The complex non-collinear magnetic orderings in $\text{Ba}_2\text{YOsO}_6$: a new approach to tuning spin-lattice interactions and controlling magnetic orderings in frustrated complex oxides

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Abstract

Frustrated magnets are one class of fascinating materials that host many intriguing phases such as spin ice, spin liquid and complex long-range magnetic orderings at low temperatures. In this work we use first-principles calculations to find that in a wide range of magnetically frustrated oxides, at zero temperature a number of non-collinear magnetic orderings are more stable than the type-I collinear ordering that is observed at finite temperatures. The emergence of non-collinear orderings in those complex oxides is due to higher-order exchange interactions that originate from second-row and third-row transition metal elements. This implies a collinear-to-noncollinear spin transition at sufficiently low temperatures in those frustrated complex oxides. Furthermore, we find that in a particular oxide $\text{Ba}_2\text{YOsO}_6$, experimentally feasible uniaxial strain can tune the material between two different non-collinear magnetic orderings. Our work predicts new non-collinear magnetic orderings in frustrated complex oxides at very low temperatures and provides a mechanical route to tuning complex non-collinear magnetic orderings in those materials.

Keywords: double perovskite, first-principles calculations, magnetic transition, frustrated magnet, complex oxides

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1. Introduction

Magnetic frustration, arising either from the geometry of crystal lattice or from the competition between different magnetic interactions, can lead to many intriguing phenomena such as complex long-range ordered states (non-collinear, chiral, etc) and disordered states (spin liquid, spin ice, etc) [1–9]. However, while frustrated magnetism is extensively studied in model calculations and experiments, first-principles studies on realistic frustrated magnetic materials are few, compared to those on normal magnets with a bipartite lattice and a dominating magnetic interaction. In particular, insights from first-principles calculations on low-temperature magnetism in frustrated complex oxides are rare [10–16].
Density-functional-theory-based first-principles study can take into account various exchange interactions, spin–orbit interaction and spin-lattice interactions in realistic materials and treat them on an equal footing, enabling us to systematically search for new magnetic phenomena in frustrated complex materials.

In this work, we study a wide range of ordered double perovskite oxides with second- or third-row transition metal elements residing on a geometrically frustrated face-centered-cubic lattice: Sr$_2$ScRuO$_6$, Sr$_2$YRuO$_6$, Ba$_2$YRuO$_6$, Sr$_2$ScOsO$_6$, Sr$_2$YOsO$_6$, and Ba$_2$YOsO$_6$. All these complex oxides are all reported in experiment to exhibit type-I collinear magnetic ordering below the respective Néel temperatures [11, 15, 17–20]. Our first-principles calculations show that at zero temperature, a number of non-collinear magnetic orderings are more stable than the type-I collinear magnetic ordering that is observed at finite temperatures. The emergence of non-collinear orderings in those complex oxides at low temperatures is due to higher-order exchange interactions that originate from second- and third-row transition metal elements. This implies that at sufficiently low temperatures there could occur a collinear-to-noncollinear spin transition in those frustrated complex oxides. Furthermore, we find that in a particular oxide Ba$_2$YOsO$_6$, experimentally feasible uniaxial strain can tune the material between two different non-collinear magnetic orderings, which reveals a mechanical approach to tuning magnetic ions and whether spin–orbit coupling is taken into account or not.

The frustrated complex oxides in this study have a double perovskite structure with a chemical formula $A_2BB'O_6$ (see figure 1(a)). Two different types of transition metal ions $B$ and $B'$ form a rock-salt ordering and therefore transition metal ions occupy a face-centered-cubic lattice (fcc), which has 'geometric frustration'. We study six double perovskite oxides which are listed in table 1. They all have one non-magnetic ion (Sc$^{3+}$ and Y$^{3+}$) and one magnetic ion (Ru$^{5+}$ and Os$^{5+}$). Experimentally, all these six complex oxides exhibit a layered collinear antiferromagnetic ordering (so-called type-I) at finite temperatures, as is shown in figure 1(b). The Néel temperatures of these six complex oxides are listed in table 1.

