

THE EFFECT OF TRANSITION METAL ON OPTOELECTRONIC PROPERTIES OF DOUBLE PEROVSKITE $\text{Sr}_2\text{CrZrO}_6$

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In this paper, we have investigated the structural, electronic, magnetic and optical properties of cubic double perovskite $\text{Sr}_2\text{CrZrO}_6$ by using the full-potential linearized augmented plane wave method (FP-LAPW), based on the density functional theory (DFT) as implemented in the WIEN2K code. The exchange correlation potentials is treated by the generalized gradient approximation (GGA), GGA+U where U is on-site coulomb interaction correction as well as modified Becke–Johnson (mBJ) which have been used to correct the potential. Calculations were performed with the Birch-Murnaghan approach to determine the equilibrium phase, lattice, bulk modulus and its pressure derivative. The results display a half-metallic ferromagnetic ground state for the cubic double perovskite $\text{Sr}_2\text{CrZrO}_6$ compound due to the strong correlation effect of transition metal Cr (3d) states with the integer value of the total magnetic moment. Furthermore, we found a direct gap (Γ - Γ) around the Fermi level, making the $\text{Sr}_2\text{CrZrO}_6$ a competent candidate for optoelectronic and spintronic applications.

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1. Introduction

Oxide half metals materials characterized by the presence of single spin direction in the Fermi level either parallel or anti-parallel to the magnetization direction have been extensively investigated due to their potential applications in the novel generation of Spin Electronics. The Half-metal (HM) materials include; Mn-doping GaAs [1, 2], rutile CrO_2 [3], spinel FeCr_2S_4 [4] and important broad class of compounds had been known as double perovskite oxides. Which have been studied since 1961s when a ferromagnetic behavior of Re-based double perovskites was reported by Longo and Ward [5]. Recently, many theoretical as well as experimental investigations were betaking to study this family of double perovskite compounds. Because the variety that, they reveal various fascinating properties such as ferroelectricity [6- 9], charge ordering, colossal magnetoresistance and superconductivity [10]. This diversity provide prospective applications in spintronic devices [11], magnetic recording [12], high-efficiency magnetic sensors [13- 15], tunnel junction [16] and solar energy. So the possible spin-electronics applications arising from the electronic structure make them a challenging subject of investigation.

The double perovskites have a general formula of $\text{A}_2\text{BB}'\text{X}_6$, where A= alkaline-earth or rare-earth metal, B and B' are different transition metals and X= oxygen or halogen [16- 20]. Their crystal structure takes the rock-salt (Na^+Cl) form [21] with a large A-cation resides in the 12 coordinate cuboctahedral hole formed by the corner-sharing $(\text{B},\text{B}')\text{X}_6$ octahedral network [22- 24]. Among these interesting family, Strontium-based compounds which are the most promising ones displaying HM behavior. At this stage, there has been a Considerable work involving both experimental and theoretical methods on $\text{Sr}_2\text{FeMoO}_6$ [15, 25- 27], $\text{Sr}_2\text{CrMoO}_6$ [27], $\text{Sr}_2\text{CrReO}_6$ [28, 29] and Sr_2CrWO_6 [25, 30]...etc. But to the best of our knowledge, up to now, very little research clarified the crystal structures, electronic and magnetic properties of $\text{Sr}_2\text{CrZrO}_6$ [12, 22] by using

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first-principles studies. Therefore, in this paper, extra calculations were done to determine the magnetic stable phases, electronic and optical properties of $\text{Sr}_2\text{CrZrO}_6$ by using the generalized gradient approximation (GGA), GGA+U as well as modified Becke-Johnson (mBJ) potential. Our results show that the magnetic phase of the compound is found to be ferromagnetic (FM) and has half metallic (HM) band structure with an energy gap of 3.359 eV computed within the mBJ corrections, which give energy gap much close to the experimental values [31]. For the optical properties, the absorption zone extended along the energy interval of E(8 to 100 eV) corresponds to λ (12,39 to 154 nm) confirms its suitability for device applications in the ultra-violet (UV) spectrum.

