Abstract Submitted
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Atomistic Monte Carlo simulations of heat transport in Si and SiGe nanostructured materials[1] IVANA SAVIC[2], Department of Chemistry, University of California at Davis, Davis, USA, DAVIDE DONADIO, Max Planck Institute for Polymer Research, Mainz, Germany, EAMONN MURRAY, Department of Chemistry, University of California at Davis, Davis, USA, FRANCOIS GYGI, Department of Computer Science, University of California at Davis, Davis, USA, GIULIA GALLI, Department of Chemistry and Physics, University of California at Davis, Davis, USA — Efficient thermoelectric energy conversion depends on the design of materials with low thermal conductivity and/or high electrical conductivity and Seebeck coefficient [1]. Semiconducting nanostructured materials are promising candidates to exhibit high thermoelectric efficiency, as they may have much lower thermal conductivity than their bulk counterparts [1]. Atomistic simulations capable of handling large samples and describing accurately phonon dispersions and lifetimes at the nanoscale could greatly advance our understanding of heat transport in such materials [2]. We will present an atomistic Monte Carlo method to solve the Boltzmann transport equation [3] that enables the computation of the thermal conductivity of large systems with both empirical and first principles Hamiltonians (e.g. up to several thousand atoms in the case of Tersoff potentials). We will demonstrate how this new approach allows one to rationalize trends in the thermal conductivity of a range of Si and SiGe based nanostructures, as a function of size, dimensionality and morphology [3]. [1] See e.g. A. J. Minnich et al. Energy Environ. Sci. 2, 466 (2009). [2] Y. He, I. Savic, D. Donadio, and G. Galli, accepted in Phys. Chem. Chem. Phys. [3] I. Savic, D. Donadio, F. Gygi, and G. Galli, submitted.

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