

## High Spin Polarization of Charge Carriers in Half-metallic-ferrimagnetic Double Perovskites $\text{Sr}_2\text{CoPtO}_6$ and $\text{Sr}_2\text{NiPtO}_6$ at Room Temperature

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**Abstract.** In the search for new half-metallic spintronics materials, with high spin polarization at room temperature, we have studied novel platinum double perovskite oxides  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$ . The structural, electronic, magnetic properties have been studied by using the self-consistent full-potential linear muffin-tin orbital (FP-LMTO) ab-initio method. Calculations are performed by mean of the local-spin-density approximation plus Hubbard parameter (LSDA+ $U$ ) method. Our results of density of states predict a half-metallic ferrimagnetic (HM-FiM) character with total spin magnetic moments of  $3.5 \mu_B$  and  $3.0 \mu_B$  per unit cell for  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$ , respectively. It is established that the FiM character is attributed to both the superexchange (SE) mechanism and localized double exchange (DE) mechanism via the  $pdd-\pi$  Co/Ni ( $e_g$ ) – O – ( $2p_z$ ) – Pt ( $e_g$ ) coupling and the latter is also believed to be the origin of the high spin polarization of  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$ .

**Keywords:** *Double perovskite oxides; Half-metallic; FP-LMTO method; LSDA+ $U$ .*

## 1. Introduction

Materials with high spin polarization of the conducting charge carriers are of great interest for spintronics [1, 2], solid-state fuel cells (SOFC), ceramic fuel cells (CFC) applications [3], and semiconductor technology [4]. In particular, the ideal materials with 100% spin polarization at room temperature describe as half-metals [5]. Such materials can be found in several materials classes; in classic mineral oxides such as  $\text{CrO}_2$  [6] or  $\text{Fe}_3\text{O}_4$  [7], in manganites such as  $\text{La}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$  and  $\text{LaSr}_2\text{Mn}_2\text{O}_7$  [8], and intermetallic Heusler alloys such as  $\text{Co}_2\text{MnGe}$  and  $\text{Co}_2\text{MnSi}$  [9], as well in the group of double perovskite oxides such as in  $\text{Sr}_2\text{CrWO}_6$  [10],  $\text{Sr}_2\text{FeMO}_6$  ( $M = \text{Mo}, \text{Re}, \text{W}$ ) [11]. Since then, special interest has been paid to double perovskite oxides that exhibit high spin-polarization and half-metallic (HM) ground state. [12,13]. HM double perovskites, which are metallic for one spin orientation while insulator for the other spin [14,15,16]. In fact, the HM property is considered to be closely related to the colossal magnetoresistance (CMR) phenomena observed in various double perovskite oxides, such as in  $\text{A}_2\text{FeMoO}_6$  ( $A = \text{Ca}, \text{Sr}, \text{and Ba}$ ) [14] and  $\text{Sr}_2\text{CrMoO}_6$  [5]. HM materials are characterized by the coexistence of metallic behavior for one electron spin and insulating behavior for the other. Their electronic density of states completely polarized at the Fermi level and the conductivity is dominated by the metallic single-spin (spin-up or spin-down) of charge carriers. Therefore, HM materials offer potential technological applications such as single-spin electron source and high-efficiency magnetic sensors.

With the objective of theoretically determining the physical effects on the chemical composition of the material due to the inclusion of magnetic elements, in this work, novel platinum based double perovskite oxides  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  have been studied. Pt is certainly an odd 5d transition metal with difficult metallurgy; however, one may remember that the platinum-cobalt alloy uses to produce strong permanent magnets. On the other hand, the role of Pt, in  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$ , is to supply spin-polarized charge carriers. Since the Pt ion is in the (4+)-valence state it supplies spin-polarized electrons per unit cell. In addition to, the Pt  $5d^6$  spin-polarized electrons are the bond (glue) and origin of the ferrimagnetism (FiM) of  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$ . Consequently, the present study supports the double exchange (DE) mechanism for the HM-FiM in  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$ . According to Hund's rules, the ionic spins configurations of the valence electrons in  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  are  $\text{Co}^{4+}$  ( $3d^5; t_{2g}^3\uparrow e_g^2\uparrow; S = 5/2$ ),  $\text{Ni}^{4+}$  ( $3d^6; t_{2g}^3\uparrow t_{2g}^1\downarrow e_g^2\uparrow; S = 2$ ) in the high spin states and  $\text{Pt}^{4+}$  ( $4d^6; t_{2g}^3\uparrow t_{2g}^2\downarrow e_g^1\uparrow; S = 1$ ) with low spin. Which are polarized antiferromagnetically with total magnetic moments of  $3.5 \mu_B$  and  $3.0 \mu_B$ , respectively. Essentially, the Pauli Exclusion Principle dictates that between two magnetic ions with half-occupied orbitals, which couple through an intermediary non-magnetic ion  $\text{O}^{2-}$ , the superexchanges ( $3d^5 - \text{O}^{2-}p - 5d^6$  and  $3d^6 - \text{O}^{2-}p - 5d^6$ ) will be strongly antiferromagnetic. However, in the Kramers-Anderson superexchange (SE) interactions, a ferromagnetic or antiferromagnetic alignment occurs between two ions with the same valence, the number of electrons [11]; while in double-exchange (DE), the interaction occurs only when one ion has an extra electron compared to the other

[12,13]. Resultantly, the FiM nature is attributed to both, the SE and the localized DE mechanisms, via the Co/Ni ( $e_g$ ) – O ( $2p$ ) – Pt ( $e_g$ ) coupling and DE is also believed to be the origin of the HM nature of  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$ .

