

Abstract Submitted  
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**Atomistic Modeling and Optimization of thermoelectric properties of SiGe nanowires**<sup>1</sup> MARIA CHAN, YING SHIRLEY MENG, TIM MUELLER, GERBRAND CEDER, Massachusetts Institute of Technology, JOHN REED, TRINH VO, ANDREW WILLIAMSON<sup>2</sup>, Lawrence Livermore National Laboratory, GIULIA GALLI, University of California, Davis — Nano-structured thermoelectric materials have been shown experimentally to have superior figure of merit compared to bulk materials. To understand the origin of this superiority, it is of interest to develop physically accurate methods to compute the thermoelectric transport coefficients of nanowires. In addition, computationally inexpensive parameterization of these physical models are needed in order for efficient sampling, e.g. in atomic configuration space, so as to design systems with optimal thermoelectric properties. We consider aspects of electron and phonon transport in SiGe nanowires. For electronic transport, we work in the diffusive regime with Boltzmann transport, combining ab initio density functional theory (DFT) calculations with a perturbative treatment of electronic scattering to obtain electronic relaxation times, conductivity and thermopower. The phonon contribution to thermal conductivity is obtained from classical equilibrium molecular dynamics simulations using the Green-Kubo formalism. Cluster expansion and effective potential techniques are used to parameterize the transport coefficients for efficient sampling and optimization.

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