

Structural, electronic and magnetic properties of a symmetrical FeReO terminated (001)-oriented slab of double perovskite Sr₂FeReO₆

Yan Zhang^{a,*}, Vincent Ji^a, Ke-Wei Xu^b

^aICMMO/LEMHE, Université Paris-Sud 11, 91405 Orsay Cedex, France

^bState Key Laboratory for Mechanical Behavior of Materials, Xian Jiaotong University, Xian 710049, Shaanxi, PR China

HIGHLIGHTS

- ▶ An outwards relaxation occurs for layer 1–layer 4 with a decreasing rumpling.
- ▶ The O atom is closer to the adjacent Re atom than to the adjacent Fe atom.
- ▶ Half-metallic nature ensures Sr₂FeReO₆ slab a potential spintronic application.
- ▶ The Fe⁺³ (3d⁵) and Re⁺⁵ (5d²) ions are in antiferromagnetic coupling.

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ABSTRACT

The structural, electronic and magnetic properties of a 9-layer symmetrical FeReO terminated (001)-oriented slab of the double perovskite Sr₂FeReO₆ have been studied by using the first-principles projector augmented wave (PAW) potential within the generalized gradient approximation (GGA) taking into account the on-site Coulomb repulsive U ($U = 2.0$ eV for Fe and 1.0 eV for Re). An outwards relaxation is observed for each layer of the first four layers and the accompanying layer's rumpling decreases successively for layer 1, layer 3 and layer 5 as well as for layer 2 and layer 4. Along the Fe–O–Re–O–Fe or Re–O–Fe–O–Re chain, the oxygen atom is closer to the adjacent Re atom than to the adjacent Fe atom. The half-metallic nature with a complete (100%) spin polarization at the Fermi level ensures that the symmetrical FeReO terminated (001)-oriented slab of the double perovskite Sr₂FeReO₆ has the potential for application in spintronic devices. The Jahn–Teller structural distortions and the outward relaxations lead to the differences between p_z state and similar p_x and p_y states, between d_{xy} state and similar d_{xz} and d_{yz} states as well as between d_{z^2} and $d_{x^2-y^2}$. The connecting charge distributions along each Fe–O–Re–O–Fe or Re–O–Fe–O–Re chain show that the hybridizations between Fe 3d and 4s, O 2s and 2p, as well as Re 5d and 6s orbitals are fairly significant.

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1. Introduction

The finding of the half-metallic (HM) ferromagnetism, large tunneling magnetoresistance (TMR) and high Curie temperature (T_c) in ordered Sr₂FeMoO₆ [1] and Sr₂FeReO₆ [2] by Kobayashi et al. in 1998 and 1999 revives the extensive study of the double perovskites discovered firstly by Ward et al. early in 1961 [3,4]. The double perovskites are a broad class of compounds with the general chemical formula A₂BB'O₆ [5], where A is an alkaline-earth-metal or rare-earth-metal atom and B and B' are the transition-metal (TM) atoms. The various choices of the A atom, and especially B and B' atoms, provide a tunable B–O–B' interaction, giving rise to

a variety of electronic properties such as metal, half-metal and insulator, as well as magnetic properties such as ferromagnetism, antiferromagnetism and ferrimagnetism [6]. The presence of two TM atoms instead of one as in a simple perovskite material is expected to give rise to far more tunability and richness of properties compared to simple perovskites ABO₃ [7,8]. Most of the double perovskites have been found to take a rock-salt crystal structure with alternate perovskite units ABO₃ and AB'O₃ along three crystallographical axes. The corners of each perovskite unit are in turn occupied by the TM atoms B and B' with oxygen atoms located in between, forming alternate BO₆ and B'O₆ octahedra. The large alkaline-earth-metal or rare-earth-metal atom A occupies the body-centered site with a 12-fold oxygen coordination in each unit.

Besides Sr₂FeMoO₆ [1,5,9–24], the second most studied member of the bulk double perovskite compounds is Sr₂FeReO₆ [2,15,17,18,20,25–31] due to its large TMR effect with a fairly high

* Corresponding author. Tel.: +33 762581599.

