

Exploring the structural, electronic, magnetic, and magneto-optical properties of double perovskites $\text{Ca}_2\text{TMIrO}_6$ (TM=Fe, Co) through first principles study

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This study is aimed at exploring the electronic, magnetic, and magneto-optical properties of double perovskites $\text{Ca}_2\text{FeIrO}_6$ and $\text{Ca}_2\text{CoIrO}_6$ with monoclinic structure (space group $P21/c$) in order to examine their potential applications in spintronic and photovoltaic devices. The calculations were done using the full-potential linearized augmented plane wave within the density functional theory. For the electronic exchange-correlation function, we used the generalized gradient approximation (GGA) and GGA+U (Hubbard potential), and spin-orbit coupling (SOC). The study showed that $\text{Ca}_2\text{FeIrO}_6$ and $\text{Ca}_2\text{CoIrO}_6$ exhibit a monoclinic structure (space group $P21/c$). The structure relaxation shows an antiferromagnetic behavior in both systems with a magnetic moment of about $6.00\mu_B$ for $\text{Ca}_2\text{FeIrO}_6$ and $4.00\mu_B$ for $\text{Ca}_2\text{CoIrO}_6$ by using GGA+U approximation. The results of GGA and GGA+U predict the half-metallic behavior of $\text{Ca}_2\text{FeIrO}_6$ and $\text{Ca}_2\text{CoIrO}_6$. The magneto-optical polar Kerr effect (MOKE) was examined by studying the variation of Kerr and ellipticity rotation. The Kerr rotation angle is 1.3° at 4.82 eV and -1.21° at 4.3 eV, and the ellipticity angle is -1.21° at 4.3 eV for $\text{Ca}_2\text{FeIrO}_6$. In the case of $\text{Ca}_2\text{CoIrO}_6$, the Kerr rotation angle is -1.04° at 4.05 eV; the significant Kerr rotation in both compounds may suggest the application of these materials in optoelectronics bias. The named compounds have a potential application in the field of spintronics and its devices, such as in optoelectronics technologies.

Key words: double perovskites, Kerr effect, optical properties, wien2k

1. Introduction:

Since the fifties of the last century, double perovskite has been the subject of many studies; the interest in these materials is due to the important electronic and magnetic properties that range from metallic, insulator, semi-conductor, superconductor to half-metallic that were discovered in $\text{Sr}_2\text{FeMoO}_6$ compounds [2, 3]. Double perovskites show significant magnetic properties. The coupling between electronic and magnetic properties, such as half metallicity with antiferromagnetic behavior, is of great interest, allowing them to be the most promising and critical multifunctional materials for use in the new generation of spintronics or optoelectronics and its devices [4]. Double-perovskite oxides have the general formula $\text{A}_2\text{B}'\text{B}''\text{O}_6$, where A is an alkaline-earth or rare-earth metal ion; B-site cations, B' and B'', are transition metals [5]. The ideal structure of double perovskite is cubic, such as in $\text{Ba}_2\text{NiOsO}_6$ [5] $\text{Ba}_2\text{TMIrO}_6$ (TM=Cr, Mn, and Fe) [7] and Ba_2BRuO_6 (B=Er, Tm) [8]. However, the small-size radius of the cation A compared with the radius size of the other ions has an important effect on the structural properties of the material. When the A-site cation radius is smaller than the ideal, the structure compensates for the cation size mismatch by tilting and rotating the $\text{B}'\text{O}_6$ and $\text{B}''\text{O}_6$ octahedral. This property is observed in many compounds with Ca, Sr, and La cations in the A-site and of monoclinic structure:

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Ca_2MnWO_6 [9], Sr_2YRuO_6 [10], Sr_2MReO_6 ($\text{M}=\text{Sc}, \text{Mn}$), Ca_2MReO_6 ($\text{M}=\text{Co}, \text{Cr}, \text{Fe}, \text{Mn}$) [11] and La_2BIR_6 ($\text{B}=\text{Mg}, \text{Mn}, \text{Co}, \text{Ni}, \text{Cu}$) [12]. Double perovskites can show both ferromagnetic (F) and antiferromagnetic (AF) behavior. This can be explained mainly by the super-exchange interaction between the neighboring transition metal ions B and B' via oxygen ions according to the Goodenough–Kanamori rule [13, 14]. Xuedong et al. [15] found that the second nearest-neighboring (2NN) Ir-Ir antiferromagnetic coupling is even stronger than the first nearest-neighboring (1NN) Ni-Ir in double perovskites $\text{Sr}_2\text{NiIrO}_6$ and $\text{Sr}_2\text{ZnIrO}_6$. $\text{Ca}_2\text{FeIrO}_6$ was synthesized by Bufaial et al. [16]. Using experiments of magnetic susceptibility and X-ray powder diffraction, they found that the $\text{Ca}_2\text{FeIrO}_6$ compounds form in a monoclinic structure, space group P21/n , with the antiferromagnetic ground state. The theoretical study using the density functional theory was done by Bhandari et al. [17], which predicts that the material should have a band gap of 0.13 eV and a significant effective magnetic moment of $6.68\mu_B$ per unit cell. Our work is aimed at studying the structural, electronic and magneto-optical properties for the monoclinic structure of double perovskites $\text{Ca}_2\text{TMIrO}_6$ ($\text{TM}=\text{Fe}, \text{Co}$).

