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Electronic structure and thermopower of Cu_3SbSe_4[1] DAT DO, Michigan State University, VIDVUDS OZOLINS, University of California, Los Angeles, S.D. MAHANTI, MAL-SOON LEE, Michigan State University, YONG-SHENG ZHANG, CHRIS WOLVERTON, Northwestern University — Cu_3SbSe_4 (Se4), a ternary derivative of the II-VI zincblende semiconductors, is a narrow band gap semiconductor (band gap $\sim$0.1 – 0.4 eV) and a promising thermoelectric. Recently, Skoug et al. [1] have measured transport properties of pure and doped Se4 (Ge and Sn substituting for Sb). They find that p-doping by 2% Sn results in optimized value of ZT=0.72 at 630 K. To understand the electronic structure and transport properties of Se4 we have carried out ab initio density functional electronic structure calculations. LDA/GGA/GGA+U approximations do not show that Se4 is a standard semiconductor. They give a resonance-like peak near the top of the valence band of width $\sim$0.5 eV. The Fermi energy for the undoped system lies below the peak, making it a pseudo-gap system, in disagreement with experiment. Non-local exchange with relaxation of Sb-Se bonds lead to the opening of a gap (0.26 eV), its origin being intimately related to the valency of Sb. Transport calculations show that Se4 is an excellent p-type thermoelectric, in agreement with experiment.

[1] Skoug et al., Sci. Adv. Mater., 3, 602 (2011).

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