Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

**Antimony arsenide: Chemical ordering and order-disorder transition in SbAs** DANIEL SHOEMAKER, Argonne National Laboratory, THOMAS CHASAPIS, Northwestern University, DAT DO, Michigan State University, MELANIE FRANCISCO, DUCK YOUNG CHUNG, Argonne National Laboratory, S. D. MAHANTI, Michigan State University, ANNA LLOBET, Lujan Neutron Scattering Center, Los Alamos National Laboratory, MERCOURI KANATZIDIS, Argonne National Laboratory — The A7 structure of the Group V elements can display chemical ordering of Sb and As, which were previously thought to mix randomly. Our structural characterization of the compound SbAs is performed by single-crystal and high-resolution synchrotron x-ray diffraction, and neutron and x-ray pair distribution function analysis. All least-squares refinements indicate ordering of Sb and As, resulting in a GeTe-type structure without inversion symmetry. This lowering of symmetry does not result in any new Bragg reflections, so high-quality scattering data are required. High-temperature diffraction studies reveal an ordering transition around 550 K. Transport and infrared reflectivity measurements, along with first-principles calculations, find that SbAs has a direct band separation larger than that of Sb or As. Because even subtle substitutions in the semimetals, notably $Bi_{1-x}Sb_x$, can open semiconducting energy gaps, a further investigation of the interplay between chemical ordering and electronic structure on the A7 lattice is warranted.

Daniel Shoemaker
Argonne National Laboratory

Date submitted: 09 Nov 2012 Electronic form version 1.4