

First-principles study of the double perovskites Sr_2XOsO_6 ($\text{X} = \text{Li}, \text{Na}, \text{Ca}$) for spintronics applications

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Abstract. We investigated double perovskite compounds of the form Sr_2XOsO_6 ($\text{X} = \text{Li}, \text{Na}, \text{Ca}$) using the full-potential linearized augmented plane wave (FP-LAPW) method. For the exchange-correlation energy, Wu and Cohen generalized gradient approximation (WC-GGA), Perdew, Burke and Ernzerhof GGA (PBE-GGA), Engel and Vosko GGA (EV-GGA), and GGA plus Hubbard U-parameter (GGA + U) were used. The calculated structural parameters are in good agreement with the existing experimental results. Calculation of different elastic constants and elastic moduli reveals that these compounds are elastically stable and possess ductile nature. The GGA + U approach yields quite accurate results of the bandgap as compared with the simple GGA schemes. The density of states plot shows that Sr-4d, Os-5d and O-2p states predominantly contribute to the conduction and valence bands. Further, our results regarding to the magnetic properties of these compounds reveal their ferromagnetic nature. In addition, these compounds seem to possess half-metallic properties, making them useful candidates for applications in spintronics devices.

Keywords. Double perovskite; FP-LAPW; Hubbard U; half-metallic; spintronics.

1. Introduction

The double perovskite compounds were discovered in the early 1950s [1]. These compounds have the general formula of $\text{A}_2\text{BB}'\text{O}_6$. The symbol A represents cations, such as the divalent ions of the alkaline earth elements, occurring in the two-fold cuboctahedral position [2]. The B and B' are small cations of the type of transition metal elements, alkali metals, alkaline earth metals and main group metals [3–7]. The double perovskites possess a wide range of interesting physical properties such as metallicity, insulation, half-metallicity, magnetoresistance, magneto-electricity, ferromagnetism and antiferromagnetism [1,8–14]. These materials are widely used in spintronics, which is a newly developing field of science, and expected to bring progressive change in the fields of data innovation and telecommunication. One of the promising applications of spintronics is the multiple-state memory devices, such as tunnelling magnetoresistance and giant magnetoresistance, whose functions totally depend on magnetization and can only be realized by using spin direction [15]. In spintronics, spin of the electrons is used as an information carrier instead of its charge [16]. These compounds with different B-cations form one of the major groups of complex perovskites and can adopt different crystalline structures [2,17,18]. Using

a group-theoretical study, Howard *et al* [19] recognized 12 different possible space groups of double perovskites. The largest subgroup of this kind of perovskites with general formula $\text{A}_2\text{BB}'\text{O}_6$ is cubic with space group $Fm\bar{3}m$ [20]. The selected B-site-ordered double perovskites Sr_2XOsO_6 ($\text{X} = \text{Li}, \text{Na}, \text{Ca}$) are all oxygen stoichiometric, in which oxygen is present at the corner of each octahedra [21]. Feng [22] studied the crystal structure of $\text{Sr}_2\text{LiOsO}_6$ by X-ray diffraction method. The crystal structure study reveals that $\text{Sr}_2\text{LiOsO}_6$ crystallizes into an ordered double-perovskite structure at room temperature with a space group of $I4/m$. However, an earlier report on $\text{Sr}_2\text{LiOsO}_6$ by Sleight *et al* [23] observed that it crystallizes in cubic phase having space group $Fm\bar{3}m$. The magnetic susceptibility and heat capacity measurements showed that it transforms to antiferromagnetic type with cooling [14,22]. Choy *et al* [24] investigated strontium-based double perovskites $\text{Sr}_2\text{LiOsO}_6$ and $\text{Sr}_2\text{CaOsO}_6$ using X-ray powder diffraction method. These compounds were found to be in cubic crystal structure with space group $Fm\bar{3}m$.

The above facts reveal that the double perovskites Sr_2XOsO_6 ($\text{X} = \text{Li}, \text{Na}, \text{Ca}$) have not yet been fully understood. To help further understand the material, we carried out theoretical calculations based on the density functional theory (DFT). In the present report, we present our results based on theoretical calculations of various properties (structural, elastic, electronic and magnetic) of the double perovskite

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compounds. On the basis of our calculations, we suggest that Sr_2XOsO_6 ($X = \text{Li, Na, Ca}$) may prove to be a promising candidate for various applications in the field of solids displaying ductile as well as ferromagnetic nature.

