Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Calculation of figure of merit for Bi_2Te_3 nanostructures[1] FABIANO OYAFUSO, Jet Propulsion Laboratory, SMITH NIELSEN, California Institute of Technology, SEUNGWON LEE, Jet Propulsion Laboratory, JAMIL TAHIR-KHELI, California Institute of Technology, PAUL VON ALLMEN, Jet Propulsion Laboratory, WILLIAM GODDARD III, California Institute of Technology — Bi_2Te_3-based materials comprise one class of promising candidates for novel thermoelectric devices, for which low/high thermal/electrical conductivity are desired. We shall present calculations highlighting the effects of reduced dimensionality on the thermoelectric figure of merit ZT for such materials, with particular emphasis on Bi_2Te_3 / Sb_2Te_3 superlattices. The calculation consists of two components, a tight-binding electronic calculation for the electrical conductivity and electronic contribution to the thermal conductivity and a Green-Kubo molecular dynamics approach for the lattice contribution to the thermal conductivity.

[1]supported by DARPA.

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Date submitted: 22 Nov 2006 Electronic form version 1.4