Half Metal Transition Driven by Doping Effects in Osmium Double Perovskite

Madhav P. Ghimire and Xiao Hu
International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science, Tsukuba 305-0044, Japan
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Using the first-principles density functional approach, we investigate Ca$_2$FeOsO$_6$, a material of double perovskite structure synthesized recently. According to the calculations, Ca$_2$FeOsO$_6$ is a ferrimagnetic Mott-insulator influenced by the cooperative effect of spin-orbit coupling (SOC) and Coulomb interactions of Fe-3d and Os-5d electrons, as well as the crystal field. When Fe is replaced with Ni, the system exhibits half metallic (HM) states desirable for spintronic applications. In [Ca$_2$Fe$_{1-x}$Ni$_x$OsO$_6$], HM ferrimagnetism is observed with $\mu_{\text{tot}} = 2\mu_B$ per unit cell for doping rate $x = 0.5$, whereas HM antiferromagnetism (HMAFM) with nearly zero spin magnetization in the unit cell for $x = 1$, respectively. It is emphasized that half metallicity is retained even with SOC effect due to the large exchange-splitting between spin-up and spin-down bands close to the Fermi level.

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I. INTRODUCTION

Double perovskite oxides have been widely investigated due to their interesting properties useful for spintronic applications.$^{12}$ With the general formula A$_2$BB’O$_6$, A is usually an alkaline earth or rare-earth element, and B and B’ are the transition metal elements, both of which are composed of edge-shared octahedra. Depending on the choice of B and B’ cations, these compounds show a variety of electrical and magnetic properties, namely metallicity, half metallicity, insulator as well as ferromagnetism, ferrimagnetism, and antiferromagnetism.$^{1}$ The discovery of room-temperature colossal magnetoresistance and half metallicity in Sr$_2$FeMoO$_6$ (where T=Mo, Re$^{35}$), multiferroicity in Bi$_2$NiMnO$_6$,$^{36}$ magneto-dielectricity in La$_2$NiMnO$_4$,$^{37}$ leads to intensive study in double perovskite materials. Recent researches have been devoted to understanding the electronic and magnetic properties of hybrid 3d-4d(5d) double perovskites which exhibit high spin polarization$^{38}$ essential for device applications at room temperature.

Half metals (HMs) are a class of materials which are metallic in one spin channel, while insulating in the opposite spin channel due to the asymmetric band structure.$^{10,12}$ HMs allow spin polarized currents to flow without any external operation, and thus are very useful for spintronics applications. The total spin-moment per unit cell is quantized in units of Bohr magneton ($\mu_B$) due to insulating state in one spin-channel. HMs have been identified in several groups of material.$^{17,20}$ Most of the experimentally available HMs are either ferromagnets (FM) or ferrimagnets (FiM) which give non-zero integer moments. It was noted that spin-polarized current can be hampered by stray fields which stabilize magnetic domain.$^{13,20}$ This drawback can be overcome by HM antiferromagnets (HMAFM), a subclass of HMs characterized further by zero spin magnetization per unit cell.$^{11,19}$ A number of materials with DP's structures have been predicted as possible candidates of HMAFMs.$^{17,22}$

Because of the recent success in synthesizing osmium oxides, osmates have been attracting significant interests yielding various unconventional phases. For instance, unusual superconductivity is observed in A$_2$Os$_2$O$_7$ (A=Cs, Rb and K)$^{31}$. Magnetically driven metal-insulator transition is found in Cd$_2$Os$_2$O$_7$,$^{12}$ and NaOsO$_3$,$^{33}$ and the ferroelectric-type structural transition has been discovered in metallic LiOsO$_3$.$^{34}$ Among the double perovskites, magnetic insulating states in Sr$_2$MOsO$_6$ (where M=Cu, Ni)$^{35}$, Mott-insulating ferromagnetic state in Ba$_2$NaOsO$_6$,$^{35}$ and half semi-metallic antiferromagnetism in Sr$_2$CrOsO$_6$,$^{37}$ are a few examples that have been reported. A newly synthesized double perovskite material Ca$_2$FeOsO$_6$ comes into our attention which is reported to be a FiM insulator driven by lattice distortion with high Curie temperature ($T_C$)$^{33}$. The crystal has unique properties suitable for spintronic device applications: Fe and Os atoms carry on opposite spin magnetizations, and octahedra exhibit strong crystal distortion which may induce strong crystal field that helps in splitting the spin-up and spin-down bands. The origin of novel FiM state with $T_C$ of 320K opens new possibility of realizing device applications at room temperature. We dope Ni atom having charge state +2 to replace Fe atom with charge state +3 to study its influence on the parent material Ca$_2$FeOsO$_6$.

