

# First-principles calculations of the electronic, magnetic and optical properties of rhenium-doped alkaline earth oxides

Nazir Ahmad Teli  and M Mohamed Sheik Sirajuddeen

Department of Physics, B.S.A Rahman Crescent Institute of Science and Technology, Chennai, India

E-mail: [nazir\\_phy\\_PhD\\_17@crescent.education](mailto:nazir_phy_PhD_17@crescent.education)

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## Abstract

The electronic, magnetic and optical properties of alkaline earth oxides XO ( $X = \text{Ca}, \text{Sr}, \text{Ba}$ ) doped with 5d transition metal rhenium (Re) were investigated by applying first-principles calculations within the treatment of density functional theory based on a full potential linearised augmented plane wave method. 5d transition metal atom Re was doped to replace Ca/Sr/Ba atoms with 12.5% concentration to form the supercells. Density of states and band structures predict half-metallic characteristics of the supercells  $X_{0.875}\text{ORe}_{0.125}$  ( $X = \text{Ca}, \text{Sr}, \text{Ba}$ ). Half-metallic band gaps were observed clearly in the spin up majority channel around the Fermi level ( $E_F$ ). Dopant 5d transition metal atom Re creates a spin magnetic moment ( $\mu_B$ ) in the supercells  $X_{0.875}\text{ORe}_{0.125}$  ( $X = \text{Ca}, \text{Sr}, \text{Ba}$ ). Optical parameters (dielectric function  $\epsilon(\omega)$ , absorption coefficient and reflectivity) were discussed. Materials exhibiting properties like absorption, reflectivity and half-metallic can be applicable for optoelectronics and spintronics devices.

Keywords: Alkaline earth oxides, electronic, magnetic, optical properties, Generalized gradient approximations (GGA) method

(Some figures may appear in colour only in the online journal)

## 1. Introduction

For two decades, the field of spintronics has held great promise and looks to exert a significant influence on future technology. Studying electron spin and the magnetic moment associated with it represents a specialized field. Devices use less energy in changing the spin as compared to generating a current for maintaining charge. In such spintronics devices, the information is transmitted through the electron's spin, offering a gateway for a new generation of spin-based devices. Giant magneto resistors and magnetic tunnel junctions are examples of spin-based devices. These spin-based devices can be used as storage devices like hard disks, magnetic field sensors, etc [1]. Half-metallic ferromagnetic materials are good candidates for spintronics applications, as was first reported by De Groot *et al* 1983 [2]. Half-metallicity was reported in other Heusler compounds by Kervan *et al* [3]. In such half-metallic materials, one of the spins (up or down) is conducting but other has a insulating/semiconducting

character, exhibiting 100% spin polarization about the Fermi level.

The main goal of the present article is to study the electronic, magnetic, half-metallic and optical properties of alkaline earth oxides XO ( $X = \text{Ca}, \text{Sr}, \text{Ba}$ ) doped with 5d transition metal rhenium (Re). Energy band gaps and the lattice constants of alkaline earth oxides were found by McLeod *et al* in 2010 [4] and compared with other theoretical and experimental works. These alkaline earth oxides are ionic crystal insulators with a wide band gap and have a significant role in industrial applications range from catalysis to microelectronics [4–7]. The half-metallic property has been reported in such oxides (CaO, MgO, SrO and BaO) doped with non-magnetic impurities [8–12] and also with magnetic impurities (transition metals) [13, 17]. Doping of nitrogen induces magnetism in the oxides [18–20]. Transition metal atoms consolidated into wide band gap oxides can enormously change their absorption properties [21, 22]. By density functional theory (DFT) calculations the structural,

electronic, optical, mechanical and thermodynamic properties of alkaline earth oxides were reported [23–29]. The optical properties (reflectivity and absorption) and band structure results of alkaline earth oxides XO ( $X = \text{Ca}, \text{Sr}, \text{Ba}$ ) were explained by exciton reflection spectra [30]. Reflectivity and imaginary parts for alkaline earth oxides have been calculated within the optical frequency range [31]. It was reported in works done by Zhou *et al* and Teli *et al* that doping of 5d transition metals in some oxides causes changes in their electronic, magnetic and optical properties [32, 33]. This is not only limited to oxides but affects other materials such as monolayer graphene and h-BN, as found by Muhammad *et al* [34, 35].

In this present work 5d transition metal atoms were doped in XO ( $X = \text{Ca}, \text{Sr}, \text{Ba}$ ) oxides with a concentration of 12.5%. The compounds were found to be half-metallic in nature. The electronic structure, magnetic and optical properties were investigated in alkaline earth oxides doped with 5d transition metal Re, which may be suitable for optoelectronics and spintronics applications.