2. Calculation method and models

The calculation of the electronic, optical and magnetic properties of the cubic double perovskite $\text{Sr}_2\text{CrZrO}_6$ compound, were performed using the full-potential linearized augmented plane wave method (FP-LAPW), based on the density functional theory (DFT) as implemented in WIEN2K code [32, 33]. The calculations of these properties are based on the self-consistent scheme by solving the Kohn-Sham equation. The exchange correlation potential was calculated within the generalized gradient approximation (GGA) [34] as well the GGA+U approximations, and by including the modified Becke-Johnson (mBJ) corrections of the potential [35] which have improved efficiently the computations of electronic and optical properties [36]. The non-overlapping muffin-tin radii (RMT) were considered to be 2.5, 1.85, 1.96 and 1.67 a.u (atomic unit) for the Sr, Cr, Zr and O atoms, respectively. The maximum angular momentum inside the muffin-tin sphere was confined to $l_{\text{max}}=10$. The cutoff parameter $R_{\text{mt}}*K_{\text{max}}$ was set to 7, where R_{mt} denotes the smallest atomic sphere radius and K_{max} is the maximum value of the wave vector K . Fourier expanded charge density was truncated at $G_{\text{max}}=12$. The number of K-points was performed at 2000 in the irreducible wedge of the Brillion zone (BZ). Concerning the structural part, the $\text{Sr}_2\text{CrZrO}_6$ double perovskite compound crystallizes in the cubic structure with space group $\text{Fm}\bar{3}\text{m}(225)$. And the atomic positions are: Sr (0.25,0.25,0.25) and (0.75, 0.75, 0.75) successive, Cr (0, 0,0), Zr (0.5, 0, 0), O (0.25, 0, 0), (0, 0.25, 0) and (0,0,0.25) (see fig.1 and 2). The formal oxidation states of Cr and Zr ions in $\text{Sr}_2\text{CrZrO}_6$ compound are 4+ oxidation states with Cr: $(\text{Cr}^{4+}(3d^2: t_{2g}^2 e_g^0))$ and Zr: $(\text{Zr}^{4+}(4d^0: t_{2g}^0 e_g^0))$ electronic configurations [12, 22]. We used the values of $U= 4\text{eV}$ and $J=0.97\text{ eV}$ [37- 43], in GGA+U calculation for the strongly correlated Cr (3d) where the U and J are on-site coulomb repulsion term and exchange term with the Hubbard U and Hund exchange J parameters, respectively [36].

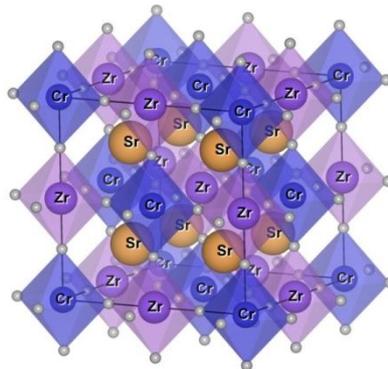


Fig.1. Crystal structure of double perovskite $\text{Sr}_2\text{CrZrO}_6$ compound

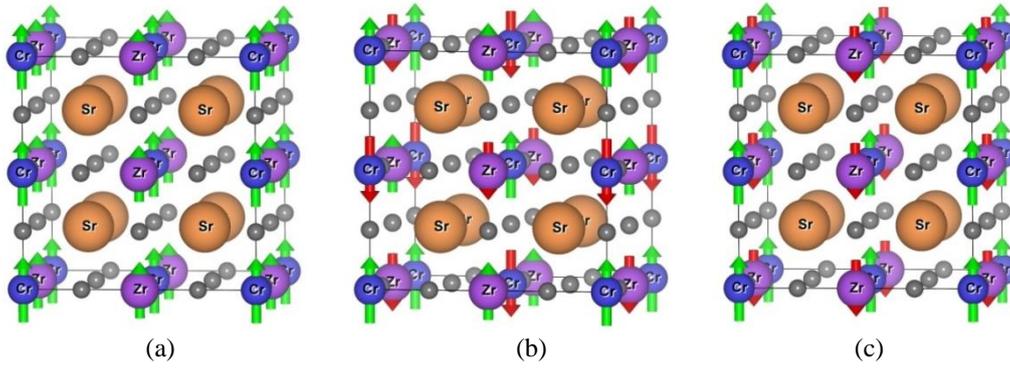


Fig. 2. Magnetic configurations: (a) ferromagnetic phase (FM), (b) antiferromagnetic phase (AFM) and (c) Ferrimagnetic phase (FiM)

