

## Study of Novel Double Perovskites $\text{La}_2\text{BB}'\text{O}_6$ ( $\text{B} = \text{V}, \text{Cr} \ \& \ \text{Sc}$ and $\text{B}' = \text{Sc}, \text{Co} \ \& \ \text{Ni}$ ) for Solar Cell Applications: A DFT study

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**Abstract:** Here we investigated the electronic, magnetic and optical properties of Novel Double Perovskites  $\text{La}_2\text{BB}'\text{O}_6$  ( $\text{B} = \text{V}, \text{Cr} \ \& \ \text{Sc}$  and  $\text{B}' = \text{Sc}, \text{Co} \ \& \ \text{Ni}$ ) using ab-initio density function theory (DFT) calculations. The GGA and GGA(+U) (Hybrid term) band structures for  $\text{La}_2\text{CrCoO}_6$ ,  $\text{La}_2\text{CrNiO}_6$ ,  $\text{La}_2\text{ScNiO}_6$ ,  $\text{La}_2\text{VNiO}_6$  and  $\text{La}_2\text{VScO}_6$  reveal metallic behavior in spin-up state, whereas, the minority spin channel has a band gap around the Fermi level ( $E_F$ ) recommend semiconducting behavior, confirm half metallicity. The GGA and GGA+U band gaps for  $\text{La}_2\text{CrCoO}_6$ ,  $\text{La}_2\text{CrNiO}_6$ ,  $\text{La}_2\text{ScNiO}_6$ ,  $\text{La}_2\text{VNiO}_6$  and  $\text{La}_2\text{VScO}_6$  are 0.95eV, 1.15eV, 1.63eV, 1.22eV & 3.54eV and 1.67eV, 1.22eV, 3.95eV, 2.0eV & 3.57eV respectively. The magnetic moments ( $\mu_B$ ) reveals that these materials are half-metallic ferromagnetic and transition metals Cr, V, Sc, Co and Ni contribute maximum to total spin magnetic moments ( $\mu_B$ ), whereas, La contributes minimum to ( $\mu_B$ ).  $\text{La}_2\text{CrNiO}_6$  (LCNO) has the maximum total spin magnetic moment,  $4.0\mu_B$ , while the total spin magnetic moment of  $\text{La}_2\text{ScNiO}_6$  (LSNO) is minimum,  $0.9\mu_B$ . Optical conductivity  $\delta(\omega)$ , for these NDPs materials are found in the range of 14,927 at 20.99eV to 11,205 at 21.55eV. The absorption coefficient  $n(\omega)$  calculated for  $\text{La}_2\text{CrCoO}_6$  has maximum value of 401.082 at 21.973eV. The optical reflectivity  $\mathcal{R}(\omega)$  for the material  $\text{La}_2\text{CrNiO}_6$  has the maximum value of 0.696 at 0.04eV, whereas the NDP material  $\text{La}_2\text{VScO}_6$  has the lowest value of 0.369 at 0.013eV via both schemes. Our investigations confirmed that these materials have high potential in ferromagnetic, spintronic, microelectronic and optoelectronic technologies. These materials can be used for solar cell applications.

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### 1. Introduction

There are different classes of perovskite which exhibit different properties such as half-metallic (HF), ferrimagnetic (FiM), ferromagnetic (FM), anti-ferromagnetic (AF), half-metallic ferromagnetic (HM-FM), half-metallic ferrimagnetic (HM-FiM), nonmagnetic (NM), ferroelectric (FE), and semiconductors (SC). One of the most important classes of perovskite

is **Novel Double Perovskites (NDPs)**. These NDPs represent a widely investigated and an interesting class of materials in solid state Chemistry and material science. They form the foundation of material science for the study of composition, structure and several chemical and physical properties, which have great importance in ferromagnetic, spintronic, microelectronic and optoelectronic technologies [1].

The general formula for novel double perovskites is commonly written as,  $A_2BB'O_6$ , where “A” being rare-earth or alkaline-earth elements, while **B** and **B'** are different transition-metal ions [2, 3]. The difference between the cations B and B', in size is critical for controlling the physical properties of novel double perovskites (NDPs) [4]. In half-metallic (HM) materials, there is a metallic behavior in minor spin channel and a well-defined band gap in the majority channel. Therefore, HM materials have following properties: (1). zero spin susceptibility; (2). quantization of magnetic moment; and (3). hundred percent spin polarization at the Fermi level [5, 6].

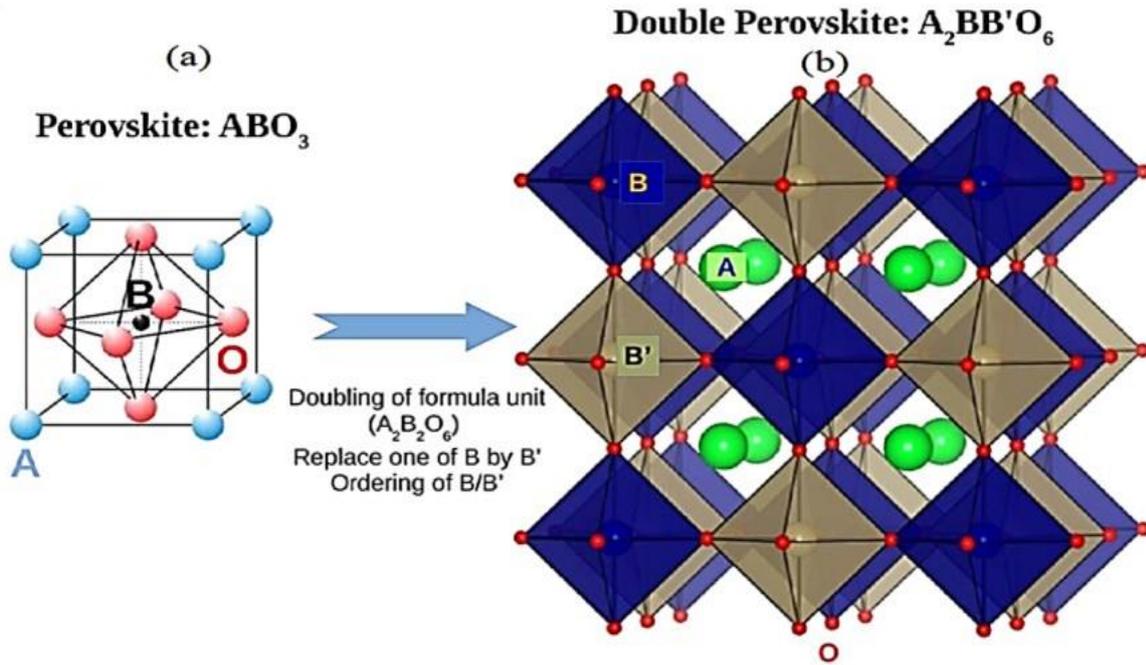
Recently, novel double perovskites (NDPs) have engrossed researchers due to their special properties in many applications. The crystal structure of novel double perovskite can be derived out of an ordinary perovskite structure  $ABO_3$  which has a wide range of properties starting from insulators to superconductors [7, 8]. The perovskite structure has a high flexibility, so almost all the elements in the periodic table can be used in the form of a perovskite crystal structure. The novel double perovskites (NDPs) compounds are composed of two simple perovskite structures (SPSs),  $ABO_3$  and  $AB'O_3$ , so the general chemical formula for novel double perovskite is  $A_2BB'O_6$ . NDPs materials are formed when the half of cations of the B site are swapped by another cation B', achieving rock salt ordering between these cations [9].

