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# Half-Metallic Ferromagnetic Double Perovskites as Promising Materials for Spintronics and Energy Devices

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## ABSTRACT

Double perovskite-like materials which include transition elements have relevance due to the technological perspectives in electronics and spintronics engineering. In this study, we report the investigations of the electronic and magnetic properties of $Sr_2CrWO_6$ and $Sr_2FeReO_6$ by using the first-principles density functional theory (DFT). The electronic and magnetic results predict proper half-metallic (HM) and ferromagnetic (FM) ground states in $Sr_2CrWO_6$ and $Sr_2FeReO_6$ with total magnetic moments of 2.0 and 3.0 $\mu_B$, respectively. Therefore, these materials seem to possess HM and FM properties, making them useful candidates for applications in spintronics and energy devices.

Double perovskite materials, which include transition elements, are relevant because of the technological perspectives in electronics and spintronics engineering. In this study, we report the research on the electronic and magnetic properties of $Sr_2CrWO_6$ and $Sr_2FeReO_6$ using first density functional density theory (DFT). The electronic and magnetic results predict suitable semi-metallic (HM) and ferromagnetic (FM) ground states in $Sr_2CrWO_6$ and $Sr_2FeReO_6$ with total magnetic moments of 2.0 and 3.0 μB, respectively. Therefore, these materials appear to possess HM and FM properties, making them useful candidates for applications in spintronics and energy devices.

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## INTRODUCTION

Respected of their requests in spintronics and energy devices, half-metallic (HM) double perovskites are appropriate based on their unique features; (i) full spin-polarization at the Fermi level ($E_F$), (ii) quantization of spin magnetic moment, and (iii) zero spin susceptibility. Some transition-metal double perovskites (TMDPs) with chemical formula $A_2MNO_6$ (A=alkali-earth; MN=transition-metals) have been recently designated to exhibit ferromagnetism (FM) and HM with (SP=100%) of conduction electrons at the $E_F$, making them promising candidates as materials suitable for spintronics technologies such as magnetic recorders, magnetic sensors, computer memories, and solar cell devices. Also, very interesting properties are detected in TMDPs family, such as magnetoresistance (MR) in ($Sr_2FeMoO_6$) and ($Sr_2FeReO_6$) [1,2], HM above room-temperature (RT) in ($A_2FeMoO_6$; A=Ca, Sr, Ba) [3,4] and ($Sr_2CrMoO_6$) [5,6] and high Curie temperature ($T_C$) [1,7]. The ordered TMDPs ($Sr_2FeMoO_6$), ($Sr_2FeReO_6$), ($Sr_2CrMoO_6$), ($Sr_2CrWO_6$), etc., are among the very few materials that allow conduction electrons of one spin direction to move through them, while blocking the electrons with opposite spin direction. In this study, the structural, electronic and magnetic properties of two Sr-based double perovskites ($Sr_2CrWO_6$ and $Sr_2FeReO_6$) are reported by using the density functional theory (DFT) calculations within the exchanged and correlated local spin density approximation (LSDA+U).

## CRYSTAL STRUCTURES

The ideal crystal structure of $Sr_2CrWO_6$ and $Sr_2FeReO_6$ can be viewed as an ordered arrangement of corner-sharing $Cr(Fe)O_6$ and $W(Re)O_6$ octahedra (6-coordinate system), alternating along the three directions of the crystal space, with the large cations $Sr^{2+}$ (12-coordinate system) occupying

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the cavities in between these octahedra. $Sr_2CrWO_6$ and $Sr_2FeReO_6$ crystallize in cubic structure with (Fm-3m) symmetry and $Cr^{3+}$–$W^{5+}$ and $Fe^{3+}$–$Re^{5+}$ systems arranged in rock-salt ordering. Their lattice parameters are a=7.8587 Å and a=7.8858 Å, respectively, around the ideal values (a=8.0 Å). Each $Cr^{3+}$ ($W^{5+}$) or $Fe^{3+}$($Re^{5+}$) is coordinated by $W^{5+}$($Cr^{3+}$) or $Re^{5+}$($Fe^{3+}$) and each has an $O^{2-}$ in between forming $Cr^{3+}/Fe^{3+}O^{2-}{}_6$ and $Re^{5+}O^{2-}{}_6$ octahedra with bond-lengths of $Cr^{3+}/Fe^{3+}$–$O^{2-}$=1.981 Å/1.949 Å and $Re^{5+}$–$O^{2-}$ =2.016 Å/1.928 Å. The atomic positions in the unit cell are $Sr^{2+}$ at 8c (¼, ¼, ¼), Cr/Fe at 4a (0, 0, 0), Re at 4b (½, ½, ½) and O at 24e (u, 0, 0), where u=0.252 and u=0.256 for Cr and Fe compound, respectively.

