Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

First-principles study of ferromagnetic coupling in $Zn_{1-x}Cr_xTe$ thin film P. JENA, QIAN WANG, QIANG SUN, Virginia Commonwealth University — Using gradient corrected density functional theory and supercell technique, we have calculated total energies, electronic structure, and magnetic properties of Cr doped ZnTe in both bulk and thin film configurations. Calculations with full geometry optimization for $Zn_{1-x}Cr_xTe$ supercell were carried out for different Cr concentrations (x=0.095, 0.143, and 0.19) and by varying the sites Cr atoms occupy. We show that the ferromagnetic phase of $Zn_{1-x}Cr_xTe$ in both bulk and thin film is energetically the most preferable state irrespective of the concentration and/or site occupation of Cr atom. The strong hybridization between Cr-3d and Te-5p states is found to be responsible for the ferromagnetic coupling - in agreement with recent experiments.

Puru Jena
Virginia Commonwealth University

Date submitted: 22 Nov 2004 Electronic form version 1.4