Electronic Band Structure analysis on newly proposed Iridium based Heusler alloys in different exchange correlation potentials.

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Abstract. Electronic band structure of newly predicted Heusler alloys Ir2VGa and Ir2VGe has been analysed using Wien 2k code. This paper is focused to understand effects on magnetism, band structure and spin polarization due to (i) Different exchange and Correlation potential and (ii) with the replacement of Ga by Ge. Structural optimization is carried out in nonmagnetic (NM) and ferromagnetic (FM) states and both the alloys are found to be stable in FM state. Band structure of both the alloys are compared in LSDA and GGA, the alloys considered are found to be metallic in both spin channels. Total magnetic moment does not obey with Slater Pauling rule. As LSDA and GGA are proved to be not accurate in estimating energy gap, calculation is repeated in modified Becke-John potential (mBJ), as it is proved to be good in many semiconductors and Half metallic Heusler alloys. In mBJ scheme, the magnetic moment of Ir2VGa and Ir2VGe is 2(μB) and 3(μB), both are Half metallic and 100% spin polarized. When Ga replaces Ge, the magnetic moment of Iridium and Vanadium is increased, Density of states at fermi level and energy Gap increases. Experimentalist support is needed to verify the results.

1. Introduction

Materials in which one spin channel is metal and other channel is semiconductor are termed as Half metals. Ferromagnetism combined with Half metals has attracted many scientists due their application Spintronics devices. Such materials which show 100% spin polarization at Fermi level, is essential for spin current in spin injection devices. Half metallic ferromagnetic materials analysed for spintronic application includes Heusler alloys[1], ferrites[2–4], rutile[5–7] perovskites[8] and dilute magnetic semiconductors[9–12]. Heusler alloy was first discovered by Friedrich Heusler, in the year 1903 in Cu2MnSn[13]. Over the century, the members of this family is increased to more than 2000, due to its diverse applications[14] in thermoelectricity[15–17], Shape memory alloys[18,19], etc.

Using Density functional theory (DFT), de Groot [20] has predicted half metallicity in NiMnSb half heusler alloys, after this many theoretical physicists have been helping experimentalist to identify best suitable alloys for various applications like spintronics, super conductors, shape memory alloys, thermoelectric field, spintronics etc. Many advanced computational codes are available to study electronic band structure and predict the properties of the alloys under consideration. Band structure analyses must be performed with utmost care, otherwise wrong prediction will lead money loss and time for experimentalist. Exchange and correlation term in Kohn-Sham equation can be treated by various methods like LSDA, GGA etc. In LSDA, local DOS is taken into consideration, but Gradient of DOS is taken into considerations in GGA.
LSDA underestimates the lattice parameter and GGA overestimates the same. Energy band gap for experimentally reported alloys was underestimated by both exchange and correlation[21]. To calculate band gap very accurately, Tran and Blaha proposed a modified version of Becke-Johnson exchange potential[22] in the year 2009[23]. The mBJ potential is semi local and orbital independent exchange correlation potential was verified by Koller by calculating energy gaps for many semiconductors[(24,25)]. Many Heusler alloys have been studied using mBJ potential for spintronic applications [26–33]. Iridium based binary alloys were widely used in GMR and TMR, memory storage devices. But Iridium based heusler alloys were not reported by theoretician except for Ir₂CrAl[34], Ir₂MnAl[35], Ir₂MnGa[36]. This motives to investigate Iridium based heusler alloys for spintronic applications.

2. Methodology

In this study, Wien2k 13.1[37] code was used for structural analysis. The multi-pole expansion of the crystal potential and electron density within atomic sphere was fixed to cutoff at l = 10. In the interstitial region the charge density and the potential were expanded as a Fourier series with wave vector G max set to 12[38]. The SCF calculations are performed for the energy convergence of 10⁻⁵ Ryd and charge convergence of 10⁻⁴e.

2.1. Computational details

Radii (in a.u) of muffin tin orbitals are 2.42 for Iridium, 2.24 for Vanadium and 2.24 for Gallium in Ir₂VGa and the same was 2.49, 2.25 and 2.24 (a.u.) for Ir, V and Ge while considering Ir₂VGe. The Rₜобщ*K_max was 7.5, where Rₜ is the smallest atomic radius and K_max is the maximum value of the reciprocal lattice vectors[27]. Calculations are carried out in a k mesh of 20x20x20 with 256k points in irreducible Brillouin zone. Core Charge leakage was set to 0.997e, by doing this Ir -4f states are considered inside the core. To treat exchange and correlation potential, LSDA, GGA and mBJ were used.