2. Computational details

The full potential linear augmented wave method (FP-LAPW) within the first principles density functional theory (DFT) implemented in the WIEN2k program [18] was applied to determine the structural, electronic, and magnetic properties of $\text{Ca}_2\text{TMIrO}_6$ ($\text{TM}=\text{Fe}, \text{Co}$). The exchange-correlation potential was described using the PBE96 form of the generalized gradient approximation (GGA) [19, 20]. The muffin-tin radii used were 2.07, 1.99, 1.99, 1.93, and 1.58 for Ca, Co, Fe, Ir, and O, respectively; we used 1000 k -points (230 k -points in the irreducible Brillouin zone), the value of separation energy is 7.180 Ry. The cut-off parameters are $\text{RMT} - k_{\text{max}} = 7$ and $\text{RMT} - G_{\text{max}} = 12$. To explore the effect of spin-orbit coupling and on-site Coulomb repulsion, (DFT+SO) and (DFT+SO+U) were introduced. The added Hubbard potential U was used with $U = 1.5$ eV for Ir and $U = 4$ eV for Co [21] and $U = 5$ eV for Fe [17]. The convergence criterion for the self-consistent calculation was 0.0001 Ry for the total energies.

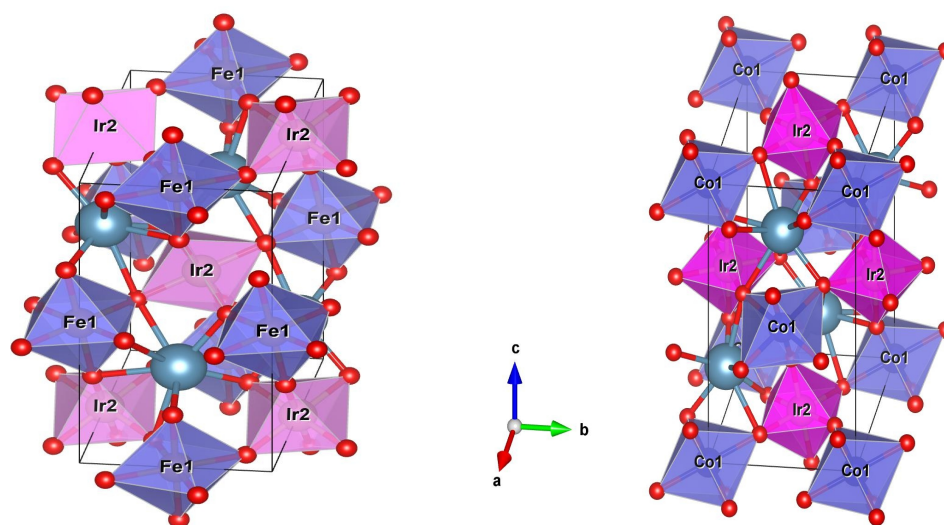


Figure 1. (Colour online) Crystal structure of double perovskite $\text{Ca}_2\text{TMIrO}_6$ ($\text{TM}=\text{Fe}, \text{Co}$).

3. Results and discussion

3.1. Structural properties

To investigate various physical properties of these compounds, we determine the stable ground states by studying the energy variation as a function of its unit cell volume. The results of the relaxation for

lattice constants and volume for both compounds are summarized in table 1, where we see that the ferrimagnetic (FIM) ground state is the most stable since the corresponding energy is minimum. As far as we know, this is the first study of these samples with a space group (P21/c), whereas the recent other works [16, 17, 21] have explored similar samples characterized by a monoclinic structure with the space group (P21/n).

Table 1. Ferromagnetic (FM) and ferrimagnetic (FIM) equilibrium ordering with lattices constants.

	Ca ₂ FeIrO ₆		Ca ₂ CoIrO ₆	
	FM	FIM	FM	FIM
E (meV) ^[1]	-1139804.2311	-1139804.2435	-1146368.9446	-1146368.9457
ΔE ^[2]		12.4		1.1
a (Å)		5.4156		5.3772
b (Å)		5.6045		5.5995
c (Å)		9.4344		9.3577
Volume (Å ³)		1569.2624		1544.5340
β		124.994°		124.632°

^[1] Total energy, ^[2] $\Delta E = E_{\text{FM}} - E_{\text{FIM}}$.