E-mail address: yan.zhang@u-psud.fr (Y. Zhang).

ferromagnetic transition temperature of about 400 K as well as highly spin-polarized transport properties at the Fermi level [2], making it a potential candidate for industrial applications in magnetoelectronic [32] and spintronics [33] devices at room temperature. However, these devices are usually constructed by two ferromagnetic slabs (e.g. double perovskites $\text{Sr}_2\text{FeMoO}_6$ and $\text{Sr}_2\text{FeReO}_6$) sandwiching a thin nonmagnetic metal (e.g. copper in a spin valve device) or a very thin insulating layer (e.g. aluminum oxide in a magnetic tunnel junction device) [33]. One of the two magnetic layers is pinned by using an antiferromagnetic layer, i.e., the magnetization in that layer is relatively insensitive to the magnetic fields. The other magnetic layer is called the “free” layer, and its magnetization can be changed by application of a relatively low magnetic field. The resistance of these devices is lowest when the magnetic moments in the two ferromagnetic layers are aligned and highest when they are antialigned. In our previous paper [31], the detailed orbital-decomposed electronic structures and magnetic properties of the bulk $\text{Sr}_2\text{FeReO}_6$ were studied by first-principles calculations using the projector augmented wave (PAW) potentials within the generalized gradient approximation (GGA). A half-metallic ferromagnetic nature was found in the bulk $\text{Sr}_2\text{FeReO}_6$, for which the octahedral crystal-field formed by the oxygen atoms around transition-metal (TM) sites splits the five-fold degenerate d states of a free TM atom into triply degenerate t_{2g} states (at lower energy) and doubly degenerate e_g states (at higher energy). The former has a smaller and the latter a larger bonding–antibonding-splitting causing the half-metallic nature that is maintained in the $\text{Sr}_2\text{FeReO}_6$ slab, a property that is essential for the industrial applications in magnetoresistive and spintronic devices. The aim of the present work is to check the electronic and magnetic properties of a $\text{Sr}_2\text{FeReO}_6$ slab.

2. Calculation method and model

The first-principles calculations are performed in a plane-wave basis set using the Vienna *ab-initio* simulation package (VASP) based on the density function theory (DFT) [34–37]. The electronic core interaction is represented by the projector augmented wave (PAW) potentials [38] which are more accurate than the ultra-soft pseudopotentials. To treat electron exchange and correlation, we chose the Perdew–Burke–Ernzerhof (PBE) [39] formulation of the generalized gradient approximation (GGA), which yields the correct ground state of the compounds. A conjugate-gradient algorithm is used to relax the atoms into their ground states, and the energies and the forces on each atom are converged within 1.0×10^{-4} eV atom $^{-1}$ and 0.02 eV Å $^{-1}$, respectively. The number of the plane waves is controlled by the cutoff energy, which in all our calculations is chosen to be 450 eV. The Sr $4s^2 4p^6 5s^2$, Fe $3d^6 4s^2$, Re $5d^5 6s^2$ and O $2s^2 2p^4$ electrons are treated as valence electrons. The Brillouin zone (B.Z) is sampled according to the Monkhorst–Pack automatic generation scheme with special k points of an $11 \times 11 \times 1$ grid, together with a Gaussian smearing broadening of 0.1 eV.

The crystal structure of the bulk double perovskite $\text{Sr}_2\text{FeReO}_6$ is a body-centered tetragonal (BCT) structure with space group $I4/mmm$, lattice constants of $a = b = 5.579$ Å and $c = 7.890$ Å [2,15,20], and the position of the bridging oxygen atom at the center between the Fe and Re atoms. The six oxygen atoms surrounding the Fe and Re sites provide the octahedral environment and the FeO_6 and ReO_6 octahedra that alternate along the [001] and [110] directions, while Sr atoms occupy the hollow space formed by the corners of FeO_6 and ReO_6 octahedra. In our previous paper [31], we optimized the structure of the bulk $\text{Sr}_2\text{FeReO}_6$. The optimized lengths of the six Fe–O bonds and the six Re–O bonds were changed to 2.008 Å and 1.937 Å, respectively, i.e. the FeO_6 octahedron is slightly larger than

the ReO_6 octahedron without obvious Jahn–Teller structural distortions for each octahedron.