## 2. Computational method

A theoretical computational approach has been implemented for investigating the electronic structure, magnetic and optical properties. A full potential linearized augmented plane wave method and WIEN2k code were applied within the framework of DFT [36–39]. Based on the generalized gradient approximations (GGA) method the exchange-correlation energy of electrons was used [40]. The separation energy was chosen to be  $-6.0$  Ry between the core states. Execution of Brillouin zone integration was introduced using a Monkhorst-Pack scheme [41, 42]. To construct the supercells a model  $2 \times 2 \times 2$  k-point mesh or grid was used. The host oxides CaO, SrO, and BaO belong to a Fm3m space group with NaCl structures. These host oxides were doped with 5d transition metal atom Re with a doping concentration of 12.5% to create the supercells. A supercell consists of 16 atoms (8 atoms of Ca/Sr/Ba and 8 atoms of oxygen) in which one atom of Ca/Sr/Ba is replaced with a 12.5% of concentration. A self-consistent field (SCF) was run to converge the energy. This iteration process stops after the energy drops lower than  $10^{-4}$  Ry and the chosen k-points are 63 k-points in the whole irreducible Brillouin zone.

## 3. Results and discussion

### 3.1. Electronic properties

In this work the lattice constants used for obtaining the electronic, magnetic and optical properties of the alkaline earth oxides XO ( $X = \text{Ca}, \text{Sr}, \text{Ba}$ ) doped with 5d metal atoms are 4.8 Å, 5.16 Å, and 5.53 Å respectively. The total density of states of the host oxides showing band gaps in both the spins (up and down) are shown in figure 1. The band gaps of host oxides CaO, SrO and BaO were measured at their highest

and lowest symmetric points and are given in table 2. As per these band gaps at Fermi level, such oxides are known to be as semiconductors or insulators depending upon the width of the band gap.

**3.1.1. CaO, SrO, and BaO doped with rhenium (Re).** The alkaline earth oxides were doped with Re 5d transition metal atoms to change the properties of the host material. The host oxides (CaO, SrO, and BaO) Ca/Sr/Ba were substituted by the transition metal atom Re with a concentration of 12.5% to form the supercells. Each supercell contains 16 atoms (8 atoms of Ca/Sr/Ba and 8 atoms of O) in which the first atom of Ca/Sr/Ba was replaced by Re. The crystal structures and atomic positions of the supercells are shown in figure 2 and table 1. The doping of Re in CaO, SrO and BaO change the characteristic of being a semiconductor/insulator into half-metallic. A half-metallic nature can be defined as when one spin for the valence band is partially filled and the other is empty (a gap). The half-metallic characteristic is confirmed from TDOS and band structures of the resulting compounds  $X_{0.875}\text{ORe}_{0.125}$  ( $X = \text{Ca}, \text{Sr}, \text{Ba}$ ). Figures 3(a), 4(a) and 5(a) show the total DOS of supercells where it is seen clearly that band gaps lie in the spin up majority channel, but in the spin down minority channels the energy bands were observed to cross the Fermi level. Therefore, it is evidenced by the density of states that the compounds display a half-metallic character. The compounds are found to exhibit semiconducting behavior in the spin up majority channel and conducting (metallic) character in the spin down minority channel. These compounds exhibit 100% spin polarization around the Fermi level ( $E_F$ ).

The contribution of Re-5d, O-2p, Ca-3s, Sr-4s, and Ba-5s orbitals in the compounds  $X_{0.875}\text{ORe}_{0.125}$  ( $X = \text{Ca}, \text{Sr}, \text{Ba}$ ) has been observed in the respective partial DOS of each compound and were shown in figures 3(b), 4(b) and 5(b). In the (spin up) majority channel of super cell  $\text{Ca}_{0.875}\text{ORe}_{0.125}$ , 5d band peaks are seen in between the band energies 1.17 eV and 2 eV in the right side of Fermi level and  $-1.68$  eV and  $-0.31$  eV in the left side of Fermi level. These 5d bands of Re pushes each other and leaving a band gap in majority spin at the Fermi level. But, in spin down minority channel, the 5d bands of Re cross the Fermi level due to hybridization of the 5d orbitals of Re. The same trend is seen in other compounds (supercells) like  $\text{Sr}_{0.875}\text{ORe}_{0.125}$  and  $\text{Ba}_{0.875}\text{ORe}_{0.125}$  but the difference was observed in the Re-orbitals at different energies. The 5d bands of  $\text{Sr}_{0.875}\text{ORe}_{0.125}$  supercell are located at  $-0.38$  eV and 0.69 eV and 5d  $\bar{}$ bands of  $\text{Ba}_{0.875}\text{ORe}_{0.125}$  are positioned at  $-0.45$  eV and 0.42 eV from either side of the Fermi level. These 5d- bands of compounds  $X_{0.875}\text{ORe}_{0.125}$  ( $X = \text{Ca}, \text{Sr}, \text{Ba}$ ) push each other leaving the band gaps in spin up majority channel whereas the 5d-Re bands of each compound cross the Fermi level because of hybridization between the 5d- orbitals. The whole contribution in forming the band gaps in (spin up) majority channel of compounds  $X_{0.875}\text{ORe}_{0.125}$  ( $X = \text{Ca}, \text{Sr}, \text{Ba}$ ) is due to 5d Re bands and same 5d Re bands were seen crossing the Fermi level in spin down minority channel. Further, as seen from the