## 2. Theory and computational details

The calculations of structural, electronic and magnetic properties for  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  were performed by using all electrons self-consistent full potential linear muffin-tin orbital (FP-LMTO) method [5,6,15] working within atomic plane wave (PLW) representation, as implemented in the LMTART code [17]. In this method, there is no shape approximation to the crystal potential. The crystal is divided into two regions; inside muffin-tin spheres, where Schrödinger's equation is solved numerically, and an interstitial region, where the wave functions are Hankel functions [17]. The local spin density approximation (LSDA) in the framework of density functional theory (DFT) is employed. For the correct description of the wave functions in the interstitial region, the spherical harmonics have been expanded to ( $L_{\text{max}} = 6$ ) for Sr, Co/Ni, Pt and O MTSs. The Brillouin zone (BZ) integration in the course of the self-consistency iterations is performed over a  $k$ -point mesh of ( $6 \times 6 \times 6$ ) with 120  $k$ -points in the irreducible part of the BZ. Double  $\kappa$  for spd LMTO basis is used, each radial function inside the spheres is matched to a Hankel function in the interstitial region, for describing the valence bands. Since the electronic configuration of elements in  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  are Sr: [Kr]  $5s^2$ , Co: [Ar]  $3d^7 4s^2$ , Ni: [Ar]  $3d^8 4s^2$ , Pt: [Xe]  $4f^{14} 5d^9 6s^1$  and O: [He]  $2s^2 2p^4$ . Therefore, the basis set consisted of the Sr (5s 4d 4p), Co/Ni (4s 3d 4p), Pt (6s 5d 6p) and O (2s 2p) LMTOs were taken as valence states and Sr (4s), Co/Ni (3p), Pt (5p 4f) as semicore states. The input of the radii (in a.u. units) of muffin-tin spheres (MTSs) for the atoms in  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  are 3.480, 1.953, 2.045 and 1.573 for Sr, Co/Ni, Pt and O, respectively.

The exchange-correlation potential used was the Barth-Hedin version of the local density approximation (LDA) [16]. Also, to treat the strong electron interaction effect in Co/Ni (3d) and Pt (5d), the LSDA+ $U$  calculations have been carried out in the Hubbard model framework [11,13,16]. By means of the option of Coulomb repulsion ( $U = 6.0$  eV) for Co/Ni (3d) and ( $U = 1.0$  eV) for Pt (5d) orbitals [6, 18]. In addition to, the value of exchange parameter ( $J = 0.89$  eV) is used for all transition metals [6,18].

## 3. Results and discussion

### 3.1 Crystal structures

The crystal structure of the double perovskite oxide with the formula  $A_2BB'O_6$  is known to be very flexible and the A, B and B' ions can be varied leading to the large number of known compounds with double perovskite oxide or related structures. Double perovskite oxides  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  crystalline at room temperature

in ordered cubic structure with space group of Fm-3m (No. 225). The lattice parameters  $a$ , oxygen positions  $u$ , unit cell volumes ( $V$ ) and bond distances are calculated theoretically and estimated from Refs. [12] and [13], see Table 1. In the unit cells of  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$ , one formula ( $Z = 1$ ), five sorts of atoms are used, and the atomic positions in fcc (Fm-3m) crystallographic are sited as Sr (8c) at  $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ , Co/Ni (4a) at  $(0,0,0)$ , Pt (4b) at  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ , O (24e) at  $(u,0,0)$ . The crystal structures are closed enough, there are no empty spheres need to introduce in the unit cells [1,3,16].

From Table 1, it is found that  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  crystallize in a cubic structure with space group of Fm-3m having an ideal lattice parameter ( $a \approx 8.0 \text{ \AA}$ ). Moreover, the crystal structures of  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  did not deviated from the ideal cubic DP. That for four reasons; (i) no displacement of the Co/Ni and Pt cations from the center of the  $\text{MO}_6$  ( $M = \text{Co}$  or  $\text{Ni}$ ) and  $\text{PtO}_6$  octahedra, their bond lengths  $M - \text{O}$  and  $\text{Pt} - \text{O}$  are approximately equal to  $2.0 \text{ \AA}$ . (ii) no displacement of the Sr cations from the cavity centers. In addition, (iii) as seen in Fig. 1, there is no distortion of the  $\text{MO}_6$  and  $\text{PtO}_6$  octahedral cages, their alternating corner bond-angles  $\text{O} - M - \text{O}$  and  $\text{O} - \text{Pt} - \text{O}$  are in the ideal value  $90^\circ$ , and (iv) no tilting of the  $\text{MO}_6$  and  $\text{PtO}_6$  octahedra in the crystals, their bond angles  $M - \text{O} - \text{Pt}$  are in the ideal value  $180^\circ$ .