The interlayer spacing of $c/4 = 7.890/4 = 1.9725$ Å is larger than that in plane of $a/4 = b/4 = 5.579/4 = 1.3948$ Å and the magnetic moments mainly come from the Fe and Re atoms of the FeReO layers, as is shown in Fig. 1, a 9-layer symmetrical FeReO terminated slab with a $2c = 15.78$ Å thickness separated by a 10 Å vacuum region in the [001] direction is used here as a supercell with basis vectors of $a_0 \times b_0 \times c_0 = 5.579 \times 5.579 \times 25.78$ Å containing 46 atoms (Sr: 8, Fe: 5, Re: 5 and O: 28). During the structure optimization, the internal coordinates of the atoms and the cell parameters are fully relaxed by using a conjugate-gradient algorithm.

3. Results and discussions

3.1. Relaxed structures

The relaxed structure of the 9-layer symmetrical FeReO terminated slab along the [001] direction of a double perovskite $\text{Sr}_2\text{FeReO}_6$ is shown in the left panel of Fig. 2. The corresponding bond lengths of the Fe–O and Re–O bonds are shown in the right panel of Fig. 2 within the (110) plane. The fractional coordinates x , y and z along the a , b and c axes, respectively, are summarized in Table 1 for all inequivalent O, Fe, Re and Sr atoms of the first five layers.

We can see that, on layer 1, the x and y fractional coordinates of the representative O atom are larger than the initial $x_0 = y_0 = 0.25$ therefore the four O atoms are closer to the central Re atom, resulting in a Re–O bond length of 1.9185 Å that is shorter than the

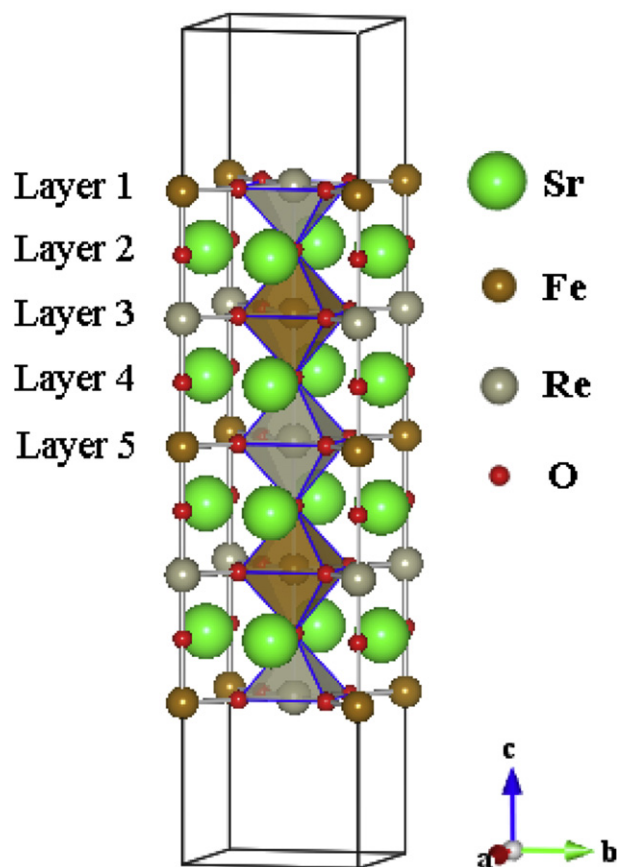


Fig. 1. The initial structure of a 9-layer symmetrical FeReO terminated (001)-oriented slab of double perovskite $\text{Sr}_2\text{FeReO}_6$.

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