3.2. Electronic properties

Total density of state (DOS) in figure 2 and partial density of state (PDOS) in figure 3 and figure 4 were computed in GGA and GGA+U approximations. Figure 2(a, c) shows that Ca₂CoIrO₆ is a metal; however, in figure 2(b, d), the Ca₂FeIrO₆ compound is half-metallic with 100% polarization (metal in the spin-up and semiconductor in the spin-down). The GGA and GGA+U approximation PDOS of Ca₂FeIrO₆ in figure 3 shows the existence of different regions. The first region located in the deeper valence band between -7.47 to 0 eV is mainly due to the d states of Ir with a small contribution of O ions. The second region is located around the Fermi level 0 to 2.55 eV, and the majority of contributions are created by the hybridization of Fe(3d)-O(2p) and Ir(5d)-O(2p). In this region, it is evident that Fe (3d) and Ir (5d) ions are responsible for the half-metallic character around the Fermi level. The third region located at the bottom of the conduction band from 2.8 eV to 4.77 eV is mainly due to the 3d states of Ir and the p states of oxygen. The upper part in the conducting band from 2.8 eV to the higher energies is due to the contributions from O (2p) and Ca (4s) states.

From figure 2(a) and figure 4, the deep part of the valence band -7 to 0 eV in Ca₂CoIrO₆ is due to the 5d states of Ir ions and 3d states of Co ions, which are dominant in this part, with a small contribution of oxygen ions. Around the Fermi level, between 0 eV and 0.95 eV, the majority of contributions are created by the hybridization of Co(3d)-O(2p) and Ir(5d)-O(2p). The Co (3d) and Ir (5d) are responsible for the half-metallic behavior around the Fermi level. In the bottom of the conduction band 2.63 to 5.54 eV, there is a hybridization between the 5d states of Ir and Co (3d) and the p states of oxygen. The upper part in the conducting band 5.92 to 8.43 eV comes from the contributions of O (2p) and Ca (4s) states. By inclusion of the on-site Coulomb interaction GGA+U, the band-gap in Ca₂FeIrO₆ is enlarged to 1.32 eV by shifting all states of unoccupied d bands upward to higher energies and lowering the energy of occupied d bands as seen in figure 2(d). However, the shape of the state density remains the same. The same observation is in the case of Ca₂CoIrO₆, where the inclusion of Hubbard-U potential leads to the change in the behavior of the material from metallic to half-metallic with a band gap of 0.107 eV in the spin-up direction. By contrast, in the spin-down direction, it presents a metallic character. This observation is similar to the other studies because the generalized gradient approximation underestimated the band gap [17, 22, 23].

3.3. Magnetic properties

The density of state calculations revealed that both compounds present a ferrimagnetic behavior. Since the magnetic moments of Fe and Co are aligned anti-parallel to that of Ir due to the hybridization between

