Origin of Ferromagnetism in pyrochlore Tl2Mn2O7 and chalcospinel CuCr2S4

Abstract:

In this talk, we present the electronic structure of two compounds, Tl2Mn2O7 and chalcospinel CuCr2S4. Using the Nth order muffin-tin obital downfolding technique, we investigate the origin of ferromagnetism in both the compounds. Based on our analysis, we establish the kinetic-energy driven mechanism to be responsible in these compounds for the experimentally observed ferromagnetism with high Curie temperatures.
For Tl2Mn2O7, we find an enhancement of Tc for moderate doping with nonmagnetic Sb and a suppression of Tc upon application of pressure, both in agreement with experimental findings.

References: T Saha-Dasgupta et. al. Phys. Rev. Lett. 96, 087205 (2006); M. De-Raychaudhury et. al., Phys. Rev. B 75, 014443 (2007); T. Saha-Dasgupta et. al.Phys. Rev. B 76, 054441 (2007