Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Thermal transport in thermoelectric skutterudites: first-principles and phenomological approaches DMITRI VOLJA, MIT, MARCO FORNARI, Central Michigan University, BORIS KOZINSKY, BOSCH LLC, DAE-HYUN WEE, BOSCH LLC, NICOLA MARZARI, MIT — The possible application of pnictogen substituted ternary skutterudites in thermoelectric devices is currently limited due to their relatively large electrical resistivity. These materials, however, exhibit thermal conductivity of the order $0.7 - 2.2$ k/Wm^{-1}K^{-1} at room temperature and may be amenable to optimization. In skutterudites at high temperatures the thermal transport is primarily dominated by anharmonic interactions of phonons. The precise evaluation of such interactions from first principles is currently a formidable task. We have analyzed the third order phonon-phonon scattering mechanisms, that arise from the anharmonicity of the interatomic potentials, and use a standard Boltzmann transport approach to derive the thermal conductivity. In our methodology we have combined first principles approaches and phenomenological interatomic potentials. We specifically studied the transport properties of $CoGe_{3/2}S_{3/2}$, $CoGe_{3/2}Te_{3/2}$ and $CoSn_{3/2}Te_{3/2}$ and provide comparison to the parental binary $CoSb_3$. We validate our approach by testing the approximations in simpler systems where full evaluation of anharmonic force constants from first-principles calculations is possible.

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Date submitted: 27 Nov 2009 Electronic form version 1.4