**Figure 1 (a)** shows the simple perovskite crystal structure  $ABO_3$  and **part (b)** shows the double perovskite structure composed of two SPSs,  $A_2BB'O_6$ . Generally, in the double perovskite structure  $A_2BB'O_6$ , the A site is occupied by the lanthanides (La) and the **B** and **B'** position are filled by the transition metal elements (V, Cr, Sc, Co, Ni, etc.) [10].

The transition metal ions (**TMI**s) at B and B' in the novel double perovskites (NDPs) show a wide range of magnetic and electronic properties. The transition metal ions are responsible for chemical flexibility and complex character, which associate with the coordination of TMI with oxygen [11].

## 2. Materials and Methods

In this research work, we used **Wien2k** software based on density functional theory (DFT). The structure optimization and all physical properties of the **NDPs**  $La_2BB'O_6$  were carried out using generalized gradient approximation (**GGA**) [12, 13] and **GGA+U** schemes. The **GG+U** (Hybrid term) is a famous approach to calculate electronic, magnetic and optical properties of transition metal oxides (strong metal system) [14, 15]. In our calculations, we used both **GGA** and **GGA+U** approaches. Furthermore, the calculations were carried out with the ‘Full potential linearized augmented plane wave (FP-LAPW) approach implemented in Wien2k code.



**Figure 1 (a)** Simple perovskite structure  $ABO_3$  **(b)** Novel double perovskite structure  $A_2BB'O_6$

The program package Wien2k allows performing electronic structure calculations of solids using Density Functional Theory. It is based on the full-potential Linearized augmented plane-wave (FP-LAPW) + Local Orbitals (LO) method, one among the most accurate schemes for band structure calculations [16].

Wien2k is an all-electronic solution scheme including relativistic effects and has many features. The radii of the muffin tin sphere for the NDPs  $La_2BB'O_6$  are taken as  $3.5a_0$  for La,  $2.0a_0$  for transition metals Cr, Sc, Co, Ni and  $1.5a_0$  for O. The self-consistent field cycle (SCF) calculations convergence is attained at 0.7 mRy as well as the convergence of charge 0.0001e. All novel double perovskites (NDPs) are in a cubic structure, making a super cell  $(2 \times 2 \times 1)$  structure and relaxed atomic position till force convergence becomes  $5 \times 10^{-3}$  eV/Å, and energy approaches to  $10^{-4}$  eV [17]. In our present calculations for better convergence of charge in the DMS, the wave cut-off value  $R_{mt}K_{max} = 6$  in the interstitial region, 4000 k-points and  $G_{max} = 24$  is taken.

### 3. Results and Discussions

The electronic, magnetic and optical properties of novel double perovskite (NDPs)  $La_2CrCoO_6$ ,  $La_2CrNiO_6$ ,  $La_2ScNiO_6$ ,  $La_2VNiO_6$  and  $La_2VScO_6$  were calculated in a periodic manner and the figures were generated using XMGRACE software. The path of k-points in the band structure (BS) and density of states (DOS) is taken as  $(\Gamma H N \Gamma P)$ . All the materials are semiconductors with spin-down channels and metallic for spin-up channels in both GGA and GGA+U (Hybrid term) schemes.

#### 3.1 Electronic Band Structure

The band structures (BS) consist of the valence band ( $V_b$ ) and the conduction band ( $C_b$ ) and in between the energy gap ( $E_g$ ), the  $V_b$  and  $C_b$  are both crowded and overlapping in the spin up channel, while there is a forbidden energy gap in the spin-down channel between them. All

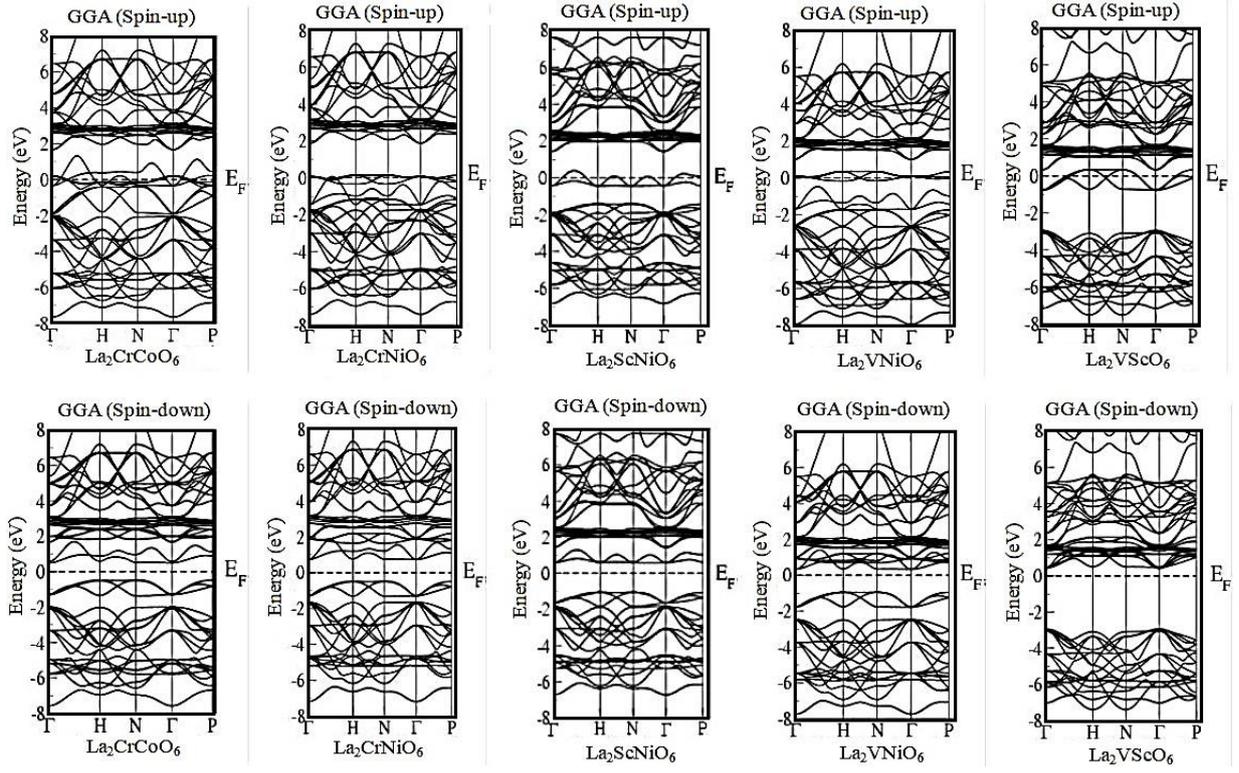
of the novel double perovskite compounds (NDPCs) of  $\text{La}_2\text{BB}'\text{O}_6$  are found to be direct band gap semiconductors because  $\text{C}_b$  minima and  $\text{V}_b$  maxima occur at the same point of symmetry in the Brillouin zone. Therefore, all NDPCs of  $\text{La}_2\text{BB}'\text{O}_6$  are metallic in the spin-up and semiconductors in the spin-down channel and are known as half-metallic novel double perovskite compounds.