3. Results and Discussions

3.1. Structural properties

We have calculated the total energy versus crystal unit cell volume with respect to the atomic positions, using both approximations GGA and GGA + U. We have found, that the FM states of $\text{Sr}_2\text{CrZrO}_6$ compound is more stable than the AFM and FiM state in both approximations GGA and GGA+U (see fig.3), the negative value of the total energy difference where $\Delta E = E_{\text{FM}} - E_{\text{X}}$ with X=AFM and FiM, indeed the $\text{Sr}_2\text{CrZrO}_6$ compound is ferromagnetic (FM) see Table.1. In order to obtain the equilibrium lattice constant and the bulk modulus for the cubic $\text{Sr}_2\text{CrZrO}_6$ in ferromagnetic phase (FM), we performed the structural optimization with minimizing the total energy by iteratively solving the Birch-Murnaghan equation of state [44] which is given as follows:

$$E(V) = E_0 + \frac{VB}{B_p} \left[\frac{(V_0/V)^{B_p}}{(B_p - 1)} + 1 \right] - \frac{BV_0}{(B_p - 1)}$$

Where: $E(V)$ represents the energy of the ground state with a cell volume V .

V_0 : is the volume in the ground state.

E_0 : is the total energy balance.

B, B_p : are bulk modulus and its derivative for the pressure.

The results for the lattice parameters, bulk Modulus, pressure derivative and the energy difference are shown in Table.1.

Table1: Calculated resultants (equilibrium lattice parameters: $a(\text{\AA})$, bulk modulus B (GPa), its pressure derivative (B') and energy difference ΔE (mev) of double perovskite $\text{Sr}_2\text{CrZrO}_6$ obtained with GGA and GGA+U.

Parameters	Approximations	a (\AA)	B (GPa)	B'	ΔE (mev)
Our work	GGA	8.0761	156.7743	4.6246	FM-AF= -13 FM-FiM= -12
	GGA+U	8.0672	156.5292	4.9865	FM-AF =2.3 FM-FiM=1.2
Other calculations	GGA+U[12]	/	/	/	-70.8
	SOC	/	/	/	-70.0
	[22]	8.0630			

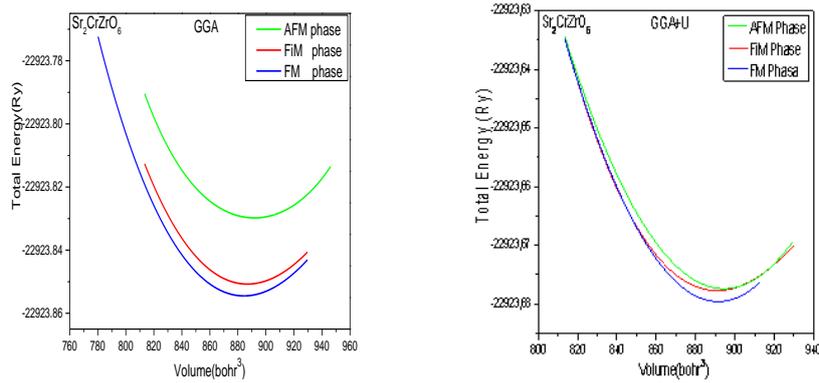


Fig. 3. Total energy change as a function of cell volume in : FM, AFM and FiM phase, using the GGA and GGA+U approximation

3.2. Electronic properties

3.2.1. Band Structure

In this part of our work, we have studied the electronic properties of Sr₂CrZrO₆ by calculating the band structure using GGA, GGA+U and mBJ approximations. Fig.4 shows the band structure of Sr₂CrZrO₆ compound for spin up and spin down channels, respectively, for an energy range between -6 and 10 (eV). In the energy interval between -1 and 1 eV, some spin-up bands cross the Fermi level (E_f). We can see also that the valence band maximum and the conduction band minimum of the spin down are located at the Γ point in the Brillouin zone, so Sr₂CrZrO₆ compound has a direct pseudo band gap ($\Gamma - \Gamma$) with different values 2.028 eV, 2.887 eV and 3.359eV for GGA, GGA+U and mBJ, respectively. From the obtained results we can conclude that this compound exhibits a Half-metallic behavior and that the U Hubbard correlation in the GGA+U influences the position of the electronic states giving a large band gap than GGA approximation [11]. The energy band gap computed by the mBJ give better results compared to GGA and GGA+U approximations and to other theoretical results using Castep code, which they found similar values ($E_g = 2.008\text{eV}$) [12].