2. Computational work

In Kohn-Sham scheme, the electron density can be obtained by summing over all the occupied states [25–27]. Full-potential linearized augmented plane wave (FP-LAPW) method [28] with different versions of generalized gradient approximation (GGA) [29–32] is used in Kohn-Shan equation. Spin polarized method, used for the calculations of ground-state properties [33] was started in the structural optimization process of the material by using the computational code wien2k [34].

In FP-LAPW scheme, unit cell of a crystal is divided into two different regions. The first region is the spherical part of atom (also called the muffin-tin region) and the second region is called interstitial region (region outside the atomic spheres). Inside each atomic sphere the potential is taken to be symmetric while it has a constant value in the interstitial region. So the Schrodinger wave equation for the spherical region can be solved by the radial wavefunction times spherical harmonics and for the interstitial region, it can be solved in the form of plane waves [28]. In the spherical region, the maximum value of the angular momentum (l_{max}) is extended

to 12. In our calculations, the R_{MT} (muffin-tin radii) values of 2.50, 1.90, 1.98, 1.98, 1.80 and 1.59 a.u. are used for Sr, Li, Na, Ca, Os and O, respectively, in order to avoid leakage of the charge from the core. A plane wave cut-off $K_{\text{max}} R_{\text{MT}} = 7$ is used for wavefunction in the interstitial region, where K_{max} shows largest k-vector and R_{MT} shows radii of the smallest muffin-tin region. For the integration of the k-space in Brillouin zone, the modified tetrahedron method [35] with 1000 k-points is used for achieving self-consistency.

3. Result and discussions

3.1 Structural properties

The double perovskite compounds Sr_2XOsO_6 ($X = \text{Li, Na, Ca}$) have face-centred cubic structure ($Fm\bar{3}m$) with four atoms per unit cell. The atomic position in the unit cell are Sr (0.25, 0.25, 0.25), X (0.5, 0.5, 0.5), Os (0, 0, 0) and O (0, 0, 0.233). In order to get the structural parameters like lattice constant, unit cell energy, optimized volume, bulk modulus and pressure derivative of the bulk modulus, the volume optimization process was carried out under the WC-GGA and PBE-GGA. In this process, unit cell energy is varied with respect to the unit cell volume using Birch-Murnaghan's equation of state [36]. The optimization plots are shown in figure 1. These plots show that the ground-state volume (also