## HALF-METALLIC PROPERTIES

**Figure 1** shows the total densities of states (TDOSs) of $Sr_2CrWO_6$ and $Sr_2FeReO_6$ with an energy-gap in spin-up of ($E_g$=2.14 eV) and ($E_g$=2.31 eV), respectively, falls between the occupied Cr/Fe (3d) and unoccupied W/Re (5d) states. From the partial densities of states (PDOSs) in **Figure 2**, it can be see that the spin-down conduction states are created mainly from the contributions of W (5d) and Re (5d) states with tiny contributions come from Cr (3d) and Fe (3d) states, respectively. The small variation between two TDOSs is due to the extra electron in Re ($5d^2$) than in W ($5d^1$). Also, since the $E_g$ produces from the antiferromagnetic coupling between Cr/Fe (3d) and W/Re (5d) states **(Figure 2)**, their peaks emerge as Cr/Fe $(3d)_\uparrow$ and W/Re $(5d)_\downarrow$ near $E_F$. Therefore, the spin-up electrons are insulating while the spin-down ones are metallic, resulting in SP = 100% of their conduction electrons at the $E_F$. Accordingly, $Sr_2CrWO_6$ and $Sr_2FeReO_6$ allow electrons of spin-down direction to move through them as though they were passing through a regular metal, while blocking electrons with spin-up direction. The obtained results of $Sr_2CrWO_6$ and $Sr_2FeReO_6$ are agreement with previous results [8,9].