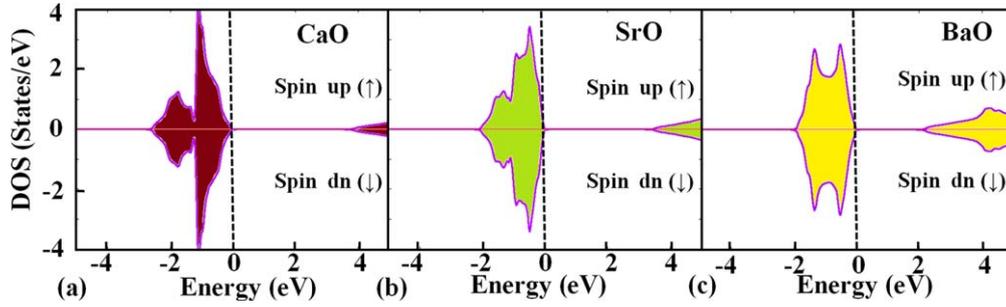


Figure 1. TDOS of XO (X = Ca, Sr, Ba).

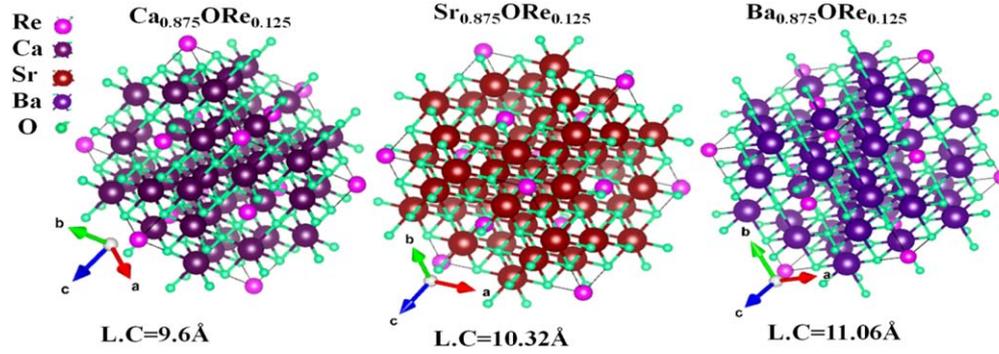


Figure 2. Crystal structures of uper cells  $X_{0.875}ORe_{0.125}$  (X = Ca, Sr, Ba).

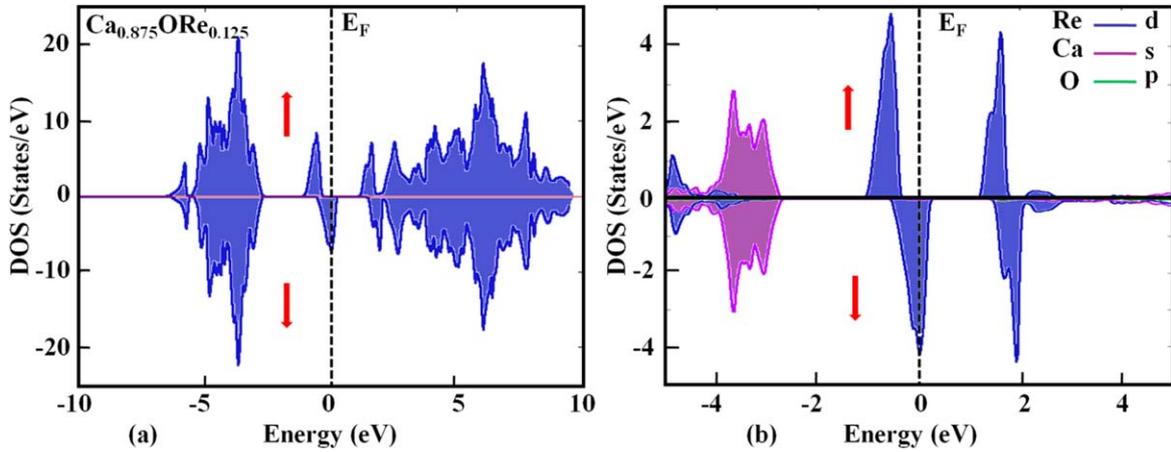


Figure 3. (a) TDOS and (b) PDOS of  $Ca_{0.875}ORe_{0.125}$ , spin (up- $\uparrow$ , down- $\downarrow$ ).

Table 1. Positions of atoms in super cells  $X_{0.875}ORe_{0.125}$  (X = Ca, Sr, Ba).