2. Computational details

We perform first-principles calculations using plane-wave basis density functional theory (DFT), as implemented in the Vienna ab initio simulation package (VASP) [22, 23]. We take into account both spin–orbit coupling (SOC) and correlation effects. We use the method proposed by Dudarev et al [24] to model Hubbard $U$ interaction. We employ a revised Perdew–Burke–Ernzerhof generalized gradient approximation (PBEsol) [25] as the exchange-correlation functional, which has been successfully applied to study second-row and third-row transition metal oxides [26, 27]. We also test other exchange-correlation functionals: local-density-approximation (LDA) and Perdew–Burke–Ernzerhof functional (PBE). All the calculations are spin-polarized (with either collinear and non-collinear magnetic ordering). We use an energy cutoff of 600 eV, and the Brillouin zone integration is performed with a Gaussian smearing of 0.05 eV and a $10 \times 10 \times 10$ $k$-mesh. The threshold of energy convergence is $10^{-6}$ eV. Throughout the calculations we use a 40-atom supercell (see figure 1(a)). For each oxide, we use its experimental structure to compare different long-range magnetic orderings. Their experimental crystal structures can be found in the references listed in table 1. Only when we study uniaxial strain, we relax the crystal structure of Ba$_2$YOsO$_6$ until each Hellmann–Feynman force component is smaller than $10^{-3}$ eV Å$^{-1}$ and the stress tensor is smaller than 1 kbar.

3. Results and discussion

For clarity, we first study Ba$_2$YOsO$_6$ as a representative example and then extend the discussion to other complex oxides. Experimentally double perovskite Ba$_2$YOsO$_6$ crystallizes in a cubic structure with a lattice constant of 8.357 Å (space group $Fm\bar{3}m$) [28]. In Ba$_2$YOsO$_6$, Y$^{3+}$ nominally has a $d^0$ occupancy and Os$^{5+}$ nominally has a $d^0$ occupancy. Due to Hund’s rule, the three electrons on Os$^{5+}$ ions fill three different $t_{2g}$ orbitals and form a core spin $S = 3/2$ [29]. The Os spins occupy a face-centered-cubic lattice, which has ‘geometric frustration’ (see figure 1(b)). The experimental Os$^{5+}$ moment is 1.65 $\mu_B$ [20], which is smaller than the atomic value $3 \mu_B$ for a $S = 3/2$ spin, due to strong hybridization of Os-5d orbitals with O-2p orbitals.

We discuss our results in two steps: in the first step we do not consider spin–orbit coupling (SOC) and in the second step we take into account SOC effects. This is to decouple the SOC effects from other intrinsic spin interactions.

3.1. Without spin–orbit coupling

Without taking into account SOC, spins are decoupled to lattice. This means that the total energy of the system only depends on relative orientations between spins. Any global
rotation of the full spin configuration with respect to lattice leads to a trivial degenerate state.

Since our 40-atom supercell includes four Os atoms that occupy a tetrahedron, we study a general four-sublattice antiferromagnetic ordering, as well as a ferromagnetic ordering for comparison. The spin configuration of a general four-sublattice antiferromagnetic ordering is schematically shown in figure 2 in which four equal-length arrows (i.e. vector spins) form a head-to-tail ring. In three-dimensional space, such a ring is characterized by two parameters θ and φ, as figure 2 shows. Thus, the four spins have the following coordinates:

\[
\begin{align*}
S_1 &= (+ \cos(\theta/2), 0, + \sin(\theta/2)) \\
S_2 &= (+ \cos(\theta/2) \cos(\pi - \phi), + \cos(\theta/2) \sin(\pi - \phi), - \sin(\theta/2)) \\
S_3 &= (- \cos(\theta/2) \cos(\pi - \phi), - \cos(\theta/2) \sin(\pi - \phi), - \sin(\theta/2)) \\
S_4 &= (- \cos(\theta/2), 0, + \sin(\theta/2)).
\end{align*}
\]

