FIRST PRINCIPALS CALCULATIONS FOR ELECTRONIC AND OPTICAL PROPERTIES OF FULL-HEUSLER ALLOYS CS_2CRGE

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Abstract - The electronic and optical properties of full-Heusler alloys Cs_2CrGe are examined in this study using FP-LAPW method based on density functional theory. Results of our calculations predict that the Hg_2CuTi-type structure is more stable than the Cu_2MnAl-type structure and the ground state of this alloy is ferromagnetic. the Density of state of Cs_2CrGe shows half metallic in spin down for the three approaches GGA and mBJ-GGA.

Keywords - Full-Heusler, FP-LAPW Method, Half Metallic, Ferromagnetic.

I. INTRODUCTION

Half metallic materials are a subject of interest due to their spintronics applications. A number of Heusler compounds, are destined to be half-metallic materials HMFs, where they are metals in one spin channel and narrow band gap semiconductors in other spin channel. The Heusler compounds have general chemical formula X_2YZ, where X and Y are transition metal elements and Z is a sp valent element, In this paper, we present a theoretical study using GGA and mBJ-GGA (modified Beck-Johnson GGA) approximations for calculating the electronic, magnetic and elastic properties of full-Heusler alloys Cs_2CrG [1].

II. STRUCTURAL PROPERTIES

Generally the full Heusler compounds crystallize to two possible structures the Hg_2CuTi and Cu_2AlMn-type. These structures can be described as consisting of four interpenetrating face-centered-cubic (fcc) lattices and has four unique crystal sites in wykoff coordinates, The cubic Hg_2CuTi-type structure space group F43m (216), while the space group of Cu_2AlMn-type is Fm3m (225). Our calculations are performed in two types of cubic structure of the Heusler: Hg_2CuTi-type, where Cs atoms occupy (4a (0,0,0), 4c (0.25, 0.25, 0.25)) sites and Cr atom occupy 4b (0.5, 0.5, 0.5) site and second type is Cu_2AlMn-type structure where Cs atoms occupy (4a (0,0,0),4b (0.5, 0.5, 0.5)) sites and Cr atom occupy 4c (0.25, 0.25, 0.25) site, and in the two types Ge atom occupy 4d (0.75, 0.75, 0.75). For the ferromagnetic (FM) state, the total energy is calculated as function of unit cell volume were fitted by Birch Murnaghan equation of state as follows [2, 3]:

$$E_T(V)=E_0 + 9B_0V_0/16[B' \{(V_0/V)^{2/3}-1\}^3+\{(V_0/V)^{2/3}-1\}^2\{6-4(V_0/V)^{2/3}-1\}^3] \quad (1)$$

The curve of total energies versus volume are shown in (Fig 1), this final confirm that the FM configuration of Hg_2CuTi-type structure has lower energy than that of the Cu_2AlMn-type structure, for that reason the FM configuration of Hg_2CuTi-type structure is considered to be stable ground state of our compound.

