Abstract Submitted
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Atomistic study of heat transport in SiGe alloys[1] IVANA SAVIC, YUPING HE, Department of Chemistry, University of California at Davis, Davis, California, USA, DAVIDE DONADIO, Max Planck Institute for Polymer Research, Mainz, Germany, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California at Davis, Davis, California, USA — Semiconductor alloys, e.g. SiGe, are considered as promising materials to build efficient thermoelectric devices [1], and atomistic modeling of heat transport in these systems may help complement and guide experiments in optimizing their efficiency. We analyze strengths and weaknesses of several atomistic approaches in modeling the thermal conductivity of SiGe alloys, and we analyze in detail their range of validity. In particular, we focus on equilibrium molecular dynamics [2], an approach based on the solution of the Boltzmann transport equation [3] and Green function techniques [4]. Applications to both bulk and nanostructured SiGe will be presented.

[1] A. J. Minnich, M. S. Dresselhaus, Z. F. Ren, and G. Chen, Energy Environ. Sci. 2, 466 (2009). [2] See e.g. D. Donadio and G. Galli, Phys. Rev. Lett. 102, 195901 (2009); Nano Lett. 10, 847 (2010). [3] See e.g. J. E. Turney, E. S. Landry, A. J. J. McGaughey, and C. H. Amon, Phys. Rev. B, 79, 064301 (2009). [4] See e.g. I. Savic, N. Mingo, and D. A. Stewart, Phys. Rev. Lett. 101, 165502 (2008).

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