

## Prediction of electronic and magnetic properties of Full Heusler Alloy – Ir<sub>2</sub>CrAl

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**Abstract:** The structural, electronic and magnetic properties were predicted for Full Heusler Alloy – Ir<sub>2</sub>CrAl using local spin density approximation as implemented in Wien2k 13.1. We analyzed and predicted that the compound can be used for spintronic application as we recognize 100% spin polarization, half metallicity and ferromagnetic with magnetic moment of 3  $\mu$ B.

**Keywords:** Heusler, Electronic Band Structure, Half Metal, Spintronic

### I. Introduction

Heusler alloys (1) with majority band metallic but minority band semiconducting are half metallic Ferro magnets (HMFs) is proposed by de Groot et al(2). If any of these HMFs exhibit 100% spin polarization at Fermi level they are identified as useful spintronic (3) materials.

The chemical formula of Heusler alloys (1) is X<sub>2</sub>YZ where X&Y are transition metals and Z atoms are from III, IV and V group elements (viz., Al, Ga, Ge, Sn, Sb, In, Bi, Tl). The structure of full Heusler alloy is L21 with space group of Fm-3-m, has four penetrating FCC sub-lattices. In this FCC structure X atoms occupy (¼,¼,¼) & (¾,¾,¾) positions, while Y atoms are at (½, ½, ½) and Z atoms at (0,0,0) as shown in figure1.

The ternary full Heusler alloys which possess half metallic character with 100% spin polarization and ferromagnetic property are of great interest for spintronic application. The electronic structure and magnetic property of Co<sub>2</sub> based Heusler compounds using LSDA+U & LSDA have been studied widely by Rai et al.(4,5). Galanakis et al.(6) have reported half metallicity in many heusler compounds and also by Hem C Kandpal(7). To our knowledge, the band structure property and magnetic property of Ir<sub>2</sub>CrAl compound have not yet been reported.

In this study we calculated the electronic structure and magnetic properties of full Heusler alloy Ir<sub>2</sub>CrAl using LSDA. We are able to predict that this compound is half metallic, ferromagnetic and also exhibits 100% spin polarization.

Subsequently we are describing the computational details in section II, structural details in section III, and summarizing result & discussions in section IV.

### II. Computational detail

An augmented plane wave plus local orbitals program for calculating crystal properties implemented in Wien2k 13.1 (8) was used. LSDA with spin polarization has been used in this study for theoretically analyzing the compound. The maximum value of lmax = 10; Rkmax = 7. In the interstitial region the charge density and potential was expanded with wave vectors up to Gmax = 12. The number of K points generated were 47; we chose to use the muffin-tin radii of 2.46 a.u. for Ir; 2.23 a.u. for Cr and 2.11 a.u. for Al.

### III. Structural Optimization ; Indentations and EQUATIONS

Since the experimental lattice parameter was not available, we used the parameter from the prediction of Micheal Gillisen(9). The volume optimization (Figure 2) was carried out to get minimum energy using SCF with energy convergence of 0.0001 Ry and charge convergence of 0.0001 e. The optimized curve is shown in figure 2. The calculated total energy was fitted into Murnaghan's equation (10).

Equation of state: (Murnaghan)

$$E=E_0 + [B*V/BP*(1/(BP-1)*(V_0/V)**BP +1)-B*V_0/(BP-1)]/14703.6$$

$$\text{Pressure}=B/BP*((V_0/V)**BP - 1)$$

Where E<sub>0</sub> is the minimum energy at 0K.

The details of optimized lattice parameter and bulk modulus is given in table 1.

The optimized lattice parameter was 1.7% less than the already predicted value. This value was used to calculate DOS, spin magnetic moment and energy band.

