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

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Abstract - In this study The electronic and elastic properties of full-Heusler alloys Cs_2CrGe are examined 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 these alloys is ferromagnetic. The total magnetic moment calculated, is an important in conformity with the Slater-Pauling curve for full-heusler alloys. Band structure of Cs_2CrGe shows half metallic in spin-dn for GGA and mBJ-GGA with an important magnetic moment which equal $4\mu_B$ which is in good agreement with the Slater-Pauling rule.

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 work, 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 [2-8]: $E_T(V)=E_0 + 9B_0V_0/16[B' \{(V_0/V)^{2/3}-1\}^3+\{(V_0/V)^{2/3}-1\}^2\{6-4(V_0/V)^{2/3}-1\}^3]$ (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.

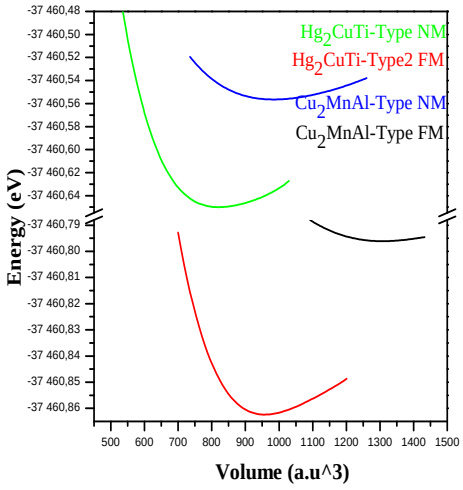


Fig.1: Volume optimization of Cs_2CrGe in Non magnetique and ferromagnetique phase in Cu_2MnAl-type and Hg_2CuTi-type structure with GGA approximation

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.

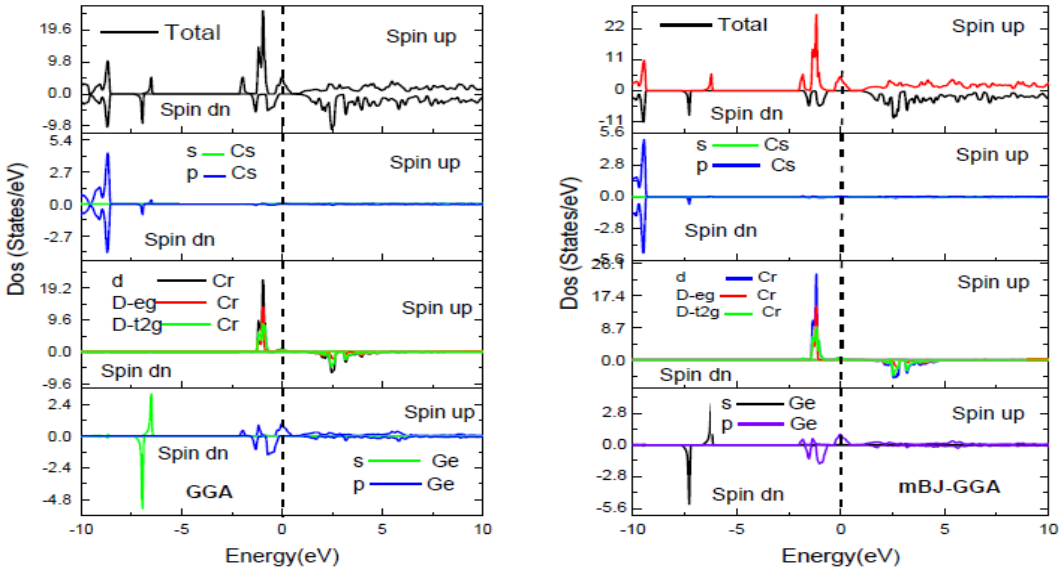


Fig.2. Spin-polarized total and partial densities of states (DOS) of Cs_2CrGe at equilibrium lattice constants using: GGA and mBJ-GGA, The Fermi level is set at zero energy.

IV. MAGNETIC PROPERTIES:

In this work, local and total magnetic moments in interstitial and spherical region for Heusler compounds Cs_2CrGe is calculated, The total spin magnetic moment present clearly integer value about $4\mu_B$ which is agreement with the Slater-Pauling rule [9] of the Hg_2CuTi-type that is described by the following formula: $\mu_{Tot} = N_V - 18$,

where μ_{tot} means the total spin magnetic moment and N_V is the total number of valence electron per cell [10-11].

For this compound Cs_2CrGe,

$$N_V = 2*(6s^1) + 3d^5 4s^1 + 3d^{10} 4s^2 1p^2 = 22$$

N_V=22 electrons, as a result $\mu_{Tot} = 4\mu_B$.

V. ELASTIC PROPERTIES:

To indicate the stability and stiffness of the compounds, we must study the elastic nature of this compounds via calculation the elastic constants C_{ij} and their related properties. So in our work we follow the method introduced by T. Charpin which consists of applying a given strain and calculated the stress and implemented in the WIEN2K package [12]. For cubic system, only three independent elastic constants C11, C12, C44 which are needed to calculate all the elastic modulus: using the following relations [13]:

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

$$G = \frac{G_R + G_V}{2} \quad (3)$$

$$G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5} \quad (4)$$

$$G_R = \frac{5(C_{11} - C_{12})\,C_{44}}{4C_{44} + 3(C_{11} - C_{12})} \quad (5)$$

Where G_V is Voigt's shear modulus corresponding to the upper bound of G values and G_R is Reuss's shear modulus corresponding to the lower bound of G values.

$$E = \frac{(C_{11} - C_{12})(C_{11} + 2C_{12})}{C_{11} + C_{12}} \quad (6)$$

$$\nu = \frac{C_{12}}{C_{11} + C_{12}} \quad (7)$$

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \quad (8)$$

where: G is the shear modulus, B is the bulk modulus, E is young's modulus, υ is Poisson's ratio and A is the anisotropy factor.

The required stability criteria [14- 15] of C11-C12 > 0, C11 > 0, C44 > 0 and (C11+C12) > 0 are found to be satisfied by Cs_2CrGe compound.

Hence indicating that it is elastically stable, by comparison of the calculated value of bulk moduli B which is obtained by fitting the total energy data versus volume in Birch Murnaghan' equation of state [16]. With the calculated results from elastic constant expression which given in Table 1 are found identical, so, this similarity validates the precision and correctness of the calculated elastic constants values of our compound.

There is another important elastic properties for several technological applications, such as the anisotropy factor (A) the Poisson ration (υ), the young Modulus (E) the shear modulus (G) [17-20].

From the Table 1 we can mention the following observations:

- The calculated factor A is smaller than 1 for this compound, which characterizes it as isotropic crystal.
- According to Pugh's criteria [21], the critical value of ratio B/ G is 1.75 i.e, if (B/ G) >1.75 the material is ductile, otherwise is brittle while for Frantsevich [22] the critical value is 2.67, so the calculated ratio B /G verifies the ductile nature of our materials.
- The Poisson's ratio (υ) of our compound is greater than 0.26, which allows us to say that according to the Frantsevich et al. [23] rule, this material is ductile.

	C11	C12	C44	G	E	B	υ	A	B/G
Cs2CrGe	43.8	0.65	9.82	2.5	7.1	15.0	0.47	0.45	5.98

CONCLUSION

In this paper, we used the FPLAPW method based on density functional theory within the GGA and mBJ-GGA to study the electronic and magnetic 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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