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Study the Electronic, Magnetic and Elastic Properties of Ir_2FeGe

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ABSTRACT

The electronic structure, magnetic and elastic properties were predicted for Full Heusler Alloy-Ir_2FeGe using local spin density approximation as implemented in Wien2k. The exchange-correlation potential is treated with the local density approximations LDA. The optimized lattice constant was 2.13% lower than the predicted value. This material is metallic and ferromagnetic. The energy level close to Fermi is mainly occupied by Ir-d and Fe-d-electrons. We accorded more attention to the elastic constants, where we have derived bulk and shear modules with employing Voigt–Reuss–Hill approach. The ferromagnetic performance of Ir_2FeGe is confirmed by the total magnetic moment of 3.50 μ_B per formula unit, where its main contribution is originated from Fe atoms.

Keywords: Ir_2FeGe full Heusler alloy; Metallic; Ab-initio calculations; Magnetic; Electronic band structure

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INTRODUCTION

Full- and half-Heusler alloys are a new class of materials that were discovered in the early 19th century [1]. Heusler alloys have a very unusual ferromagnetism and very important because of their interesting and varied magnetic properties [2,3]. The Full- and half-Heusler alloys have a big family of Multifunctional materials for spintronics devices [4]. Shape memory alloys [5], superconducting materials [6], and thermoelectric materials [7]. Heusler alloys have Slater-Pauling behavior [8]. The ordered Full Heusler compounds with stoichiometric composition X_2YZ are ternary compounds, where X and Y are transition metals and Z is a group II, IV or V element [9]. Crystallize in type structure "regular" (Cu_2MnAl, L_{21} prototype) with space group $Fm\bar{3}m$ $N^0: 225$, the atoms are located at the Wyckoff coordinates: with atoms at $X_1(1/4, 1/4, 1/4)$, $X_2(3/4, 3/4, 3/4)$, $Y(1/2, 1/2, 1/2)$, and $Z(0, 0, 0)$ [9], as shown in Figure 1. GilleBen [10] has theoretically predicted and reported many Heusler full and half compounds, and the Ir_2FeGe compound is part of this prediction. We report here for the first time. The objective of this study is to predict the structural parameters, electronic structure, magnetic properties and elastic properties of Ir_2FeGe Heusler alloy by using the first-principles calculations of the full-potential linearized augmented plane wave (FP-LAPW) method. This document is organized as follows: computational details are described in Section 2, the results are discussed in Section 3, and finally, gives the conclusions.

COMPUTATIONAL METHOD

In this study, we have used the first-principle calculations of density functional theory [11,12] based on FPLAPW method is implemented in Wien2k code [13]. The exchange correlation potential was treated by using the local density approximation (LDA) proposed by Perdew and Wang [14]. It calculates the self -consistent solution of the equations of Kohn and Sham [15]. The cutoff parameter is $R_{mt} * K_{MAX}=7$ (where R_{mt} is the smallest radius of the muffin-tin spheres and K_{MAX} is the largest reciprocal lattice vector used in the plane wave expansion). The Muffin Tin radius of Ir, Fe and Ge are 2.20 a.u, 2.00 a.u and 2.00 a.u respectively in such a way that the muffin-tin spheres do not overlap. The number of k-points chosen is 1500 in the Brillouin zone [16,17], but only 101 irreducible points have been generated. In these calculations the energy separation is -6.0 Ry for the compound used between the valence states and the core states. The basic functions are expanded into spherical harmonic functions inside the muffin-tin sphere and Fourier series in the interstitial region. The maximum value of the angular momentum, *l*max=10 is taken for the wave function expansion inside the muffin tin spheres. The electronic configurations for the compound of the system studied are: Ir((Xe)$4f^{14}5d^{7}6s^{2}$), Fe((Ar) $3d^{6}4s^{2}$), Ge ((Ar): $4s^{2}3d^{10}4p^{2}$), and CrySDen [18], package has been used to plot the crystal structure of Ir_2FeGe and is shown in Figure 1.