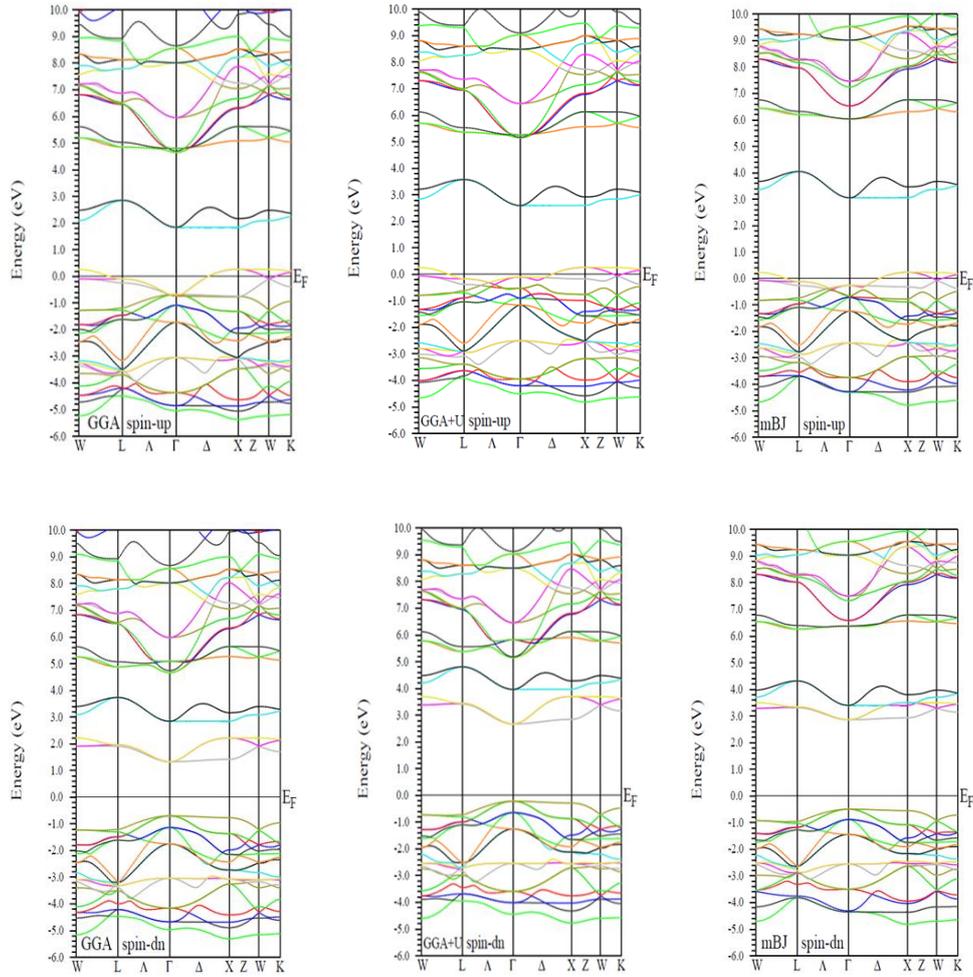


Fig. 4: Band structure for double perovskite $\text{Sr}_2\text{CrZrO}_6$ compound with approximations GGA, GGA+U and mBJ.

3.2.1. Density of states (DOS)

To view the contribution of the different states of electron for $\text{Sr}_2\text{CrZrO}_6$ compound in the band structure, the total and partial density of states using the GGA, GGA + U and mBJ approximations are shown in fig.5 respectively. The DOS of $\text{Sr}_2\text{CrZrO}_6$ shows half-metallic behavior in good agreement with previously reported calculations [12, 22]. Hence, our calculations show the half metallic behavior in $\text{Sr}_2\text{CrZrO}_6$ compound for each approximation GGA, GGA+U and mBJ. We can see clearly the metallic behavior of $\text{Sr}_2\text{CrZrO}_6$ in spin-up, because the overlap between the valence and the conduction band by the Cr- t_{2g} orbital, however, in spin-down the $\text{Sr}_2\text{CrZrO}_6$ has an insulating behavior. The Dos in the region between -5eV and Fermi level, is dominated by the O-2p states and the conduction band region is mainly composed by the doubly degenerate e_g of Cr (Cr- d_{eg}) and by the triply, doubly degenerate of Zr (Zr- t_{2g} and Zr- eg) states. On the other hand the contribution of Sr (3d) is clear in this region.