We first perform spin-polarized DFT-PBEsol calculations using the experimental structure of Ba$_2$YO$_5$O$_6$ (see table S1 in section I of supplementary materials (stacks.iop.org/JPhysCM/31/445803/mmedia) for its structural parameters). Then we discuss U dependence and exchange-correlation functional dependence. We compute the total energy of the ferromagnetic ordering and different four-sublattice antiferromagnetic orderings (collinear, coplanar, non-collinear non-coplanar etc.). Our spin-polarized DFT-PBEsol calculations find that three distinct antiferromagnetic states as well as ferromagnetic ordering are stabilized in Ba$_2$YO$_5$O$_6$. They are shown in figure 3. Figure 3(a1) is a collinear antiferromagnetic state in which all the spins are either parallel or anti-parallel (θ = 180°, referred to as $E_1$). For simplicity, we use $E$ to refer to a state as well as the energy of that state. Figure 3(a2) is a coplanar antiferromagnetic state in which all four spins lie in the same plane; one pair of anti-parallel spins is orthogonal to another pair of anti-parallel spins ($\theta = 0°, \phi = 90°$, referred to as $E_2$). Figure 3(a3) is a non-collinear non-coplanar state in which every two spins form an identical angle ($\theta = \arccos(\frac{1}{2}) \approx 71°, \phi = 90°$, referred to as $E_3$). Figure 3(a4) is a ferromagnetic state (referred to as $E_{FM}$). Figure 3(b) shows that the non-collinear non-coplanar state ($E_3$) has the lowest total energy, followed by the coplanar state ($E_2$) and then followed by the collinear state ($E_1$). The ferromagnetic state ($E_{FM}$) has much higher energy than all antiferromagnetic orderings, which indicates that the nearest-neighbor exchange coupling is antiferromagnetic in nature.

Next, we discuss Hubbard U dependence and exchange-correlation functional dependence. The correlated ion in Ba$_2$YO$_5$O$_6$ is Os$^{5+}$. While the accurate value of Hubbard U on Os is not known, we expect that it does not exceed 5 eV because Os is a third-row transition metal element [30, 31]. We repeat the previous calculations using different values of U$_{Os}$ ranging from 0 to 5 eV. The results are shown in figure 3(b). We find that while the energy difference between the three antiferromagnetic orderings decreases with U$_{Os}$, the energy sequence $E_3 < E_2 < E_1 < E_{FM}$ does not change with Hubbard U$_{Os}$. On the other hand, the magnitude of Os-projected magnetic moment increases with U (from m$_{Os}$ = 1.8 $\mu_B$ at U$_{Os}$ = 0 eV to m$_{Os}$ = 2.5 $\mu_B$ at U$_{Os}$ = 5 eV). Experimentally m$_{Os}$ = 1.65 $\mu_B$ in Ba$_2$YO$_5$O$_6$ [20] and the U$_{Os}$ = 0 result is the closest to the experimental value. This is consistent with previous studies showing that in spin-polarized DFT calculations, the exchange splitting in PBEsol exchange-correlation functional is sufficiently large [32, 33]. Turning on a Hubbard U impairs the agreement between experiment and theory. We therefore use U$_{Os} = 0$ eV in the remainder of the paper. In addition, we study the effect of different exchange-correlation functionals on the energy sequence of the four magnetic orderings. We compare the energy differences $\Delta E$ obtained by spin-polarized DFT calculations using PBEsol, PBE and LDA calculations. Figure 3(c) shows that the energy sequence $E_3 < E_2 < E_1 < E_{FM}$ does not change in all the calculations, indicating that our results are robust.

Figure 4 shows the total density of states and projected densities of states of Ba$_2$YO$_5$O$_6$ in the lowest-energy non-collinear non-coplanar magnetic ordering ($E_3$), calculated

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Table 1. A list of magnetically frustrated complex oxides in this study. FM and AFM-I refer to ferromagnetic ordering and type-I antiferromagnetic ordering, respectively. Note that the notations of space groups in this table are taken from the respective references directly.

| Material         | Magnetic ion | d Shell | Space group      | Magnetic transition | Reference          |
|------------------|--------------|---------|------------------|---------------------|--------------------|
| Sr$_2$ScRuO$_6$  | Ru$^{3+}$    | 4$d^3$  | $I\bar{2}/m$ (300 K) | AFM-I, $T_N \sim 60$ K | [17]               |
| Sr$_2$YRuO$_6$   | Ru$^{3+}$    | 4$d^3$  | $P2_1/n$ (293 K)  | AFM-I, $T_N \sim 26$ K | [18]               |
| Ba$_2$YRuO$_6$   | Ru$^{3+}$    | 4$d^3$  | $Fm\bar{3}m$ (4.2 K) | AFM-I, $T_N \sim 37$ K | [19, 21]           |
| Sr$_2$ScOsO$_6$  | Os$^{3+}$    | 5$d^3$  | $P2_1/n$ (3.5–300 K) | AFM-I, $T_N \sim 92$ K | [11]               |
| Sr$_2$YO$_5$O$_6$| Os$^{3+}$    | 5$d^3$  | $P2_1/n$ (2.9–300 K) | AFM-I, $T_N \sim 53$ K | [15]               |
| Ba$_2$YO$_5$O$_6$| Os$^{3+}$    | 5$d^3$  | $Fm\bar{3}m$ (3.5–290 K) | AFM-I, $T_N \sim 69$ K | [20]               |