We have performed first-principles density-functional calculations on Ca$_2$FeOsO$_6$ (CFOO). It is found that CFOO is a FiM Mott insulator with total angular moment $\mu_{\text{tot}} = 4\mu_B$ per unit cell of [Ca$_2$FeOsO$_6$]. This material is interesting in the sense that the topmost valence states close to Fermi level ($E_F$) are exclusively spin-down bands contributed from 5d electrons of Os atoms, and the element Fe has no influence on the electronic state near $E_F$. Therefore, replacing Fe by 3d elements with more than five valence electrons one can make a fine control on charge and spin. Specifically, we consider the replacement of Fe atom by the Ni atom which shows interesting properties desirable in spintronics.
FIG. 1. Double perovskite structure of [Ca$_2$FeOsO$_6$]$_2$ and [Ca$_2$NiOsO$_6$]$_2$. The red (blue) arrows indicate the direction of Fe/Ni(Os) spins along the $a$ direction which is the easy axis.

We find that the material [Ca$_2$Fe$_{1-x}$Ni$_x$OsO$_6$]$_2$ is HM-FIM with $\mu_{\text{tot}} = 2\mu_B$ at $x = 0.5$ and nearly compensated HMAFM with $\mu_{\text{tot}} = 0.3\mu_B$ at $x = 1$. The interplay among Coulomb repulsion, SOC and the crystal field plays an important role in this material.

The organization of this paper is as follows: Section II describes the details on crystal structure and methods. Section III presents the results on the parent material [Ca$_2$FeOsO$_6$]$_2$, while Sec. IV discusses the results on the possibility of obtaining half metallicity in the doped materials [Ca$_2$Fe$_{1-x}$Ni$_x$OsO$_6$]$_2$. Section V contains the discussions and the conclusions are drawn in Sec. VI.

II. CRYSTAL STRUCTURES AND METHODS

In the double perovskite [Ca$_2$FeOsO$_6$]$_2$ (CFOO), the transition metal Fe and Os occupy B and B’ sites in an ordered way. The crystal structure of CFOO shown in Fig. 1 falls in the space group $P2_1/n$ with monoclinic-distortion. It has structural distortions due to the tilting and rotation of the two corner-sharing FeO$_6$ and OsO$_6$ octahedra.

The electronic and magnetic structure calculations were performed within density-functional theory (DFT) by using the full-potential linearized augmented plane wave plus local orbital method implemented in the WIEN2k code. The atomic sphere radii $R_{\text{MT}}$ were 2.17, 1.99, 1.99, 2.0 and 1.64 Bohr for Ca, Fe, Ni, Os and O respectively. A set of 1000 $k$-points were used in the full Brillouin zone. The standard generalized-gradient approximation (GGA) exchange-correlation potential within the PBE-scheme were used with Coulomb interaction $U$ of 5eV for Fe/ Ni) and 1.5eV for Os, respectively. Spin-orbit coupling is considered via a second variational step using the scalar-relativistic eigenfunctions as basis. We checked different magnetic configurations of Fe, Ni and Os sites and found that the FiM structure shown in Fig. 1 is the ground state consistent with the experiments.

III. PARENT MATERIAL [Ca$_2$FeOsO$_6$]$_2$

In CFOO, the transition element Fe nominally takes the charge state $+3$ with $3d^5$ configuration. These five valence electrons occupy the $t_{2g}$ and $e_g$ orbits resulting to a high-spin (HS) state of Fe. On the other hand, Os takes the charge state $+5$ with $5d^5$ configuration, where three valence electrons occupy the $t_{2g}$ orbits giving rise to HS state.

To gain insight into the electronic properties of CFOO, the spin-resolved total and partial density of states (DOS) in spin-up and spin-down channels are shown in Fig. 2. According to first-principles calculations, there is an energy gap of $\sim 0.8$eV at $E_F$, indicating clearly that CFOO is a Mott insulator. This result is consistent with the recent experimental report of the insulating state in CFOO. Fe-3$d$ (i.e., $t_{2g}$ and $e_g$) states in spin-up channel are fully occupied and remain deep in the valence region, whereas the states in spin-down channel lies in the conduction region. Unlike Fe, Os-5$d$ (i.e., $t_{2g}$) states are located in the conduction region with a broad peak for spin-up channel indicating the empty states, whereas in spin-down channel they occupy the topmost valence
Ni doping corresponds to addition of three extra electrons to the system. Since the charge states of Fe(+3) and Ni(+2) differ from each other, the Os atom interacting with Fe has a charge state +5 and 5d\(^{5}\) configuration while the other one interacting with Ni has +6 charge state and 5d\(^{2}\) configuration, to maintain charge neutral in the system. Thus, Ni doping will influence the system by (i) shifting the Os bands towards the conduction region, and (ii) compensating magnetic moment by 2\(\mu_{B}\) per each Fe replacement. In this way, one can modify the material to design the desired HMFiM and HMAFM.

