Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Structure and physical properties of Antimony Asenide: a first principle study[1] DAT DO, S. D. MAHANTI, Department of Physics and Astronomy, Michigan State University — The group V elements, Sb, As and Bi have attracted renewed attention especially after the discovery of the strong topological insulator $Bi_{1-x}Sb_x$. While the mixing of group V elements are thought to be random, recently, Shoemaker et al., arXiv:1210.1986 [cond-mat.mtrl-sci], using single-crystal and high-resolution synchrotron x-ray diffraction, and neutron and x-ray pair distribution function analysis, show that SbAs has chemical ordering. Here we present a detailed theoretical study of the structure and physical properties of SbAs. Our cluster expansion calculation predicts the existence of the chemical ordering, in agreement with experiment. The electronic structure calculations reveal that SbAs is a semimetal with a pseudo gap. We also discuss the similarities and differences of SbAs with its two end-members Sb and As and the Sb-Bi system (bulk), and compare the surface electronic structures of all these systems.

[1]This work is partially supported by Center for Revolutionary Materials for Solid State Energy Conversion, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences - DE-SC0001054

Dat Do
Department of Physics and Astronomy, Michigan State University

Date submitted: 09 Nov 2012 Electronic form version 1.4