Abstract Submitted for the MAR11 Meeting of The American Physical Society

Nanodopant Induced Band Modulations and Electronic Transport Properties in $AgPb_mSbTe_{2+m}$ -type Thermoelectric Nanocomposites¹ YI ZHANG, CHANGFENG CHEN, Physics Department and HiPSEC, University of Nevada, Las Vegas, XUEZHI KE, Department of Physics, East China Normal University, China, JIHUI YANG, Electrochemical Energy Research Lab, GM R&D Center, PAUL KENT, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — The remarkable performance of many novel thermoelectric materials is attributed to their nanosized inclusions. By extensive first-principles calculations we show the distinct band structure modulation in $AgPb_mSbTe_{2+m}$ (LAST)-type nanocomposites. A band gap widening and conduction band minimum splitting process resulting from the nanodopants is discovered for a series of nanocomposites. Boltzmann transport calculations demonstrate that this process leads to a pronounced change in the high temperature electronic transport. The effects of different substitutional elements and atomistic orderings are discussed. Our results provide new understanding of nanosized doping in thermoelectric materials and narrow gap semiconductors.

¹This work is supported by DOE Agreements DE-FC52-06NA26274 and DE-FC26-04NT42278. The computation resource (CRAY-XT5) of the NCCS and the CNMS in ORNL are sponsored by DOE.

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Date submitted: 26 Nov 2010

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