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Figure 2. A general four-sublattice antiferromagnetic spin configuration in three-dimensional space. The four spins (equal-length vector) form a head-to-tail ring with the two green spins in one plane and the other two yellow spins in another plane. The ring formed by the four spins is characterized by two angles $\theta$ and $\phi$. Here, $\theta$ is the angle between the two green spins, and $\phi$ is the angle between the two planes.
by spin-polarized DFT-PBEsol method. The other magnetic orderings have similar densities of states. Close to the Fermi level are dominating Os-$t_{2g}$ states, while Os-$e_g$ states are much higher than the Fermi level. Therefore, the low-energy physics can be well described by Os-$t_{2g}$ states which form a $S = 3/2$ core spin.

Now we repeat the spin-polarized DFT-PBEsol calculations on the other five complex oxides and find the same energy sequence $E_3 < E_2 < E_1 < E_{FM}$ between the three antiferromagnetic orderings and the ferromagnetic ordering (see figure 5). Turning on Hubbard $U$ on Ru or Os does not qualitatively change the results. This implies that the underlying spin interaction could be universal to this class of frustrated magnets. Considering that the spins of Os$^{5+}$ and Ru$^{5+}$ are large ($S = 3/2$), we construct the spin interaction using a classical vector-spin model. The simplest nearest-neighbor classical Heisenberg interaction predicts that all four-sublattice antiferromagnetic orderings on a fcc-lattice are continuously degenerate [34]. This is clearly at odds with the DFT results that all three stable antiferromagnetic orderings have different energies. The second nearest-neighbor Heisenberg interaction is trivial in our DFT calculations since we use a 40-atom
supercell which includes four magnetic ions. For a given magnetic ion, the other three magnetic ions in the cell are its nearest-neighbors on a fcc lattice. Its second nearest-neighbors are in fact the periodic images in the adjacent cell. Therefore, the second nearest-neighbor interaction is a constant in our results (figure 5).

A common beyond-Heisenberg spin interaction is the nearest-neighbor biquadratic interactions and 4-spin ring interactions, which have been shown to be important in complex oxides [35–38]. They also have a larger inter-site hopping matrix elements due to stronger hybridization between transition metal elements and oxygen. A common beyond-Heisenberg spin interaction is the nearest-neighbor biquadratic interactions and 4-spin ring interactions, which have been shown to be important in complex oxides [35–38]. They also have a larger inter-site hopping matrix elements due to stronger hybridization between transition metal elements and oxygen.

\[ H = H_{\text{Heisenberg}} + H_{\text{quad}} + H_{\text{ring}} + H_0 \]

where \( |S_i| = 1 \) is a vector-spin, \( N \) is the number of spins and \( E_0 \) is a reference energy. First we consider a general four-sublattice antiferromagnetic Hamiltonian on a fcc lattice and insert equation (1) into equation (2), we obtain:

\[ \frac{E}{N} = -2J_1 + (a_1 + a_2) \left( \frac{13}{4} - \cos \theta + \frac{7}{4} \cos(2\theta) \right) + 2 \cos \left( \frac{\theta}{2} \right) \cos(2\phi) + E_0. \]  

The nearest-neighbor Heisenberg interaction (\( J_1 \)-term) does not depend on \( \theta \) and \( \phi \), indicating a continuous degeneracy, as we mentioned above. The nearest-neighbor biquadratic and 4-spin ring interactions are additive on a fcc lattice, indicating that we can combine the two interactions with one coefficient \( \alpha_1 = a_1 + a_2 \). Equation (3) have three extremal solutions, which exactly correspond to the collinear state (\( E_1 \)), the coplanar state (\( E_2 \)) and the non-collinear non-coplanar state (\( E_3 \)). Their total energies are:

\[ E_1/N = -2J_1 + 2a_1 + E_0 \]

\[ E_2/N = -2J_1 + 2a_1 + E_0 \]

\[ E_3/N = -2J_1 + \frac{2}{3} a_1 + E_0. \]  

For a positive \( J_1 \) and a positive \( a_1 \), equations (4) and (5) find an energy sequence \( E_3 < E_2 < E_1 < E_{FM} \), irrespective of the values of \( J_1 \) and \( a_1 \). This reproduces our spin-polarized DFT results (figure 5).