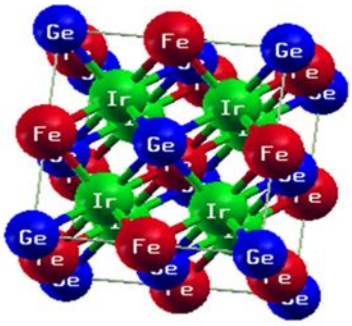


Figure 1. Crystal Structure of Ir_2FeGe

RESULTS AND DISCUSSION

Structural Properties

As the experimental lattice parameter was not available, we used Micheal Gillisen's prediction parameter [10]. The volume optimization was performed to obtain the minimum total energy using a SCF calculation with an energy convergence of 0.0001 Ry. Figure 2 is presented the energy total as a function of volume for the compound Ir_2FeGe, Calculated total energy was adjusted from the Murnaghan equation [19]. The calculated structural parameters of

Ir_2FeGe in the Cu_2MnAl-type structure such as the lattice constant (a), bulk modulus (B), and its pressure derivative (B) are listed in Table 1. The equilibrium lattice constant optimized of Ir_2FeGe is 5.96 $\overset{0}{\mathrm{A}}$, this value is 2.13% lower than the predicted value [10].

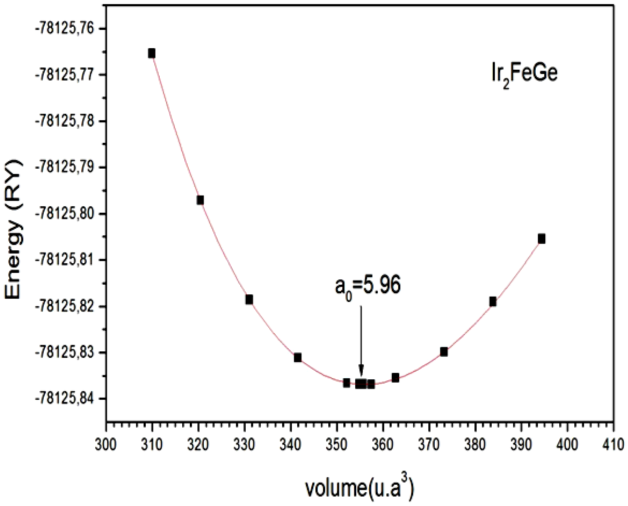


Figure 2. Total Energy Vs Volume of Ir_2FeGe

Table 1. Calculated equilibrium lattice constants $a(\overset{o}{A})$, bulk modulus B (GPa), and its first derivative B', Equilibrium Energy of Ir_2FeGe.

	$a(\overset{o}{A})$	**B (Gpa)**	**B'**	$\Delta a(\overset{o}{A})$	**E(RY)**
Ir_2FeGe	5.96	269.235	4.77	0.13	-78123.8
Previous [10]	6.09				

Magnetic Moment

The Slater–Pauling (SP) rule for the X_2YZ Heusler family describes the relationship between the N_V of a compound and its measurable magnetic moment values. To find the magnetic momentum per cell unit, we use the rule given by Kubler et al. [19] $M_t = N_V - 24$, M_t: magnetic moment per cell unit, N_V is the accumulated number of valence electrons in the cell unit. Roofer, Pauling and Friedel have observed that this behavior is applicable to 3d transition metals and alloys [20-22], and it was then applied to semi-metallic cubic Heusler materials [23]. In our compound, the valence Ir_2FeGe is equal to 30. So 30-24=6. For this compound, the magnetic moment is different from an integer, the value obtained not satisfying the Slater-Pauling rule, which confirms the metallic character for this compound. The total and partial moment is given in Table 2. The contribution to the magnetic moment comes mainly from Fe as predicted in the DOS diagram. This confirms the magnetic nature of the Ir_2FeGe phase. The calculated magnetic moment was 4.37% lower than the predicted value [10].