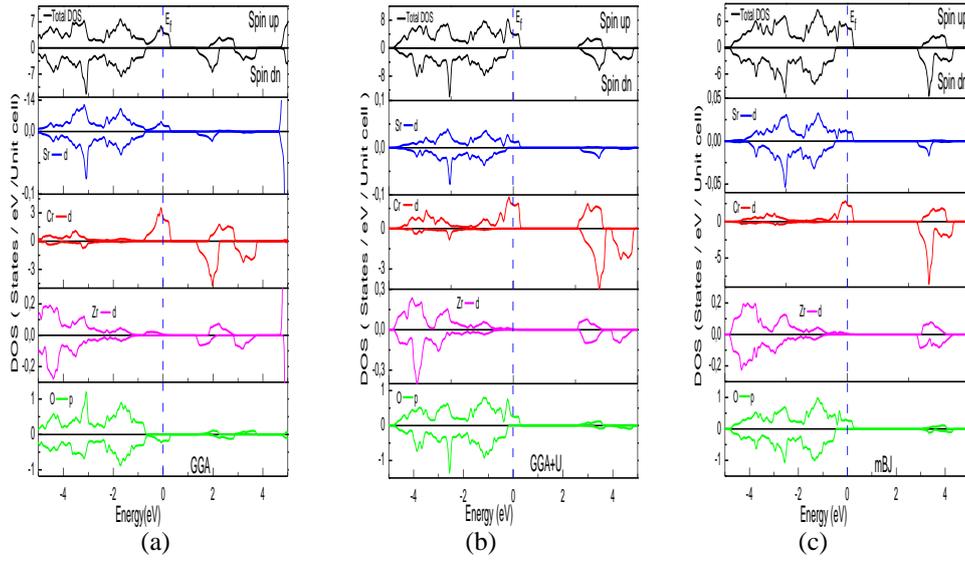


Fig.5: Total and partial density of states for double perovskite $\text{Sr}_2\text{CrZrO}_6$ compound
(a) GGA, (b) GGA+U, (c) mBJ approximations

3.3. Magnetic properties

The magnetic moment in Bohr Magneto (μ_B) of Sr, Cr, Zr and O atoms, as well as the total and interstitial magnetic moment for each approximations GGA, GGA+U and mBJ are shown in table.2. The stable magnetic state of $\text{Sr}_2\text{CrZrO}_6$ is calculated on the basis of optimization for each configuration magnetic; ferromagnetic (FM), anti-ferromagnetic (AFM) and ferrimangetic (FiM), whereas for the self-consistent field (SCF) FM, AFM, and FiM, the calculations have been performed by double cell. So, the spin of Cr and Zr are paralleled in FM configuration, but in AFM configuration, the spin of one Cr and Zr atoms is set up while the other spin is down, for FiM configuration, the moments of Cr and Zr are antiparallel and of different magnitude (fig.2). We found the stable ground state energy in ferromagnetic (FM) system comparing to anti-ferromagnetic and ferromagnetic states. See (table.1 and fig.3), this ferromagnetism observed in cubic $\text{Sr}_2\text{CrZrO}_6$ double perovskite is created by the double exchange mechanism [11, 36]. The total magnetic moment of $\text{Sr}_2\text{CrZrO}_6$ compound have integer values using GGA, GGA+U and mBJ, which confirms the half metallic nature of our compound.

Table2: Moment magnetic (in Bohr Magneto μ_B) for several sites of double perovskite $\text{Sr}_2\text{CrZrO}_6$ using GGA, GGA+U and mBJ approximations. And compared with orther calculations

Site	GGA	GGA+U	mBJ	Other calculations	
				[12]	[22]
μ^{Sr}	0.002	0.002	0.003	/	/
μ^{Cr}	1.863	2.141	2.043	1.904	2.80
μ^{Zr}	0.008	0.009	0.020	0.034	-0.022
μ^{O}	-0.028	-0.070	-0.062	/	/
μ^{int}	0.029	0.276	0.303	/	/
μ^{cell}	1.999	2.009	2.000	2.000	/