The calculated band gaps in the spin-down channels using the GGA method are 0.945, 1.150, 1.632, 1.225 and 3.545eV for  $\text{La}_2\text{CrCoO}_6$ ,  $\text{La}_2\text{CrNiO}_6$ ,  $\text{La}_2\text{ScNiO}_6$ ,  $\text{La}_2\text{VNiO}_6$  and  $\text{La}_2\text{VScO}_6$ , respectively. The calculated band gaps in the spin-down channels using the GGA+U method are 1.667, 1.221, 3.950, 2.008 and 3.577eV for  $\text{La}_2\text{CrCoO}_6$ ,  $\text{La}_2\text{CrNiO}_6$ ,  $\text{La}_2\text{ScNiO}_6$ ,  $\text{La}_2\text{VNiO}_6$  and  $\text{La}_2\text{VScO}_6$ , respectively. All the calculated band gaps are in good agreement with previous theoretical results, also discussed in **Table 1** [17, 18].

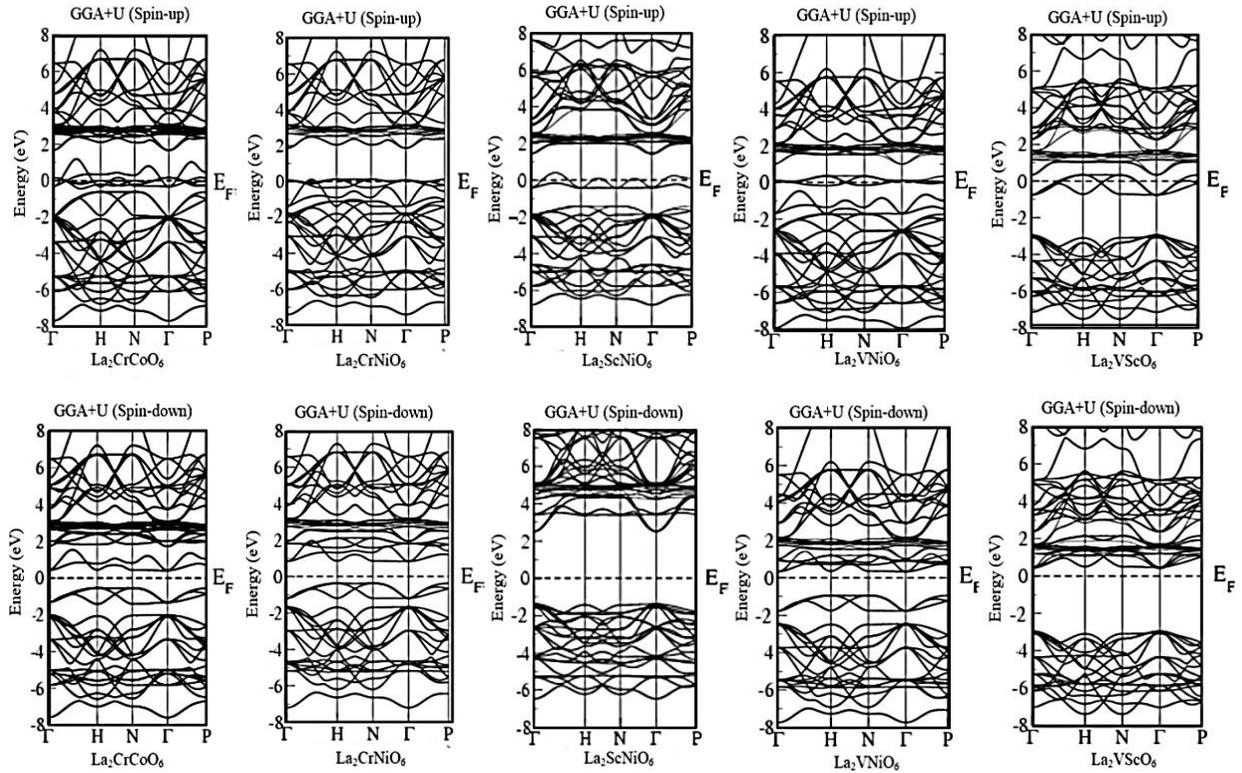
**Table 1** Comparison of calculated electronic band gaps with previous electronic structure findings.

#	NDPs	GGA (Current)		GGA (+U)Current		GGA (Other)		GGA (+U) Other	
		Spin Up	Spin dn	Spin Up	Spin dn	Spin Up	Spin dn	Spin Up	Spin dn
1.	$\text{La}_2\text{CrCoO}_6$	Metallic	<b>0.945</b>	Metallic	<b>1.667</b>	Metallic	<b>0.934</b>	Metallic	<b>0.773</b>
2.	$\text{La}_2\text{CrNiO}_6$	Metallic	<b>1.150</b>	Metallic	<b>1.221</b>	Metallic	<b>1.140</b>	Metallic	<b>1.110</b>
3.	$\text{La}_2\text{ScNiO}_6$	Metallic	<b>1.632</b>	Metallic	<b>3.950</b>	Metallic	<b>1.631</b>	Metallic	<b>1.497</b>
4.	$\text{La}_2\text{VNiO}_6$	Metallic	<b>1.225</b>	Metallic	<b>2.008</b>	Metallic	<b>1.214</b>	Metallic	<b>1.116</b>
5.	$\text{La}_2\text{VScO}_6$	Metallic	<b>3.545</b>	Metallic	<b>3.577</b>	Metallic	<b>3.555</b>	Metallic	<b>3.682</b>

Figures 2 and 3 show all NDPCs band structures using GGA and GGA (+U) (hybrid term) techniques respectively.



**Figure 2** Band structures of NDPs  $\text{La}_2\text{BB}'\text{O}_6$  using GGA in both Spin-up and Spin-down channels.



**Figure 3** Band structures of NDPs  $\text{La}_2\text{BB}'\text{O}_6$  using GGA (+U) in both Spin-up and Spin-down channels.

