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Electronic structure and transport properties of high performance thermoelectrics $AgPb_mSbTe_{2+m}$[†] D. I. BILC, S. D. MAHANTI, Michigan State University, Department of Physics and Astronomy, East Lansing, MI 48824, U.S.A., M. G. KANATZIDIS, Michigan State University, Department of Chemistry, East Lansing, MI 48824, U.S.A. — *Ab initio* electronic structure calculations based on gradient corrected density functional theory were performed on a class of novel quaternary compounds $AgPb_mSbTe_{2+m}$,[2] which were found to be excellent high temperature thermoelctrics with large figure of merit $ZT \sim 2.2$ at 800K.[3] These systems form in the rock-salt structure similar to the well known two component system PbTe where Ag and Sb occupy Pb sites. We find that resonant states appear near the top of the valence and bottom of the conduction bands of bulk PbTe when Ag and Sb replace Pb. These states can be understood in terms of modified Te-Ag(Sb) bonds. We find that the electronic structure near the gap depends sensitively on the microstructural arrangements of Ag-Sb atoms. The common feature of these microstructural arrangements is that they have a more rapidly increasing density of states (DOS) near the gap as compared to bulk PbTe due to the appearance of distinct resonant states. The effect of the increased DOS on the transport properties (electrical conductivity and thermopower) will also be discussed. 2. K. F. Hsu *et. al.*, Science **303**, 818, (2004). 3. D. I. Bilc *et. al.*, Phys. Rev. Letters **93**(14), 146403, (2004). [†]Supported by the Office of Naval Research (Contract No. N00014-02-1-0867 MURI program).

Daniel I Bilc
Michigan State University,
Department of Physics and Astronomy,
East Lansing, MI 48824, U.S.A.

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