3.4 optical properties

In order to know the different ways which light interacts with the double perovskite $\text{Sr}_2\text{CrZrO}_6$ compound we have presented the optical properties, based on the complex dielectric function: $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$, to describe the polarization response of the material to an

electromagnetic radiation. Where ω is the angular frequency and $\epsilon_1(\omega)$, $\epsilon_2(\omega)$ are the real and imaginary parts of $\epsilon(\omega)$, respectively. Kramers-Kronig relation is used to calculate the real and imaginary parts of dielectric function $\epsilon(\omega)$ [11]. Several optical properties such as absorption coefficient $\alpha(\omega)$ and reflectivity $R(\omega)$ can be calculated based on the complex dielectric function [45]:

$$\alpha(\omega) = \frac{2\pi\omega}{c} \sqrt{\frac{-R_e(\omega) + |\epsilon|}{2}} \quad (1)$$

$$R(\omega) = \frac{(n-1)^2 + K}{(n+1)^2 + k} \quad (2)$$

The absorption coefficient $\alpha(\omega)$ and reflectivity $R(\omega)$ were calculated at the equilibrium lattice constant using GGA, GGA+U and mBJ approximations. In fig.6 and fig.7 we have plotted the computed results for $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ for both directions of spin respectively, from fig.6 we can observe that some peaks decreases to the minimum values, with negative numbers in the low energies localized at 0.65eV and 1.52eV for GGA+U and GGA approximation respectively for the spin-up, in other direction of the spin this peaks are localized at 25.20 eV, 24.5 eV and 24.9 eV for GGA, GGA+U and mBJ respectively. The negative values of $\epsilon_1(\omega)$ correspondent the energy region show the entirely reflected with the incident electromagnetic waves, so the $\text{Sr}_2\text{CrZrO}_6$ material shows metallic behavior [11]. The computed results for the imaginary part $\epsilon_2(\omega)$ are shown in fig.7. This imaginary part determines the absorption properties of the $\text{Sr}_2\text{CrZrO}_6$ material. The calculated imaginary part exhibit three peaks in the spin down, the first is localized at 8eV, 7.28 eV and 4.6 eV for GGA, GGA+U and mBJ respectively, the second is limited in 24.98 eV, 24.2 eV and 23.9 eV for GGA, GGA+U and mBJ respectively and the third occurs on energy equal 32.31eV, 31.6 eV and 31.84 eV for GGA, GGA+U and mBJ respectively. These peaks are affected by the transition from the valance band (VB) to the conduction band (CB) [44].

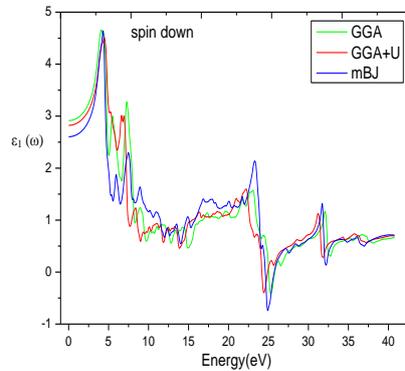


Fig.6: Real party (ϵ_1) of dielectric functions of double perovskite $\text{Sr}_2\text{CrZrO}_6$ for spin spin down.

The results of absorption coefficient are displayed in Fig.8 for different directions of spin. It is clearly seen that the absorption near to 3.35eV (fundamental absorption), corresponds to the electronic transitions from the valance band (VB) to the conduction band (CB). The $\text{Sr}_2\text{CrZrO}_6$ double perovskite compound has robust absorption in two regions, the first between [22.44 eV, 26.55 eV] and the second between [31.06 eV, 33.12eV]. In the region between [3.35 eV, 22.44 eV] we observe the appearance of different peaks from different electronic transitions. So, the $\text{Sr}_2\text{CrZrO}_6$ double perovskite compound is appropriate for device applications in the major part of the spectrum, especially in ultraviolet.

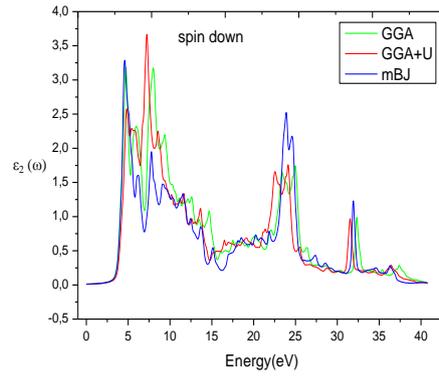


Fig. 7. Imaginary party (ϵ_2) of dielectric functions of double perovskite Sr_2CrZrO_6 for spin down.