Atoms	Positions			Atoms	Positions		
	X	Y	Z		X	Y	Z
Re1	0	0	0	O <sub>1</sub>	1/4	1/4	1/4
Ca <sub>1</sub> /Sr <sub>1</sub> /Ba <sub>1</sub>	1/2	0	0	O <sub>2</sub>	3/4	1/4	1/4
Ca <sub>2</sub> /Sr <sub>2</sub> /Ba <sub>2</sub>	1/4	1/4	0	O <sub>3</sub>	0	0	1/4
Ca <sub>3</sub> /Sr <sub>3</sub> /Ba <sub>3</sub>	3/4	1/4	0	O <sub>4</sub>	1/2	0	1/4
Ca <sub>4</sub> /Sr <sub>4</sub> /Ba <sub>4</sub>	1/4	0	1/4	O <sub>5</sub>	0	1/4	0
Ca <sub>5</sub> /Sr <sub>5</sub> /Ba <sub>5</sub>	3/4	0	1/4	O <sub>6</sub>	1/2	1/4	0
Ca <sub>6</sub> /Sr <sub>6</sub> /Ba <sub>6</sub>	0	1/4	1/4	O <sub>7</sub>	1/4	0	0
Ca <sub>7</sub> /Sr <sub>7</sub> /Ba <sub>7</sub>	1/2	1/4	1/4	O <sub>8</sub>	3/4	0	0

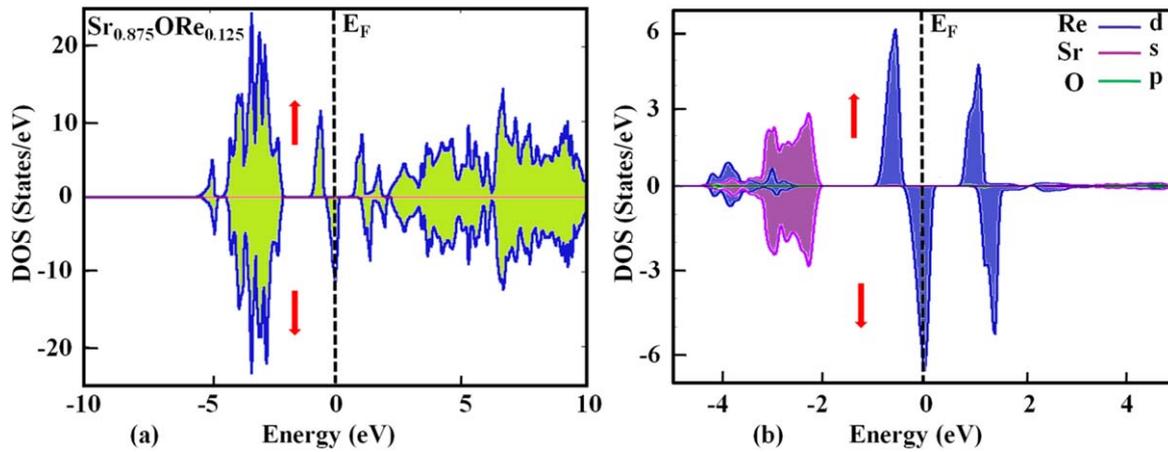


Figure 4. (a) TDOS and (b) PDOS of  $\text{Sr}_{0.875}\text{ORE}_{0.125}$ , spin (up- $\uparrow$ , down- $\downarrow$ ).

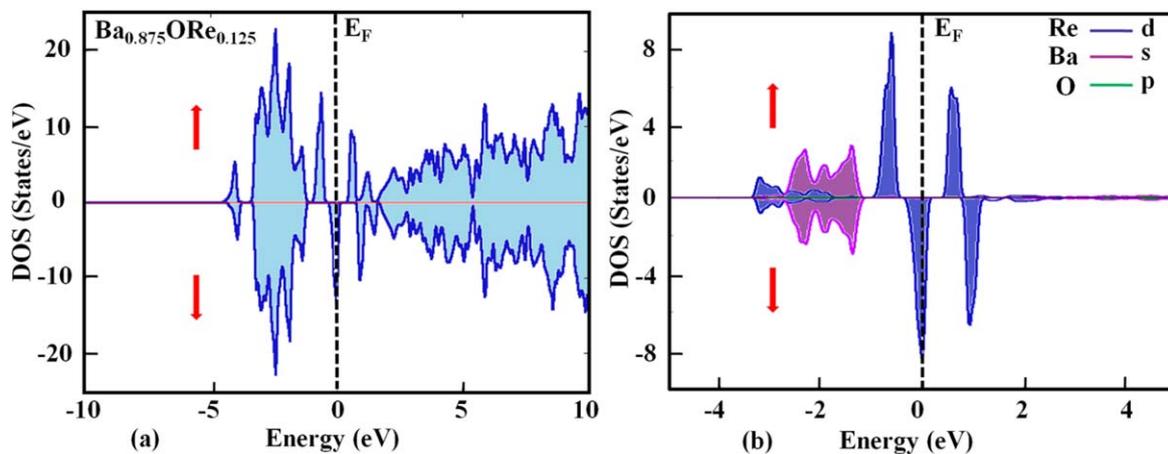


Figure 5. (a) TDOS and (b) PDOS of  $\text{Ba}_{0.875}\text{ORE}_{0.125}$ , spin (up- $\uparrow$ , down- $\downarrow$ ).