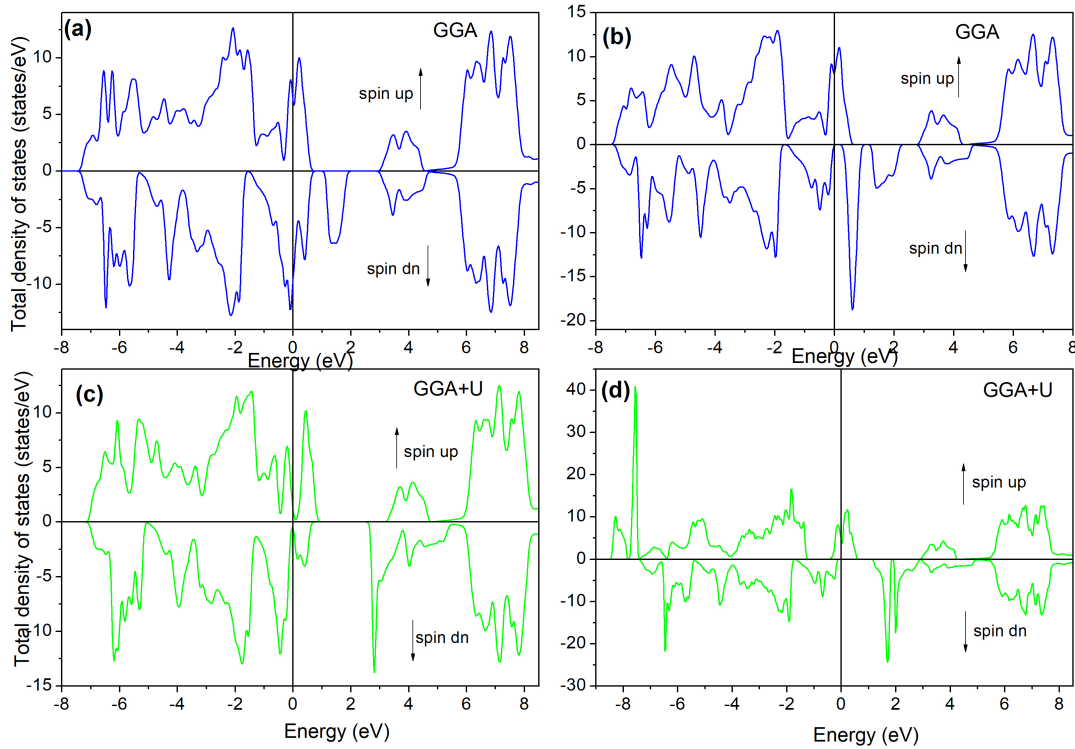


Figure 2. (Colour online) Total densities of states: $\text{Ca}_2\text{CoIrO}_6$ (a, c) using GGA and GGA+U, $\text{Ca}_2\text{FeIrO}_6$ (b, d) using GGA and GGA+U.

the Co and Fe ($3d$) states and Ir ($5d$) states on the one hand, and O ($2p$) on the other hand. Further, the values of the magnetic moments are not equal; this behavior can be explained via the super-exchange interaction through oxygen ions [13, 14].

The magnetic moments of Fe and Co ions represent the main contributors to the total magnetic moment of the two compounds, which is estimated at $3.62\mu_B$ and $2.44\mu_B$, respectively, as shown by the results of the calculations listed in table 2.

The magnetic moment on oxygen atoms is generated from oxygen vacancies [24], and Ca atoms carry a negligible magnetic moment. The magnetic moments within GGA and GGA+U methods summarized in table 2 show that the magnetic moment of $\text{Ca}_2\text{FeIrO}_6$ is $6.02\mu_B$. This value is relatively great due to the large spin-orbit and Coulomb interaction in ($3d$) and ($5d$) transition metals, whereas the magnetic moment of $\text{Ca}_2\text{CoIrO}_6$ is $3.72\mu_B$. These values are increased when we include the on-site Coulomb interaction with $4\mu_B$ for $\text{Ca}_2\text{CoIrO}_6$. The calculated total and partial magnetic moments on $\text{Ca}_2\text{FeIrO}_6$ and $\text{Ca}_2\text{CoIrO}_6$ for the magnetization along the c -axis are shown in table 2.

3.4. Magneto-optical properties

The studied double perovskite materials exhibit a large spin-orbit coupling and are characterized by important electronic properties such as half-metallic with ferrimagnetic behavior. The semi-conducting behavior has an essential role in the optical transfer properties; thus, it has an interesting MO effect. In industry, materials with huge MO effects are of great interest for use as devices in the fields such as optical telecommunications, reading the heads in data, visualization, sensors, or other optoelectronic devices. Many compounds have been studied, such as Sr_2FeWO_6 , which has the maximum polar Kerr rotation of 3.87° [24], and $\text{Ba}_2\text{B}'\text{RuO}_6$ ($\text{B}'=\text{Er, Tm}$) with a huge magneto-optical Kerr effect angle of 17.7° and 5.6° in the infrared region [8]. Currently, no study presents the magneto-optical properties of the compounds included in this study. Therefore, we first focused on the magneto-optical Kerr effect of these materials by