2.2. Structural optimization of Ir₂VZ (Z=Ga, Ge)

Structural optimization of Ir₂VZ (Z=Ga, Ge) alloys have been performed in nonmagnetic (NM) and Ferromagnetic (FM) states using LSDA and GGA as exchange correlation potentials. The calculated total energy versus volumes were fitted into Birch–Murunaghan equation of state[39] to obtain the optimized lattice parameter. Total Energy vs Volume of Ir₂VZ (Z=Ga, Ge) alloys for NM and FM states were plotted and are presented in Fig 1a & b. These figures show that Ir₂VZ (Z=Ga, Ge) alloys have minimum energy in FM state and hence stable in ferromagnetic state. The optimized lattice parameter along with bulk modulus in both exchange correlation potentials are given in Table 1.

| Table 1. Optimized structural properties of Ir₂VGa, Ir₂VGe in LSDA & GGA. |
|-------------------|-------------------|-------------------|-------------------|
| Parameter         | Ir₂VGa            | Ir₂VGe            |
|                   | LSDA  | GGA  | Ref[40] | LSDA  | GGA  | Ref[40] |
| Lattice parameter Å | 6.0094 | 6.1276 | 6.115 | 6.0537 | 6.1679 | 6.145 |
| Bulk modulus (Gpa) | 275   | 242.7 | -     | 257   | 220  | -     |

From the table, it is observed that the deviation in optimized lattice parameter values are less than 1 % from the reference value. In both LSDA and GGA method of calculation, the optimized lattice parameter of Ir₂VGe is greater than that of Ir₂VGa and this is due to the decrease in atomic radius and increase in electronegativity of Ge; however, it follows the same trend as that of the reference lattice parameter.
values. Bulk modulus value decreases by 6% when Ga replaces Ge. The experimental bulk modulus or other theoretical values are not available, so the values presented here is purely predictive. I compared the values with similar compounds Co2VGa(201Gpa) and Co2VGe(205Gpa)[41] and found to be higher than that of these compounds indicating hard materials. Optimization calculation is not performed in mBJ as it does not have exchange energy functional it has only exchange potential functional.[42]

3. Result and Discussion

3.1. Magnetism of Ir2VZ (Z=Ga, Ge) in LSDA, GGA and mBJ
The total magnetic moment per unit cell for full Heusler alloys can be obtained using the Slater-Pauling rule, \( M = (N_v - 24) \mu_B \) Where \( N_v \) is the number of valence electrons per unit cell. For Ir2VGa and Ir2VGe,
the number of valence electrons per unit cell is 26 and 27 respectively. Hence, the expected magnetic moment per unit cell is 2 \( \mu_B \) and 3 \( \mu_B \) for \( \text{Ir}_2\text{VGa} \) and \( \text{Ir}_2\text{VGe} \) respectively.

The calculated total and partial magnetic moment of individual elements are reported in Table 2. On comparing the magnetic moments obtained in LSDA and GGA scheme, the total magnetic moment is high in GGA, due to the variation in lattice parameter. When Ga is replaced with Ge, the total magnetic moment as well as magnetic moment of Ir and V increases, this can be attributed change in lattice constant, which lead to the less overlap between d orbitals and exchange interaction is high[43]. In case of \( \text{Ir}_2\text{VGa} \) the magnetic moment of Ir and V are ferromagnetically coupled with each other whereas Ga is ferrimagnetically coupled with them. In case of \( \text{Ir}_2\text{VGe} \), Ir, V and Ge are ferromagnetically coupled with each other. In case of \( \text{Ir}_2\text{VGa} \), the calculated magnetic moment in GGA scheme is in agreement with that reported by Gilleßen[40]. Gilleßen[40] has reported a magnetic moment of 1.97 for \( \text{Ir}_2\text{VGa} \). For \( \text{Ir}_2\text{VGe} \), the magnetic moment is 2.99 in present studied which agrees very well with Slater -Pauling rule, but Gilleßen[40] has reported 0.0 for \( \text{Ir}_2\text{VGe} \). The integral magnetic moment of 2 \( \mu_B \) and 3 \( \mu_B \) are obtained respectively for \( \text{Ir}_2\text{VGa} \) and \( \text{Ir}_2\text{VGe} \) compounds in GGA+ mBJ scheme. The integral magnetic moment is indication of half metallicity in the alloys considered.