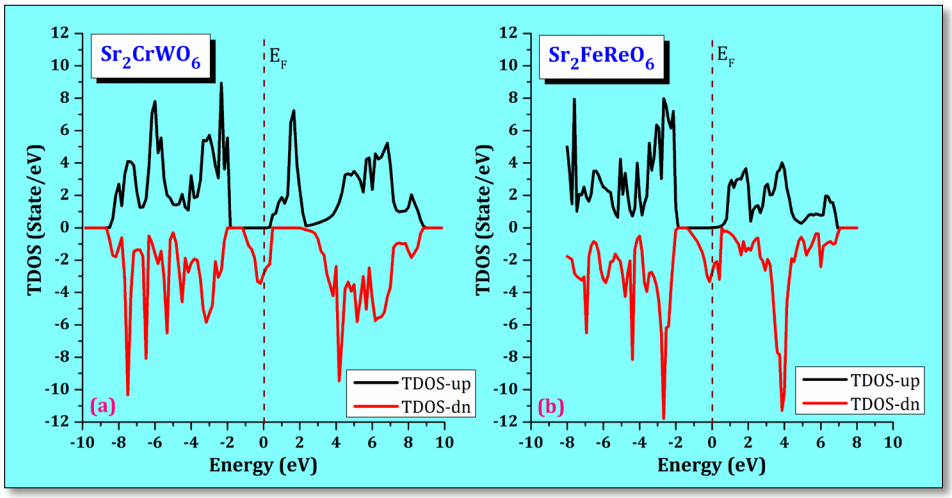


**Figure 1.** TDOSs for (a) $Sr_2CrWO_6$ and (b) $Sr_2FeReO_6$, ($E_F$=0.0 eV).

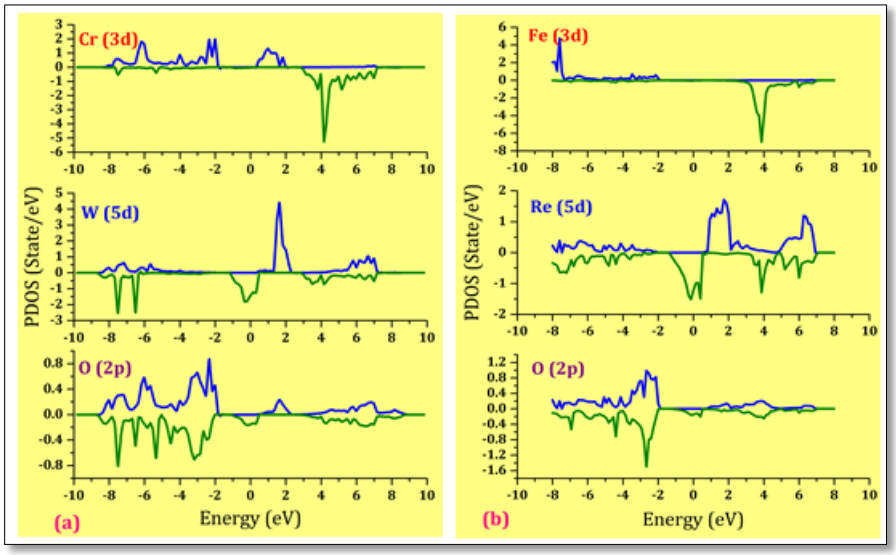


**Figure 2.** PDOSs for (a) $Sr_2CrWO_6$ and (b) $Sr_2FeReO_6$.

## FERROMAGNETIC PROPERTIES

The most contributions to the electronic and magnetic structures of $Sr_2CrWO_6$ and $Sr_2FeReO_6$ come from the super-exchange interaction (SEI) between the energetic orbitals of 3d and 5d in $Cr^{3+}$ ($3d^3$)/$Fe^{3+}$ ($3d^5$) and W ($5d^1$)/Re ($5d^2$), respectively. The spin configurations of ground states in two compounds are stabilized in $Cr^{3+}$ ($3d^3$; $t_{2g}^3\uparrow e_g^0\uparrow$; S=3/2 $\mu_B$) and $W^{5+}$ ($5d^1$; $t_{2g}^1\uparrow e_g^0\uparrow$; S=1/2 $\mu_B$); $Fe^{3+}$ ($3d^5$; $t_{2g}^3\uparrow e_g^2\uparrow$; S=5/2 $\mu_B$) and $Re^{5+}$ ($5d^2$; $t_{2g}^2\uparrow e_g^0\uparrow$; S=2/2 $\mu_B$). Thus, the ferromagnetic structures can be assigned primarily to the SEI between Cr/Fe and W/Re via intermediated O atoms in 180° long-chain paths; Cr ($3d\text{-}t_{2g}^3\uparrow e_g^0\uparrow$)–O ($2p_\pi$)–W ($5d\text{-}t_{2g}^1\downarrow$) and Fe ($3d\text{-}t_{2g}^3\uparrow e_g^2\uparrow$)–O ($2p_\pi$)–Re ($5d\text{-}t_{2g}^2\downarrow$). Where, the band filling of spin-up and spin-down sub-orbitals in $t_{2g}$ and $e_g$ govern these interactions. The calculated magnetic moments for $Sr_2CrWO_6$ are $M_{Cr}$=2.919 $\mu_B$, $M_W$=–1.044 $\mu_B$ with a total magnetic moment per unit cell of $M_{Tot.}$=1.878 $\mu_B$, in agreement with the LSDA+U value $M_{Tot.}$=2.01 $\mu_B$ [10,11] and theoretical (S=2 $\mu_B$). For $Sr_2FeReO_6$, $M_{Fe}$=4.578 $\mu_B$, $M_{Re}$=–1.344 $\mu_B$ and $M_{Tot.}$=3.184 $\mu_B$, also in agreement to the LSDA+U result, $M_{Tot.}$=3.06 $\mu_B$ [8] and theoretical (S=3 $\mu_B$). The obtained 100% SP, HM and FM features in $Sr_2CrWO_6$ and $Sr_2FeReO_6$ makes them suitable for many potential applications like spintronics, where the spin currents are utilized as well as charge currents.

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