Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

**On the role of nanostructure on the thermal conductivity of skutterudite thermoelectrics**[1] MARCO FORNARI, Central Michigan University, DMITRI VOLJA, JIVTESH GARG, Massachusetts Institute of Technology, DAE-HYUN WEE, Ewha Womans University, BORIS KOZINSKY, Robert Bosch LLC, NICOLA MARZARI, University of Oxford — One of the most effective strategies to improve the thermoelectric figure of merit in skutterudites is to reduce thermal conductivity via alloying, filling, or nanostructuring. The latter is most effective when the dimension of the domains is comparable in size to the mean free path of the dominant heat-conducting phonons. In bulk, pristine semiconductors and insulators thermal conductivity and phonons' mean-free paths can nowadays be calculated fully from first-principles from the anharmonic terms in the ionic displacements. We show here our results for the lattice thermal conductivity of several compounds with the skutterudite structure, obtained from the Boltzmann transport equation using phonon lifetimes determined from density functional calculations. We will also discuss the effect of fourth-order terms, albeit as obtained using phenomenological approaches. Last, we comment on the interplay between the different length scales for the nanostructured domains and the relevant heat-carrying phonons.

[1]Support from Robert Bosch LLC/MIT Energy Initiative.

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Date submitted: 09 Dec 2010 Electronic form version 1.4