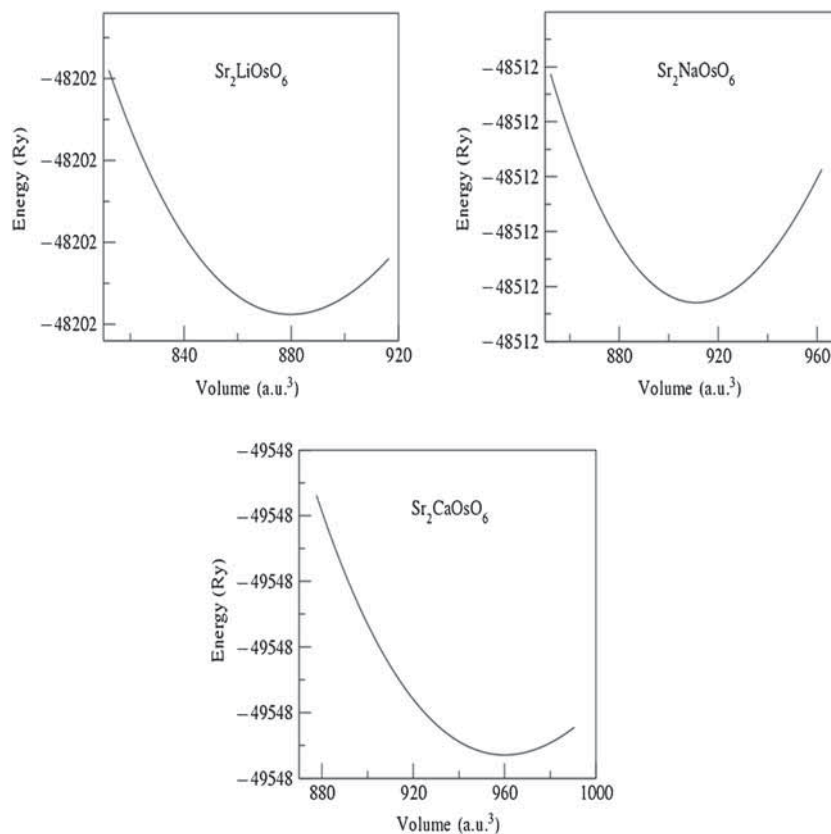


Figure 1. Optimization plots showing energy vs. volume for $\text{Sr}_2\text{LiOsO}_6$, $\text{Sr}_2\text{NaOsO}_6$ and $\text{Sr}_2\text{CaOsO}_6$.

called stable volume) for any compound of Sr_2XOsO_6 is the one at which the total energy is minimum. From the stable volume, the ground-state parameters such as the unit cell length (α_0), optimized volume (V), bulk modulus (B) and its pressure derivative (B') and energy (E) were calculated. Table 1 shows the comparison of the structural parameters with the experimental results for Sr_2XOsO_6 ($X = Li, Na, Ca$). It can be seen from the table that the lattice constant increases in varying X from Li to Ca. This increase is due to the change in the atomic size of the cations, since the atomic size increases from Li to Na to Ca. Our calculated data of the lattice constant (α_0) with PBE-GGA scheme are in fair agreement with the available experimental results. Table 1 shows that the bulk modulus of Sr_2LiOsO_6 is larger than Sr_2NaOsO_6 and Sr_2CaOsO_6 , indicating that Sr_2LiOsO_6 is harder than the other two compounds. In this study, majority of the parameters like optimized volume, bulk modulus and unit cell energy are calculated for the first time, and no theoretical as well as experimental data is available for comparison.

3.2 Elastic properties

Elastic properties of matter provide information upon which one can construct its physical model. These properties show a

material response to an applied macroscopic stress. For cubic compounds, only three constants (C_{11} , C_{12} and C_{44}), known as elastic constants, are required for complete characterization of their elastic properties [37]. Using these constants we have the capacity to know about a material that is under stress, misshapes and afterward comes back to its unique shape when the stress is released. To know these constants we need to calculate the value of stress tensor for a small strain with the help of wien2k package. For Os-based double perovskite Sr_2XOsO_6 ($X = Li, Na, Ca$), we have performed the DFT calculations in order to find out its elastic properties. Also, the following restrictions were followed for the elastic stability of the cubic compounds [38]:

$$\frac{1}{3}(C_{11}+2C_{12}) > 0, C_{44} > 0, \frac{1}{2}(C_{11}-C_{12}) > 0, C_{12} < B < C_{11}. \quad (1)$$

If these criteria are satisfied, compounds are said to be elastically stable. In addition, these elastic constants are related to different mechanical parameters through the following expressions:

$$E = \frac{9GB}{3B + G}, \quad (2)$$

Table 1. Structural parameters of Sr_2LiOsO_6 , Sr_2NaOsO_6 and Sr_2CaOsO_6 along with available data.

	Present (GGA)		Experimental	Other calc.
	WC-GGA	PBE-GGA		
<i>Sr₂LiOsO₆</i>				
α_0 (Å)	7.9531	8.0491	7.860 ^{a,b} , 7.855 ^c	—
V (Å ³)	125.7208	130.3273		
B (GPa)	154.3866	142.4391		
B'	5.0000	5.0000		
E	-48196.02	-48202.08		
<i>Sr₂NaOsO₆</i>				
α_0 (Å)	8.0536	8.1434	8.130 ^{a,b}	—
V (Å ³)	130.5441	134.9637		
B (GPa)	152.9712	140.4047		
B'	4.5948	5.0000		
E	-48505.50	-48511.82		
<i>Sr₂CaOsO₆</i>				
α_0 (Å)	8.1780	8.2869	8.210 ^{a,b} , 8.227 ^c	—
V (Å ³)	136.6896	142.2226		
B (GPa)	155.7424	136.5520		
B'	5.0015	5.0000		
E	-49541.37	-49547.97		

^aRef. [22], ^bRef. [23], ^cRef. [24].

