Magnetic configurations in cubic Bi$_2$MnFeO$_6$ alloys from first-principles

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We expand our study on cubic BiFeO$_3$ alloys presented in [K. Koumpouras and I. Galanakis, J. Magn. Magn. Mater. 323, 2328 (2011)] to include also the BiMnO$_3$ and Bi$_2$MnFeO$_6$ alloys. For the latter we considered three different cases of distribution of the Fe-Mn atoms in the lattice and six possible magnetic configurations. We show that Fe and Mn atoms in all cases under study retain a large spin magnetic moment, the magnitude of which exceeds the 3 $\mu_B$. Their electronic and magnetic properties are similar to the ones in the parent BiMnO$_3$ and BiFeO$_3$ compounds. Thus oxygen atoms which are the nearest-neighbors of Fe(Mn) atoms play a crucial role since they mediate the magnetic interactions between the transition metal atoms and screen any change in their environment. Finally, we study the effect of lattice contraction on the magnetic properties of Bi$_2$MnFeO$_6$.

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INTRODUCTION

Spintronics brought to the center of the scientific research new materials with exotic properties \cite{1, 2}. The latest addition to these materials are the so-called multiferroics which combine several ferroic orders like ferromagnetism, ferroelectricity, ferroelasticity etc \cite{3, 4}. Among them exist some compounds which combine electric and magnetic order exhibiting the magnetoelectric effect \cite{5}. These alloys have several potential applications like magnetic-field sensors and electric-write magnetic-read random-access memories \cite{6, 7}. Magnetic order and ferroelectricity have different origins \cite{8, 9, 10} and thus the materials exhibiting the magnetoelectric effect are few and the coupling between the magnetic and electric properties is weak. An alternative route to achieve a strong coupling could be the growth of thin film heterostructures and several advances have been made towards the magnetic control of ferroelectricity \cite{11, 12, 13, 14} and the electric control of thin film magnetism \cite{11, 12, 13, 14}.

Among the most studied single-component multiferroic compounds are the bismuth ferrite and the bismuth manganite, BiFeO$_3$ and BiMnO$_3$. Bulk BiFeO$_3$ crystalizes in a perovskite-like pseudocubic structure instead of a ferrite one \cite{15} and bulk BiMnO$_3$ prefers a monoclinic lattice \cite{16}. BiFeO$_3$ is a ferroelectric G-type antiferromagnet \cite{15} while BiMnO$_3$ is a ferromagnet presenting no net spontaneous polarization \cite{17, 18, 19}. A Jahn-Teller distortion corresponding to an elongation of the oxygen octahedron surrounding the Mn atom induces a polar order in BiMnO$_3$ and G-type antiferromagnetism appears as in BiFeO$_3$; this new multiferroic state is close in energy to the ferromagnetic non-polar ground state \cite{20, 21, 22}. Several first-principles calculations have been carried out to study the properties of both bulk BiFeO$_3$ \cite{23} and BiMnO$_3$ compounds \cite{24, 25}. We refer readers to Ref. \cite{26} for an overview of the literature on both compounds. Since the single-component crystals like BiFeO$_3$ present only a weak magnetoelectric effect, an alternative route to achieve a more strong effect has been proposed to be the growth of heterostructures where epitaxial strain can enhance the phenomenon \cite{27, 28}. Doping has been also proposed to enhance the performance of such structures \cite{29, 30, 31}. Towards such heterostructures, multilayers consisting of alternating layers of BiFeO$_3$ and BiMnO$_3$ have been proposed where the ferroelectricity of BiFeO$_3$ couples to the ferromagnetic order in BiMnO$_3$ through epitaxial strain and a nanoscale checkboard from first-principles has been recently proposed for several lattice structures \cite{32}. Simple doping of BiFeO$_3$ with Mn leads to an antiferromagnetic coupling of the Mn spin moments to the Fe ones \cite{33}.