We note that Hubbard \( U \) on Ru or Os atoms can change the magnitude of the coefficients \( J_1 \) and \( \alpha \) by \( J_1 \propto U^2 \) and \( \alpha_1 \propto U^2 \). However, Hubbard \( U \) can not change the sign of \( J_1 \) and \( \alpha \). A positive \( J_1 \) and a positive \( \alpha_1 \) always lead to the energy sequence \( E_3 < E_2 < E_1 < E_{FM} \). On the other hand, as we increase the Hubbard \( U \) on Ru or Os, the energy difference between the four magnetic orderings gets smaller as equations (4) and (5) indicate. This is consistent with the spin-polarized DFT+U results shown in figure 3(b).

3.2. With spin–orbit coupling

Ru and Os are heavy elements and their SOC cannot be neglected. We perform spin-polarized DFT-PBEsol+SOC calculations to study SOC effects on the zero-temperature magnetic orderings in those complex oxides. Similarly we first study Ba2YO4Os3 as a representative example and then extend the discussion to the other five oxides.

The effects of SOC are to couple Os 5d and 4f orbits to the crystal lattice. This means that those magnetic orderings which would be degenerate without SOC now have different energies due to their different orientations with respect to the crystal lattice, i.e. the presence of SOC induces anisotropic exchange interaction and leads to more different complex magnetic orderings [44, 45]. Our spin-polarized DFT-PBEsol + SOC calculations find that in Ba2YO4Os3, there are nine stable antiferromagnetic orderings, which are explicitly shown in figure 6. Similar to the results of DFT calculations without SOC, we classify

\[ \text{Figure 6. Nine stable antiferromagnetic orderings found in Ba}_2\text{YO}_4\text{Os}_3 \text{ from spin-polarized DFT-PBEsol calculations with spin–orbit coupling (PBEsol+SOC). (a) Two collinear antiferromagnetic orderings: (a1) referred to as } E_{1a}; \text{ (a2) referred to as } E_{1b}. (b) Four coplanar antiferromagnetic orderings: (b1) referred to as } E_{2a}; \text{ (b2) referred to as } E_{2b}; \text{ (b3) referred to as } E_{2c}; \text{ (b4) referred to as } E_{2d}. (c) Three non-collinear non-coplanar antiferromagnetic orderings: (c1) referred to as } E_{3a}; \text{ (c2) referred to as } E_{3b}; \text{ (c3) referred to as } E_{3c}. \]
as collinear non-coplanar states (three different states, labelled as $E_1$, $E_2$, and $E_3$). After SOC is taken into account, the two lowest energy states are a non-collinear non-coplanar state $E_{a1}$ and a coplanar state $E_{a2}$. The energy of $E_{a1}$ is set as the zero energy.

Figure 7. Energy sequence in ascending order of the nine stable antiferromagnetic orderings found in Ba$_2$YOsO$_6$ from spin-polarized DFT-PBEsol+SOC calculations. The two lowest energy states are a non-collinear non-coplanar state $E_{a1}$ and a coplanar state $E_{a2}$. The energy of $E_{a1}$ is set as the zero energy.

These nine magnetic orderings into three cases: collinear states (two different states, labelled as $E_{a1}$ and $E_{b1}$), coplanar states (four different states, labelled as $E_{a2}$, $E_{a3}$, $E_{a4}$, $E_{a5}$) and non-collinear non-coplanar states (three different states, labelled as $E_{a6}$, $E_{a7}$, $E_{a8}$). It is straightforward to check that if we turn off SOC, the two collinear magnetic orderings $E_{a1}$ and $E_{b1}$ would be degenerate, and the four coplanar magnetic orderings ($E_{a2}$, $E_{a3}$, $E_{a4}$, $E_{a5}$) would also be degenerate in DFT calculations. Figure 7 shows the energy sequence sorted in ascending order for these nine stable antiferromagnetic orderings in Ba$_2$YOsO$_6$. After SOC is taken into account, we find that the two lowest-energy magnetic orderings are a non-collinear non-coplanar state $E_{a3}$ and a coplanar state $E_{a2}$, both of which are more stable than the experimentally observed type-I collinear ordering ($E_{a1}$ and $E_{b1}$). This result is robust and does not depend on the choice of exchange-correlation functionals, the comparison between different exchange-correlation functionals is provided in section II of supplementary materials.

