

Electronic and magnetic properties of MnSnAs_2

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We have also synthesized MnSnAs_2 single crystals using the vertical temperature gradient solidification method. The crystal structure of MnSnAs_2 is chalcopyrites, which are “genealogically” related to the more familiar tetrahedrally-coordinated zinc-blende materials, with lattice constants of $a=5.794 \text{ \AA}$ / $c=11.365 \text{ \AA}$. Using the experimentally determined lattice constants and crystal structure, we carried out first principles electronic structure calculations, using the full-potential linearized augmented plane wave (FLAPW) method in the local density approximation (LDA). The lowest total energies were observed for the AFM state, indicating that AFM ordering in the system is energetically favored at 0 K. We find that MnSnAs_2 is *metallic* in the electronic calculation. Interestingly, MnSnAs_2 exhibited ferromagnetism with $T_C = 328 \text{ K}$ and a magnetic moment per Mn at 5K of $2 \mu_B$. In this presentation we will discuss electronic, electrical, and magnetic properties of newly synthesized chalcopyrite MnSnAs_2 compound.