**Table 1. The optimized crystal structure data of  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$ ,  $M = \text{Co}, \text{Ni}$**

Compound	$\text{Sr}_2\text{CoPtO}_6$	$\text{Sr}_2\text{NiPtO}_6$
Crystal symmetry	Cubic (Fm-3m)	Cubic (Fm-3m)
Lattice parameters; $a$ ( $\text{\AA}$ )	7.562	7.680
Oxygen position O ( $u$ )	0.247	0.250
Unit cell volume $V$ ( $\text{\AA}^3$ )	435	453
Tolerance factor $t$	1.038	1.024
$d_{(\text{Sr}-\text{O})}$	2.679	2.715
$d_{(M-\text{O})}$	1.870	1.922
$d_{(\text{Pt}-\text{O})}$	1.918	1.866

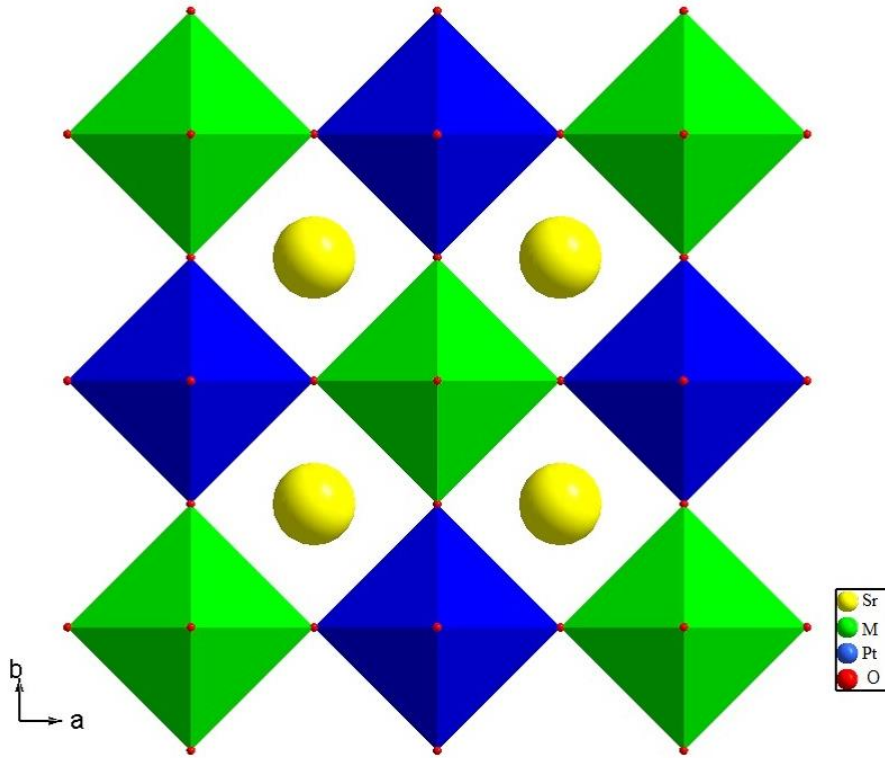


Fig. 1. 2D ( $ab$  plane) crystal structure of double perovskite oxides  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  in ( $Fm\text{-}3m$ ) space group, M refers to Co (3d) and Ni (3d) atoms. The bond angle of  $\text{MO}_6$  (green) and  $\text{PtO}_6$  (blue) octahedra is in the ideal value ( $M - O - Pt = 180^\circ$ ). Sr atoms site in the caves between the  $\text{MO}_6 - \text{PtO}_6$  octahedra.

### 3.2 Electronic and magnetic properties

The calculated densities of states (DOSs) for  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  have been performed using the LSDA+ $U$  calculation method, at room temperature, and the results of DOSs are given in Figs. 2, 3, 4, and 5. In all figures, the upper and lower curves represent the spin-up and spin-down densities of states per unit cell, respectively. Horizontal axis stands for the energy relative to the Fermi energy ( $E - E_F$  (eV)), so the Fermi level is situated at ( $E_F = 0.0$  eV). Figs. 2 and 3 illustrate the separated total densities of states (TDOSs), while the accumulated of TDOSs and Co/Ni (3d), Pt (5d), and O (2p) partial densities of states (PDOSs) of  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  are shown in Figs. 4 and 5, respectively.