| Magnetic moment per unit cell (\( \mu_B \)) | \( \text{Ir}_2\text{VGa} \) | \( \text{Ir}_2\text{VGe} \) |
|-------------------------------------------|-----------------|-----------------|
| \( \mu_{\text{tot}} \)                     | 1.87            | 1.98            | 2.00            | 2.717          | 2.99            | 3.00            |
| \( \mu_{\text{Ir}} \)                      | 0.266           | 0.279           | 0.265           | 0.477           | 0.55            | 0.578           |
| \( \mu_{\text{V}} \)                       | 1.17            | 1.27            | 1.38            | 1.45            | 1.57            | 1.69            |
| \( \mu_{\text{Z}} \)                       | 0.0088          | -0.0007         | -0.0094         | 0.0654          | 0.05            | 0.248           |

3.2. Electronic band structure and Half Metallicity of \( \text{Ir}_2\text{VZ} \) (Z=Ga, Ge) in LSDA, GGA and mBJ.

Electronic band structures are plotted along the high symmetry directions in the Brillouin Zone. The spin polarized band structure plot along with total Density of States (DoS) of \( \text{Ir}_2\text{VGa} \), \( \text{Ir}_2\text{VGe} \) using LSDA, GGA and mBJ as exchange correlation potential are presented in Fig 2a, b, c & Fig 3a, b, c respectively. From band structure plot Fig 2a of \( \text{Ir}_2\text{VGa} \) in LSDA scheme it is observed that Fermi energy level passes through conduction band in both majority and minority spin channels. Thus, the alloy is of metallic in nature.

In majority spin up channel, one can observe a pseudo gap at 0.6eV below the Fermi energy level. In minority spin channel, pseudo gap exits at 0.2eV below the Fermi energy level. In the band structure plot of \( \text{Ir}_2\text{VGa} \) using GGA (Fig 2b) as exchange correlation potential, the same metallic behaviour is observed in spin up channel. In spin down channel, spin gapless semiconductor with vanadium-d level passing along the Fermi energy level is observed.

Considering the band structure of \( \text{Ir}_2\text{VGa} \) Fig 2c in mBJ scheme, it is observed that majority spin up channel is metallic in nature. The pseudo band gap presents in the spin up channel in LSDA and GGA scheme is found to be absent in mBJ scheme.
Figure 2 a. Band structure of Ir$_2$VGa in LSDA – Spin up (left), Total DoS (Center) & spin down (Right)

Figure 2 b. Band structure of Ir$_2$VGa in GGA – Spin up (left), Total DoS (Center) & spin down (Right)

Figure 2 c. Band structure of Ir$_2$VGa in mBJ – Spin up (left), Total DoS (Center) & spin down (Right)
Figure 3a. Band structure of Ir$_2$VGe in LSDA – Spin up (left), Total DoS (Center) & spin down (Right)

Figure 3b. Band structure of Ir$_2$VGe in GGA – Spin up (left), Total DoS (Center) & spin down (Right)

Figure 3 c. Band structure of Ir$_2$VGe in mBJ – Spin up (left), Total DoS (Center) & spin down (Right)
This is due to the fact that mBJ scheme focusses on exchange correlation energy rather than on potential involved[26]. But spin down channel Fermi energy level passes through the gap, exhibiting semiconducting nature. Thus, Ir₂VGa is half metallic in mBJ exchange energy. An indirect band gap of 0.2eV along the Γ and X point of the Brillouin zones. Similar half metallicity has been observed and reported by D P. Rai [26] for Co₂VSb alloy with mBJ scheme. The change in band structure in LSDA and GGA scheme is attributed to change in lattice parameter. In three schemes Fermi energy level are different, the shift in fermi level changes the occupied level at Fermi energy level.