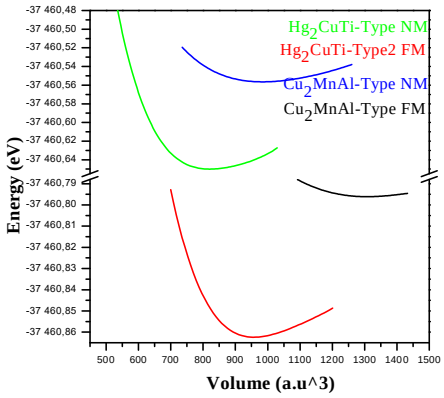
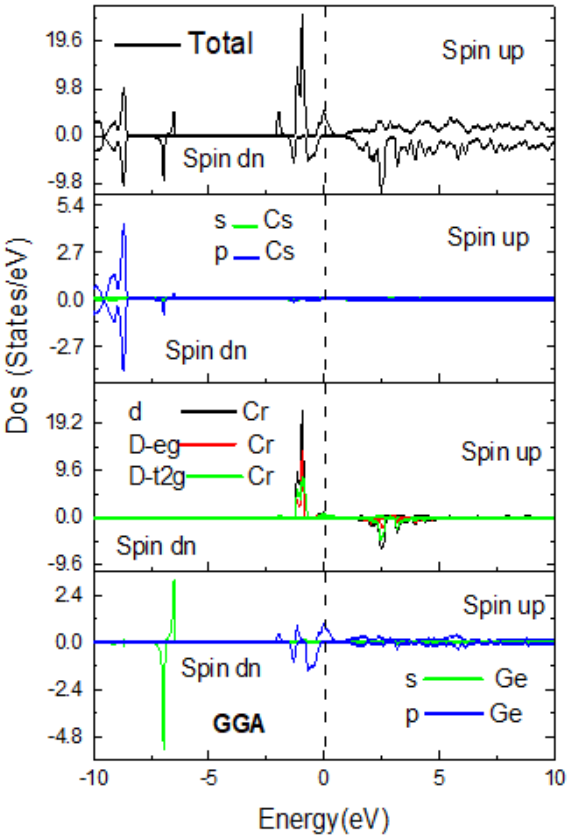


Fig.1: Volume optimization of Cs_2CrGe in Non magnetique and ferromagnetique phase in Cu_2MnAl-type and Hg_2CuTi-type structure with GGA approximation

III. DENSITY OF STATE

The corresponding density of states total and partial of states, TDOS and PDOS, for Cs_2CrGe obtained using GGA, mBJ+GGA are presented in Figs. 4(a, b, c). We have plotted the partial density of states (DOS) of Cr D-eg and D-t2g, (Cs) Ge-s and (Cs) Ge-p electrons for the spin-up and spin-down. The upper part of each curve shows the majority spin densities and the lower one the minority spin densities. In general way, the curves of total DOS are nearly identical for the three used approximations. According to Fig.4, we observed from the total density of states for GGA and mBJ-GGA the half metallic nature of Cs_2CrGe. The majority spin bands are strongly metallic, for the three approaches, a peak is observed at Fermi level. We can divide the area outside occupied by the different states into three separate regions: in the area where the energy is less than about -2 eV, we observed peaks of

hybridization between the states Cs-p and Ge-p , in the region between -2 eV and 0.5 eV, we have hybridization between the states of Cs-p, Cr-D-t2g, Cr-p and Ge-p; we noted that the contributions of the atom Cr and Ge are very large compared to Cs atom which is quite low. For higher energies than 0.5 eV, hybridization occurs between the Ge p-states, Cs-p and the contribution of Cr atom is low detected. The minority spin our compound is semiconductor-like around the Fermi level, the Fermi level is at 0 eV is located in a gap of energy and that for the three approximations used GGA, GGA+ U and GGA + mBJ. The width of the gap is very small with the GGA calculation and becomes very important in applying the potential mBJ. In the valence area we detected some peaks energies resulting to contribution of states Cs-p and Ge-p states, we note that the presence of Cr atom states are negligible. In conduction region a large extended in space where states of Cs-p and Ge-p hybridize. In particular, the minority Cr (d) orbitals are more hybridized than the majority states; the spin-down channel has semiconductor behavior, through the Fermi level, while the spin-up evidence a conductor feature. The conduction band in spin-up channel is mainly composed of Ge (p) character which hybridizes well with the Cr (d) states; this hybridization is responsible for the half metallic noticed in Cs_2CrGe which allows us to use this compound in spintronics applications.