We perform first-principles calculations to check the above idea for replacement rate \(x = 0.5\) in \([\text{Ca}_2\text{Fe}_{1-x}\text{Ni}_x\text{OsO}_6]_2\). As shown in Fig. 3, Fe-3d states in spin-up channel are fully occupied lying deep in the valence region, whereas for spin-down channel they remain in the conduction region. The Ni-3d bands are also occupied in spin-up channel while the spin-down bands are partially occupied with a localized peak at -1.8eV below \(E_F\). The remaining bands appear in the conduction region. This happens because five out of eight \(d\) electrons from Ni occupy the spin-up channel and the three remaining electrons go to spin-down channel to fill the \(t_{2g}\) orbits. Due to repulsive interaction from spin-down Ni-3d electrons, Os-\(t_{2g}\) electrons which were originally lying at the topmost valence region in the parent material (see Fig. 2) shift towards the conduction region crossing \(E_F\) (see Fig. 5(b)). As the results, the Os-\(t_{2g}\) states crossing \(E_F\) form a continuous band and give rise to metallic state below \(E_F\). As observed in Fig. 2(d), oxygen bands below \(E_F\) in both spin-channels hybridize with the Fe-3d and Os-5d states. This is caused due to octahedral distortions, where three sorts of oxygen positions with different Fe(Os)-O bond-lengths appear.

The magnetic property of CFOO is of particular interests. At the ground state obtained from first-principles calculations, Fe couples antiferromagnetically with Os. The calculated total moment (\(\mu_{\text{tot}}\)) is 4.0\(\mu_B\) per unit cell (see Table I). In an ionic picture, each Fe ion carries moment +5\(\mu_B\) while Os ion carries -3\(\mu_B\), giving rise to \(\mu_{\text{tot}} = 2 \times (+5\mu_B) + 2 \times (-3\mu_B) = 4\mu_B\) in \([\text{Ca}_2\text{FeOsO}_6]_2\), consistent with the first-principles calculations.

IV. DOPED MATERIALS \([\text{Ca}_2\text{Fe}_{1-x}\text{Ni}_x\text{OsO}_6]_2\)

The above properties makes CFOO a promising candidate for exploring possible HM states with fine control on charge and magnetic moments. HM states can be achieved in CFOO by doping 3\(d\) transition metals having valence electron larger than five. To be specific, we consider the B-site modification by replacing one Fe atom with Ni in \([\text{Ca}_2\text{FeOsO}_6]_2\), an element having charge state +2 with 3\(d^8\) configuration. Out of eight valence electrons five occupy the \(t_{2g}\) and \(e_g\) orbits of spin-up channel while the remaining three occupy the \(-t_{2g}\) orbits in spin-down channel giving rise to a moment of 2\(\mu_B\) per Ni atom.

FIG. 3. Density of states for \([\text{Ca}_2\text{Fe}_{0.5}\text{Ni}_{0.5}\text{OsO}_6]_2\) in spin-up (↑) and spin-down (↓) channels: (a) total, (b) Fe-3\(d\)/Ni-3\(d\) states, (c) Os-5\(d\) states, and (d) three inequivalent oxygen-2\(p\) states.

FIG. 4. Density of states for \([\text{Ca}_2\text{NiOsO}_6]_2\) in spin-up (↑) and spin-down (↓) channels: (a) total, (b) Ni-3\(d\) states, (c) Os-5\(d\) states and (d) three in-equivalent oxygen-2\(p\) states.
FIG. 5. Band structures for doping rate (a) $x = 0$, (b) $x = 0.5$ and (c) $x = 1$ in $[\text{Ca}_2\text{Fe}_{1-x}\text{Ni}_x\text{OsO}_6]_2$ for spin-up (red) and spin-down (black) channels.

for spin-down channel. Hence, with spin-up channel insulating and spin-down channel metallic, the material is a half metal.