From the TDOS in Figs. 2 and 3, one can clearly see that the  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  are half-metallic. Since an energy gap of about  $E_g = 2.0$  eV

(from -1.75 eV to 0.25 eV) between the occupied bands is observed in spin-up of TDOS, while a finite band in spin-down of TDOS is expanded from -1.0 eV to 0.50 eV through the  $E_F$ , resulting as HM nature in  $Sr_2CoPtO_6$  material. Similarly, in  $Sr_2NiPtO_6$ , the energy gap of about  $E_g = 1.20$  eV (from -0.12 eV to 1.08 eV) between the occupied bands is observed in spin-up of TDOS, while a finite band in spin-down of TDOS is expanded from -2.92 eV to 0.68 eV through the  $E_F$ . Thus, our results of the TDOSs predict HM character for two double perovskite oxides. It is observed that the conduction-band, in spin-down of TDOSs, in  $Sr_2NiPtO_6$  ( $\Delta W = 3.60$  eV) is broader than in  $Sr_2CoPtO_6$  ( $\Delta W = 1.50$  eV). This may be attributed to the additional electron in Ni (3d) double perovskite;  $Ni^{4+}$  ion has six electrons in 3d orbit ( $3d^6$ ) while  $Co^{4+}$  one has less electron in 3d orbit ( $3d^5$ ).

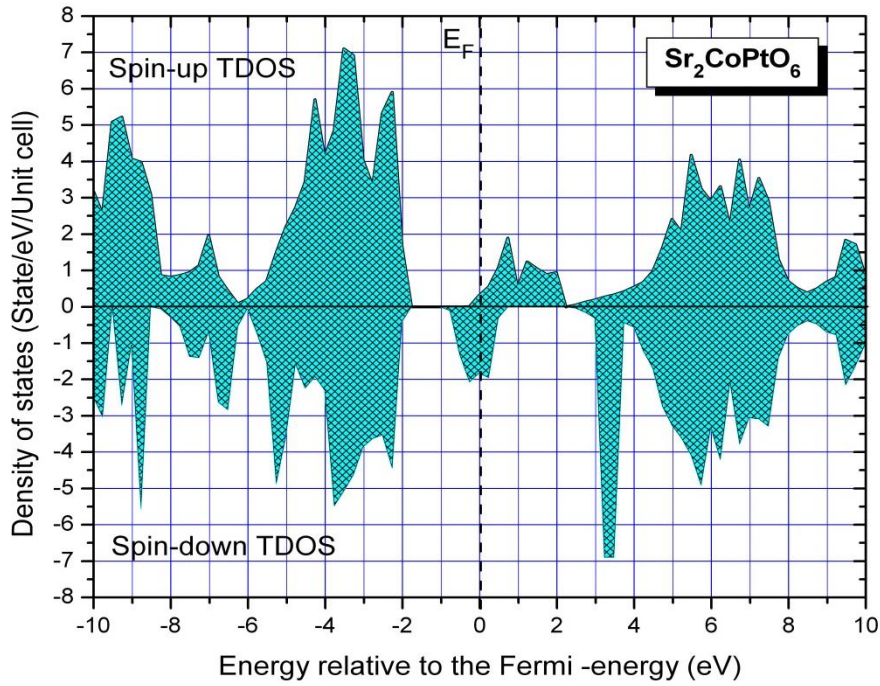


Fig. 2. Total density of states of  $Sr_2CoPtO_6$  from LSDA+ $U$  calculations

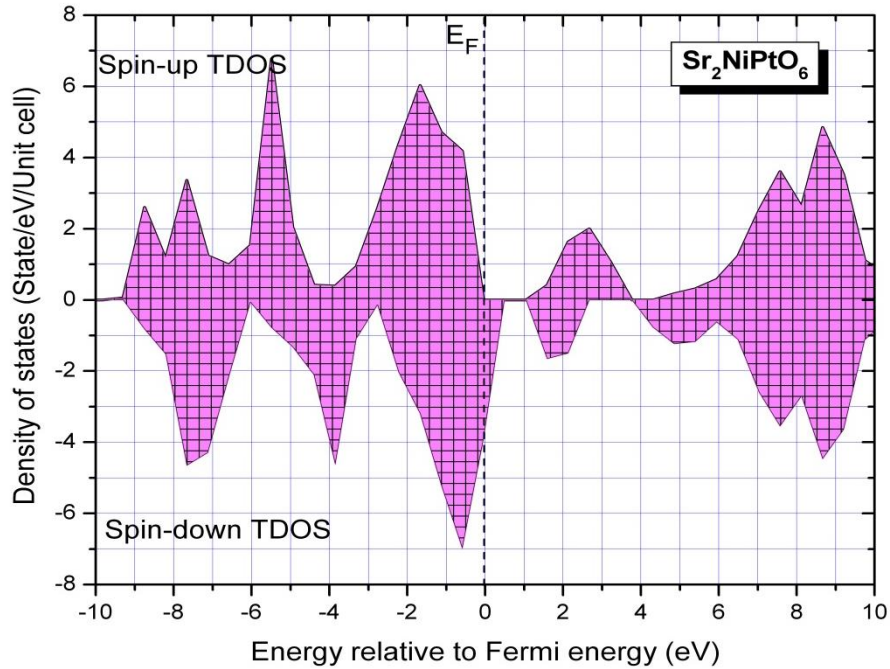


Fig. 3. Total density of states of  $\text{Sr}_2\text{NiPtO}_6$  from LSDA+ $U$  calculations

