Rev. B 87, 104111 (2013) [3] Tianli Feng and Xiulin Ruan, Phys. Rev. B 93, 045202 (2016)

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