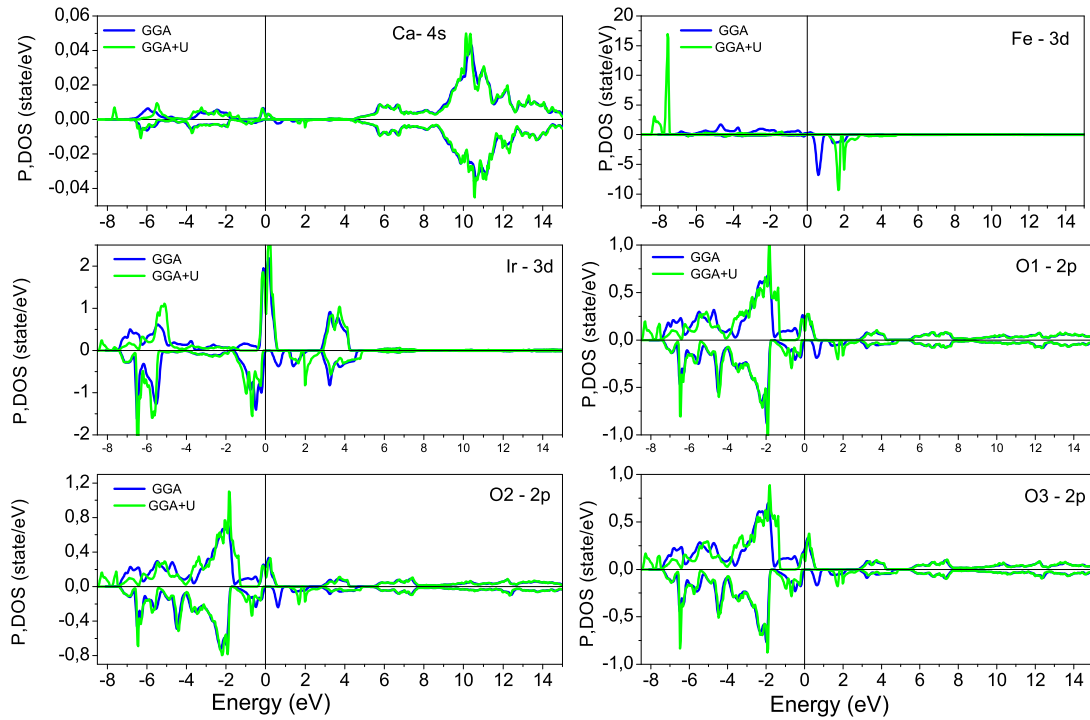


Figure 3. (Colour online) The projected density of states using GGA and GGA+U approximation at antiferromagnetic configuration utilizing ($U_{\text{Fe}} = 5$ eV, $U_{\text{Ir}} = 1.5$ eV) of $\text{Ca}_2\text{FeIrO}_6$.

Table 2. The calculated total and partial magnetic moments (in units of Bohr's magneton, μ_B) with band gap spin up (\uparrow)/spin down (\downarrow) in eV for $\text{Ca}_2\text{FeIrO}_6$ and $\text{Ca}_2\text{CoIrO}_6$.

	$\text{Ca}_2\text{FeIrO}_6$				$\text{Ca}_2\text{CoIrO}_6$			
	M_{Fe}	M_{Ir}	M_{tot}	gap	M_{Co}	M_{Ir}	M_{tot}	gap
GGA	3.62	-0.66	6.02	$\uparrow 0 \downarrow 0.383$	2.44	-0.66	3.72	$\uparrow 0 \downarrow 0$
	3.48 ^a	-0.55 ^a	6.00 ^a					
GGA+U	4.14	-0.88	6.00	$\uparrow 0 \downarrow 1.34$	2.62	-0.42	4	$\uparrow 0.107 \downarrow 0$
	4.12 ^a	-0.87 ^a	5.99 ^a		2.743 ^b	-0.431 ^b	2 ^b	$\uparrow 0.09^b \downarrow 0$

^(a)[17], ^(b)[21]

performing theoretical calculations. The magnetization in polar Kerr effect is perpendicular to the surface of the sample and parallel to c -axis. The linear response of a system due to an external electromagnetic field with a small wave vector can be described with the complex dielectric function:

$$\begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & 0 \\ -\epsilon_{xy} & \epsilon_{xx} & 0 \\ 0 & 0 & \epsilon_{zz} \end{pmatrix}, \quad (3.1)$$

where ϵ_{xx} and ϵ_{zz} are the diagonal components and ϵ_{xy} is the off-diagonal components of the dielectric tensor. The optical conductivity tensor is related to the dielectric tensor by the equation:

$$\epsilon_{\alpha\beta}(\omega) = \delta_{\alpha\beta} + \frac{4\pi i}{\omega} \sigma_{\alpha\beta}(\omega),$$