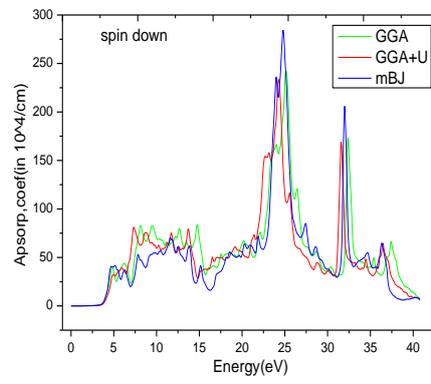


Fig.8. Absorption coefficient of double perovskite Sr_2CrZrO_6 for spin-down.

Fig. 9 displays the computed results of optical reflectivity $R(\omega)$, from this curve, the reflectivity reaches a maximum values in the energy range between [22.29 eV, 27.11 eV] through 38.91% for spin down and different peaks can also be observed in other regions, from 3.35 to 22.29 eV and from 29.11 to 39.65 eV.

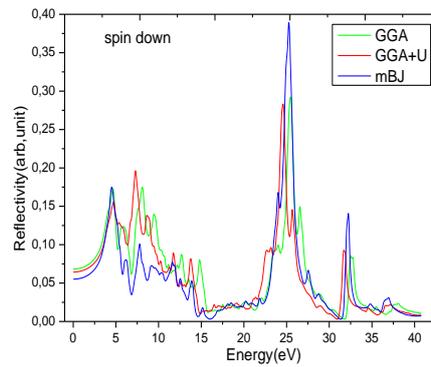


Fig.9: The reflectivity of double perovskite Sr_2CrZrO_6 for spin-down

4. Conclusion

In the present work, we have investigated the structural, electronic, magnetic and optical properties of the cubic double perovskite Sr_2CrZrO_6 , using the GGA, GGA+U and mBJ

approximations based on FP-LAPW method as implemented in the WIN2K code. The structural, electronic and magnetic properties are in a good agreement with other calculations. We obtain a direct gap (Γ - Γ) around the Fermi level for the spin down direction, whereas for the spin up direction there is an overlapping of the valence band and the conduction one, for each approximation GGA, GGA+U and mBJ. The half-metallic nature of this compound is observed.

The densities of states and magnetic properties show that $\text{Sr}_2\text{CrZrO}_6$ is ferromagnetic by the double exchange mechanism. Finally, the results of the dielectric function, optical reflectivity and absorption coefficient confirm undoubtedly the usefulness of the cubic double perovskite $\text{Sr}_2\text{CrZrO}_6$ compound for different applications in the ultraviolet spectrum.