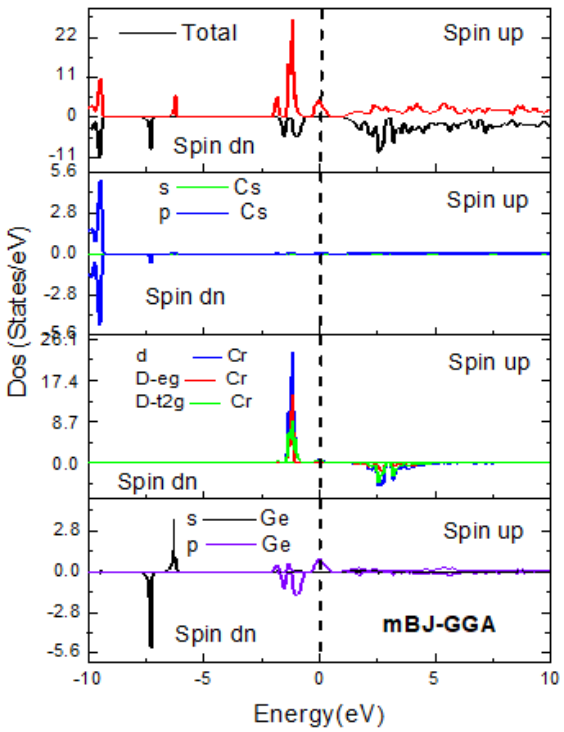


Fig.2. Spin-polarized total and partial densities of states (DOS) of Cs_2CrGe at equilibrium lattice constants using: GGA and mBJ-GGA, The Fermi level is set at zero energy.

IV. OPTICAL PROPERTIES

In this work, we have studied the optical properties, which is extremely important for the identification of the internal structure of our material. Our compound Cs_2CrGe is a half-metallic ferromagnetic like the other Heusler alloy [4].

It's shown the metallic behavior in the majority spin channel and semiconductor behavior in the minority of spin channel. For this, we have two contributions to optical properties, namely intraband for majority spin and interband for minority spin channel, to arrive at a correct interpretation of optical spectra in this compound.

4.1 Absorption coefficient:

The absorption edge corresponds to the transition of the electrons from the top of the valence band to the bottom of the conduction band. In our calculations, the absorption coefficient is illustrated by considering the intereband and intraband transitions in the minority and majority spin respectively.

The absorption coefficient is given by the following formula [5,6]:

$$\alpha(\omega)=\frac{\sqrt{2}\omega}{c}\left(\sqrt{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)}-\varepsilon_1(\omega)\right)^{1/2} \quad (2)$$

The imaginary part $\varepsilon_2(\omega)$ of dielectric function is used to calculate the absorption coefficient.
The polarization response similarities are taken into account in absorption (Fig.3). As shown in this Fig.3 an important peak situated at 14.06 eV explains the important ultraviolet absorption of maximum light at this wave length.

However, the peak located at 2.85 eV correspond to visible absorption, while for the majority spin of absorption, the peak situated at 0,28 eV correspond to infrared, so our compound Cs_2CrGe highlights the transparent nature in the electromagnetic spectra.

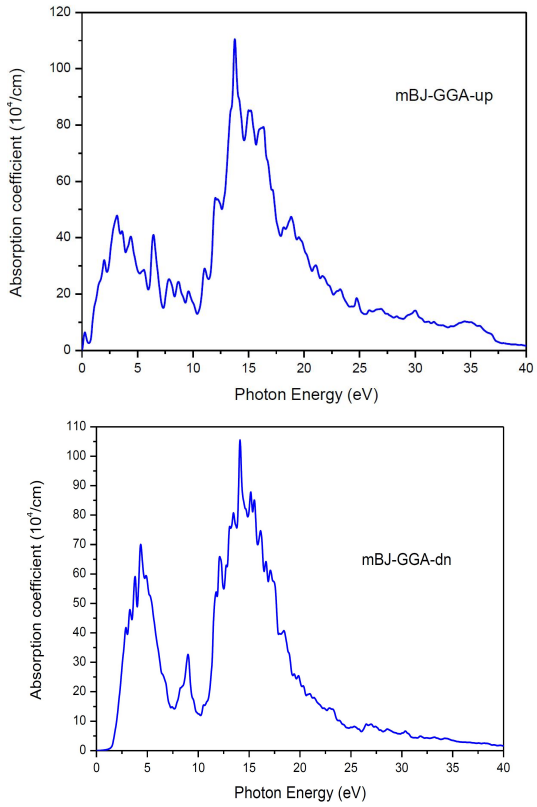


Fig.3. Calculated values of optical coefficient $\alpha(\omega)$ for (a) majority spin and (b) minority spin by addding the two kinds of transitions, ineterband trnasition and intraband transition.

