Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Thermoelectric properties of Quintuple Layer Bi_2Te_3[1] ROGER LAKE, FERDOWS ZAHID, University of California Riverside — Motivated by recent experimental results,[2] we derive the thermoelectric parameters of a Bi_2Te_3 film of one quintuple layer thickness. Our results show approximately ten times increase in the figure of merit (ZT) for the thin film (ZT = 7.2) compared to that for the bulk (ZT = 0.68). The large enhancement in ZT results from the change in the distribution of the valence band density of modes brought about by the quantum confinement in the thin film. Our theoretical model uses ab initio electronic structure calculations as implemented in the VASP software package combined with a Landauer approach for calculating the linear-response transport coefficients. We employ two fitting parameters: a rigid shift of the conduction and valence bands to match the known bulk bandgap (i.e. a 'scissors operator'), and an energy independent electron mean free path for the phonon scattering inside the device. With these two fitting parameters, our results show excellent agreement with the known experimental values for bulk Bi_2Te_3.

[1]Supported by the MARCO Center FENA
[2]D. Teweldebrhan, V. Goyal and A. A. Balandin, Nano Lett. 10, 1209 (2010); D. Teweldebrhan, V. Goyal, M. Rahman, and A. A. Balandin, Appl. Phys. Lett. 96, 053107 (2010); Y. Zhang et al., Nat. Phys. 6, 584 (2010).

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Date submitted: 23 Nov 2010 Electronic form version 1.4