Table 2. The calculated values of total and partial magnetic moments for the Ir_2FeGe

	μ^{total}	μ^{Ir}	μ^{Fe}	μ^{Ge}	$\mu^{Intestinal}$	μ^{V}
Ir_2FeGe	3.5	0.36	2.62	0.0091	0.41	30
Previous [10]	3.66					

Electronic Properties

Band structure: We calculated the electronic band structure of Ir_2FeGe at equilibrium lattice parameter in different highs points of symmetry in the Brillouin zone, for majority and minority band of alloy Ir2FeGe. Figure 3 show an overlap has been found between the valence bands and the conduction bands at the E_F level, along X-W direction in both canal up and down, and the absence of a bandgap which clearly indicates the metallic character. From Figure 3, it is clear the Ir-4d and Fe-3d bands are dominating at the Fermi level. It is clear that the low-energy region below -3 eV consists mainly of the states s and p of the electrons of atoms Ge and the band structure is almost identical for both directions of spin. The scattered upper bands are due to the strong hybridization of the d states of Ir and Fe, including a contribution of the states p of Ge in the occupied states of valence. The electrons p of the atom Ge hybridize with p electrons of Ir and Fe atoms.

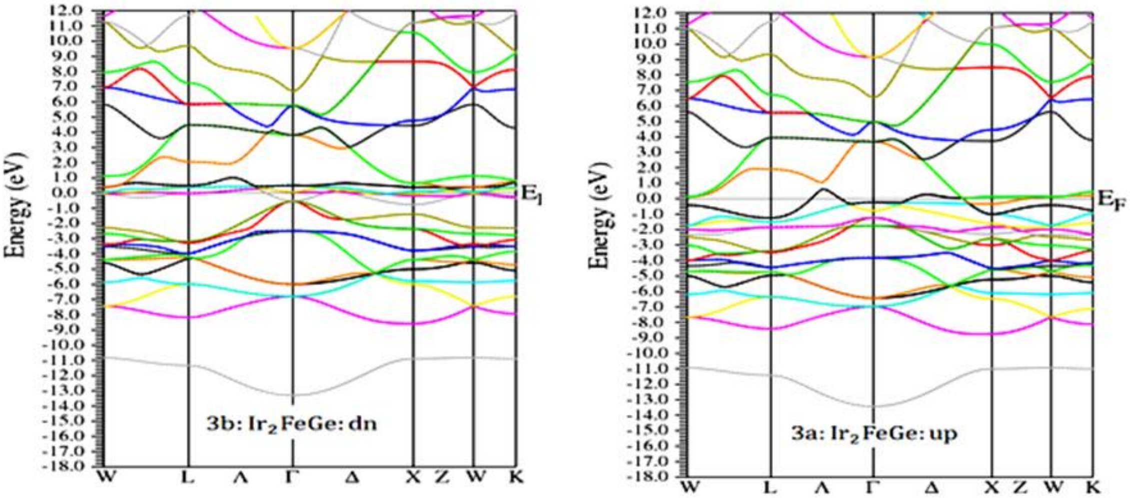
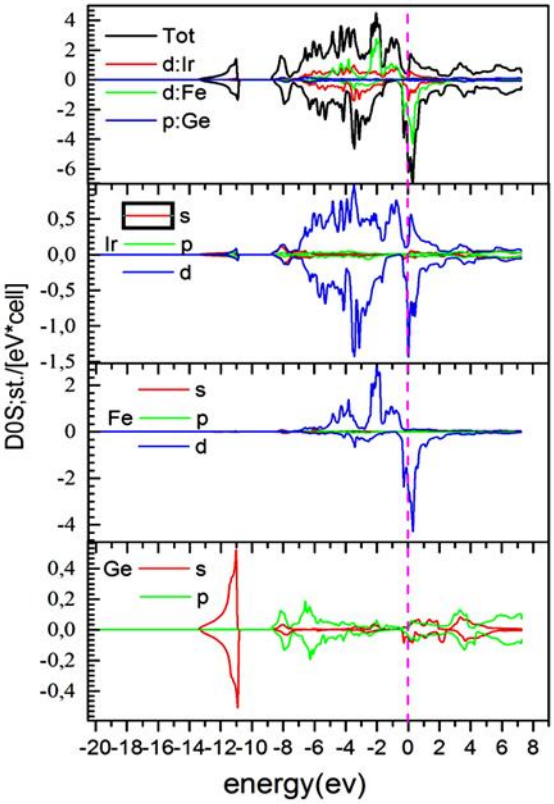