4.2 Refractive index:

The refractive index of a material is very helpful optical parameter to determine the propagation of light through the optical medium. In this study we have illustrated our results by considering the interband and intraband transition in both majority and minority spin channels. The complex refractive index $\tilde{n}(\omega)$ is expressed as [6-7]:

$$\tilde{n}(\omega) = n(\omega) + ik(\omega) \qquad (3)$$

The real as well as imaginary parts of refractive index can be express in terms of complex dielectric functions, by the following expressions:

$$n(\omega) = \frac{1}{\sqrt{2}}\left[\left\{\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2\right\}^{\frac{1}{2}} + \varepsilon_1(\omega)\right]^{\frac{1}{2}} \qquad (4)$$

$$k(\omega) = \frac{1}{\sqrt{2}}\left[\left\{\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2\right\}^{\frac{1}{2}} - \varepsilon_1(\omega)\right]^{\frac{1}{2}} \qquad (5)$$

The real part of the complex refractive index n(x) describes the ordinary refractive index while the imaginary part k(x), still known under the name of extinction coefficient interprets photon energy loss as propagates through the medium In Fig.4, the refractive index n(ω) is plotted, the static refractive index n(0) is recorded as 2.16 eV, the maximum value of the refractive index (2.72) at 2.03 eV.The extinction coefficient k(ω) is presented in the same figure (Fig.4), this final show to us the local maximum of k(ω) (1.59) at 4.30 eV. For this compound, as the values of the refractive index is greater than 1 the photon entering this material is slowed down by interactions with the electrons in the material.

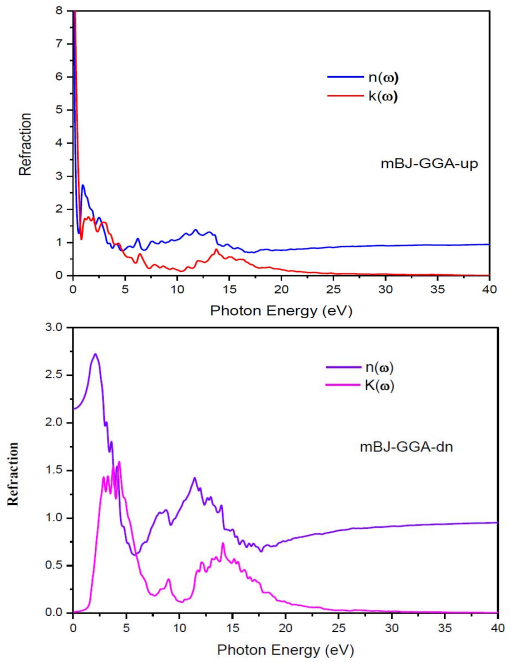


Fig.4. The refractive index spectra, N(ω) for (a) majority spin and (b) minority spin using the two types of transitions, ineterband trnasition and intraband transition.

CONCLUSION

In this work, we used the FPLAPW method based on density functional theory within the GGA and mBJ-GGA to study the electronic and optical properties of the cubic full-Heusler Cs_2CrGe. The spin-polarized calculations confirm that the structure is best described in the stable ferromagnetic Hg_2CuTi-type structure, moreover this half-metallic character probably makes these compounds promising

candidates for applications in spintronic, The optical properties, such as the absorption and refractive index, were examined in the energy range from 0 eV to 40 eV, revealed that our compound highlights the transparent nature in the electromagnetic spectra.

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