Next, we test the other five complex oxides and compare the non-collinear non-coplanar state $E_{a3}$ and the coplanar state $E_{a2}$ to the experimentally observed type-I collinear ordering ($E_{a1}$ and $E_{b1}$). We find similar results (see figure 8) that at zero temperature, the type-I collinear magnetic ordering is not the most stable one; both the non-collinear non-coplanar state ($E_{a3}$) and the coplanar state ($E_{a2}$) have lower energies. This implies that in those complex oxides there could occur an entropy-driven collinear-to-noncollinear magnetic transition at sufficiently low temperatures.

Finally, we notice that the $\Delta E$ between $E_{a2}$ and $E_{a3}$ of Ba$_2$YOsO$_6$ is extremely small (about 0.10 meV/f.u.), indicating these two antiferromagnetic orderings are almost degenerate. This is an accidental degeneracy, which is not protected by symmetry and strongly depends on materials, as figure 8 shows. While antiferromagnetic orderings are difficult to control due to the vanishing of net moments, the near-degenerateness between the two complex antiferromagnetic orderings implies that mechanical strain may tune Ba$_2$YOsO$_6$ from one magnetic ordering to another. Here we consider uniaxial strain, since experimentally amplified piezoelectric actuators can generate continuously tunable uniaxial strain up to 1% [46, 47]. Such uniaxial strain has been successfully applied to Sr$_2$RuO$_4$ to enhance its superconducting transition temperatures [46, 48] and tune its resistivity in the vicinity of van Hove singularities [47]. Uniaxial strain has also been proved to be effective in manipulating the magnetic degrees of freedom in BaFe$_2$As$_2$ [49].

Since we need to study strain effects, we perform structural optimization for Ba$_2$YOsO$_6$ using spin-polarized DFT-PBEsol+SOC method and obtain an optimized lattice constant of 8.368 Å, which is in good agreement with the experimental value (within about 0.2% difference). We calculate the energy difference between the coplanar state $E_{a2}$ and the non-collinear non-coplanar state $E_{a3}$ in Ba$_2$YOsO$_6$ when one of its lattice constant $a_1$ is under strain while the other two lattice constants as well as internal coordinates are fully relaxed. Figure 9 shows $E_{a2} - E_{a3}$ as a function of uniaxial strain $\varepsilon_{x1}$ which is defined as:

![Figure 9](image-url)
where \(d_0\) is the theoretical lattice constant in equilibrium obtained from spin-polarized DFT-PBEsol+SOC calculations. We find that uniaxial tensile strain favors the non-collinear non-coplanar state \(E_{3\alpha}\) while sufficient uniaxial compressive strain can make the coplanar state \(E_\beta\) more stable. The critical strain is about 0.1% of uniaxial compression, which is achievable by using piezoelectric actuators [46–48].

4. Conclusions

In conclusion, we perform first-principles calculations on a wide range of magnetically frustrated complex oxides and predict that at zero temperature, a number of non-collinear magnetic orderings are more stable than the type-I collinear magnetic ordering that is observed at finite temperatures. Those non-collinear magnetic orderings are induced and stabilized by nearest-neighbor biquadratic interactions, which become pronounced in materials that contain second-row and third-row transition metal elements. It implies that at sufficiently low temperatures, a collinear-to-noncollinear magnetic transition can occur probably due to entropy effects. We test different exchange-correlation functionals, various correlation strengths on magnetic ions and presence/absence of spin–orbit coupling. We find that our conclusions are robust. We also demonstrate that a particular complex oxide \(\text{Ba}_2\text{YOsO}_6\) is in the vicinity of the phase boundary between two non-collinear magnetic orderings. Experimentally feasible uniaxial strain can tune the material across the magnetic phase boundary, with uniaxial tensile strain energetically favoring the non-collinear non-coplanar ordering \((E_{3\alpha})\), and uniaxial compressive strain making the coplanar ordering \((E_{\beta})\) more stable.

Our prediction of zero-temperature four-sublattice magnetic orderings in those frustrated complex oxides (with detailed orientation of magnetic moments) should provide new targets for future neutron scattering measurements at very low temperatures. Our work also shows that tunable uniaxial strain can control complex non-collinear magnetic orderings in \(\text{Ba}_2\text{YOsO}_6\), providing an example to studying spin-lattice interactions in frustrated oxides. We hope our theoretical calculations can stimulate new experimental study on magnetic properties of those materials.

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Data availability statement

The data that support the findings of this study are openly available in [50].

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