#### IV. Figures and Tables

Lattice Constant $a_0$ (Å)			Bulk Modulus B (GPa)	Equilibrium Energy (Ry)
Previous	present	$\Delta(a_0)$		
6.069(9)	5.9648	0.105	270.9268	-73974.051777

Table1: Lattice Constant, Bulk Modulus, Equilibrium Energy

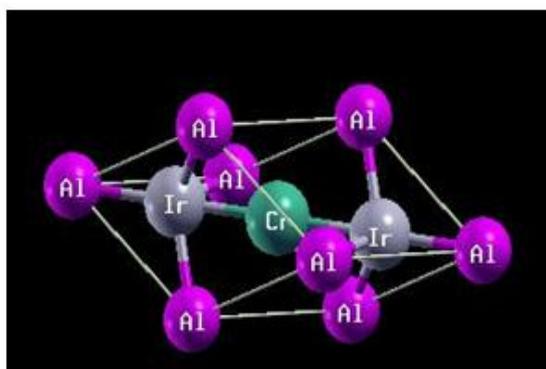


Fig 1: Unit Cell Structure of Ir2CrAl

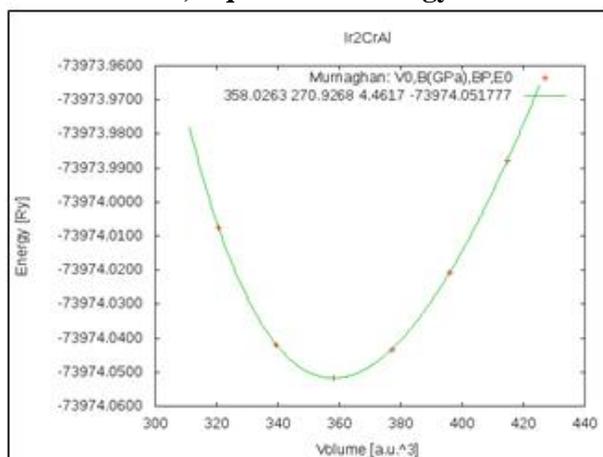


Fig 2: Volume Optimization of Ir2CrAl

Energy	Gap(eV)	Spin	polarization
$E_{max}(\Gamma)$	$E_{min}(X)$	$\Delta E$	$p_{\uparrow}(E_f)$ $p_{\downarrow}(E_f)$ P %
0.18	0.12	0.3	50.27 0.00 100

Table2 Energy gap and spin polarization

Magnetic Moment Of Ir2CrAl				
Previous (9)	Present – Calculated			
	Ir	Cr	Al	Total
3.00	0.22191	2.390	0.00006	3.00

Table3 Total and partial magnetic moment

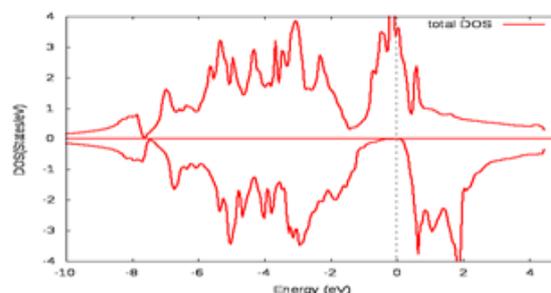
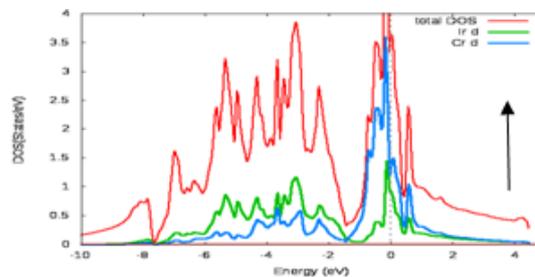
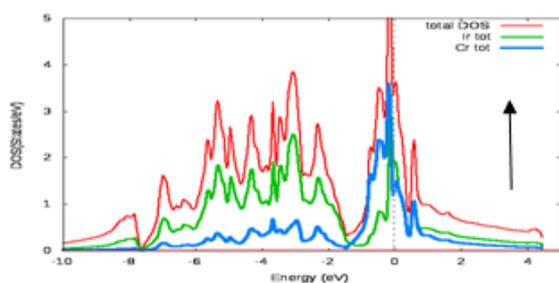


