Electronic Structure and Magnetic Properties of Fe_2YAl (Y = Ti, Cr, Mn, Cu) Heusler Alloys

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Abstract: In this paper we were reported electronic structure and magnetic properties of Fe_2YAl (Y = Ti, Cr, Mn, Cu) Heusler alloys by using SPRKKR package. In order to calculate the ground state properties and to determine the more stable structure for the Fe_2YAl (X = Ti, Cr, Mn, Cu) compounds, we have used the energy minimization procedure. The calculated magnetic moment underestimates from experimentally obtained values and the calculated magnetic moment by Slater Pauling rule. Fe_2CrAl band structure calculations indicate metallic behavior in the majority spin band, while an energy band gap of 0.401eV is observed at the Fermi energy level in the minority spin band. In the case of Fe_2MnAl, both band structure calculations and the DOS indicate metallic behavior in the majority spin band, while an energy band gap of 0.42 eV is observed in minority spin band**.**

IndexTerms **– Heusler alloys, Density Functional Theory, SPRKKR, Electronic Structure Properties, Magnetic Properties.**

I. INTRODUCTION

During the last few years a lot of attention was paid to Heusler alloys due to their wide range of properties which are potentially used in magnetic and electronic industries (Graf et al. 2016; Jain et al. 2017, Chandra et al. 2018, Chandra et al. 2018a). Heusler alloys are intermetallic compounds with the general formula X_2YZ or XYZ. Here, X and Y are transition metals and Z is an element of the III-V groups. Among them Fe-based alloys have aroused the great interest in the development of electronic devices used around the world, such as mobile phones, computers, memory devices, inductor, transformers and other nano electronic components. In this work, the detail electronic structure properties of Fe_2YAl (Y= Ti,Cr, Mn, Cu) (Fm-3m) structure have been investigated by first-principles calculations. It is recognized that the density functional theory (DFT) has been successfully applied to the first-principles calculations of ground state properties of various materials. During the last years many experimental groups have tried to synthesize them mainly in the form of thin films.

The Fe_2TiAl is a very important in the area of aeronautics and astronautics because Fe_2TiAl has high melting temperature, low density, good environmental resistance, high thermal conductivity, attractive modulus, etc (Adebambo et al, 2016). Also, most Fe-based full-Heusler alloys with chemical formula Fe_2MnZ have been predicted to be half-metallic (Jain et al. 2014, Fujii et al, 1995). Structure and magnetic properties of $Fe_{2+x}Mn_{1-x}Al$ Heusler compounds have been investigated by experimentalists and theoreticians (Paduani et al. 2007, Buchelnikov et al. 2014). These interesting magnetic materials are considered to be very promising for technological applications. Sharma and Pilani investigated the electronic, magnetic optical properties of Fe_2YAl (Ti, V and Cr) and observed that these properties changes with atomic configuration of Heusler alloys (Sharma and Pilani, 2013). They were observed that for the majority spin state Fe_2CrAl compound has high density of states and shows 100% spin polarization in the vicinity of the Fermi level. The total magnetic moment is consistent with Slater-Paulings rule and in excellent agreement with the experimental data. According to most reviews the half metallicity in Fe based Heusler alloys makes to them to serve as alternative materials for spintronics devices (Adebambo et al, 2016).

II. COMPUTATIONAL

We have performed the self consistent band calculations in the generalized gradient approximations (GGA) for full-relativistic mode using SPRKKR package (Ebert, 2012). Perdew, Burke, and Ernzerhof exchange correlation potential has been used for calculation. The equilibrium lattice constants of all these alloys are obtained by minimum energy optimization. About 4000 k-points and 40 energy points were used in SPR-KKR and basis functions up to l = 3 were included.

The full-Heusler compounds generally crystallize in two possible structures: the Hg_2CuTi-type $L2_1$ structure and the Cu_2MnAl-structure. $L2_1$ structure is represented by the generic formula X_2YZ, where X and Y denote transition metal elements and Z is s–p element. The structure is composed off our interpenetrating face-centered cubic (fcc) lattices with positions described with the Wyckoff coordinates as: A (0, 0, 0), B (1/4, 1/4, 1/4), C (1/2, 1/2, 1/2) and D (3/4, 3/4, 3/4). The Cu_2MnAl-type full-Heusler compound as the structure where the X atoms occupy the (A, C) sites, while in Hg_2CuTi-type structure the (A, B) sites are occupied by X atoms. In this work the calculations are done for Cu_2MnAl type $L2_1$ order Fe_2YAl (Y = Mn, Cr, Cu, Ti. The crystal structure is shown in fig.1

