

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Sorting Category: 06.11.5 (C)

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 ($T = \text{Ti}, \text{V}, \text{Cr}, \text{Mn}, \text{Fe}$). 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.

Prefer Oral Session
 Prefer Poster Session

Paul Larson
pml6@cwru.edu
Case Western Reserve University

Date submitted: 30 Nov 2004

Electronic form version 1.4