Moreover, to discuss the role of Co/Ni (3d) and Pt (5d) ionic bands in the properties of  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$ . Since the energy gap in the spin-up results from the antiferromagnetic coupling between Co (3d) and Pt (5d), as seen in Figs. 4 and 5, it may be called an antiferromagnetic coupling gap which in consistency with SE mechanism proposed by D.D. Sarma for double perovskite oxide  $\text{Sr}_2\text{FeMoO}_6$  [14]. In contrast, as shown in Figs. 4 and 5, the  $E_F$  lies in the partially filled spin-down bands of Co (3d)/Ni (3d), Pt (5d), and O (2p) hybridization states. The low spin of Pt ( $5d^6 S = 1/2$ ) couples antiferromagnetically to the high spin of Co (3d) ( $S = 5/2$ ) [19] and Ni (3d), resulting HM-FiM ground state. Here, as possible explanation is a competitive between the DE (ferromagnetic) and the SE (antiferromagnetic). Therefore, the FiM coupling is attributed to the LSE Co ( $e_g$ )/Ni (3d) – O ( $2p_\pi$ ) – Pt ( $e_g$ ) hybridization, see Fig. 6, in accordance with the Goodenough-Kanamori and Kramers-Anderson superexchange interactions [7, 20]. Since the Co/Ni (3d) spin-up bands are filled and the Co/Ni (3d) spin-down bands are unfilled, only the Pt (5d) spin-down orbitals would hybridize with the open Co/Ni (3d) spin-down orbital for lowering the kinetic energy.

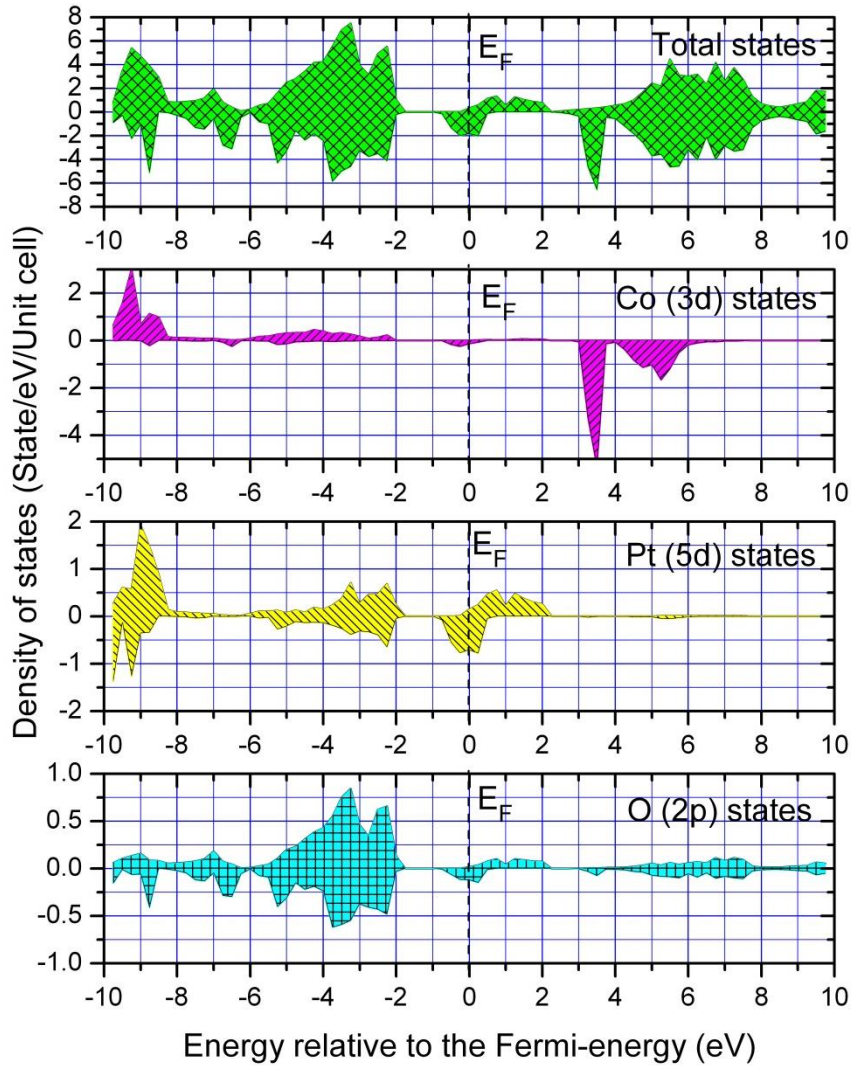


Fig. 4. Total and partial densities of states, Co (3d), Pt (5d) and O (2p), in Sr<sub>2</sub>CoPtO<sub>6</sub>