Let us now focus to the most interesting case of replacement rate $x = 1$, where both Fe atoms are replaced by Ni atoms within unit-cell. From the first principles calculations the FiM ground state is $\sim 135\text{meV}$ less than the first excited AFM state. Due to the presence of Ni atom alone on the B-site, Os atom fully attains the charge state +6 with $d^2$ configuration unlike in the parent material $[\text{Ca}_2\text{FeOsO}_6]_2$. For Ni of $d^8$, three $t_{2g}$ and two $e_g$ orbits in spin-up channel and three $t_{2g}$ orbits in spin-down channel are occupied. For Os of $d^2$, only two $t_{2g}$ orbits in spin-down channel are occupied. The system is then expected to favor half metallicity with full compensation of total moment. As revealed by the DOS shown in Fig. 4, Ni-3$d$ states are fully occupied in spin-up channel by five electrons and the remaining electrons go to occupy the $t_{2g}$ orbits in spin-down channel. This is evident with the occupation of Ni-3$d$ states in the valence region with a localized peak at -1.6eV below $E_F$. The unoccupied $e_g$ band appears far in the conduction region. The Os-5$d$ states are almost empty in spin-up channel but has partial occupation with a band crossing $E_F$ in spin-down channel. This is caused mainly by the spin-down electrons of Ni which push the Os-$t_{2g}$ states up towards the conduction region. Thus, two of the $t_{2g}$ states of Os atom remain in the valence region while the unoccupied state moves to the conduction region crossing $E_F$ (see also Fig. 5(c)). Due to crystal distortion, gap could not open-up among the $t_{2g}$ states of Os atom which results in metallic state in spin-down channel. Oxygen 2$p$ states are found to hybridize strongly with Os-5$d$ states near $E_F$ in both spin channels. Thus, with spin-up channel insulating and spin-down channel metallic, the system turns to a HM as clearly seen in Fig. 4.

As summarized in Table I, two replaced Fe atoms take away $\mu \simeq 2\mu_B$, and the charge transfer in two Os atoms associated on doping reduces $\mu \simeq 2\mu_B$ further, resulting in compensation of total moment to zero. The results obtained by first-principles calculations are consistent with the ionic picture. These features can also be seen from the spin-density isosurface plot in Fig. 5(b). With the zero total moment and HM property, the material $[\text{Ca}_2\text{NiOsO}_6]_2$ should be a HMAFM. However, SOC induces an orbital moment of $\sim 0.17\mu_B$ across Os resulting in the total moment of $0.3\mu_B$ per unit cell. Hence the material may be called a nearly compensated half metal.

TABLE I. Moments per atom of Fe[Ni] and Os, one set of three in-equivalent oxygen atoms and unit cell ($\mu_{\text{tot}}$) for replacement rate $x$ in $[\text{Ca}_2\text{Fe}_{1-x}\text{Ni}_x\text{OsO}_6]_2$ from first-principles calculations. The unit of moments is the Bohr magneton $\mu_B$. The contributions from individual atoms are within muffin-tins while the total angular moment includes those from interstitial regime.

| $x$ | Fe [Ni] | Os | O | $\mu_{\text{tot}}$ |
|-----|---------|----|---|------------------|
| 0   | 4.13    | -1.6 | -0.11 | 4.0 |
| 0.5 | 4.13 [1.68] | -1.36 | -0.15 | 2.0 |
| 1   | [1.68]  | -1.09 | -0.14 | 0.3 |

V. DISCUSSIONS

In order to give a clear picture on how doping changes the electronic structure for $x = 0$, 0.5 and 1 in $[\text{Ca}_2\text{Fe}_{1-x}\text{Ni}_x\text{OsO}_6]_2$, band structure plots are shown in
Os on the other hand shows the $t_{2g}$ characters. The full replacement of Fe with Ni shows an active $e_g$ like orbitals (see Fig. 6(b)). The size of the Os-$t_{2g}$ isosurface reduces in the doped material due to one electron less than in the parent material.

First-principles calculations on magnetic anisotropy energy indicates $a$ axis of the crystal as the easy axis (see Fig. 1) with anisotropy energy of $\sim 2$meV and $\sim 4$meV per unit cell for Ca$_2$FeOsO$_6$ and Ca$_2$NiOsO$_6$ respectively.

Robustness of half metallicity is checked for doping rate $x = 1$ by considering the (i) antisite disorder and (ii) surface effects with a vacuum of 20Å along 001. We have confirmed that the HM state remains stable in both configurations.

In the present work, HMAFM and HMFiM have been derived from the same parent material. Thus, using them in an integrated system, one can construct a useful device for spintronics applications without suffering from the problem of lattice mismatching.

VI. CONCLUSIONS

Based on the first-principles density functional approach, we propose material tailoring on a Mott insulator [Ca$_2$FeOsO$_6$]$_2$ with double perovskite structure exploiting the cooperative effect from Coulomb interaction, spin-orbit coupling and the crystal field. It is demonstrated that replacing Fe by Ni, one can achieve several half metals. Especially, [Ca$_2$NiOsO$_6$]$_2$ is found to be a nearly compensated half metals, which is ideal for spintronic applications. It is emphasized that the large exchange splitting between spin-up and spin-down bands at the Fermi level retains the half metallicity even in presence of strong spin-orbit coupling.

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