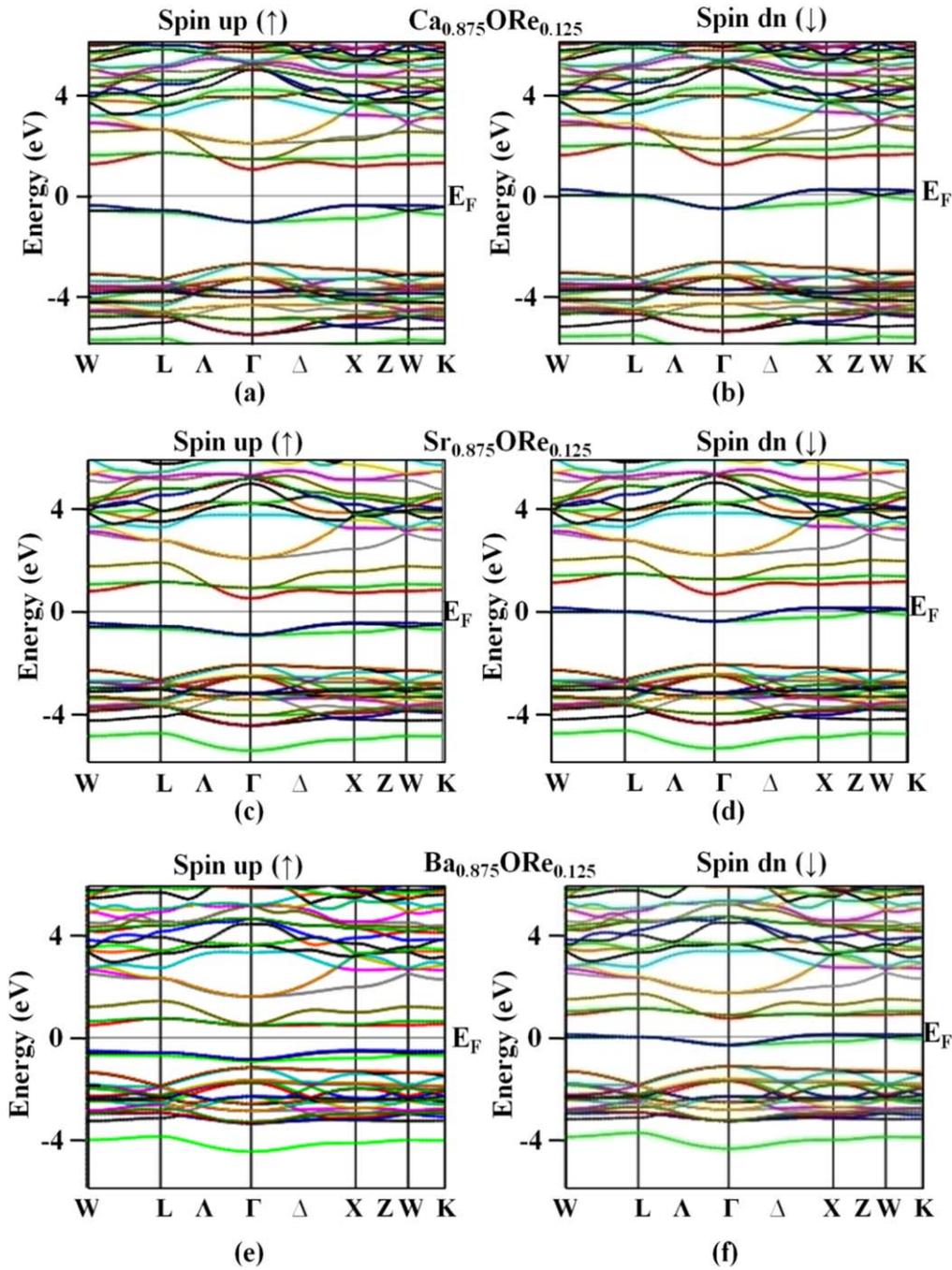
partial DOS of each supercell, the O-2p, Ca-3s, Sr-4s, and Ba-5s orbitals do not contribute directly towards the creation of the band gap in one of the spins. Therefore, half-metallicity in the compounds originates only from 5d Re orbitals.

Both spins of the electronic band structure (spin up and spin down) of the compounds  $\text{X}_{0.875}\text{ORE}_{0.125}$  ( $\text{X} = \text{Ca}, \text{Sr}, \text{Ba}$ ) are plotted and shown in figure 6. Band gaps have been found to occur in the spin up majority channel only, whereas the energy bands cross the Fermi level in the spin down minority channel predicting half-metallicity of the compounds  $\text{X}_{0.875}\text{ORE}_{0.125}$  ( $\text{X} = \text{Ca}, \text{Sr}, \text{Ba}$ ). The energy band gaps were determined between the highest symmetric valence bands at X and lowest symmetric conduction bands at  $\Gamma$ . All the three compounds (super cells)  $\text{X}_{0.875}\text{ORE}_{0.125}$  ( $\text{X} = \text{Ca}, \text{Sr}, \text{Ba}$ ) show indirect energy band gaps in (spin up) majority channel. These indirect band gaps were calculated and are given in table 2.

