Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Suppresion of ferromagnetism in $Zn_xCr_{1-x}Te$: A DFT study
JUAREZ L.F. DA SILVA, National Renewable Energy Lab, 1617 Cole Blvd., Golden, CO 80401, USA, GUSTAVO M. DALPIAN, Centro de Ciencias Naturais e Humanas, Universidade Federal do ABC, Santo Andre, SP, Brazil, SU-HUAI WEI, National Renewable Energy Lab, 1617 Cole Blvd., Golden, CO 80401, USA — The possibility to control the charge and spin degrees of freedom independenlty in diluted magnetic semiconductos (DMS) provides an opportunity in the realization of spintronic devices. Therefore, there is a great desire to understand the physical parameters that control T_C in DMS. In this talk, we will report a density functional theory study of $Zn_xCr_{1-x}Te$ and $Ga_xCr_{1-x}As$, which show interesting carrier dependence of the T_C. We found that the stability of ferromagnetism (FM), which is calculated with respect the anti-ferromagnetic (AFM) phase, can be controlled by p- and n-type co-doping. For randomly distributed Cr, the maximum FM stability is found to be at ≈ 1.25 holes per magnetic ion. Furthermore, we studied the formation of magnetic Cr precipitates by analysing the binding energy of two Cr atoms in the host semiconductors. Our results indicate that a simple Coulomb binding picture cannot provide a consistent explanation for the formation of Cr-rich aggregates. Instead, we show that the variation of Cr-Cr binding energy can be discribed quite well using the band coupling model [G. M. Dalpian, S.-H. Wei, X. G. Gong, A. J. R. da Silva, and A. Fazzio, Solid State Commun. **138**, 353 (2006)].

Juarez L. F. Da Silva
National Renewable Energy Lab

Date submitted: 22 Nov 2007 Electronic form version 1.4