Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Magnetic properties of Cr_3Te_4 doped with transition metals: An *ab intio* study NABIL AL-AQTASH, The Hashemite University, RENAT SABIRIANOV, University of Nebraska at Omaha — We report density functional theory (DFT) study of the magnetic properties of Cr_3Te_4 doped with transition metals (TM) (Co, Fe, Ni, V and Mn), TM ions doped in Cr sites, Cr_{3-x} $(TM)_xTe_4$ (x = 0.5 and 1). We performed screening of the exchange coupling interaction and magnetization modifications upon the substitution of Cr by 3d-transition metals at various Cr sites in the Cr_3Te_4 structure. Our calculation show that Cr_3Te_4 has ferromagnetic coupling and large magnetization (Magnetization per unit cell is 18.24μB). Magnetocrystalline anisotropy (MAE) of this material is also large (MAE= 1.67MJ/m^3). Our calculations show that the increase in interlayer spacing strengthen ferromagnetism of Cr_3Te_4. Doping with Mn increases Cr_3Te_4 magnetization, but reduces the exchange coupling energy which means reducing Curie temperature (T_c). We find that doping with 3d-TM elements decreases the magnetocrystalline anisotropy energies (MAE) of Cr_3Te_4.

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Date submitted: 06 Nov 2015 Electronic form version 1.4