From the Band structure plot of Ir₂VGe in LSDA and GGA (Fig 3a, b) schemes, it can be observed that Fermi energy level passes through conduction band in both the spin channels. Thus, exhibiting metallicity. A small pseudo gap is present below the Fermi energy level in spin up channel. In spin down channel, vanadium-d levels are present at the Fermi energy level. Analysis of band structure plot of Ir₂VGe in mBJ scheme (Fig 3 c) shows that. Ir₂VGe is halfmetallic due to its metallic nature in spin up channel and semiconducting nature in spin down channel. An indirect band energy gap of 0.4eV is obtained in mBJ calculation. As Ga is replaced by Ge, band gap increases similar trend is observed in Co₂VGa and Co₂VGe[44].

Thus, both alloys exhibit half metallicity and ferromagnetism in mBJ scheme.

3.3. Spin Polarization of Ir₂VZ (Z=Ga, Ge) in LSDA, GGA and mBJ.

The spin polarization can be calculated using the following formula

\[ P(E_F) = \frac{\rho \uparrow (E_F) - \rho \downarrow (E_F)}{\rho \uparrow (E_F) + \rho \downarrow (E_F)} \]  

Where \( \rho \uparrow \) and \( \rho \downarrow \) are the DoS (density of States) in spin up and spin down channels respectively.

For the practical use of material in spintronics application, 100% spin polarization is an essential condition. To get 100% spin polarization, density of states in any one spin channel should be zero. The electron spin polarization at fermi energy is studied for Ir₂VZ (Z=Ga, Ge) alloys in LSDA, GGA and mBJ schemes. DoS at Fermi energy level, percentage of polarization and energy gap are reported in table 3.

| Table 3. DoS at Fermi energy level, percentage of polarization and energy gap of Ir₂VGa, Ir₂VGe. |
|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|
| Alloys | \( \rho \uparrow (E_F)/\text{Ry} \) | \( \rho \downarrow (E_F)/\text{Ry} \) | P% | Energy Gap [eV] |
| Ir₂VGa | LSDA | 37.09(2.72/eV) | 10.75(0.79/eV) | 55.05 | -- |
|       | GGA  | 57.19(4.205/eV) | 4.35(0.32/eV) | 85.86 | -- |
|       | mBJ  | 46.92(3.45/eV) | 0.00 | 100 | 0.2 |
| Ir₂VGe| LSDA | 73.53(5.40/eV) | 40.20(2.95/eV) | 29.3 | -- |
|       | GGA  | 66.14(4.86/eV) | 2.17(0.159/eV) | 93.68 | -- |
|       | mBJ  | 56.81(4.177/eV) | 0.00 | 100 | 0.4 |

For Ir₂VGa alloy, the calculated spin polarization is found to be 55% and 85% in LSDA and GGA scheme respectively. In mBJ 100% spin polarization is observed, due to zero density of states at Fermi energy level.

In Ir₂VGe, percentage of spin polarization at Fermi energy level is 29.3% and 93.68 % in LSDA and GGA respectively. In LSDA, heavy DoS is observed in both spin channel. In GGA, DoS is reduced in both the spin channel. In mBJ, DoS is further reduced, which lead to the 100% spin polarization.
The reason for the different percentage of spin polarization in different exchange correlation potential and the effect of main group element can be understood from the partial DoS of each constituent element. The partial DoS of Ir, V, Ga and Ge are presented in Fig 4, 5 and 6.

First, the partial density of states (PDoS) in LSDA scheme for Ir$_2$VGa and Ir$_2$VGe are, compared to understand the influence of main group element. Figure 4a, b presents the PDoS of Ir$_2$VGa and Ir$_2$VGe in LSDA scheme. When Ga is replaced with Ge, the density of states increases drastically (ref table 3) reason can analysed from Fig 4a, b. In spin up DoS of Ir$_2$VGa, Vanadium d -states, Ir -d states and Ga s, p states have contributed.

In spin down states, few states Ir d-eg and p states of Ga are present in the fermi energy level. This indicates hybridization between Ir and Ga thus affecting half metallicity. In case of Ir$_2$VGe, main contribution to spin up DoS is from Vanadium d-states next is from Ir, and least from Ge- s states. It is evident that Ge has redistributed the d electron states of Ir and V.

