Abstract Submitted
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Ab-initio investigation of thermal transport in alloyed and nanostructured materials[1] DMITRI VOLJA, Massachusetts Institute of Technology, Department of Materials Science and Engineering, Cambridge, MA, BORIS KOZINSKY, Robert BOSCH LLC Research and Technology Center, Cambridge MA, JIVTESH GARG, Massachusetts Institute of Technology, Department of Materials Science and Engineering, Cambridge, MA, MARCO FORNARI, Central Michigan University, Department of Physics, Mount Pleasant, MI, NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne — A whole spectra of intriguing physical properties appears in conventional materials when structural features reach nanoscale. Since thermal conductivity is controlled by the heat carriers' mean free paths, it becomes of paramount importance to understand and engineer the role of alloying and nanostructuring on transport coefficients. First-principles calculations often provide accurate microscopic parameters, but at significant computational cost even for ideal, perfect systems. We present a hybrid classical-quantum method to compute thermal conductivity from both harmonic and anharmonic terms using Boltzmann transport formalism. We combine first-principles calculations of harmonic terms and force-field calculations of third-order and fourth-order force constant. Results for SiGe will be discussed to show the validity of approach. We also discuss the effects of nanostructuring by introducing boundary scattering contributions, as well as mechanisms of filler rattling in thermoelectric skutterudites.

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