Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

First-Principles Studies of Earth-Abundant Tetrahedrite Thermoelectrics YI XIA, FEI ZHOU, VIDVUDS OZOLINS, UCLA — Recent experiments have shown inexpensive and naturally occuring tetrahedrite-based materials that exhibit a thermoelectric figure of merit near unity. These compounds are typically of the form $Cu_{12-x}M_xSb_4S_{13}$, where M is a transition metal, such as Zn or Fe, for a wide range of x. Using density-functional theory calculations, the ternary phase diagram and various defect formation energies are calculated. Furthermore, the electronic structure, phonon spectrum and thermoelectric properties are investigated. We observe metallic behavior and strong lattice anharmonicity of stoichiometric $Cu_{12}Sb_4S_{13}$. In addition, doping with transitional metals Zn or Fe increases both resistivity and anharmonicity. The theoretical calculations are in good agreement with experimental measurements.

Yi Xia
None

Date submitted: 09 Nov 2012 Electronic form version 1.4