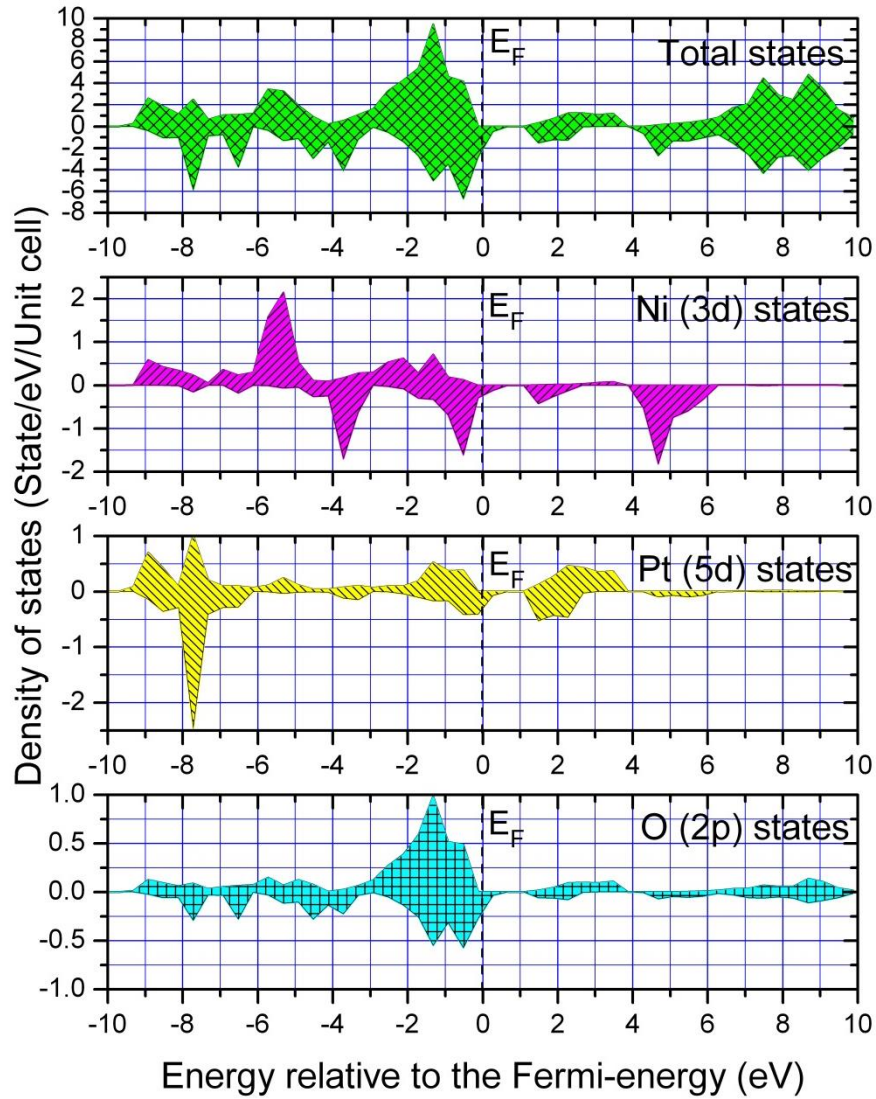


Fig. 5. Total and partial densities of states, Ni (3d), Pt (5d) and O (2p), in  $\text{Sr}_2\text{NiPtO}_6$

The itinerancy and FiM, Fig. 6, arise from a spin polarized conduction mechanism in which ordering and electronic configuration of the transition metal

cations play a critical role. Structurally, the Co/Ni (3d) and Pt (5d) transition metal cations are ordered in an alternating rock-salt manner within a double perovskite lattice. Electronically, the Co/Ni (3d) cations have large spin magnetic moments  $S = 5/2$  and  $S = 2$  for  $\text{Co}^{4+}$  and  $\text{Ni}^{4+}$ , respectively, whereas the Pt (5d) cation usually has  $S = 1$ . Equal spin magnetic moments of the 3d and 5d cations could result in a so-called half-metallic antiferromagnetic (HM-AFM), where completely spin-polarized conduction occurs in a zero ( $S = 0$ ) magnetization materials. Candidate HM-AFM double perovskite materials, for example  $\text{SrLaCoRuO}_6$  where both high-spin  $\text{Co}^{2+}$  and  $\text{Ru}^{5+}$  cations have ( $S = 3/2$ ) [21]. However, previous studies showed that these materials order antiferromagnetically with two opposed  $\text{Co}^{2+}$  [ $\text{Co}^{2+}\uparrow(3d) - \text{O}^{2-}(2p) - \text{Co}^{2+}\downarrow(3d)$ ] and two  $\text{Ru}^{5+}$  [ $\text{Ru}^{5+}\uparrow(4d) - \text{O}^{2-}(2p) - \text{Ru}^{5+}\downarrow(4d)$ ] spin sublattices. On the other hand, HM-AFM nature have been observed in double perovskite  $\text{Sr}_2\text{OsMoO}_6$  [22]. This material showed 100% spin-polarization of conduction electrons crossing the Fermi level without showing a net magnetization ( $M = 0$ ). The origin of HM-AFM in  $\text{Sr}_2\text{OsMoO}_6$  attributes to both superexchange and localized double exchange mechanisms via the [ $\text{Os}^{2+}\uparrow(5d) - \text{O}^{2-}(2p) - \text{Mo}^{2+}\downarrow(4d)$ ] coupling.