Figure 3. Band Structure of Ir_2FeGe

Density of states: The total projected (DOST) and partial (DOSP) densities between -20 and 8 are shown in Figure 4 and the Fermi level is taken as the source of the energy. The analysis of the figures of the total and partial density of Ir_2FeGe indicates a non-zero density at the Fermi level and the absence of the forbidden band Eg, which allows us to deduce that this material is metallic in nature. Fe-3d orbitals have a maximum conduction in contribution band and contribute closer to the Fermi level. One can understand that the density of states (DOS) at the Fermi level is mainly due to the Ir-4d and Fe-3d states, Germanium does not contribute to DOS at Fermi Level. Moreover, the d states of Ir and d of Fe have an exchange interaction around the Fermi level. it is also lucid from this figure that the compound Ir_2feGe, has a very strong magnetic character, this is visible thanks to the antisymmetry of the states of a majority and a minority, although the contribution of Fe is more significant, despite the fact that there is only one Fe but two atoms of Ir.



(4a)

Figure 4. Total DOS of Ir_2FeGe

Charge density: The calculation of the electronic charge density which is generally presented in a plane where in one direction, informs us about the charge transfer and therefore about the nature of the bond in the material, namely the ionic or covalent nature of the bond. Thus, to visualize the character of the Ir2FeGe bonds, we calculated the charge density as a contour located in the basal plane (110). Figure 4 shows the outline of the charge density of Ir_2FeGe in their face-centered cubic structure, it can be seen that for the compound Ir_2FeGe there is a high electron density between the Ir atoms (electronegativity of Ir=2.2) and their near neighbor Fe (electronegativity of Fe=1.83), and Ge (electronegativity of Ge=2.01), whose explanation seems to come mainly from the covalent nature of the Ir-Ge bond, which is responsible for the high value of the compressibility modulus. The analysis of the interactions between the atoms within the Ir_2FeGe compound show that there is an ionic bond between the Ir and Fe atoms. If we proceed to a more in-depth analysis, we observe on the one hand an almost spherical distribution of the Ir, Fe and Ge atoms and the existence of charge transfer from the Fe atom to the Ir atom (electronegativity of Ir=2.2), that because of the greatness of the electronegativity of the latter, so he attracts the electrons to form a stable byte, whence it constitutes an ionic bond. The compound becomes an ionic compound and an electrical conductor which has a high melting point (Figure 5).

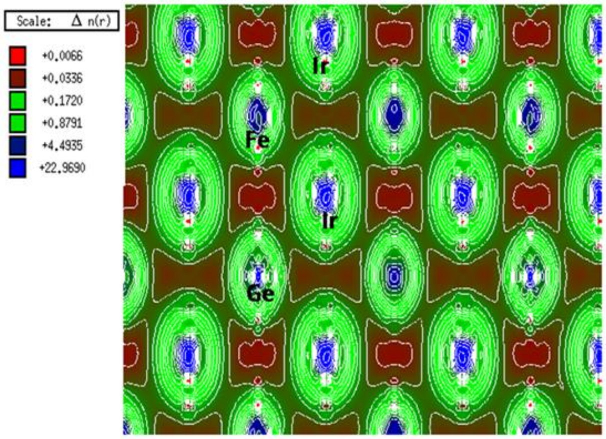


Figure 5. Electron Density Plot of Ir2FeGe

Elastic Properties and Mechanical Stability

The elastic properties have an important role by giving useful knowledge on the nature of the bonding between the neighboring atomic planes, the elastic constants are used to define the mechanical stability of the deformation of the crystal face. They are the proportionality coefficients relating the applied strain to the stress, which describes the response of the material, its strength, and mechanical stability under compression [24,25]. In a cubic crystal, the mechanical stability is obtained when the following conditions on the elastic constants (C_{11}, C_{12}, and C_{44}) are satisfied $C_{11} + 2C_{11} > 0, C_{44} > 0, C_{11} - C_{12} > 0, C_{12} < B < C_{11}$ [24-26].

The computations of elastic constants of Ir_2FeGe are shown in Table 3. It can be said that the Ir_2FeGe compound is mechanically stable because all these elastic constants are positive and satisfied for the stability conditions of crystal lattice [24-26]. C_{11} and C_{12} describe the response of the crystal to unidirectional compression, while C_{44} is proportional to the shear modulus and can be used as a measure of shear deformation [25]. The value of C_{11} is greater than C_{44} of 80.52%. It reveals that Ir_2FeGe has more compressive strength than shear deformation. It can be seen from Table 3 that the calculated bulk modulus at zero pressure from elastic constants is 1.28% higher than that obtained by total energy optimization, our results show that the value of the constant C_{11} is larger than the other constants. So we can say that the length change resistance is the most important in this compound.