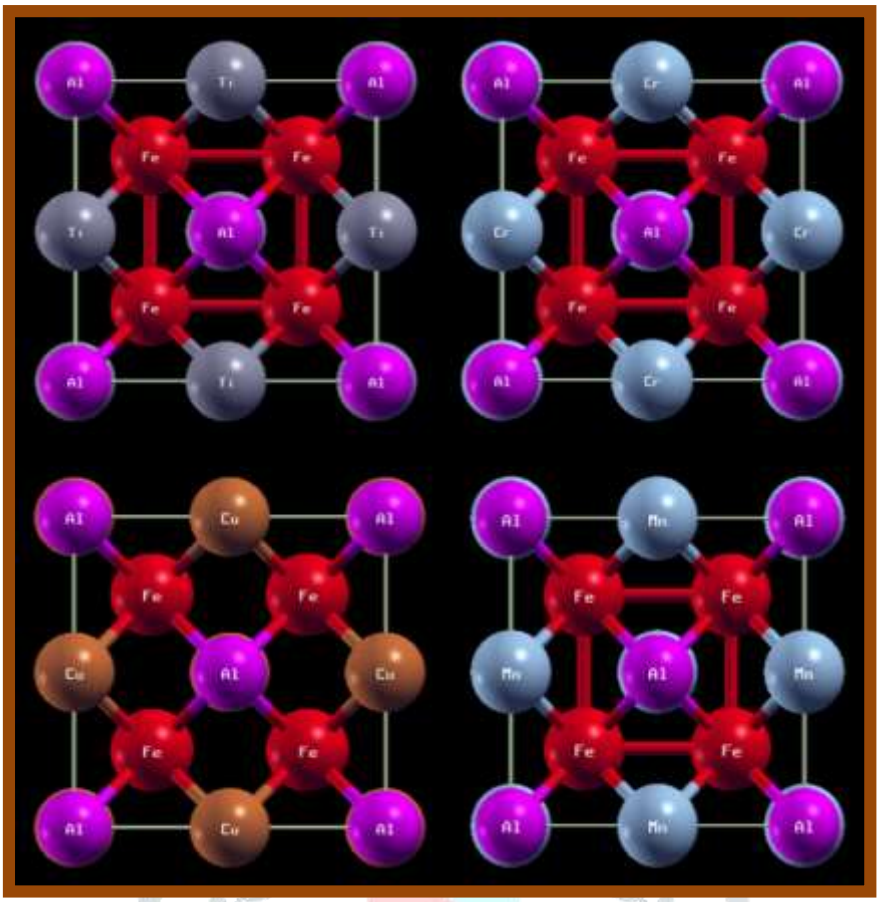

Fig. 1: Xcrysdens Crystal structure view of Fe_2YAl (Y=Ti, Cr, Mn and Cu)

III. RESULTS AND DISCUSSION

In order to calculate the ground state properties and to determine the more stable structure for the Fe_2YAl (X = Ti, Cr, Mn, Cu) compounds, we have used the energy minimization procedure. In this procedure, the total energies are calculated for Cu_2MnAl phases for the different volumes around the equilibrium cell volume, where the plots of the calculated total energies versus reduced volume for these compounds are given in Fig. 2(a) to 2(d). The calculated total energies are fitted to the Gaussian equation peak fitting to determine the minimized equilibrium lattice constant. In addition, the calculated equilibrium parameters, converged energy and Fermi energy are given in Table 1, which also contains results from earlier theoretical works. On the whole, our computed ground state parameters are in good agreement with previous results in the literature. More precisely, our calculated values of the lattice constant are slightly underestimated (overestimated) as compared to their corresponding theoretical values.

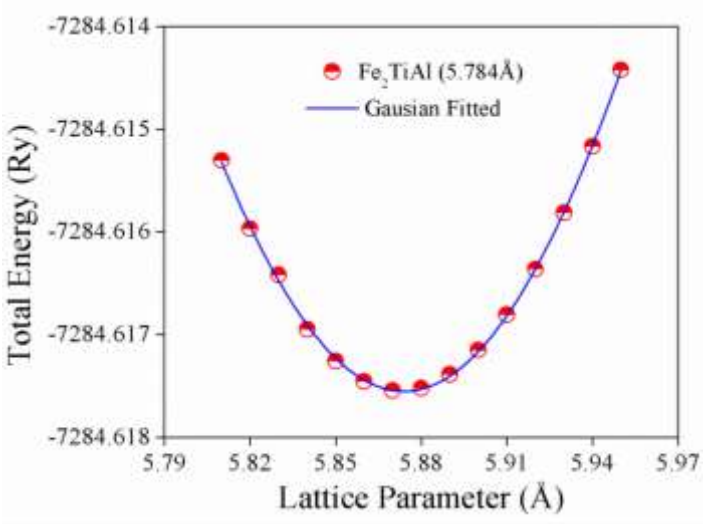

Fig. 2(a): Optimization of the lattice parameter for Fe_2TiAl compounds.