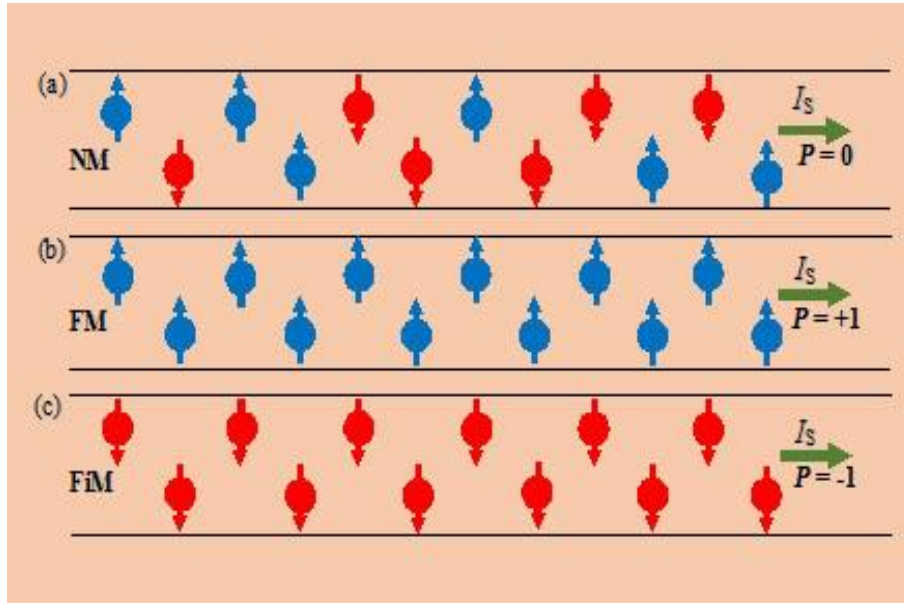


Fig. 6. Schematic diagram for the spin current ( $I_s$ ) in double perovskite oxide materials, along the x-axis. (a) Random oriented spins of conduction electrons in nonmagnetic (NM) materials with non-spin-polarization ( $P = 0$ ), (b) high spin-polarized current with only spin-up in ferromagnetic (FM) materials with ( $P = +1$ ) and (c) high spin-polarized current with only spin-down in ferrimagnetic (FiM) materials with ( $P = -1$ ). The spin orientations of conduction electrons are conserved only in the  $\pm z$ -direction.

The partial spin magnetic moments of double perovskite oxides  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  are calculated at room temperature and found to be  $3.80 \mu_B$  for Co (3d) and  $-0.30 \mu_B$  for Pt (5d) ions; Co and Pt are polarized antiferromagnetically. Therefore, a total spin magnetic moment of  $3.50 \mu_B$  per unit cell is obtained, which is consistent with the HM character of  $\text{Sr}_2\text{CoPtO}_6$ . While for  $\text{Sr}_2\text{NiPtO}_6$ , the partial spin magnetic moments are found to be  $3.91 \mu_B$  for Ni (3d) and  $-0.82 \mu_B$  for Pt (5d) ions with total spin magnetic moment of  $3.0 \mu_B$  per unit cell.

**Table 2. Partial and total spin magnetic moments for double perovskite oxides  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$ , calculated by LSDA+ $U$  method.**

Ion	$\text{Sr}_2\text{CoPtO}_6$	$\text{Sr}_2\text{NiPtO}_6$
Sr	0.02	0.01
Co/Ni	3.80	3.91
Pt	-0.30	-0.82
O	-0.02	0.02
Total	3.50	3.00