### 3.2. Magnetic properties

5d transition metal atoms (Re) substituted in alkaline earth oxides creates a magnetic moment in the supercells  $\text{X}_{0.875}\text{ORE}_{0.125}$  ( $\text{X} = \text{Ca}, \text{Sr}, \text{Ba}$ ). The total spin-magnetic

moment of the supercells including the contribution of each atom in creation of magnetic moment in the compounds (super cells) is given in table 3. The spin-magnetic moment of the host (un-doped) compounds (CaO, SrO, and BaO) is nearly about zero but the spin magnetic moment increases by doping of 5d transition metal atom Re in the supercells. The spin magnetic moment in compounds is due to spinning of electrons. The valence electronic configuration of the atoms is Ca-{Ar} 4s<sup>2</sup>, Sr-{Kr} 5s<sup>2</sup>, Ba-{Xe} 6s<sup>2</sup>, O-{He} 2s<sup>2</sup>, 2p<sup>4</sup> and Re-{Xe} 4f<sup>14</sup> 5d<sup>5</sup> 6s<sup>2</sup>. In super cells, the creation of magnetic moment is due to valence electrons. So from electronic configuration, it was observed that Re has more valence electrons as compared to other atoms which specify its effect would be more. The magnetic moment value is greater for Re atom in the super cell as compared to other atoms. So, it means that the transition metal atoms play an important role in producing magnetism in the alkaline earth oxides. 5d transition atom Re and oxygen have positive values while as alkaline earth atoms (Ca, Sr and Ba) tend to create negative magnetic moment values. Therefore, the transition metal atoms Re and oxygen (O) have a positive effect while the alkaline earth atoms append negative effect.



**Figure 6.** Band structures of  $\text{Ca}_{0.875}\text{ORe}_{0.125}$  (a)  $\uparrow$  (b)  $\downarrow$ ,  $\text{Sr}_{0.875}\text{ORe}_{0.125}$  (c)  $\uparrow$  (d)  $\downarrow$  and  $\text{Ba}_{0.875}\text{ORe}_{0.125}$  (e)  $\uparrow$  (f)  $\downarrow$ .

**Table 2.** Band gaps of the undoped and doped compounds.

Compounds	Band gap-(eV)	Band gap-(eV) (Previous work)
CaO	3.85	3.66 <sup>a</sup> , 2.91 <sup>b</sup> , 15.5 <sup>c</sup>
SrO	3.53	3.33 <sup>a</sup> , 3.44 <sup>b</sup> , 12.8 <sup>c</sup>
BaO	2.14	2.12 <sup>a</sup> , 2.44 <sup>b</sup>
$\text{Ca}_{0.875}\text{ORe}_{0.125}$	1.5	—
$\text{Sr}_{0.875}\text{ORe}_{0.125}$	0.93	—
$\text{Ba}_{0.875}\text{ORe}_{0.125}$	1.1	—

<sup>a</sup> [43]

<sup>b</sup> [44]

<sup>c</sup> [45]