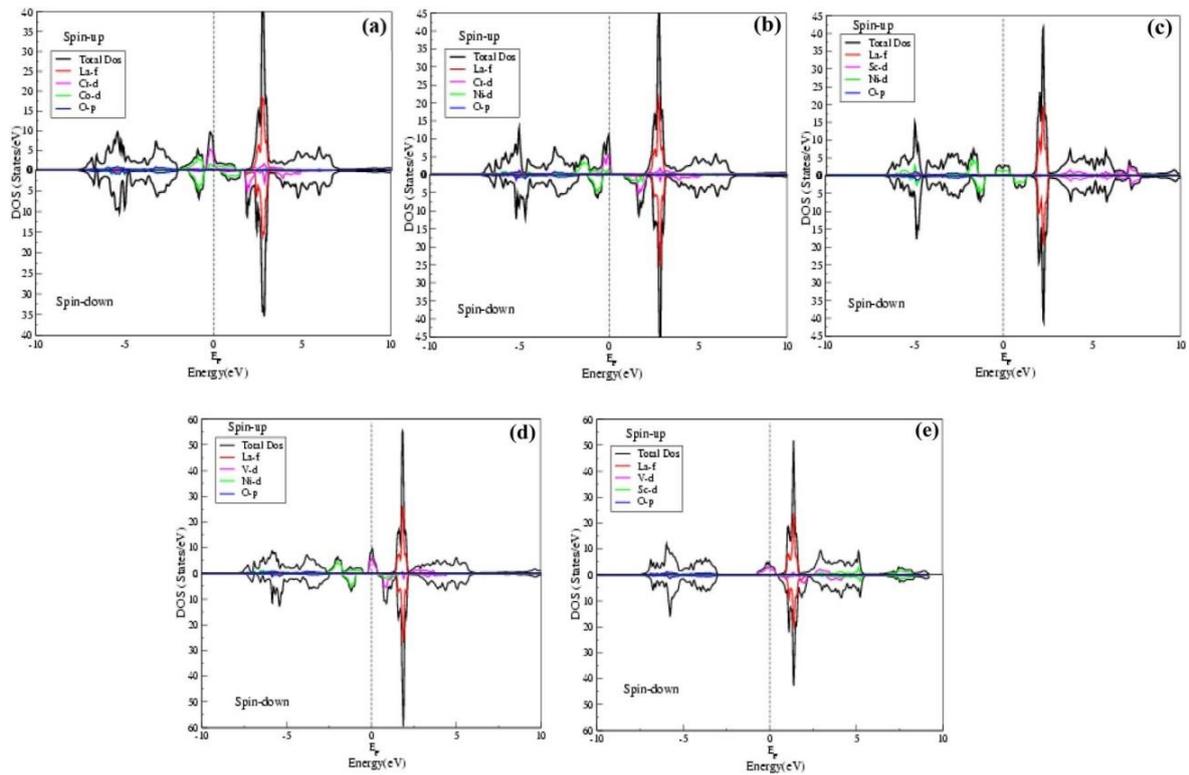
### 3.2. Density of States

The behaviors of the Band Structures (BS) and Electronic Distributions (States) of the  $\text{La}_2\text{CrCoO}_6$ ,  $\text{La}_2\text{CrNiO}_6$ ,  $\text{La}_2\text{ScNiO}_6$ ,  $\text{La}_2\text{VNiO}_6$  and  $\text{La}_2\text{VScO}_6$  materials were calculated by total density of states (TDOS) by GGA and GGA (+U) schemes as shown in Fig. 2 and 3. The total density of states (TDOS) calculations show that in all the compounds a maximum contribution above the Fermi level ( $E_F$ ), arises due to Tot-La in the spin-up as well as spin-down states. The valence and conduction bands overlapping in the spin-up channel validates the metallic behavior, whereas there is a clear gap between the valence and conduction bands for the spin-down channel displaying semiconducting behavior, hence confirming that all these compounds are half-metallic (HM). The main reasons for the half metallicity are p-d hybridization and double exchange. The stronger p-d hybridization in these compounds leads to the p-state being pushed above the Fermi level  $E_F$  in the spin-up channel, while the band extends in the spin-down channel with  $E_F$  exhibiting the double exchange effect, referred to as half metallicity. In the case of  $\text{La}_2\text{CrNiO}_6$  La-f has maximum contribution, whereas below the Fermi level there is a small contribution from Cr-d and Ni-d to the total density of states (TDOS) and the peak value of the total density of states (TDOS) in the conduction band is nearly 48 (states per eV) at 3eV.

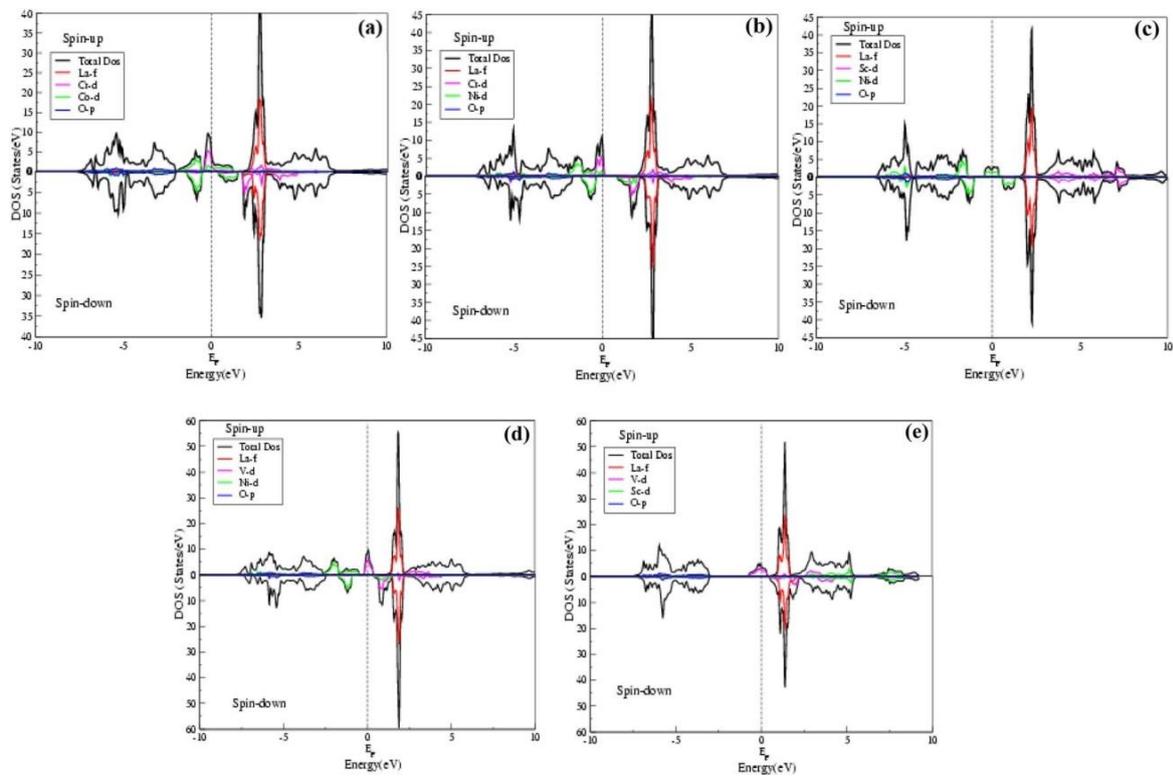
The density of states of the Half-Metallic Novel Double Perovskites HM-NDPs describe the behavior of the band structures, the electronic distribution is described in the form of the total density of states (TDOS) using GGA and GGA+U, as shown in Figures 4(a-e) and 5(a-e). All the NDPs Materials are metallic for the spin-up channel and semiconductors for the spin-down channel in both the GGA and GGA (+U) schemes. The valance band ( $V_b$ ) and conduction band ( $C_b$ ) overlaps for the spin-up channel and for the spin-down channel there is an energy gap ( $E_g$ ) between them. The negative side of energy describes  $V_b$ , while the positive energy side shows  $C_b$ , separated by the Fermi level  $E_F$ .

