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Atomic Ordering and Gap Formation in Ag-Sb Based Ternary Chalcogenides[1] S.D. MAHANTI, KHANG HOANG, JAMES R. SALVADOR, Michigan State University, MERCOURI G. KANATZIDIS, Northwestern University — Ag-Sb based ternary chalcogenides are important in optical phase change and thermoelectric applications. Although discovered almost 50 years ago and thought to be semiconductors, a fundamental understanding of their electronic structures had been lacking. We report *ab initio* electronic structure studies using density functional theory (DFT) to explain their observed atomic structures, the physics of gap formation and their low-energy properties. Total energy calculations yield theoretical atomic structures which are consistent with experiment. Ag/Sb ordering is found to have a huge impact on the electronic structure near the Fermi energy. It gives pseudogap structure in some ordered structures, and either a pseudogap or a gap in others. For the lowest energy structures, as one goes from Te to Se to S, the (indirect) band gap goes from being negative to positive. Transport properties of $AgSbTe_2$ can be understood in terms of a small intrinsic band gap and extremely shallow impurity states. The calculated negative band gap in this compound can be ascribed to the defficiency of DFT.

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