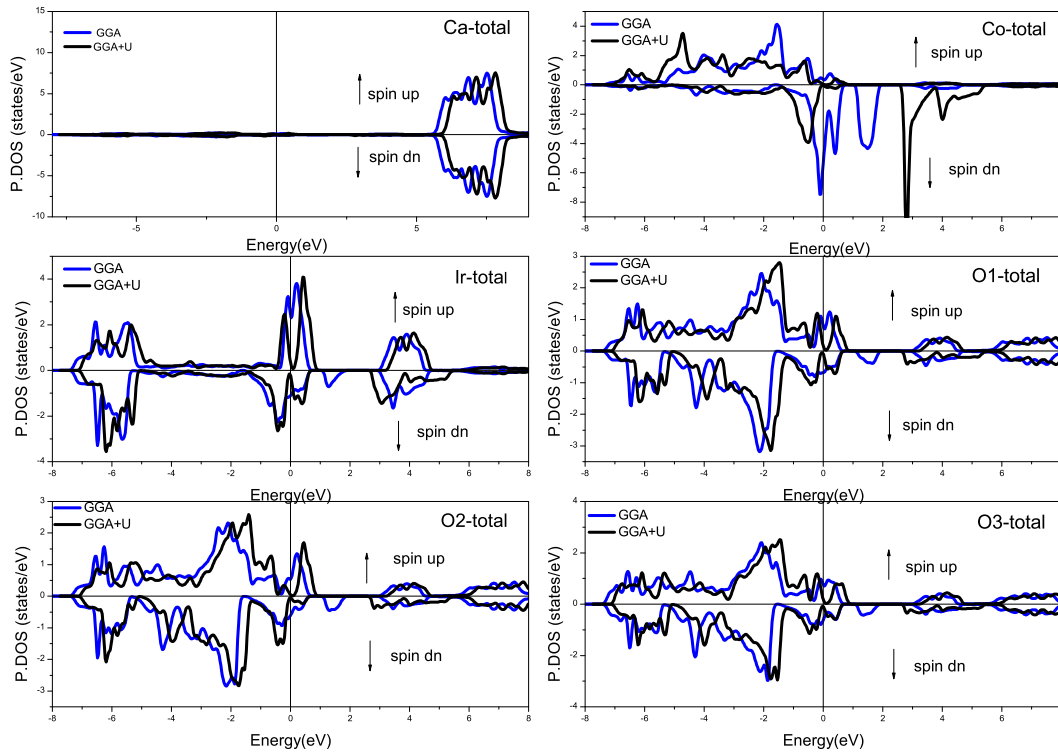


Figure 4. (Colour online) The projected density of states using GGA and GGA+U approximation at antiferromagnetic configuration utilizing ($U_{Co} = 5$ eV, $U_{Ir} = 1.5$ eV) of Ca_2CoIrO_6 .

where:

$$\sigma_{\alpha\beta}(\omega) = \frac{-ie^2}{m^2\hbar V} \sum_k \sum_{mm'} \frac{f(E_{mk}) - f(E_{m'k})}{\omega_{mm'}} \frac{\Pi_{m'm}^\alpha \Pi_{mm'}^\beta}{(\omega - \omega_{mm'} + i\gamma)}, \quad (3.2)$$

where, $\Pi_{m'm}^\alpha$ and $\Pi_{mm'}^\beta$ are the optical dipolar matrix elements, $f(E_{mk})$ is the Fermi function, $E_{m'k}$ and E_{mk} are Kohn-Sham energies at the position k for two bands m', m respectively, so that $\hbar\omega_{mm'} = E_{mk} - E_{m'k}$, and γ is the lifetime parameter [26]. The magneto-optical absorption is described by the imaginary part of the non-diagonal elements of the conductivity tensor. The Kerr rotation θ_k and Kerr ellipticity ϵ_k were related to the optical conductivity by the relation given as [27, 28]:

$$\theta_k + i\epsilon_k = \frac{-\sigma_{xy}}{\sigma_{xx}\sqrt{1 + (2\pi i/\omega)\sigma_{xx}}}.$$

Figure 5 presents the Kerr rotation and ellipticity. We can see a peak of Kerr $\theta_k = -0.97^\circ$ at 0.1 eV and ellipticity rotation $\epsilon_k = -0.45^\circ$ at 0.28 eV with RCP dominance of polarized light for Ca_2FeIrO_6 , while for Ca_2CoIrO_6 , Kerr rotation $\theta_k = -0.23^\circ$ at 0.11 eV and $\epsilon_k = -0.11^\circ$ at 0.31 eV with RCP dominant. In this region of low energy, the Kerr rotation peaks are induced by the plasma resonance due to the metallic behavior of the compounds, as mentioned in the study of Feil and Haas [29]. We have the main peak of 1.3° located at an incident photon energy of 4.82 eV (with large width of 1.38 eV) in Kerr rotation, and the main peak of -1.21° at 4.3 eV in ellipticity rotation for Ca_2FeIrO_6 . For Ca_2CoIrO_6 the main peaks are -1.1° at 4.46 eV (ellipticity rotation) and -1.04° at 4.05 eV (Kerr rotation). Because of the Kramers-Kronig relation, we observe an alternation in the sign of θ_k and ϵ_k . The calculated Kerr rotation was compared with other compounds as Ca_2FeWO_6 that have $\theta_k = 1.32^\circ$ at 1.89 eV and Ca_2FeReO_6 with $\theta_k = 1.04^\circ$ at 1.43 eV [25]. These large values of Kerr rotation in the range of 4.5 to 5 eV may suggest the potential application of these materials in ultraviolet laser light magneto-optical effect devices.