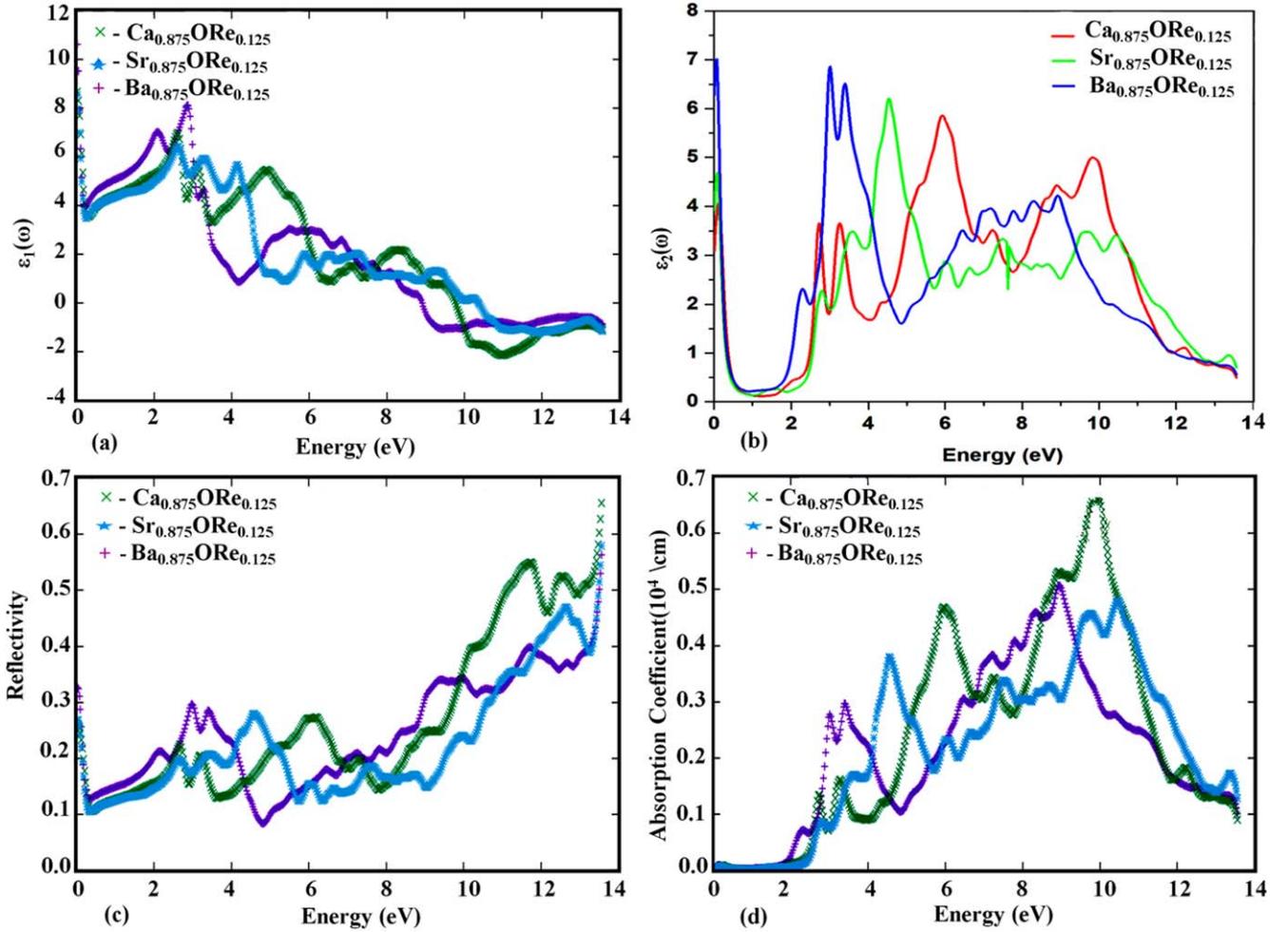
### 3.3. Optical properties of doped compounds

Optical properties of the materials are generally determined from the complex dielectric function

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega). \quad (1)$$

Wherein  $\varepsilon_1(\omega)$  is the real part of the dielectric function and  $\varepsilon_2(\omega)$  is the imaginary part of the dielectric function.

Dielectric function  $\varepsilon(\omega)$  offers two transitions, an intraband and an interband. However, in this study there is no addition of intraband transition contribution and only the interband contribution is prepended. Based on the DFT calculations, the imaginary part  $\varepsilon_2(\omega)$  can be determined by



**Figure 7.** (a) Real part  $\epsilon_1(\omega)$  of the dielectric function. (b) Imaginary part  $\epsilon_2(\omega)$  of the dielectric function. (c) Reflectivity and (d) absorption coefficient of  $X_{0.875}ORE_{0.125}$  (X = Ca, Sr, Ba) compounds.

**Table 3.** Spin magnetic moment ( $\mu_B$ ) of supercells  $X_{0.875}ORE_{0.125}$  (X = Ca, Sr, Ba).

Atoms in compounds	$Ca_{0.875}ORE_{0.125}$ ( $\mu_B$ )	$Sr_{0.875}ORE_{0.125}$ ( $\mu_B$ )	$Ba_{0.875}ORE_{0.125}$ ( $\mu_B$ )
Interstitial	0.16761	0.19183	0.14848
1 Re	0.73260	0.75303	0.84923
2 Ca/Sr/Ba	-0.00794	-0.00578	-0.00777
3 Ca/Sr/Ba	-0.00345	-0.00224	-0.00255
4 Ca/Sr/Ba	-0.00329	-0.00216	-0.00248
5 Ca/Sr/Ba	-0.00345	-0.00224	-0.00255
6 Ca/Sr/Ba	-0.00329	-0.00216	-0.00247
7 Ca/Sr/Ba	-0.00345	-0.00224	-0.00253
8 Ca/Sr/Ba	-0.00330	-0.00216	-0.00244
9 O	0.00102	-0.00034	0.00555
10 O	0.00102	-0.00034	0.00555
11 O	0.02094	0.01286	0.00089
12 O	0.02094	0.01286	0.00089
13 O	0.02094	0.01286	0.00093
14 O	0.02094	0.01286	0.00093
15 O	0.02095	0.01287	0.00092
16 O	0.02095	0.01287	0.00092
Total	0.99973	1.00237	0.99150

using below relation (2) and from which real part  $\varepsilon_1(\omega)$  of the dielectric constant could be calculated by applying Kramers–Kronig relation [46–48]:

$$\varepsilon_2(\omega) = \left(\frac{2\pi e}{m\omega}\right)^2 \frac{1}{\pi} \times \sum_{v,c} \left\{ \int_{BZ}^{BZ} d^3k |M_{cv}(k)|^2 \delta[E_c(k) - E_v(k) - h\omega] \right\} \quad (2)$$