In a recent publication (Ref. \cite{34}) we have presented extended first-principles calculations, employing the Quantum-ESPRESSO \cite{35} ab-initio electronic structure method in conjunction with the Generalized-Gradient Approximation (GGA) in the Perdew-Burke-Erzenhof formulation \cite{36}, on the electronic and magnetic properties of BiFeO$_3$ alloy as a function of the lattice constant in the case of the cubic perovskite structure (see figure 1 in Ref. \cite{34}), where the heavy cations (Bi) occupy the corners of the cube, oxygen atoms the center of the faces and the Fe atom is at the center of the cube. Fe atoms alone form a cubic cell and the considered 2x2 unit cell in our calculations contained eight primitive cells and thus eight Fe atoms. We studied four possible magnetic arrangements: one ferromagnetic (F-type) and three antiferromagnetic (A-type, C-type and G-type). We found that all four types of magnetic order are close in energy and for a lattice constant of the primitive cell larger than 3.888 Å the G-type antiferromagnetism becomes more stable than the ferromagnetic state. The density of states (DOS) and the spin magnetic moments of the Fe atoms, which are responsible for the magnetic properties, showed similar behavior in all possible magnetic states since magnetic interactions are
mediated by oxygen atoms. Bi atoms showed no contribution to magnetism while the magnetic properties of the oxygen atoms depended strongly on their local environment since they are located at the midpoints between neighboring iron atoms.

We expand the study in Ref. 35 to cover also the case of Mn substitution for Fe in BiFeO$_3$ motivated by the work in Ref. 27 since the coexistence of Fe and Mn cations seems to lead to new multiferroic materials. We have concentrated our interest on the electronic and magnetic properties of the resulting compounds employing the same electronic structure method as in Ref. 35 and calculations details are similar. We have chosen to study a case with equal number of Fe and Mn atoms (denoted as Bi$_2$MnFeO$_6$) using the same 2x2 unit cell as in Ref. 35. Thus now we have four Fe atoms and four Mn atoms per unit cell. There are several ways to distribute the Fe and Mn atoms and in panel (a) of Fig. 1 we present the three cases which we have considered. In the I-case we have a layered structure consisting of alternating pure Fe and pure Mn layers along the [001] direction. In the II-case we have alternating pure Fe and pure Mn layers along the [110] direction and in III-case along the [111] direction. In I-case each Fe(Mn) atom has four Fe(Mn) and two Mn(Fe) atom as nearest transition-metal neighbors while in II-case each Fe(Mn) atom has two Fe(Mn) and two Mn(Fe) atom as nearest transition-metal neighbors.

![FIG. 1: Fe and Mn atoms in Bi$_2$MnFeO$_6$ form a cubic lattice. In (a) we present the three distributions of Mn and Fe atoms which we considered and in (b) the possible magnetic configurations (vectors pointing up correspond to positive spin magnetic moments and vectors pointing down to negative moments). Notice that there are now two possible A-type antiferromagnetic structures: (i) A1 where atoms belonging to neighboring planes along the [001] direction have antiparallel spin magnetic moments, and (ii) A2 when this occurs along the [100] directions. For the same reason there are two C-type antiferromagnetic configurations along the [110] (C1) and along the [101] (C2) directions.](image)

| TABLE I: Absolute values of the atom-resolved spin magnetic moments in $\mu_B$ for all cases and for all magnetic configurations under study. Results are for a lattice constant of the primitive unit cell (see Fig. 1 in Ref. 35) of 14.7 a.u. (3.888 Å). In case III the A1 and A2 structures are equivalent due to symmetry reasons and the same is valid also for the C1 and C2 configurations. |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| BiFeO$_3$       | BiMnO$_3$       | I-case          | II-case          | III-case         |
| Fe   | Mn | Fe | Mn | Fe | Mn | Fe | Mn | Fe | Mn | Fe | Mn |
| F    | 2.98 | 3.63 | 2.99 | 3.48 | 3.18 | 3.39 | 3.31 | 3.22 |
| A1   | 3.26 | 3.53 | 3.24 | 3.49 | 3.37 | 3.27 | 3.40 | 3.26 |
| A2   | 3.26 | 3.39 | 3.30 | 3.35 | 3.35 | 3.40 | 3.26 |
| C1   | 3.53 | 3.41 | 3.57 | 3.32 | 3.51 | 3.37 | 3.59 | 3.31 |
| C2   | 3.51 | 3.40 | 3.58 | 3.32 | 3.52 | 3.39 | 3.59 | 3.31 |
| G    | 3.65 | 3.24 | 3.68 | 3.22 | 3.68 | 3.21 | 3.68 | 3.18 |
RESULTS AND DISCUSSION