For NDP  $\text{La}_2\text{CrCoO}_6$  in the spin-down channel, the main contribution in  $V_b$  is due to the Co-d orbital. The minor contribution of Cr-d is detected in the  $V_b$  and some crowded peaks of O-p are also detected but too far from the edge of the  $V_b$ . Inside the  $C_b$  the Co-d is also found to be dominant near the edge and the major contribution of La-f is detected in the form of the high peaks shown in Figure 4(a-b) in GGA and GGA+U, respectively. For the NDP  $\text{La}_2\text{CrNiO}_6$  in the spin-down channel, the  $V_b$  mostly consists of the Ni-d orbital and the  $C_b$  consists of the Ni-d, Cr-d and La-f orbitals, as shown in Figure 5 (a-b).

Similarly, we observed that in the case of the  $\text{La}_2\text{ScNiO}_6$  (LSNO),  $\text{La}_2\text{VNiO}_6$  (LVNO) and  $\text{La}_2\text{VScO}_6$  (LVSO) materials (Fig.4(c-e) and 5(c-e)) there is a small contribution of Ni-d to the total density of states (TDOS) below the  $E_F$ , while above the  $E_F$  there is a maximum contribution of La-f to the (TDOS). Furthermore, there is a negligible contribution of the O-p to the (TDOS) below the  $E_F$  and a small contribution of Sc-d and V-d in the conduction bands, for both the spin-up and spin-down channels. The density of states (DOS) are nearly same for both type of calculations and the maximum value of the DOS above the Fermi level  $E_F$  is at approximately 1.25eV [18].The TDOS of the all NDPs are shown in Figure 4 (a-e) and Figure 5 (a-e).



**Figure 4 (a-e)** TDOS of all NDPs materials calculated by GGA scheme.



**Figure 5 (a-e)** TDOS of all NDPs materials calculated by GGA (+U) scheme.

### 3.3. Magnetic Properties

The magnetic properties of Novel Double Perovskites (NDPs) materials were investigated by both GGA and GGA (+U) calculations and carried out in spin polarization manner. The GGA calculation, for d-state electrons of transition metals with oxides in the spinal compounds are not strongly co-related to the standard band theory structure, which keep them near the Fermi level ( $E_F$ ). Therefore we use GGA (+U) calculation for the transition metals d-state electrons, by choosing an appropriate U, which splits the band structure of the materials but the total magnetic moments still remain the same. And the energy gaps ( $E_g$ ) from 0.945, 1.150, 1.632, 1.225 and 3.545eV reach to 1.667, 1.221, 3.950, 2.008 and 3.577eV respectively, for spin-down channels.

The magnetic moments of all NDPs are given in the Table 2 and 3 by GGA and GGA (+U) schemes respectively. According to the results, all the five compounds are half-metallic ferromagnetic (HM-FM). The transition metals Cr, Co, Ni, Sc and V contribute maximum part to total spin magnetic moments. For  $\text{La}_2\text{CrCoO}_6$  and  $\text{La}_2\text{CrNiO}_6$ , the transition metal (Cr) has maximum contribution to total spin magnetic moments of these compounds, while Lanthanum (La) has minimum contribution. And for  $\text{La}_2\text{ScNiO}_6$  and  $\text{La}_2\text{VNiO}_6$  there is maximum contribution of Nickel (Ni) to their total spin magnetic moments. And in the case of NDP  $\text{La}_2\text{VScO}_6$  the transition metal Vanadium (V) has the maximum contribution, to total spin magnetic moment of  $\text{La}_2\text{VScO}_6$ . In these five materials, the NDP  $\text{La}_2\text{CrNiO}_6$  has the maximum total spin magnetic moment equal to  $4.0\mu_B$ , while the total spin magnetic moment of  $\text{La}_2\text{ScNiO}_6$  is minimum and equal to  $0.9\mu_B$  [17, 18].

**Table 2** The magnetic moments ( $m^{S1}$  to  $m^{S5}$ ) and  $m^{\text{Intst}}$  of NDPs calculated by GGA scheme

#	NDPs	$m^{\text{Intst}}$	$m^{S1}$	$m^{S2}$	$m^{S3}$	$m^{S4}$	$m^{S5}$	$m^{\text{Cell}}$
1	$\text{La}_2\text{CrCoO}_6$	<b>0.27150</b>	0.01201	2.32582	0.18412	0.01326	0.01290	<b>2.88359</b>
2	$\text{La}_2\text{CrNiO}_6$	<b>0.28269</b>	0.01420	1.99849	1.38930	0.04885	0.05090	<b>4.00017</b>
3	$\text{La}_2\text{ScNiO}_6$	<b>0.01170</b>	0.00220	0.04520	0.77638	0.02802	0.02834	<b>0.99828</b>
4	$\text{La}_2\text{VNiO}_6$	<b>0.15326</b>	0.01338	0.89250	1.48145	0.06907	0.06982	<b>2.97139</b>
5	$\text{La}_2\text{VScO}_6$	<b>0.42797</b>	0.07356	1.42382	0.03688	0.00487	0.00447	<b>2.00820</b>

**Table 3** The magnetic moments ( $m^{S1}$  to  $m^{S5}$ ) and  $m^{\text{Intst}}$  of NDPs calculated by GGA (+ U) scheme

#	NDPs	$m^{\text{Intst}}$	$m^{S1}$	$m^{S2}$	$m^{S3}$	$m^{S4}$	$m^{S5}$	$m^{\text{Cell}}$
1	$\text{La}_2\text{CrCoO}_6$	<b>0.32371</b>	0.02128	2.38831	0.15488	0.01886	0.01511	<b>3.00761</b>
2	$\text{La}_2\text{CrNiO}_6$	<b>0.26399</b>	0.01282	1.97414	1.40242	0.05606	0.05715	<b>4.00693</b>
3	$\text{La}_2\text{ScNiO}_6$	<b>0.01631</b>	0.00239	0.01728	1.31964	0.05725	0.05270	<b>1.00007</b>
4	$\text{La}_2\text{VNiO}_6$	<b>0.15399</b>	0.01325	0.89531	1.48322	0.06848	0.06922	<b>2.97283</b>
5	$\text{La}_2\text{VScO}_6$	<b>0.42984</b>	0.07343	1.42780	0.03685	0.00532	0.00506	<b>2.01050</b>

