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Electronic structure and magnetic properties of transition-metal doped Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3 for diluted magnetic semiconductors
PAUL LARSON, WALTER LAMBRECHT, Department of Physics, Case Western Reserve University, 10900 Euclid Ave, Cleveland, OH 44106 — The semiconducting tetradymite-structure materials Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3 serve as the basis for high-performance room-temperature thermoelectric devices. Recently, it was found that these materials act as diluted magnetic semiconductors (DMS) with $T_c \sim 10$ K using a few percent doping of transition metal atoms (T = Ti, V, Cr, Mn, Fe). Electronic structure calculations have been performed using the full-potential linear muffin-tin orbital (FP-LMTO) method to understand these materials magnetic properties. The T atoms substitute at the much larger Bi/Sb sites which leads to isolated atomic-like states with very little crystal-field splitting and approximately 3+ valence. This leads to a high spin state with the magnetic moments essentially following Hund's rule. The position of the T $3d$ states in the band gap will be investigated by analysis of the density of states (DOS). The effects of lattice relaxation and the magnetic interaction of T atoms in the unit cell will also be investigated.

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