We will start our discussion from the case of BiMnO$_3$. In Table I we have gathered the spin magnetic moments in $\mu_B$ for the transition metal atoms for all cases under study and for a lattice constant of the primitive cell of 3.888Å. We have also included in the first column the values for BiFeO$_3$ from Ref. 35. Note that for BiMnO$_3$ and BiFeO$_3$ the A1 and A2 as well as the C1 and C2 antiferromagnetic configurations defined in Fig. I are degenerated. If we look at the spin magnetic moments Mn in BiMnO$_3$ posses in general a very high spin magnetic moment which reaches the 3.63 $\mu_B$ in the ferromagnetic case and varies between 3.24 and 3.53 $\mu_B$ in the antiferromagnetic configurations comparable to the values for Fe in BiFeO$_3$. The only noticeable difference for the two alloys concerns the ferromagnetic case (F-type) where Fe has a spin moment of about 3 $\mu_B$ quite smaller than all other cases. Mn has one valence electron less than Fe and thus in order to understand the behavior of its spin magnetic moment with respect to Fe we have to look at the density of states (DOS) presented in Fig. 2 for Mn and Fe in BiMnO$_3$ and BiFeO$_3$, respectively, for all four magnetic configurations under study. In the F- and A-configurations the large exchange splitting of the Mn d-states pushes the minority bands slightly higher in energy with respect to Fe while for the latter part of the extra electron occupies minority-spin states near the Fermi level leading to smaller Fe spin magnetic moments with respect to Mn. In the C- and G-configurations Mn presents a minority-spin pick pinned exactly at the Fermi level but this cannot explain the behavior of the spin magnetic moments in these cases. In the same figure we present with yellow shaded region the triple degenerated t$_{2g}$ states. The latter are higher in energy with respect to the t$_{2g}$ states due to the crystal field effect. The e$_g$ orbitals (d$_{xz}$ and d$_{yz}$) point towards the neighboring oxygen atoms and thus energetically are unfavorable with respect to the t$_{2g}$ orbitals (d$_{xy}$, d$_{xz}$ and d$_{yz}$) which point in the intermediate space, since in the latter case the Coulomb repulsion with the electrons occupying the oxygen p-orbitals is smaller. In the minority-spin band of Mn the e$_g$ states are not presented since they are slightly over the upper bound of the energy axis. In the majority-spin band the e$_g$ states are partially occupied while for Fe the are completely occupied and thus Mn has a slightly smaller spin magnetic moment for the C- and G-configurations. Finally we should shortly discuss the other atoms in these two compounds. Bi atoms are heavy and their role is to yield the electric polarization when the lattice is distorted while due to symmetry their spin magnetic moment is almost zero and thus their contribution to the magnetic properties can be neglected. Oxygen atoms as discussed in Ref. 35 for BiFeO$_3$ are located at the midpoints between neighboring transition-metal atoms. If the two Fe atoms had antiparallel moments the oxygen atom in the middle has a zero spin magnetic moment due to symmetry, otherwise its spin moment was about 0.15 $\mu_B$ due to the hybridization between the O-p and Fe-t$_{2g}$ orbitals. Manganese t$_{2g}$-orbitals hybridize with the oxygen p-orbitals much weaker and as a result oxygen atoms in BiMnO$_3$, when both Mn neighboring atoms have parallel spin moments, exhibit spin magnetic moments of one order of magnitude smaller than in BiFeO$_3$ (the larger obtained value is about 0.03 $\mu_B$ in the ferromagnetic configuration). Thus in BiMnO$_3$ the magnetic properties are entirely localized at the Mn sites.