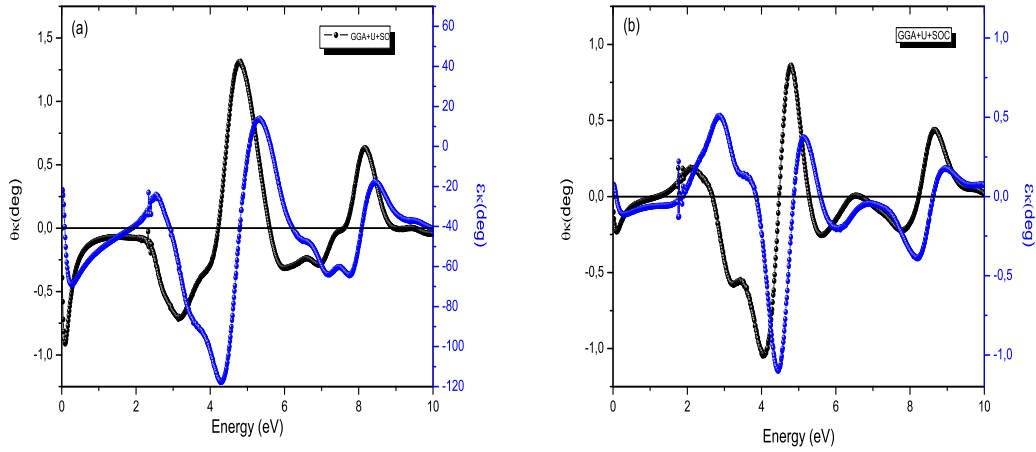


Figure 5. (Colour online) The calculated polar Kerr angle θ_k and Kerr ellipticity ϵ_k as a function of photon energy (eV): (a) for $\text{Ca}_2\text{FeIrO}_6$ and (b) for $\text{Ca}_2\text{CoIrO}_6$.

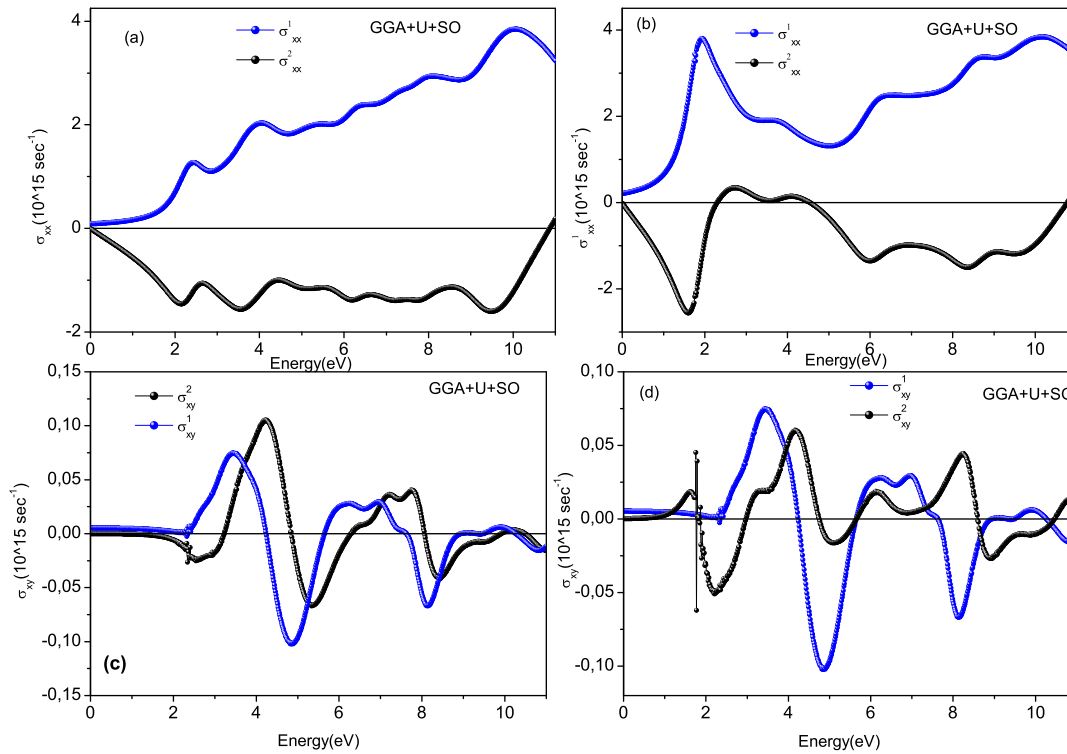


Figure 6. (Colour online) (a) and (b) represent the absorption σ_{xx}^1 and dispersive σ_{xx}^2 of optical conductivity, (c) and (d) off-diagonal optical conductivity σ_{xy}^1 and σ_{xy}^2 as a function of photon energy (eV) $\text{Ca}_2\text{FeIrO}_6$ and $\text{Ca}_2\text{CoIrO}_6$, respectively.