Table 3. Elastic constant $C_{ij}(Gpa)$, the bulk modulus B(Gpa), shear modulus G(Gpa), Young's modulus E(Gpa), anisotropy factor (A), Poisson's ratio v, and the bulk-modulus-to-shear-modulus ratio, for the Ir_2FeGe.

	C_{11}	C_{12}	C_{44}	A	E	B	G	V	B/G
Ir_2FeGe	394.74	221.73	76.89	0.88	224.67	272.73	82.44	0.36	3.31

The modulus B, the shear modulus G, Young's The modulus E, the Poisson ratio for $\mathrm{Ir_2FeGe}$ get from the individual elastic constants by the Hill approximation, this approximation is based on the approaches of Reuss and Voigt, with $\mathrm{B_H = B_v = B_R = (C_{11} + 2C_{12})/3}$ (Hill'sbulk modulus) and et $\mathrm{G = (G_V + G_R)/2 = G_H}$(Hill's shear), [25,27,28], These results are presented in Table 3. The Young's modulus E and the Poisson's ratio ν are determined by the relations:

$\mathrm{E = 9BG/(3B + G)}$ et $\mathrm{\nu = (3B - 2G)/2(3B + G)}$ [25,27,28], with Bulk modulus B determine the resistance of a material to volume change by applied pressure [25]. For cubic material, the shear modulus (G) is related to the second-order elastic constants [29], the Shear modulus G measures resistance of material to the plastic deformation [29], whereas the Young’s modulus is an important parameter which is defined as the ratio of the tensile stress to the tensile strain [30]. It is used to provide a measure of the stiffness of the solid. The larger the value of the Young’s modulus E, the stiffer is the material [30]. From Table 3 it can be said that the $\mathrm{Ir_2FeGe}$ compound has good rigidity because of the high value of the Young's modulus. According to Frantsevich et al. [31], Metals with a Poisson's ratio of about $1/3$ are ductile, whereas metals with a Poisson's ratio less than $1/3$ are deduced as being fragile, so the compound $\mathrm{Ir_2FeGe}$ is a ductile compound. We notice that there are no available data to compare with our results of elastic constants, bulk and shear modulus. The obtained elastic constants are used to compute the anisotropy parameter (A) [27,30], which is given by the relation: $\mathrm{A = 2C_{44}/(C_{11} - C_{12})}$, is an important physical quantity which tells about the structural stability and it is highly correlated with the possibility of inducing micro-cracks in the materials. we get the anisotropy parameter $\mathrm{A = 0.88}$ this result indicates that the elastic properties of $\mathrm{Ir_2CrGe}$ are highly anisotropic. We can say that if:

A < 1, the material is the most rigid along the axis of the cube $< 100 >$,

A $>$ 1 is the most rigid along the diagonals of the body $< 111 >$ [32].

We observe, according to the results found ($\mathrm{A = 0.08} < 1$, and thus the $\mathrm{Ir_2FeGe}$ is most rigid along the axis of the cube $< 100 >$ in a structure of L21. From the Criterion of Pugh [33] the B/G ratio is 3.31 for $\mathrm{Ir_2FeGe}$ The value is an index of ductility of the studied material since she is larger than 1.75 this result indicated that the compound is ductile.

CONCLUSIONS

In summary, we optimized the volume to find a stable minimum energy configuration and we have also investigated the electronic, elastic, and magnetic properties of the $\mathrm{Ir_2FeGe}$ of Heusler alloy, using the first principles calculations of the full potential linearized augmented plane wave (FP-LAPW) method. The band structure of this material is of a metallic character for both spin orientations. State density analysis gives a detailed explanation of the contribution of the atomic characters of different orbitals in the energy bands. the compound studied satisfies Born's criteria for mechanical stability. The origin of magnetism in this alloy of Heusler comes mainly from transition metal Fe.

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