Table 2. Elastic parameters (in GPa) of double perovskites Sr_2XOsO_6 ($X = Li, Na, Ca$).

Compounds	C_{11}	C_{12}	C_{44}	B	G	E	ν	A	B/G	$C_{12}-C_{44}$
Sr_2LiOsO_6	293.58	101.18	71.35	165.32	80.43	207.62	0.29	0.74	2.06	29.83
Sr_2NaOsO_6	293.20	84.57	67.16	154.12	80.17	204.96	0.28	0.64	1.92	17.41
Sr_2CaOsO_6	331.19	77.47	63.35	162.04	83.98	214.84	0.28	0.50	1.93	14.12

$$B = \frac{C_{11} + 2C_{12}}{3}, \quad (3)$$

$$\nu = \frac{3B - 2G}{2(3B + G)}, \quad (4)$$

$$A = \frac{2C_{44}}{C_{11} - C_{12}}. \quad (5)$$

Table 3. Calculated bandgap energies (in eV) of Sr_2XOsO_6 (X = Li, Na, Ca) along with experimental results.

Compounds	Present			
	WC-GGA	PBE-GGA	EV-GGA	GGA + U
$\text{Sr}_2\text{LiOsO}_6$	1.32	1.39	1.59	1.90
$\text{Sr}_2\text{NaOsO}_6$	1.24	1.30	1.51	1.83
$\text{Sr}_2\text{CaOsO}_6$	1.38	1.46	1.81	2.24

In Equation 2, ‘ E ’ is the Young’s modulus. Table 2 shows the calculated value of E , suggesting that $\text{Sr}_2\text{CaOsO}_6$ is stiffer than $\text{Sr}_2\text{LiOsO}_6$ and $\text{Sr}_2\text{NaOsO}_6$ due to the high value of the Young’s modulus. In Equation 3, ‘ B ’ is the bulk modulus that measures the resistance of a substance to its uniform compression. The Poisson’s ratio ‘ ν ’ in Equation 4 provides information about the bonding forces present in solid materials. For central force solids, the Poisson’s ratio has a limit of 0.25 to 0.5 [39]. From the data listed in table 2, it is clear that our calculated Poisson’s ratio lies in this range, suggesting that the bonding forces are of central type for all these compounds. Elastic anisotropy (A) is the property of a material,