![Figure 4 Partial DoS of Ir, V, Ga & Ge in LSDA for (left) Ir$_2$VGa and (right) Ir$_2$VGe](image-url)
This may be due to the electronegativity Ge has increased the bonding between Ir, V and Ge.[35] When spin down states of Ir₂VGe is compared with Ir₂VGa, it is observed that Ge has pushed the Ir-d-eg and V-d-t²g states to fermi energy level, thereby increasing DoS in Spin down states. In LSDA both alloys did not show spin polarization as explained in magnetism as well by band structure analysis.

As calculation performed using LSDA as exchange correlation potential is proved to underestimate lattice constant as well as energy gap in many 3d Heusler alloys[43,45,46]. The spin polarization analysis is carried out using GGA and in GGA+mBJ.

First, the comparison of PDoS of Ir, V and Ga of Ir₂VGA in GGA and mBJ scheme. PDoS of Ir and V d-eg, d-t²g states and Ga s, p states are presented in Fig5. Ir d-states splits up into d-eg and d-t²g states. Ir d-eg states splits predominately into three peaks, two in spin up channel and one in spin down channel. In spin up channel, V-d states splits in to d-eg and d-t²g states both the states lie on the fermi level. From Ga PDoS, it is observed that both sand p states lie at fermi level in spin up channel,

![Graphs showing partial density of states](image-url)
but in spin down channel p states is present. Thus Ir-d-eg states and Ga-p states were present and alter the half metallicity.

In mBJ scheme, it is evident that exchange splitting has been enhanced in spin up channel for all three elements and in spin down no states lies at fermi energy level. This is due to the shift of fermi energy. Ir2VGa is metallic in spin up channel due to presence of Ir, V and Ga states at fermi energy level. In spin down channel Ir, V and Ga states are shifted away from fermi level and creates energy gap. Thus, in mBJ scheme Ir2VGa is half metallic, same is supported in magnetism and band structure discussion presented above.

Figure 6 Ir2VGe – Partial DoS of Ir, V, Ge in (left) GGA and (right) in mBJ.
Y axis: DoS (States / eV)
Figure 6 represent PDoS of Ir, V and Ge of Ir$_2$VGe in GGA and mBJ scheme. It is observed that the inclusion of one more electron in replacement of Ga by Ge has affected the symmetry states of Ir - d, but V d-state states are not affected. This may be due to the strong electronegativity of Ge states and forms bond with Ir states. From PDoS of Ir and Ge, it is clear that Ir-d states and Ge s and p states present at the fermi level in spin down states indicating strong hybridization between Ge and Ir. In GGA PDoS, it is observed Ir$_2$VGe is metallic in both spin channel. On repeating the calculation in GGA +mBJ, both spin up and spin down level are changed drastically. Ir and V -d states distributed in spin up channel are shifted below the fermi level and in spin down channel shifted above fermi level creating an energy gap. p and s states of Ge is pushed above the fermi level. In spin up channel the d level of Ir and V, s p band of Ge cross the fermi level indicating metallic nature. In spin down channel, there exists a wide gap indicating semiconducting nature. Thus, Ir$_2$VGe is half metallic in mBJ scheme. Same was explained in magnetism and band structure.

4. Conclusions.
In summary, First Principle Calculations are performed on predicted Heusler alloys Ir$_2$VGaand Ir$_2$VGe using Wien 2k code. Structural properties were analysed using LSDA, GGA and mBJ correlation functions. A detailed comparison between LSDA, GGA and mBJ was carried out in explain magnetism, band structure and spin polarization. Our calculations show that both alloys are stable in Ferro magnetic state. In LSDA as well as in GGA the two alloys did not exhibit Half metallic character. As per Slater - Pauling rule integral magnetic is not obtained LSDA and GGA. In GGA+ mBJ, both alloys show metallic nature in spin up and semiconducting in spin down. The integral magnetic moment of 2μB for Ir$_2$VGa and 3μB for Ir$_2$VGe is obtained. Energy gap of Ir$_2$VGa is 0.2eV and Ir$_2$VGe is 0.4 eV.

The influence on main group element in magnetism and half metallicity is discussed using PDoS. Experimentalist support is needing to verify the energy gap and magnetism for implementing the alloys for spintronic applications. Ir and V are strongly correlated transition metals, in future calculation will be extended with Hubbard potential.

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