Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Pressure-driven changes in electronic structure of $BiCoO_3$[1] SUDIPTA KANUNGO, TANUSRI SAHA-DASGUPTA, S.N Bose National Centre for Basic Sciences — Using first-principles DFT based calculations, carried out on the recently measured crystal structure data [Oka et.al. J.Am.Chem.Soc.132, 9438 (2010)], we study the changes in the electronic structure of $BiCoO_3$ between the ambient-pressure and the high-pressure conditions. Our study shows that the application of high pressure drives the high-spin-to-low-spin transition at the Co site. The obtained results for the ambient pressure phase shows C-type AFM alignment of Co high spins, while the electronic structure at the high-pressure phase shows the presence of a finite energy gap at E_f in contrast with previously reported metallic or semimetallic character with low-spin state of Co. This semiconducting behavior in the nonmagnetic $BiCoO_3$ with LS state of Co is found to be driven by the presence of the $GdFeO_3$ type of orthorhombic distortion which arises due to finite mixing of Bi lone-pair states with O-p states, as opposed to previously predicted cubic or tetragonal symmetry of the high-pressure. The ambient pressure phase shows an order of magnitude larger energy gap arising due to the AFM alignment of Co in the high-spin state than the energy gap at the high pressure phase, explains the observed 3-order of magnitude jump in resistivity.

[1]Ref: Sudipta Kanungo and T. Saha-Dasgupta, Phys.Rev.B 83,104104(2011)

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Date submitted: 26 Oct 2011 Electronic form version 1.4