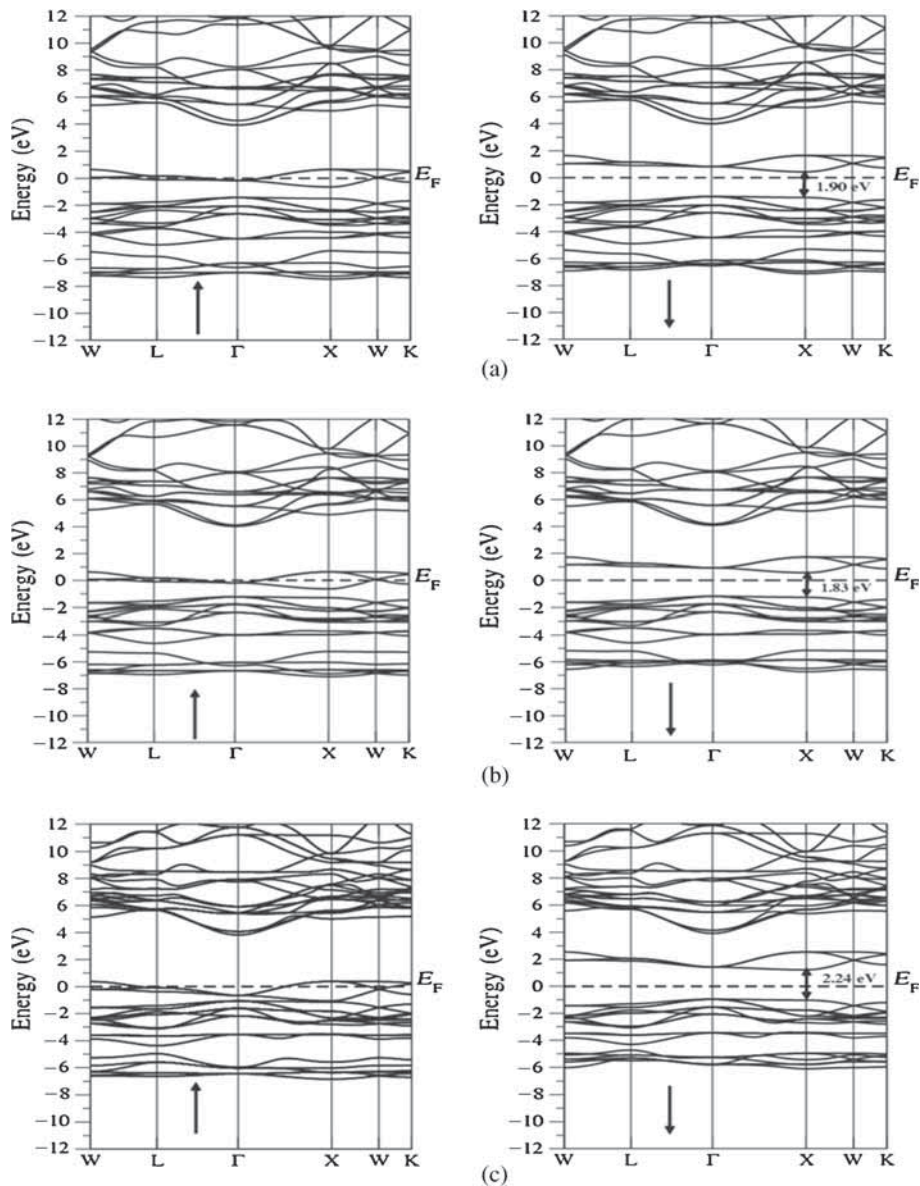


Figure 2. Band structure of the double perovskite (a) $\text{Sr}_2\text{LiOsO}_6$, (b) $\text{Sr}_2\text{NaOsO}_6$ and (c) $\text{Sr}_2\text{CaOsO}_6$ in both spin-up and -down modes, calculated using GGA + U.

which is directionally dependent. If its value is 1, the material shows isotropic behaviour, while for all other values the material is anisotropic [40]. Table 2 shows that Sr_2NaOsO_6 and Sr_2CaOsO_6 are more elastically anisotropic as compared with Sr_2LiOsO_6 .

Ductility and brittleness come in the category of elastic properties and can be determined using the elastic constant (C_{ij}), Cauchy's pressure ($C_{12}-C_{44}$), Pugh's index of ductility (B/G) and the Poisson's ratio ' ν '. If the Cauchy's pressure is negative, the material has a brittle nature, while