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} p \int_0^\infty \frac{\omega_0 \varepsilon_2(\omega_0)}{\omega_0^2 - \omega^2} d\omega_0. \quad (3)$$

Having a good description of  $\varepsilon_2(\omega)$  (imaginary) part with energies, the  $\varepsilon_1(\omega)$  (real) part of the dielectric function can be calculated. In this work imaginary part as well as  $\varepsilon_1(\omega)$  (real) part of the dielectric function were determined within energy range 0–14 eV. Figures 7(a) and (b) show the  $\varepsilon_1(\omega)$  (real) and  $\varepsilon_2(\omega)$  (imaginary) parts of dielectric relation  $\varepsilon(\omega)$  for the compounds  $X_{0.875}ORe_{0.125}$  ( $X = Ca, Sr, Ba$ ). The peaks are seen in between the energy range 0–5 eV for real part  $\varepsilon_1(\omega)$  of dielectric function  $\varepsilon(\omega)$ . The highest peak values of  $\varepsilon_1(\omega)$  for compounds ( $Ba_{0.875}ORe_{0.125}$ ,  $Ca_{0.875}ORe_{0.125}$ ,  $Sr_{0.875}ORe_{0.125}$ ) are 10.8, 8.8 and 8.6. It has been observed from the graph of the real part  $\varepsilon_1(\omega)$  versus energy that  $\varepsilon_1(\omega)$  values decrease towards negative values which indicates that the electromagnetic wave (incident light) is entirely reflected within this region. The  $\varepsilon_2(\omega)$  (imaginary) part of the  $\varepsilon(\omega)$  (dielectric function) is an essential part which helps to measure the absorptive character, interband transitions and also defines the direct relationship with the band structure.

Reflectivity versus energy curves of the compounds ( $Ba_{0.875}ORe_{0.125}$ ,  $Ca_{0.875}ORe_{0.125}$ , and  $Sr_{0.875}ORe_{0.125}$ ) are shown in figure 7(c). It has been observed from the curves that the reflectivity values increases as the energy gets increased. From reflectivity curves the peak values are seen in between the energy range (12–14 eV) which means at higher energy, higher are the reflectivity values (peaks). Therefore, by increasing the energy from 0 to 14 eV the reflectivity would be more. As per the reflectivity curves, the peak values of the compounds are located at 13.6 eV and in this energy range 12–14 eV the absorption is less and compounds show the interband transition of the photons in this region.

Optical absorption has a direct relationship with the  $\varepsilon_2(\omega)$  (imaginary) part of the  $\varepsilon(\omega)$  (dielectric function). Figure 7(d) shows the plotted curves of absorption coefficient versus energy. High peak values of absorption coefficients for compounds  $Ba_{0.875}ORe_{0.125}$ ,  $Ca_{0.875}ORe_{0.125}$ , and  $Sr_{0.875}ORe_{0.125}$  are found to lie between energy ranges 9–11 eV. The absorption coefficient values increase to peak values as the energy increases to a high value. Then absorption coefficient values decreases after reaching peak value which suggests that optical absorption decreases and the reflectivity increases. Therefore, the doped compounds are predicted to exhibit both properties like absorption and reflectivity and such compounds can be used in optoelectronic devices.

## 4. Conclusion

A FPLAPW method has been used to examine the electronic structure, magnetic and optical properties of the alkaline earth oxides XO ( $X = Ca, Sr, Ba$ ) doped with 5d transition metal atom Re within the treatment of density functional theory. It has been found that doped compounds exhibit half-metallicity. The half-metallic property is clearly seen in the DOS and band structures of doped compounds  $X_{0.875}ORe_{0.125}$  ( $X = Ca, Sr, Ba$ ). From partial DOS of the doped compounds the contribution of 5d orbitals is observed which gives formation of band gaps in the spin up majority channel around the Fermi level. Total spin magnetic moment of the supercells  $Ca_{0.875}ORe_{0.125}$ ,  $Sr_{0.875}ORe_{0.125}$  and  $Ba_{0.875}ORe_{0.125}$  is given as  $0.99973\mu_B$ ,  $1.00237\mu_B$  and  $0.99150\mu_B$  respectively. The optical parameters dielectric constants (real and imaginary), reflectivity and absorption of the compounds have been calculated and shown. Compounds exhibiting electronic, magnetic and optical properties can be used in spintronics and optoelectronic applications.

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## Data availability

The authors of this research paper acknowledge the availability of data for all the scientific deliberations in this work.

## ORCID iDs

Nazir Ahmad Teli  <https://orcid.org/0000-0002-8909-1265>

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