### 3.4. Optical Properties

#### 3.4.1. Optical Conductivity

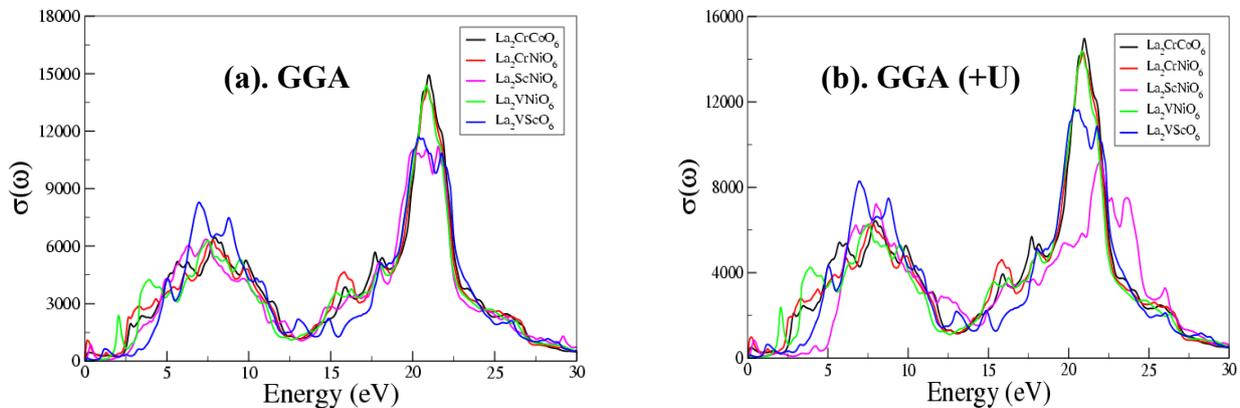
We have calculated the optical properties of the half-metallic ferromagnetic ordered novel double perovskites (NDPs) materials  $\text{La}_2\text{CrCoO}_6$ ,  $\text{La}_2\text{CrNiO}_6$ ,  $\text{La}_2\text{ScNiO}_6$ ,  $\text{La}_2\text{VNiO}_6$  and  $\text{La}_2\text{VScO}_6$ , including the optical conductivity  $\delta(\omega)$ , absorption coefficient  $\alpha(\omega)$ , refractive index  $n(\omega)$  and optical reflectivity  $\mathcal{R}(\omega)$  for various energies (in eV), via the GGA and GGA (+U) techniques. The optical conductivity is calculated by the equation:

$$\delta(\omega) = \mathbf{J}(\omega) / \mathbf{E}(\omega) \dots\dots\dots (1)$$

The calculated optical conductivity  $\delta(\omega)$  is illustrated in Figure. 6 (a-b) and values of the optical conductivity are listed in **Table 4**, which shows that the optical conductivity varies from 11,205 to 14,927.  $\text{La}_2\text{CrCoO}_6$  has the maximum value of 14,927 at 20.9eV, while  $\text{La}_2\text{ScNiO}_6$  has the minimum value of 11,205 at 21.5eV. The values of the optical conductivity calculated by using GGA scheme for the  $\text{La}_2\text{CrCoO}_6$ ,  $\text{La}_2\text{CrNiO}_6$ ,  $\text{La}_2\text{ScNiO}_6$ ,  $\text{La}_2\text{VNiO}_6$  and  $\text{La}_2\text{VScO}_6$  NDPs are 14,927, 14,181, 11,205, 14,377 and 11,680 at 20.993eV, 20.911eV, 21.565eV, 20.830eV and 20.367eV respectively. Similarly, the calculated values of optical conductivity  $\delta(\omega)$  via GGA (+U) scheme for the  $\text{La}_2\text{CrCoO}_6$ ,  $\text{La}_2\text{CrNiO}_6$ ,  $\text{La}_2\text{ScNiO}_6$ ,  $\text{La}_2\text{VNiO}_6$  and  $\text{La}_2\text{VScO}_6$  NDPs materials are 14,958, 14,317, 9,286, 14,377 and 11,680 at 20.99eV, 20.91eV, 22.0eV, 20.83eV and 20.36eV correspondingly. The results obtained for the optical conductivity  $\delta(\omega)$  are comparable with previous investigations calculated by both schemes [17, 18].

**Table 4** The calculated values of Optical Conductivity of NDPs via GGA and GGA (+U)

#	NDPs	GGA		GGA (+U)	
		$\delta(\omega)$	E(eV)	$\delta(\omega)$	E(eV)
1	$\text{La}_2\text{CrCoO}_6$	14,927	20.993	14,958	20.990
2	$\text{La}_2\text{CrNiO}_6$	14,181	20.911	14,317	20.912
3	$\text{La}_2\text{ScNiO}_6$	11,205	21.565	9,286	22.000
4	$\text{La}_2\text{VNiO}_6$	14,377	20.830	14,377	20.830
5	$\text{La}_2\text{VScO}_6$	11,680	20.367	11,680	20.367



