It should be noted that we have used GGA+U method in the present study as GGA calculations are unable to yield an insulating state. Our optimized lattice parameters are a= 9.62 Å, b= 5.50 Å and c= 9.74 Å(unit cell volume of 490.21 Å^3). The corresponding experimental values are 9.49 Å, 5.45 Å and 9.57 Å respectively[9] (unit cell volume of 471.13 Å^3). The calculated monoclinic angle β between vectors **a** and **c**, is 108.15°, which is slightly overestimated with respect to the experimental one (107.60°).

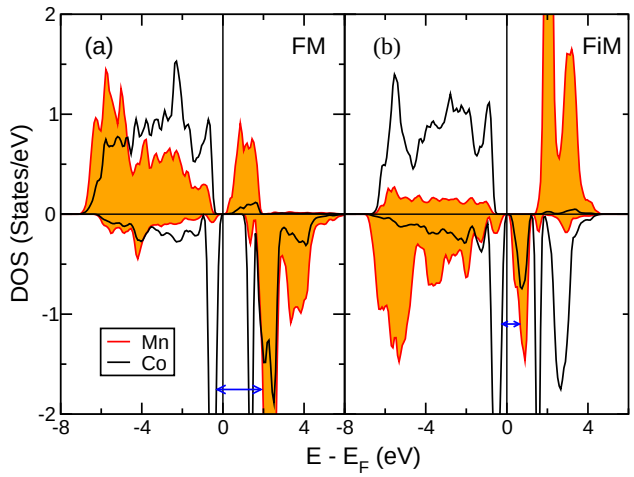

FIG. 2: (Color online) Mn and Co DOSs projected on d-orbitals for (a) FM and (b) FiM configurations. The horizontal blue lines indicate separation between the occupied Co and unoccupied Mn states in the minority spin. See text for details.

In Fig. 2, we show the density of states (DOS) obtained by GGA+U method for the ferromagnetic and ferrimagnetic (FiM) states. The choice of our U values opens up a band gap of around 0.3 eV in the FM state. The top of the valence band is dominated by Co-d and O-p states (not shown) while the Mn states are pushed about 1 eV below the Fermi energy. On the other hand the bottom of the conduction band is due to Mn-d and O-2p states. A comparison of the total energies of iso-structural FM and FiM structures yields that the FM state is 163 meV/f.u. lower in energy compared to the FiM state. The magnetic moment of Co (both in 2a and 2b sites) is found to be 2.5 μ_B, while Mn carries a magnetic moment of 3.2 μ_B, yielding a magnetic moment of 6 μ_B/f.u. in the FM state. The analysis of orbital projected charges in both FM and FiM magnetic structures shows that Co is in a high spin state with around 7 d electrons (Co^{2+} state), while the Mn sphere contains around 5 d electrons. It seems that Mn is in an oxidation state which is associated with an ionicity of about 2+ rather than 4+, which is the expected ionic state from the counting of oxidation states. This deviation from the expected ionicity may

$$Z^*_{Bi}: \begin{pmatrix} 4.51 & 0.18 & 0.32 \\ 0.21 & 4.71 & -0.35 \\ -0.14 & -0.10 & 4.98 \end{pmatrix}, \begin{pmatrix} 4.55 & 0.18 & 0.30 \\ 0.26 & 4.77 & -0.41 \\ -0.09 & 0.0 & 4.95 \end{pmatrix}$$

$$Z^*_{Co}: \begin{pmatrix} 2.81 & 0.00 & 0.26 \\ 0.00 & 2.47 & 0.00 \\ \boxed{0.02} & 0.00 & 2.84 \end{pmatrix}, \begin{pmatrix} 2.83 & 0.00 & 0.34 \\ 0.00 & 1.64 & 0.00 \\ \boxed{1.15} & 0.00 & 2.74 \end{pmatrix}$$

$$Z^*_{Mn}: \begin{pmatrix} 3.31 & 0.58 & -0.32 \\ 0.74 & 4.25 & 0.47 \\ -0.37 & \boxed{0.07} & 4.05 \end{pmatrix}, \begin{pmatrix} 3.80 & 0.29 & -0.41 \\ 0.67 & 4.05 & 0.17 \\ 0.21 & \boxed{0.62} & 4.39 \end{pmatrix}$$

$$Z^*_{O}: \begin{pmatrix} -3.37 & -0.19 & -0.14 \\ -0.20 & -2.28 & 0.14 \\ 0.33 & 0.57 & -2.26 \end{pmatrix}, \begin{pmatrix} -3.35 & 0.08 & 0.06 \\ -0.18 & -2.27 & 0.15 \\ 0.23 & 0.42 & -2.29 \end{pmatrix}$$

TABLE I: Born effective charges of Bi, Co, Mn and O (one in the Co-O-Mn chain) for FM (left) and FiM (right) configurations.

be attributed to the low symmetry structure and small Mn-O bond lengths. Similar ill-defined oxidation states of Mn and O were mentioned by Ciucivara *et. al*[6] for an iso-structural compound Bi_2NiMnO_6. The structural analysis shows that in the FM state, $\angle Mn-O-Co(2a)$ is equal to 159.45° while the angle $\angle Mn-O-Co(2b)$ is 150.83° giving an average $\angle Mn-O-Co$ angle of 155.14°. In both the Mn-O-Co chains, the Co-O bond is about 0.18 Å longer than the Mn-O bond. This clearly indicates that the Mn-O bond is stronger in comparison with Co-O bond, which is reflected in the DOS where we see that more Mn-d states are pushed down below the Fermi level.

We have computed a spontaneous electronic polarization of 5.88 $\mu C/cm^2$ in the FM state by Berry phase method. A 4×4 array of strings containing 32 k-points has been used to obtain the electronic polarization, which is non-zero only along the short-axis **b** in agreement with the C2 symmetry of the crystal. Our estimated value is close to what has been measured for Bi_2NiMnO_6 thin films. Unfortunately, we are unable to find an experimental value for BCMO.

Now we discuss the effect of magnetic structure on the BEC matrices shown in Table 1. It is observed that they are quite anisotropic due to the highly distorted structure of the compound and there are significant differences in BEC's for FM and FiM states for Co and Mn. Both diagonal and off-diagonal components of BEC matrices of Co and Mn are different in FM and FiM states, with major changes observed for $(Z^*)_{31}$ and $(Z^*)_{32}$ components (shown in box) of Co and Mn BEC's respectively. These changes may be attributed to the changes in electronic DOS's in two magnetic states, where, e.g., the energy separation between the occupied Co and unoccupied Mn t_{2g} states in the minority spin channel (Fig. 2) is decreased significantly in FiM state compared to the FM state. According to Ghosez *et al.*[15], the expression for BEC has the energy separation in the denominator and hence a reduction of this value should increase BEC significantly. A relatively small change occurs in the di-