According to Hund's rules, the ionic spins configurations of the valence electrons in  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  are:  $\text{Co}^{4+}$  ( $3d^5$ ;  $t_{2g}^3\uparrow e_g^2\uparrow$ ;  $S = 5/2$ ),  $\text{Ni}^{4+}$  ( $3d^6$ ;  $t_{2g}^3\uparrow t_{2g}^1\downarrow e_g^2\uparrow$ ;  $S = 2$ ), in high spin states, and  $\text{Pt}^{4+}$  ( $4d^6$ ;  $t_{2g}^3\uparrow t_{2g}^2\downarrow e_g^1\uparrow$ ;  $S = 1$ ) with low spin, polarized antiferromagnetically with theoretical total magnetic moments of  $3.5 \mu_B$  and  $3.0 \mu_B$ , respectively. Furthermore, from Fig. 4, the Co (3d) states show a large exchange splitting of about 3.9 eV, while the Pt (5d) states show a small exchange splitting of about 1.2 eV. Most of the O (2p) PDOS is located between  $-9.7$  eV and  $-1.7$  eV and between  $-0.8$  eV and  $+2.1$  eV crossing  $E_F$ . Whereas, for  $\text{Sr}_2\text{NiPtO}_6$ , Fig. 5, the exchange splitting of Ni (3d) states is about 4.2 eV and of Pt (5d) states is very small, about 1.1 eV. Here, the contributions of O (2p) states are located between  $-9.0$  eV and  $+0.3$ , and between  $+1.2$  eV and  $4.3$  eV in conduction band.

#### 4. Conclusions

In summary, we have performed LSDA+ $U$  calculations for the novel platinum double perovskite oxides  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  by using the self-consistent full-potential linear muffin-tin orbital (FP-LMTO) method. The DOS-results predict a half-metallic ferrimagnetic character with high spin polarization at room temperature. The total spin magnetic moment of for  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  are  $3.5 \mu_B$  and  $3.0 \mu_B$  per unit cell, respectively. The fully spin polarized conducting property of double perovskite oxides  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  is associated with intensive peaks in the TDOSs and PDOSs of Co (3d- $e_g$ )/ Ni (3d- $e_g$ ) and Pt (5d-  $e_g$ )

spin-down states (HM) closed to the Fermi level. It obtained that the electronic configurations of Co/Ni and Pt ions interchange between two oxidation states with stable electronic configurations  $\text{Co}^{2+} - \text{Pt}^{6+}$  to  $\text{Co}^{3+} - \text{Pt}^{5+}$  and similarly for  $\text{Ni}^{2+} - \text{Pt}^{6+}$  to  $\text{Ni}^{3+} - \text{Pt}^{5+}$ . The present study suggests that a kinetic energy of double exchange interaction, through the  $pdd-\pi$  Co ( $e_g$ )/ Ni ( $3d-e_g$ ) - O ( $2p\pi$ ) - Pt ( $e_g$ ) coupling, is operative to produce a high spin polarization with HM-FiM character in  $\text{Sr}_2\text{CoPtO}_6$  and  $\text{Sr}_2\text{NiPtO}_6$  double perovskite oxide materials.

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**الاستقطاب المغزلي العالي لحاملات الشحنة في البيروفسكيتات المزدوجة  $Sr_2CoPtO_6$  و  $Sr_2NiPtO_6$  التي تتصف بخاصية نصف معدنية-فيريمغناطيسية عند درجة حرارة الغرفة**

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**ملخص البحث.** في البحث عن مواد جديدة ذات إلكترونات مغزليه نصف المعدنية، مع الاستقطاب المغزلي العالي لإلكترونات التوصيل عند درجة حرارة الغرفة، درسنا أكاسيد البيروفسكيت المزدوج التي تحتوي بصورة أساسية على عنصر البلاتين،  $Sr_2CoPtO_6$  و  $Sr_2NiPtO_6$ . وقد درست الخصائص التركيبية، الإلكترونية والمغناطيسية باستخدام المبادئ الأولية لطريقة الجهد الكلي الخطي الكعك المداري (FP-LMTO) المتسقة ذاتياً. يتم تنفيذ العمليات الحسابية باستخدام تقريب الكثافة المحلية المغزليه بالإضافة إلى بارامتر طاقة فيرمي (LSDA+U). النتائج التي تحصلنا عليها لكثافة الحالات تتنبأ بطابع نصف معدني فيرميمغناطيسي (HM-FIM) بمجموع عزم مغزلي مغناطيسي  $3.5 \mu_B$  و  $3.0 \mu_B$  لكل وحدة خلية من مركبات  $Sr_2CoPtO_6$  و  $Sr_2NiPtO_6$ ، على التوالي. ثبت أن خاصية FIM تعزى إلى كل من آلية التأثير المتبادل الفائق (SE) والتبادل المحلي المزدوج (DE) عن طريق اقتران إلكترونات المدارات المحلية للعناصر الانتقالية مع بعضها البعض خلال إلكترونات أيونات الأكسجين  $O(2p_p) - Co/Ni(e_g)$ . وهذا الأخير يعتقد أيضاً أنه أصل الاستقطاب المغزلي العالي لإلكترونات التوصيل في  $Sr_2CoPtO_6$  و  $Sr_2NiPtO_6$ .

**كلمات المفتاحية:** أكسيد البيروفسكيت المزدوج، نصف معدني، طريقة (FP-LMTO)، حسابات (LSDA+U)