Probably the most interesting from the three cases of possible atomic distributions of Fe and Mn atoms presented in Fig. I is the I-case where we have along the
FIG. 3: (Color online) Fe and Mn d-resolved DOS for the I-case (see atoms distribution if Fig. 1) for all six magnetic configurations. Notice that in all cases the positive DOS values correspond to the majority states (e.g. in the A1 and A2 cases the majority states are the spin-up for the Fe atoms and the spin-down for the Mn atoms).

[001] directions successive layers of pure Fe and pure Mn atoms. In Table I we have gathered the spin magnetic moments for all magnetic configurations under study and in Fig. 3 the Fe- and Mn-resolved DOS. Note in each magnetic configuration all Fe(Mn) atoms have the same magnitude of the spin magnetic moment (only its orientation varies) and thus the same DOS shape. We present the absolute value of the spin magnetic moments and in Fig. 3 the positive DOS values correspond to the majority-spin electrons in order to make comparison between the various cases easier to follow. We will start our discussion from the spin magnetic moments presented in Table I. Our first remark is that both Fe and Mn spin moments are very close to their values in the parent BiFeO$_3$ and BiMnO$_3$ alloys, respectively. Moreover the A1 and A2 as well as the C1 and C2 antiferromagnetic configurations correspond to almost identical spin magnetic moments. Thus, as discussed in Ref. 35, we can conclude that the oxygen atoms play a crucial role. Although themselves possess very small spin magnetic moments they bridge the transition-metal atoms and they mediate the magnetic interactions playing a shielding role for the Fe and Mn atoms. Each Fe(Mn) atom has now 4 Fe(Mn) atoms as nearest transition-metal neighbors instead of 6 in the perfect alloys and the other two have been substituted by Mn(Fe) atoms. But this change in the environment is screened by the intermediate oxygen atoms and the spin moments of the transition-metal atoms are only marginally affected. This discussion is also reflected in the DOS presented in Fig. 4. For each magnetic configuration the Fe- and Mn-resolved DOS are almost identical to the ones for the parent BiFeO$_3$ and BiMnO$_3$ alloys in Fig. 2 and all the details shown in Fig. 2 are present also in the DOS in Fig. 3; e.g. in both figures Fe in the F-case presents a double pick structure in the minority-spin band and the Fermi level is pinned exactly between these two picks while in the G-configuration there two distinct minority-spin picks corresponding to the $t_{2g}$ and $e_g$ states.

For the II- and III-cases of the Fe-Mn distribution we include the spin magnetic moments in Table I and the DOS in Fig. 4. We do not present the A2 and C2 cases in the figure since for the II-case they are similar to the A1 and C1 magnetic configurations while for the III-case as mentioned in the introduction we cannot distinguish between the A1(C1) and A2(C2) cases due to the symmetry of the lattice presented in Fig. 1. In II-case we...
have [001] chains of pure Fe and pure Mn or equivalently we can describe the structure as successive layers of pure Fe and pure Mn along the [110] direction. With respect to the I-case now each Fe(Mn) atom has only 2 nearest-neighboring transition metal atoms of the same chemical species instead of 4. In the III-case, which can be envisaged as alternating layers of pure Fe and pure Mn along the [111] direction all nearest neighbors are of the other chemical type, e.g. each Fe atom has 6 nearest-neighboring Mn atoms. Thus although the magnetic interactions are mediated by the oxygen atoms the effect on the spin magnetic moments is larger especially for the ferromagnetic (F-type) alignment of the spin moments. As the number of Mn neighbors increases the Fe spin magnetic moment in the F-case increases from 2.99 $\mu_B$ in the I-case to 3.18 $\mu_B$ in the II-case and 3.31 $\mu_B$ in the III-case. Simultaneously the Mn spin magnetic moment drops from 3.48 $\mu_B$ in the I-case to 3.22 $\mu_B$ in the III-case. For the antiferromagnetic cases under study the influence on the spin magnetic moments is smaller and for the G-type antiferromagnetism spin magnetic moments are unaltered by the variation of the Fe-Mn distribution. Overall even in the F-case the change in the magnitude of the spin magnetic moments is quite small; less than 0.3 $\mu_B$. The behavior of the spin magnetic moments is also reflected on the DOS presented in Fig. 4. In the II-case both Fe- and Mn-resolved DOS for all magnetic configurations under study are similar to the I-case. In the III case the only noticeable difference concerns Fe in the ferromagnetic case where the two picks at the Fermi level in the minority-spin band have merged in one broad large pick due to the influence of the exclusively Mn neighbors and this is also the only case where the variation of the spin-magnetic moment is noticeable reaching the 0.3 $\mu_B$ with respect to the I-case.