**Figure 6 (a-b)** Optical Conductivity of NDPs materials in both schemes.

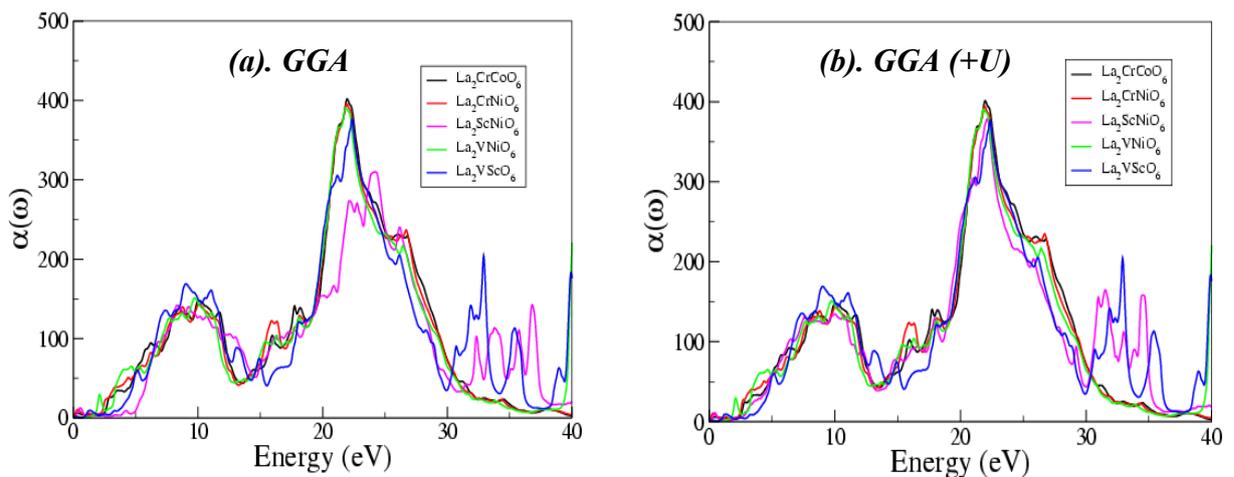
### 3.4.2. Absorption Coefficient

We have determined the absorption coefficient  $\alpha(\omega)$  for all materials  $\text{La}_2\text{CrCoO}_6$ ,  $\text{La}_2\text{CrNiO}_6$ ,  $\text{La}_2\text{ScNiO}_6$ ,  $\text{La}_2\text{VNiO}_6$  and  $\text{La}_2\text{VScO}_6$  by using GGA and GGA (+U) techniques. The absorption coefficient  $\alpha(\omega)$  calculated for  $\text{La}_2\text{CrCoO}_6$  (LCCO) has maximum value of 401.082 at energy equal to 21.973eV. It means that this material has more potential to absorbed incident photons and can be used for the absorption purposes in many optical devices. While the absorption coefficient of  $\text{La}_2\text{VScO}_6$  (LVSO), is minimum as compared to other materials. Therefore its absorption power for incident photons will be least and may be less useful for optical applications than others four materials. The absorption coefficients calculated by GGA and GGA (+U) processes, are nearly same for all the compounds. For each NDP material, the maximum value of absorption coefficient is in the energy range of (21 to 22.5eV). The absorption coefficients calculated for  $\text{La}_2\text{VNiO}_6$  is ( $\alpha=390.602$ ) exactly same, in both schemes for same value of energy ( $E=21.837\text{eV}$ ). The obtained values of absorption coefficient of all NDPs are given in **Table 5** and illustrated in **Figure 7 (a-b)**.

**Table 5** The absorption coefficients of NDPs calculated by GGA and GGA (+U) schemes.

#.	NDPs	GGA		GGA (+U)	
		$\alpha(w)$	$E(eV)$	$\alpha(w)$	$E(eV)$
1.	$\text{La}_2\text{CrCoO}_6$	401.082	21.973	401.871	21.973
2.	$\text{La}_2\text{CrNiO}_6$	394.128	21.918	395.603	21.918
3.	$\text{La}_2\text{ScNiO}_6$	378.128	22.136	376.096	22.204
4.	$\text{La}_2\text{VNiO}_6$	390.602	21.837	390.602	21.837
5.	$\text{La}_2\text{VScO}_6$	376.535	22.354	376.535	22.535

The given below figures further illuminate the absorption coefficients  $\alpha(\omega)$  of novel double perovskites (NDPs) materials using both schemes i.e. GGA and GGA (+U).



**Figure 7 (a-b)** Absorption Coefficients of NDPs materials in both **GGA & GGA (+U)** schemes.

### 3.4.3. Refractive Index

In optics the index of refraction or refractive index  $n(\omega)$  of an optical medium is a dimensionless number that describes how light, or any other radiation, propagates through that medium. It is defined as, the ratio of the speed of a light in a vacuum,  $C = 3 \times 10^8$  m/s, and the phase velocity ( $v$ ) of light in the medium and given by:

$$n = C/V \dots \dots \dots (2)$$

Where “C” is the speed of light in a vacuum and “v” is the phase velocity of the light in the medium. The refractive index is a critical feature of semiconductors, revealing the amount of light bent or refracted. The GGA and GGA(+U) calculations report higher values of the refractive index  $n(\omega)$  for  $\text{La}_2\text{CrCoO}_6$ ,  $\text{La}_2\text{CrNiO}_6$ ,  $\text{La}_2\text{ScNiO}_6$ ,  $\text{La}_2\text{VNiO}_6$  and  $\text{La}_2\text{VScO}_6$  materials of 6.005 (at 0.013 eV), 9.602 (at 0.038 eV), 4.928 (at 0.122 eV), 3.943 (at 0.013 eV) and 3.979 (at 0.013eV), and 6.322 (at 0.013eV), 8.732 (at 0.013 eV), 4.614 (at 0.149eV), 3.820 (at 0.019eV) and 3.979 (at 0.013eV), indicating their potential use in optoelectronic applications, primarily in electronic displays, such as LCDs, OLEDs, and quantum dot light-emitting diodes (QD-LEDs) televisions. Now, permanence and inkjet-printing fabrication of QD-LEDs are being tested for future commercialization. **Table 6** shows the refractive indices  $n(\omega)$  of all the NDPs materials in (eV).

**Table 6** Refractive indices of novel double perovskites NDPs calculated via GGA and GGA (+U) techniques.

#	NDPs	GGA		GGA (+U)	
		$n(\omega)$	E(eV)	$n(\omega)$	E (eV)
1	$\text{La}_2\text{CrCoO}_6$	6.005	0.013	6.322	0.013
2	$\text{La}_2\text{CrNiO}_6$	9.602	0.038	8.732	0.013
3	$\text{La}_2\text{ScNiO}_6$	4.928	0.122	4.614	0.149
4	$\text{La}_2\text{VNiO}_6$	3.943	0.013	3.820	0.019
5	$\text{La}_2\text{VScO}_6$	3.979	0.013	3.979	0.013

