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Electronic origins of the magnetic phase transitions in zinc-blende Mn chalcogenides

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Precise first-principles spin-polarized total-energy and band-structure calculations have been per-formed for the zinc-blende Mn chalcogenides with the use of the local-spin-density (LSD) approach. We find that the LSD is capable of identifying the correct magnetic-ground-state structure, but it overesti-mates the ordering temperature T& and the valence-band exchange splitting h~. The discrepancy is at-tributed to the overestimation by LSD of the p-d coupling. Adjusting this coupling by an external poten-tial and fitting its parameters to the s- and p-band exchange splitting in MnTe alone, we find that T& =73, 90, and 128 K, respectively, for MnTe, MnSe, and MnS, in good agreement

with

6112 SU-HUAI WEI AND ALEX ZUNGER 48

integration is performed using 10 special k-points for the
zinc-blende structure and equivalent k-points for all the
other structures. '

The muffin-tin (MT) size we used for
Mn and Te are 2.59 a.u. The local magnetic moments

p
are integrated inside the muon-tin spheres. %"e estimate our convergence error in AEz;„„and

p at

2 meV and

0.05 pz per Mn atom,

48 ELECTRONIC ORIGINS OF THE MAGNETIC PHASE... 6113

TABLE

48 ELECTRONIC ORIGINS OF THE MAGNETIC PHASE... 6115

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