Finally, we have also studied the effect of a smaller lattice constant for the I-case and in Table II we present the obtained results for a lattice constant of 3.703 Å, which is about 4.8 % smaller than the 3.888 Å used in all previously presented results. Already in Ref. 35 we had shown that contracting the lattice of BiFeO$_3$ leads to an important decrease of the spin magnetic moment which in the G-type antiferromagnetism is less than 1 $\mu_B$ with respect to the 3.65 $\mu_B$ in Table II for the larger lattice constant. Also in the case of Mn in BiMnO$_3$ the Mn spin magnetic moment decreases with the contraction of the lattice although the decrease is not as dramatic as in BiFeO$_3$. This picture is also reflected in the layered I-case of Bi$_2$MnFeO$_6$ which we studied. In the I-case the Fe atoms keep a large number of Fe nearest-neighbors and its spin magnetic moment exhibits an even larger decrease than in the case of BiFeO$_3$. Especially in the G-type antiferromagnetism the Fe spin magnetic moments attend a low of only 0.25 $\mu_B$ being at the edge of being non-magnetic. On the contrary Mn atoms keep a high value of their spin magnetic moment which exceeds the 2.8 $\mu_B$ in all cases and thus, as in the case of BiMnO$_3$, Mn magnetic properties are less affected by the contraction of the lattice.

### SUMMARY AND CONCLUSIONS

We expand our study in Ref. 35 to the case of Bi$_2$MnFeO$_6$ alloys. First we have studied the BiMnO$_3$ alloy for various magnetic configurations and we have shown that, as was the case for BiFeO$_3$, Mn atoms exhibit high values of their spin magnetic moment, the magnitude of which exceeds the 3 $\mu_B$ in all cases under study. The small difference between the Fe and Mn spin magnetic moments can be easily explained by the position of the $e_g$ states with respect to the $t_{2g}$ states which lie lower in energy due to the crystal field effect. We took into account three different possible distributions for the Fe and Mn atoms in Bi$_2$MnFeO$_6$ and studied one ferromagnetic and five possible antiferromagnetic alignments of the spin magnetic moments. Both Fe- and Mn-resolved magnetic and electronic properties are only marginal sensitive to the various distributions of the atoms and show properties close to Fe and Mn atoms in the parent BiFeO$_3$ and BiMnO$_3$ alloys, respectively. Also among the various magnetic configurations the spin moments show small variation and their magnitude is always larger than 3 $\mu_B$. Thus oxygen atoms which are the nearest-neighbors of Fe(Mn) atoms play a crucial role since they mediate the magnetic interactions between the transition metal atoms and they screen any change in their environment. Finally we have shown that contracting the lattice leads to a large decrease in the spin magnetic moments of the Fe atoms as in BiFeO$_3$ studied in Ref. 35 while the Mn atoms retain a large portion of their spin magnetic moment.

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|        | BiFeO$_3$ | BiMnO$_3$ | Bi$_2$MnFeO$_6$ (I-case) |
|--------|-----------|-----------|--------------------------|
| Fe     | 2.32      | 3.05      | 2.21                     |
| Mn     | 3.22      | 2.93      | 2.10                     |
| Fe     | 1.87      | 1.07      | 2.17                     |
| Mn     | 3.05      | 3.11      | 3.11                     |
| G      | 0.98      | 2.53      | 0.25                     |
|        |           |           | 2.84                     |
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