Fig.3. Total DOS



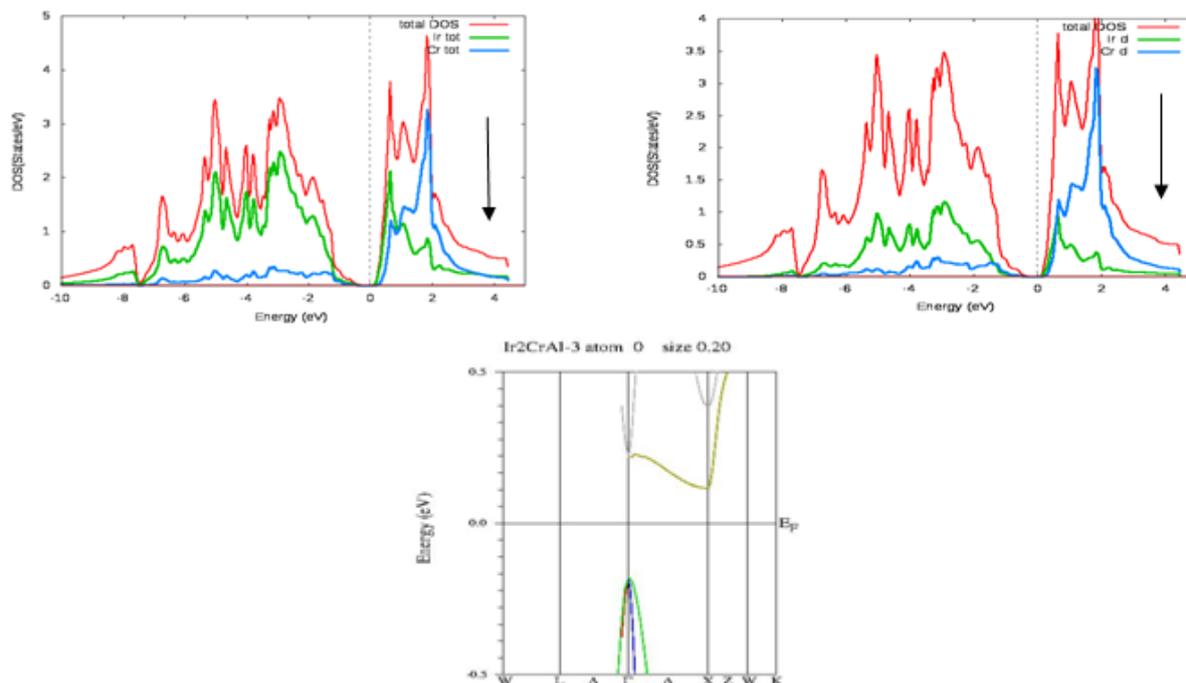


Fig 5. Energy band diagram

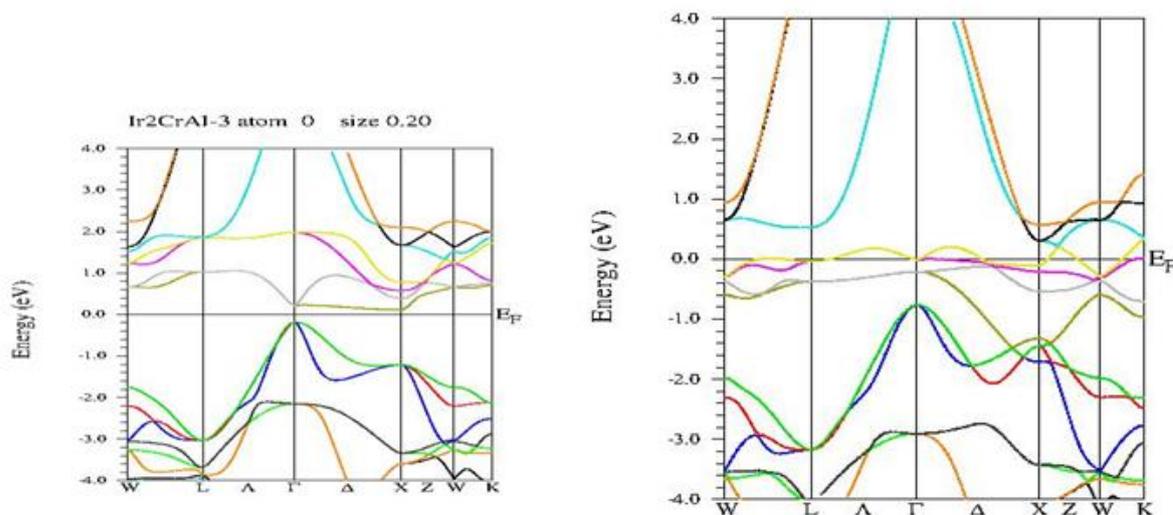


Fig 6. Energy band diagrams

## V. Conclusion

### Spin polarization and half metallicity.

The value of electron spin polarization at Fermi level place an important role to use the compound in scientific and technological areas. The spin polarization of paramagnetic and anti-ferromagnetic material vanishes below the magnetic transition temperature. For ferromagnetic material P is given by(12)

$$P = \frac{N\uparrow(E_F) - N\downarrow(E_F)}{N\uparrow(E_F) + N\downarrow(E_F)}$$

where  $N\uparrow(E_F)$  and  $N\downarrow(E_F)$  are the spin dependent density of states at the ( $E_F$ ) .

The DOS at Fermi level for spin up state is 50.27 and for spin down states is 0. Thus the calculation for the compound Ir2CrAl shows that its 100% spin polarized at  $E_F$  the details are given in table-2. Figure (3) and

(4) summarizes the results of DOS plot. From (4 a,b) graph we find that in spin up state, the contribution to total DOS is mainly from Cr atom. The d states of Cr atom contribution are more than the Ir d states as in graph (4a,b). But in spin down states Figure(4c,d) both Ir and Cr d states contribution is zero.

The energy band diagram for spin up and spin down states were plotted for range of -4 eV to 4 eV as shown in figure (6a,b)). In fig (5) we identify the indirect band gap along  $\Gamma$ -X symmetry with gap of 0.3 eV in spin down states and Fermi level is pinned up in the gap. In majority of states the energy levels indicate metallic character. For half metals, the formation of energy gap was discussed by Galanakis et.al (6) for co<sub>2</sub> and Rh<sub>2</sub> based compounds. Our values are also lie in the same range as Ir<sub>2</sub>MnAl (9) the energy gap is 0.351eV.