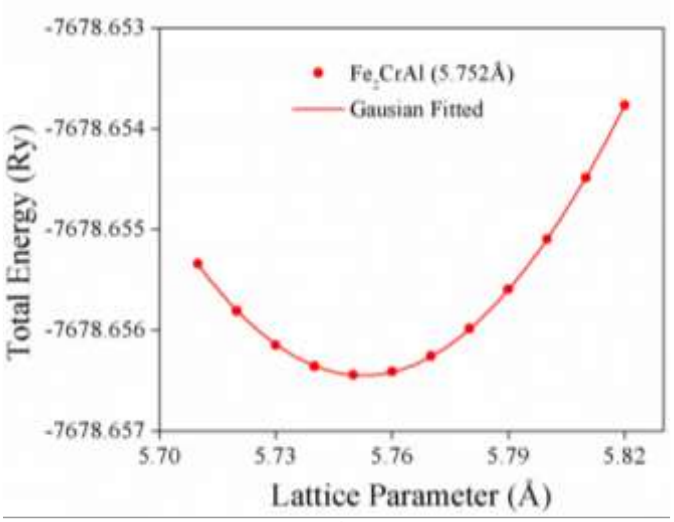

Fig.2(b): Optimization of the lattice parameter for Fe_2CrAl compounds

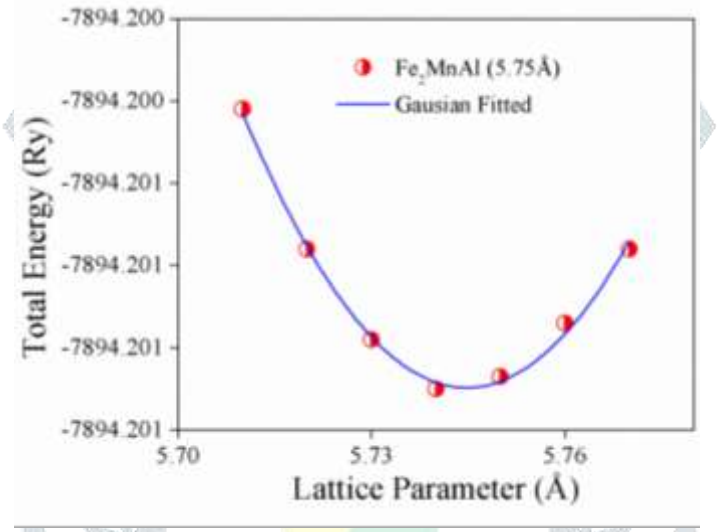

Fig. 2(c): Optimization of the lattice parameter for Fe_2MnAl compounds.

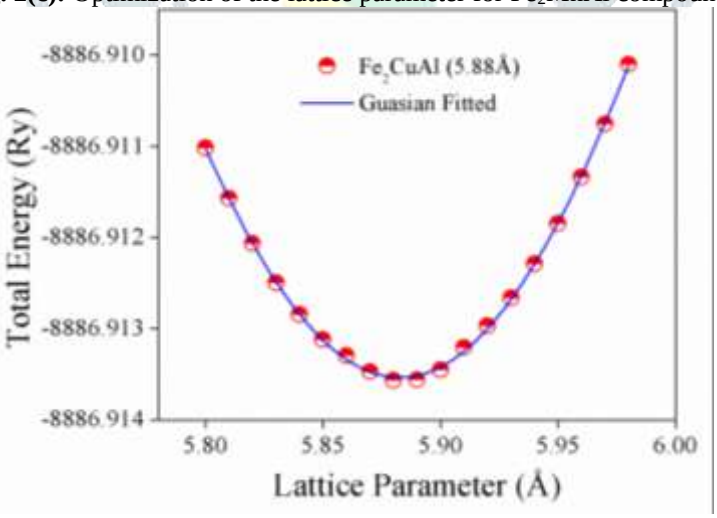

Fig.2(d): Optimization of the lattice parameter for Fe_2CuAl compounds.