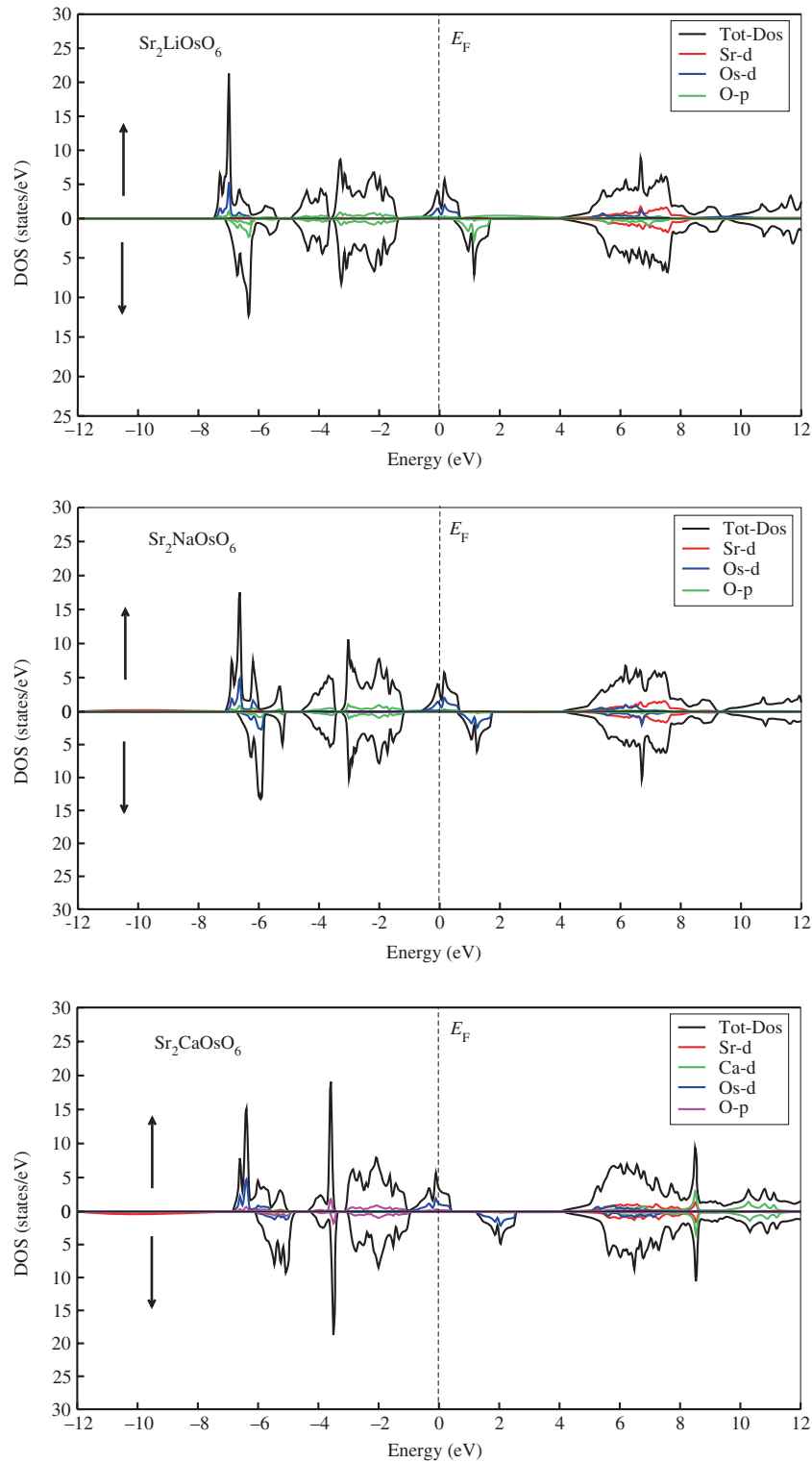


Figure 3. Density of states (DOS) plots for double perovskites Sr_2LiOsO_6 , Sr_2NaOsO_6 and Sr_2CaOsO_6 in both the spin directions.

Table 4. Magnetic moments (in μ_B) of the interstitial region, individual atoms and total cell for the double perovskites Sr_2XOsO_6 ($X = Li, Na, Ca$).

Compounds	m^{Inst}	m^{Sr}	$m^{Li/Na/Ca}$	m^{Os}	m^O	m^C
Sr_2LiOsO_6	0.32981	0.00919	0.00011	0.58433	0.00948	0.98949
Sr_2NaOsO_6	0.31291	0.00935	0.00070	0.65219	0.00339	1.00483
Sr_2CaOsO_6	0.53766	0.01134	0.00933	1.24068	0.01616	1.90728

for positive value the material possesses ductile nature [40]. From the data listed in table 2, it is clear that the Cauchy's pressure is positive for all these compounds, which highlights that these compounds are ductile in nature. Similarly, another index responsible for ductility and brittleness of a material is the B/G ratio. A critical value of the B/G ratio, 1.75, is used to separate the ductile materials from brittle materials. Materials having values higher than 1.75 are categorized as ductile, while those with B/G ratios lower than 1.75 are regarded as brittle [38]. In our calculated data, the B/G ratio for all the compounds is greater than 1.75, which reveals the ductile nature of these compounds. Poisson's ratio ' ν ' is another criterion used for the ductility and brittleness of a compound. If its value is greater than 0.26 the material possesses ductile nature otherwise the material behaves in a brittle manner. Table 2 shows that the Poisson's ratio for all these compounds is greater than 0.26, which reveals that these compounds are ductile in nature. According to our knowledge, no theoretical or experimental data exist regarding the elastic properties of these compounds with which we can compare our work. We believe that our work can provide stimulus for further research in this direction in the future.