### Magnetic Properties.

In order to predict the total spin magnetic moment of Hmfs we should use Slater Pauling rule. Slater Pauling rule is given by  $m_{\text{HMF}} = n_{\text{V}} - 6$ .for magnetic moment per atom. To find magnetic moment per unit cell we use the rule given by Kubler et al.(11)  $m_{\text{H}} = N_{\text{V}} - 24$ .where  $m_{\text{H}}$  magnetic moment per unit cell,  $N_{\text{V}}$  is the accumulated number of valence electrons in unit cell.. The magnetic moment per unit cell should be an integer.

In our compound Ir<sub>2</sub>CrAl valence is 27. So  $27 - 24 = 3$ , which is in good agreement with Slater Pauling rule. The total and partial moment is given in table(3). The contribution to magnetic moment is mainly from Cr as predicted in DOS plot magnetic moment of Ir is very less and of Al is negligible. The calculated magnetic moment is in good agreement with previous (9) prediction.

### Conclusion

We performed volume optimization to find stable minimum energy configuration. The DOS ,energy band structure and magnetic moment of Ir<sub>2</sub>CrAl were calculated using LSDA. The investigation reveals that Ir<sub>2</sub>CrAl has 100% spin polarization. The energy gap in spin down states indicates that it is semiconducting and in spin up states it is metallic. Calculated integral magnetic moment indicates also supports Half metallic ferromagnet.

Thus Ir<sub>2</sub>CrAl is a good spintronic material

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