Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Optical, electronic and transport properties of tetrahedrites SIMON KOHL, Karlsruhe Institute of Technology, JASON VIELMA, DAVID FOSTER, GUENTER SCHNEIDER, Oregon State University — Doped Tetrahedrites $Cu_{12-x}TM_xSb_4S_{13}$ (TM=Fe,Mn,Zn) have recently attracted interest as thermoelectric materials. We present an ab-initio study based on density functional theory of the optical, electronic and transport properties of these materials. We find in $Cu_{12-x}Zn_xSb_4S_{13}$: 1. the band-gap can be tuned through chalcogenide substitution and the optical absorption is very large making tetrahedrites attractive also as solar absorber materials. A point defect study of the Zn rich tetrahedrite (x=2) based on supercell calculations indicates p-type conductivity and Cu-Zn antisite defects are the dominant acceptor defect with Cu-vacancies also contributing. The calculated hole concentration is much larger than what is expected from conductivity measurements. We discuss these results in the context of the observed unusual, variable range hoping like electronic transport properties. Finally we present results of thermopower calculations based on semiclassical Boltzmann theory and discuss the applicability of these approach for tetrahedrites.

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Date submitted: 15 Nov 2013 Electronic form version 1.4