References

- [1] M. Shirai, T. Ogawa, I. Kitagawa, N. Suzuki, *J. Magn. Magn. Mater.* **177–181**, 1383 (1998).
- [2] J.H. Park, S.K. Kwon, B.I. Min, *Physica B* **281–282**, 703 (2000).
- [3] K. Schwarz, *J. Phys. F: Met. Phys.* **16**, L211 (1986).
- [4] M.S. Park, S.K. Kwon, S.J. Toun, B.I. Min, *Phys. Rev. B* **59**, 10018 (1999).
- [5] J. Longo and R. Ward, *J. Am. Chem. Soc.* **83**, 2816 (1961).
- [6] J.G. Bednorz, K.A. Muller, *Phys. Rev. Lett.* **52**, 2289 (1984).
- [7] S.M. Yang, S.J. Moon, T.H. Kim, Y.S. Kim, *Curr. Appl. Phys.* **14**(5)(2014) 757–760.
- [8] A. S. Milošević, V. M. Lalić, S. Zoran, S. Popović, F. R. Vukajlović, *Opt. Mater.* **35**(10), 1765 (2013).
- [9] H. F. Li, G. H. Zhang, Y. Zheng, B. Wang, W. J. Chen, *Acta Mater.* **76**(1), 472 (2014).
- [10] Z. Ali, Iftikhar Ahmad, B. Amin, M. Maqbool, G. Murtaza, I. Khan, M. J. Akhtar, F. Ghaffor. *Physica B* **406**, 3800 (2011).
- [11] B. Bouadjemi, S. Bentata, A. Abbad, W. Benstaali. *Solid State Communications* **207**, 9 (2015).
- [12] Y. P. Liu, H. R. Fuh, Z. R. Xiao, Y. K. Wang. *Journal of Alloys and Compounds* **586**, 289 (2014).
- [13] J. H. Park, E. Vescovo, H. J. Kim, C. Kwon, R. Ramesh, T. Venkatesan, *Nature (London)* **392**, 794 (1998).
- [14] W.E. Pickett, J.S. Moodera, *Phys. Today* **54**, 39 (2001).
- [15] K.I. Kobayashi, T. Kimura, H. Sawada, K. Terakura, Y. Tokura, *Nature (London)* **395**, 677 (1998).
- [16] C. M. Bonilla, D. A. Landinez, J. Arbey, E. Vera Lopez, J. Roa-Rojas, *Phys. B* **398**, 208 (2007).
- [17] Q. Zhang, Z.F. Xu, J. Liang, J. Pei, H.B. Sun. *Journal of Magnetism and Magnetic Materials* **354**, 231 (2014).
- [18] Guoyan Huo, Xin Ren, Lili Qian, Ning Zhang, Shuang Liu, Xu Yan. *Journal of Magnetism and Magnetic Materials* **343**, 119 (2013).
- [19] J. Cheng, Z.Q. Yang, *Phys. Status Solidi B* **243**(6), 1151 (2006).
- [20] Hong-Tay-Jeng, G.Y. Guo, *Phys. Rev. B* **67**, 094438 (2003).
- [21] M. Musa Saad H.-E, M. El-Hagary. *Journal of Magnetism and Magnetic Materials* **360**, 229 (2014).
- [22] Salah Eldin Ashamallah Yousif, O.A. Yassin. *Physica B* **406**, 2038 (2011).
- [23] A. Souidi, S. Bentata, W. Benstaali, B. Bouadjemi, A. Abbad, T. Lantri. *Materials Science in Semiconductor Processing* **43**, 196 (2016).
- [24] Hong-Tay-Jeng, G.Y. Guo, *Phys. Rev. B* **67**, 094438 (2003). *Deng. Solid State Communications* **191**, 70 (2014).
- [25] H.T. Jeng, G.Y. Guo, *Phys. Rev. B* **67**, 094438 (2003).
- [26] T.S. Chan, R.S. Liu, G.Y. Guo, S. F. Hu, J.G. Lin, J.M. Chen, C.-R. Chang, *Solid State Commun.* **133**, 265 (2005).
- [27] Wu. Hua, *Phys. Rev. B* **64**, 125126 (2001).
- [28] H. Kato, T. Okuda, Y. Okimoto, Y. Tomioka, *Phys. Rev. B* **69**, 184412 (2004).

- [29] C.Q. Tang, Y. Zhang, J. Dai, Solid State Commun. **133**, 219 (2005).
- [30] J.B. Philipp et al., Phys. Rev. B **68**, 144431 (2003).
- [31] S. Menezla, A. Kadri, K. Zitouni, A. Djelal, M. Djrmouni, A. Hllouche, A.Zaaoui. Super lattices and Microstructures **88**, 18 (2015).
- [32] K. Schwarz and P. Blaha, Computational Materials Science. **28**, 259 (2003).
- [33] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, J. Luitz, WIEN2K-An Augmented plane wave & Local Orbital Program for Calculating Crystal Properties (Techn. Universitat Wien, Austria, 2001).
- [34] J.P. Perdew, et al, Phys.Rev.Lett. **100**, 136406 (2008).
- [35] F. Tran, P. Blaha, Phys. Rev. Lett. **102**, 226401 (2009)
- [36] A. Abbad, W. Benstaali, H. A. Bentounes, S. Bentata, Y. Benmalem, solid state communications **228**, 36 (2016).
- [37] R. Von Hemlholt, J. Wecker, B. Holzapfel, L. Shultz, K. Samwer, Phys. Rev. Lett. **71**, 2331 (1994).
- [38] Hua Wu, Phys. Rev.B **64**, 125126 (2001).
- [39] Horng-TayJeng, G.Y. Guo, Phys. Rev. B **67**(094438), 1 (2003).
- [40] C.Q. Tang, Y. Zang, J. Dai, Solid State Commun. **133**, 219 (2005).
- [41] Q.F. Li, X.F. Zhu, L.F. Chen, J. Phys. Condens. Matter **20**(255230), 1 (2008).
- [42] A. Ciucivara, B. Sahu, L. Kleinman, Phys. Rev. B **76**, 064412 (2007).
- [43] L. Bi, A.R. Taussig, H. Kim, L. Wang, G.F. Dionne, D. Bono, K. Persson, Phys. Rev. B **78**, 104106 (2008).
- [44] F. D. Murnaghan, Proc. Natl. Acad. Sci. USA **30**, 5390 (1994).
- [45] A. Meziani, D. Heciri, H. Belkhir. Physic B **406**, 3646 (2011).