Table 1 Obtained Lattice Parameters, Converged Energy and Fermi Energy

Sample	Lattice Parameter (Å)	Converged Energy (Ry)	Fermi Energy (Ry)
Fe_2TiAl			
Calculated	5.874	-7284.61756	0.756
Prev. Rep. Theo.	5.778[a]	----	----
Prev. Rep. Exp.	5.858[a]	----	----
Fe_2CrAl			

Calculated	5.752	-7678.65639	0.817
Prev. Rep. Theo.	5.610[a]	----	----
Prev. Rep. Exp.	5.811[a]	----	----
Fe_2MnAl			
Calculated	5.650	-7894.18490	----
Prev. Rep. Theo.	5.830[b]	----	----
Prev. Rep. Exp.	5.850[c]	----	----
Fe_2CuAl			
Calculated	5.883	-8886.91348	0.722
Prev. Rep. Theo.	----	----	----
Prev. Rep. Exp.	5.830[d]	-----	----

[a](Shreder et al, 2005), [b](Azar et al, 2012), [c](Vinesh et al, 2009), [d](Gilleßen & Dronskowski, 2010)

Fig. 3 (a, b, c, d) shows DOS for Fe_2YAl (Y =Ti, Cr, Mn, Cu) majority and minority spin bands respectively and Fig. 4 (a, b, c d) shows band structures of all samples. In the DOS of Fe_2TiAl, the majority and minority spin densities shows metallic behavior. The band structure calculation is in good agreement (Fig. 5a and b) with DOS (Fig. 6a) as both majority and minority spin bands show metallic behavior. These calculations show that Fe_2TiAl has metallic nature. In the case of Fe_2CrAl, both band structure calculations (Fig. 4b) and the DOS (Fig. 3b) indicate metallic behavior in the majority spin band, while an energy band gap of 0.401eV is observed at the Fermi energy level in the minority spin band. The majority spin conduction bands cross the Fermi level, while there is an energy gap at all points shows at the Fermi level for the minority spin bands.

In the case of Fe_2MnAl, both band structure calculations (Fig. 4c) and the DOS (Fig. 3c) indicate metallic behavior in the majority spin band, while an energy band gap of 0.42 eV is observed at the Fermi energy level in the minority spin band. In the case of Fe_2CuAl, both band structure calculations (Fig. 4d) and the DOS (Fig. 3d) indicate metallic behavior in the majority spin band and the minority spin band. The values of total and partial spin magnetic moments of Fe_2YAl (Y=Ti, Cr, Mn, Cu) have been calculated are summarized in Table 5.2. The obtained values of magnetic moment are underestimated with the Slater–Pauling curve (SPC) for full Heusler alloys.