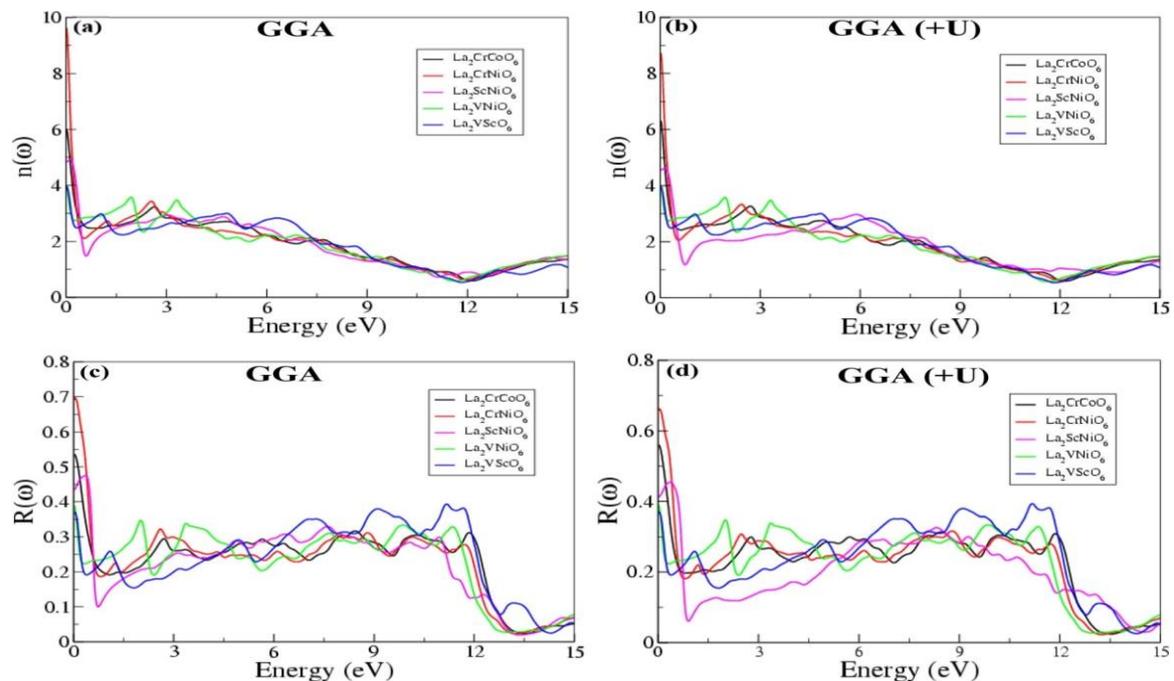
The refractive index  $n(\omega)$  calculated for  $\text{La}_2\text{CrNiO}_6$  has the maximum value of 9.602 at 0.038eV, whereas a minimum value of 3.943 at 0.013eV is reported for the  $\text{La}_2\text{VNiO}_6$  NDP, as compared to the other materials. There is no large deference between the refractive indices  $n(\omega)$  calculated by GGA and GGA (+U). The refractive indices measured for the  $\text{La}_2\text{VNiO}_6$  and  $\text{La}_2\text{VScO}_6$  materials are nearly the same at 0.013eV in the GGA scheme. The refractive indices  $n(\omega)$  of  $\text{La}_2\text{CrCoO}_6$  and  $\text{La}_2\text{ScNiO}_6$  are equal to 6.0 and 4.9 at 0.013eV and 0.122eV, respectively. The values of refractive indices observed for all NDPs materials are non-linear. Initially there is a sharp increase and then a decrease with increasing energy(eV), etc., which is in good agreement with previously reported theoretical and experimental results related to 2D double perovskites [17-18]. Refraction is an important characteristic of a substance for its use, in many optical devices. The index of refraction  $n(\omega)$  determines how much light is refracted, or bent, when entering in a material. These NDPs materials may be used for many components of an optical instrument such as solar cells, driving mirrors, slide projectors, cameras and telescopes etc. **Fig.8 (a-b)** represents the refractive indices  $n(\omega)$  of all NDPs in (eV).

### 3.4.4. Optical Reflectivity

The optical reflectivity  $\mathcal{R}(\omega)$  values in relation to the incident energy calculated by the GGA and GGA (+U) shown in **Fig. 8 (c and d)** confirm the reflective nature of these materials. The optical reflectivity is the ratio of the energy of a wave reflected from a surface to the energy possessed by the wave striking the surface. The GGA and GGA (+U) values of the reflectivity  $\mathcal{R}(\omega)$  for all NDPs given in **Table 7** indicate that the surfaces of these materials are smooth and have an ordered crystalline structure. Among all of these materials, the NDP  $\text{La}_2\text{CrNiO}_6$  has the maximum value of 0.696 at 0.04eV, whereas NDP  $\text{La}_2\text{VScO}_6$  has the lowest value of 0.369 at 0.013eV in both the GGA and GGA (+U) schemes. Table 7 and figure 8 (c-d) represent the  $\mathcal{R}(\omega)$  of all the NDPs materials in (eV).

**Table 7** Optical reflectivity of novel double perovskites NDPs calculated via GGA and GGA (+U) schemes.

#	NDPs	GGA		GGA (+U)	
		$\mathcal{R}(\omega)$	E (eV)	$\mathcal{R}(\omega)$	E (eV)
1	$\text{La}_2\text{CrCoO}_6$	0.534	0.040	0.558	0.042
2	$\text{La}_2\text{CrNiO}_6$	0.696	0.040	0.662	0.040
3	$\text{La}_2\text{ScNiO}_6$	0.475	0.036	0.454	0.038
4	$\text{La}_2\text{VNiO}_6$	0.389	0.013	0.389	0.013
5	$\text{La}_2\text{VScO}_6$	0.369	0.013	0.369	0.013



**Figure 8 (a-b)** Refractive index  $n(\omega)$  and **(c-d)** reflectivity  $\mathcal{R}(\omega)$  of the  $\text{La}_2\text{CrCoO}_6$ ,  $\text{La}_2\text{CrNiO}_6$ ,  $\text{La}_2\text{ScNiO}_6$ ,  $\text{La}_2\text{VNiO}_6$  and  $\text{La}_2\text{VScO}_6$  materials calculated by the GGA and GGA(+U) processes.

#### 4. Conclusions

In this research, we investigated the influence of 3d transition metals inclusion at the B (V, Cr and Sc) and B' (Sc, Co and Ni) sites of the 2D  $\text{La}_2\text{BB}'\text{O}_6$  novel double perovskites NDPs on the electronic, magnetic, and optical properties. Full structural optimization was carried out by using the full-potential Linearized augmented plane wave (FP-LAPW) technique as implemented in Wien2K software. The results are in good agreement with previously reported work. The electronic band structures in the spin-up and spin-down states reveal that all of these NDPs materials are half-metallic. In the case of the spin-up channel,  $\text{La}_2\text{CrCoO}_6$ ,  $\text{La}_2\text{CrNiO}_6$ ,  $\text{La}_2\text{ScNiO}_6$ ,  $\text{La}_2\text{VNiO}_6$  and  $\text{La}_2\text{VScO}_6$  display metallic behaviors, while they display non-metallic features in the spin-down channel. The calculated density of states gives a detailed explanation of the band structure and the electronic distributions of these materials drawn in terms of the total density of states verify the half-metallic nature. The pd-hybridizations, double exchange correlations (strong-correlation correction (GGA (+U))), ground-state energies and calculated total magnetic moments ( $2.9\mu_B$ ,  $2.0\mu_B$ ,  $0.9\mu_B$ ,  $4.0\mu_B$  and  $2.8\mu_B$ ) of these materials confirm the ferromagnetic behavior. Therefore, the overall nature of these materials is half-metallic ferromagnetic (HM-FM).

We have calculated the optical conductivities and absorption coefficients, and their maximum values are 14,927 (at 20.993eV) and 401.08 (at 21.973eV) for the NDP material  $\text{La}_2\text{CrCoO}_6$  respectively. The refractive index and optical reflectivity calculations reveal that  $\text{La}_2\text{CrNiO}_6$  has the highest values of 9.602 at 0.038eV and 0.696 at 0.04eV, where as  $\text{La}_2\text{VNiO}_6$  has the lowest values of 3.943 at 0.013eV and 0.389 at 0.013eV, compared to all the other materials. The fully spin-polarized strong magnetic element induces the weak magnetic element, and slightly increases the positive (or negative) magnetic moment; therefore it is regarded as the main cause of the half-metallic (HM) properties. In summary, based on our calculations, we discovered that 2D  $\text{La}_2\text{BB}'\text{O}_6$  novel double perovskites NDPs with 3d transition metals incorporated at the B (V, Cr and Sc) and B' (Sc, Co and Ni) sites have potential applications in spintronic, multifunctional and optoelectronic devices.

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