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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 μ_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.

The double perovskite materials, here 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 appropriate semi-metallic (HM) and ferromagnetic (FM) ground states in Sr_2CrWO_6 and Sr_2FeReO_6 with magnetic total 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.

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].

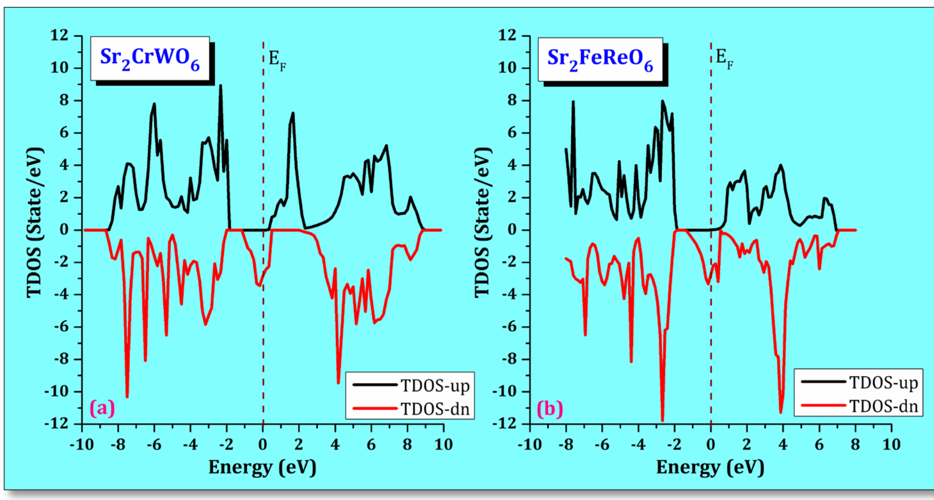

Figure 1. TDOSs for (a) Sr_2CrWO_6 and (b) Sr_2FeReO_6, (E_F=0.0 eV).

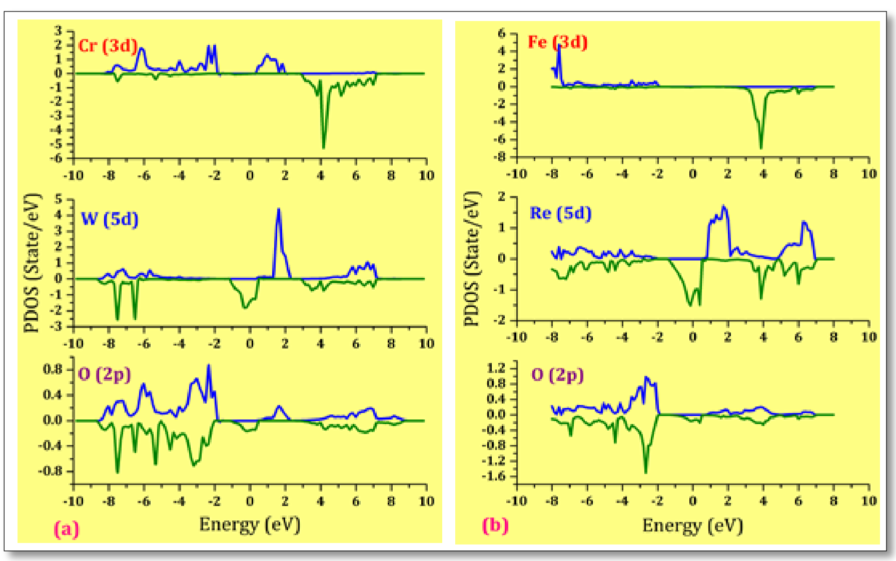

Figure 2. PDOSs for (a) Sr_2CrWO_6 and (b) Sr_2FeReO_6.

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 μ_B) and W^{5+} ($5d^1$; $t_{2g}^1{}_{\uparrow}$ $e_g^0{}_{\uparrow}$; S=1/2 μ_B); Fe^{3+} ($3d^5$; $t_{2g}^3{}_{\uparrow}e_g^2{}_{\uparrow}$; S=5/2 μ_B) and Re^{5+} ($5d^2$; $t_{2g}^2{}_{\uparrow}$ $e_g^0{}_{\uparrow}$; S=2/2 μ_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-$t_{2g}^3{}_{\uparrow}$ $e_g^0{}_{\uparrow}$)–O ($2p_\pi$)–W (5d-$t_{2g}^1{}_{\downarrow}$) and Fe (3d-$t_{2g}^3{}_{\uparrow}$ $e_g^2{}_{\uparrow}$)–O ($2p_\pi$)–Re (5d-$t_{2g}^2{}_{\downarrow}$). 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 μ_B, M_W=–1.044 μ_B with a total magnetic moment per unit cell of $M_{Tot.}$=1.878 μ_B, in agreement with the LSDA+U value $M_{Tot.}$=2.01 μ_B [10,11] and theoretical (S=2 μ_B). For Sr_2FeReO_6, M_{Fe}=4.578 μ_B, M_{Re}=–1.344 μ_B and $M_{Tot.}$=3.184 μ_B, also in agreement to the LSDA+U result, $M_{Tot.}$=3.06 μ_B [8] and theoretical (S=3 μ_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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