3.3 Electronic properties

To determine the band structure of the selected compounds, we have performed spin polarized DFT calculations under the WC-GGA, PBE-GGA, EV-GGA and GGA + U method. The WC-GGA, PBE-GGA and EV-GGA underestimate the bandgaps and misplace the energy levels of the Os-5d state (not shown). However, when GGA + U method is applied, the compounds Sr_2XOsO_6 ($X = Li, Na, Ca$) show half-metallic nature with overlapping bands in spin-up direction and semiconducting behaviour in the spin-down direction. In the spin-down state the energy level Os-5d moves towards conduction band, thereby creating a bandgap across the Fermi level. The calculated bandgap energies in spin-down state are quoted in table 3. For Sr_2LiOsO_6 compound, the calculated band structure plots are shown in figure 2a. It is clear from the plots that the compound is metallic in spin-up mode and a wide gap semiconductor in spin-down state, with a half-metallic bandgap of 0.43 eV. For Sr_2NaOsO_6 , the plots are displayed in figure 2b showing metallic behaviour in spin-up mode and semiconducting behaviour in spin-down mode. The calculated half-metallic bandgap for Sr_2NaOsO_6 is 0.55 eV. The band structure of Sr_2CaOsO_6 is shown in figure 2c. In spin-up state, it has metallic character with overlapping bands across the Fermi level and in spin-down state

it has semiconducting nature with a half-metallic bandgap of 1.21 eV.

To further clarify the band structure, we calculated the DOS plots for Sr_2XOsO_6 ($X = Li, Na, Ca$) as shown in figure 3. The calculated DOS for Sr_2XOsO_6 ($X = Li, Na, Ca$) are plotted in the energy range of -12 to 12 eV. The main contribution to the conduction band maximum of all the compounds seems to be due to the Sr-4d, Ca-3d, Os-5d and O-2p orbitals. From the plots, it is clear that there are three different bands in the energy range of -7 to -1 eV in the valence band region. The lowest band is due to the Os-5d and O-2p states. The band next to it is purely due to the O-2p state. The band which crosses the Fermi level in spin-up mode is mainly due to the Os-5d state; however, in spin-down mode there is a bandgap of 1.90, 1.83 and 2.24 eV across the Fermi levels for Sr_2LiOsO_6 , Sr_2NaOsO_6 and Sr_2CaOsO_6 , respectively. In conduction band, the occupied region is from 4 to 12 eV. This region is mostly occupied by Sr-4d and Os-5d states; however, a minor contribution also comes from the p-state of the oxygen.

3.4 Magnetic properties

To investigate the magnetic nature of Sr_2XOsO_6 ($X = Li, Na, Ca$), we carried out the spin polarized DFT calculations with GGA + U scheme. We found that these compounds possess ferromagnetic nature. The main source of magnetization in these compounds is the unfilled Os-5d orbital. Further investigation of the Os-5d state shows that it is the partially filled t_{2g} orbital which is responsible for ferromagnetism in all these compounds. The total magnetic moments of a cell, m^c , of each of these compounds as well as their individual atomic magnetic moments are quoted in table 4. Our calculations reveal that the magnetic moments of strontium for Sr_2XOsO_6 ($X = Li, Na, Ca$) are 0.009, 0.009 and 0.01 μ_B , respectively. In each compound, the magnetic moments of all the spheres have the same direction, so they strongly support each other. Also, the data in table 4 show that the compound containing 'Ca' in the B-site, Sr_2CaOsO_6 , has a high value of magnetic moment suggesting a strong ferromagnetic nature. Moreover, in all the three type of compounds, the osmium contributes largely in the total spin magnetic moment.

4. Conclusions

We calculated the structural, elastic, electronic and magnetic properties of strontium-based double perovskites Sr_2LiOsO_6 ,

Sr_2NaOsO_6 and Sr_2CaOsO_6 using the full-potential method within the framework of DFT. The calculated lattice parameters are in reasonable agreement with the existing experimental results. Most of the structural parameters are calculated for the first time by using WC-GGA and PBE-GGA. All these compounds show elastic stability and are found to be ductile in nature. Investigation of the electronic properties reveals that these compounds are half-metallic in nature. We have observed that GGA + U method tends to give better results for electronic band structure of these compounds, as compared with the simple GGA schemes. From the band structure, it is concluded that the energy bandgap in spin-down state increases as X is replaced by Li, Na and then Ca in Sr_2XOsO_6 . Analysis of the density of states shows that Os-5d state plays the main role in half-metallicity of the said compounds. Furthermore, the calculated magnetic moments reveal the ferromagnetic nature of these compounds.

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