In the region of energy higher than 3.0 eV, the Kerr and ellipticity rotation peaks originate from the quite significant off-diagonal optical conductivity element. Figure 6 presents the calculated diagonal (the real part σ_{xx}^1 and the imaginary part σ_{xx}^2) and the off-diagonal (the real part σ_{xy}^1 and imaginary

part σ_{xy}^2) optical conductivity for both compounds in the range from 0 to 10 eV. In figure 6(a), we plotted the absorption spectra (the real part) and dispersive of the optical conductivity. We note that the band gap starts around 1.8 eV. In the region higher than 3.0 eV, the peaks in the two spectra are at the same positions; they originate from the p - d inter-band transition [30]. The off-diagonal optical conductivity σ_{xy}^1 and σ_{xy}^2 are related to Kerr and ellipticity rotation. The main peak in the imaginary part of the off-diagonal optical conductivity is due to the principal inter-band transitions at all points.

4. Conclusion

The structural, electronic, magnetic, and magneto-optical properties of double perovskites $\text{Ca}_2\text{CoIrO}_6$ and $\text{Ca}_2\text{FeIrO}_6$ with monoclinic structure (space group $P21/c$) have been investigated using the first-principles DFT within the GGA and GGA+U approximation. We showed that the configuration with ferrimagnetic coupling is the most stable. GGA and GGA+U computations predict the half-metallic behavior for $\text{Ca}_2\text{FeIrO}_6$ and $\text{Ca}_2\text{CoIrO}_6$. The band gap was enlarged for $\text{Ca}_2\text{FeIrO}_6$ from 0.383 eV to 1.34 eV by including Hubbard-U electron correlation. In the case of $\text{Ca}_2\text{CoIrO}_6$, the band gap is opened and presents the value of about 0.107 eV. Both compounds exhibit important electronic and magnetic properties that may suggest potential applications in spintronic devices. We predict a huge Kerr and ellipticity rotation $\theta_k = 1.3^\circ$ at 4.82 eV for $\text{Ca}_2\text{FeIrO}_6$ and -1.1° at 4.46 eV for $\text{Ca}_2\text{CoIrO}_6$, which made them potential candidates for application in ultra-violet optoelectronic devices and hence promising multifunctional materials.

Acknowledgements

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Дослідження структурних, електронних, магнітних і магнітооптичних властивостей подвійних перовскітів $\text{Ca}_2\text{TMIrO}_6$ (TM=Fe, Co) за першими принципами

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Вивчаються електронні, магнітні та магнітооптичні властивості подвійних перовскітів $\text{Ca}_2\text{FeIrO}_6$ і $\text{Ca}_2\text{CoIrO}_6$ моноклінної структури (просторова група $P21/c$) з метою оцінки можливості їх потенційного застосування у спінтронних та фотоелектричних пристроях. Обчислення проведено з використанням повнопотенціального методу лінеаризованих приєднаних плоских хвиль в рамках теорії функціоналу густини. Для електронної обмінно-кореляційної функції використано узагальнені градієнтні наближення (GGA) та GGA+U (з потенціалом Габбарда), а також спін-орбітальний зв'язок (SOC). Виявлено, що $\text{Ca}_2\text{FeIrO}_6$ і $\text{Ca}_2\text{CoIrO}_6$ мають моноклінну структуру (просторова група $P21/c$). Релаксація структури в наближенні GGA+U виявила антиферромагнітну поведінку в обидвох системах з магнітними моментами близько $6.00\mu_B$ для $\text{Ca}_2\text{FeIrO}_6$ та $4.00\mu_B$ для $\text{Ca}_2\text{CoIrO}_6$. Результати наближень GGA і GGA+U передбачають напівметалічну поведінку $\text{Ca}_2\text{FeIrO}_6$ та $\text{Ca}_2\text{CoIrO}_6$. Магнітооптичний полярний ефект Керра (МОКЕ) досліджувався шляхом вивчення змін в обертаннях поляризацій Керра та поляризації еліптичного типу. Для $\text{Ca}_2\text{FeIrO}_6$ кут повороту Керра складає 1.3° при 4.82 eV і -1.21° при 4.3 eV, а кут еліптичності -1.21° при 4.3 eV. Для $\text{Ca}_2\text{CoIrO}_6$ кут повороту Керра становить -1.04° при 4.05 eV; значне обертання в обидвох сполуках може вказувати на можливе застосування цих матеріалів в оптоелектричних схемах. Досліджені сполуки можуть потенційно використовуватись в оптоелектронних технологіях у спінтронних пристроях.

Ключові слова: подвійні перовскіти, ефект Керра, оптичні властивості, WIEN2k