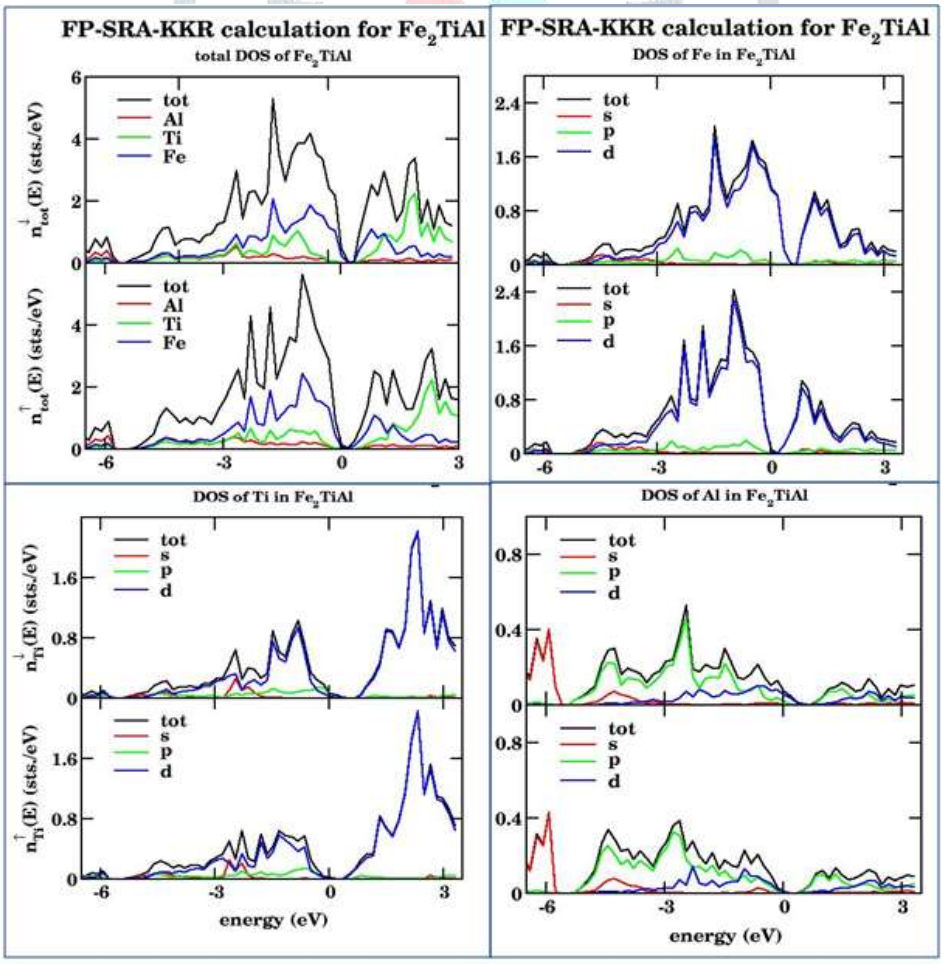

Fig. 3(a): Total and partial density of states of Fe_2TiAl

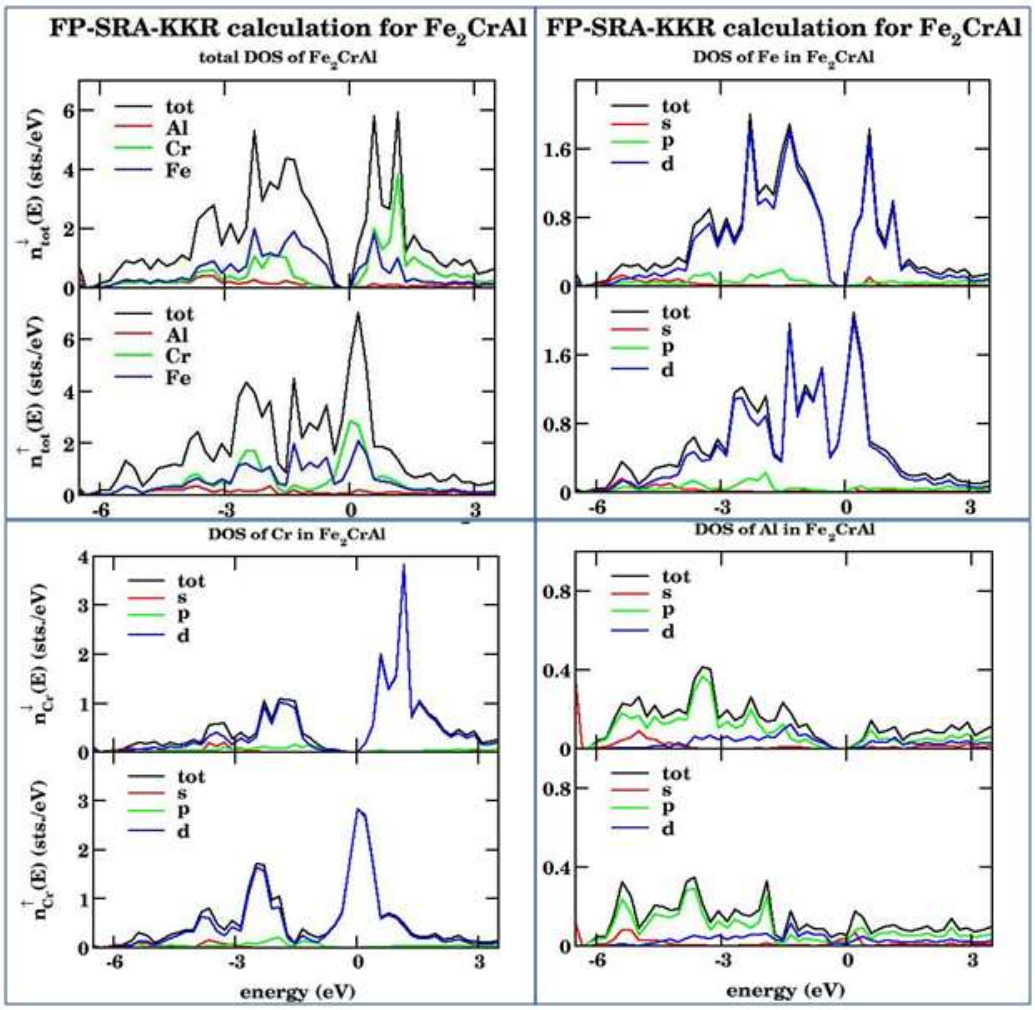

Fig. 3(b): Total and partial density of states of Fe_2TiAl

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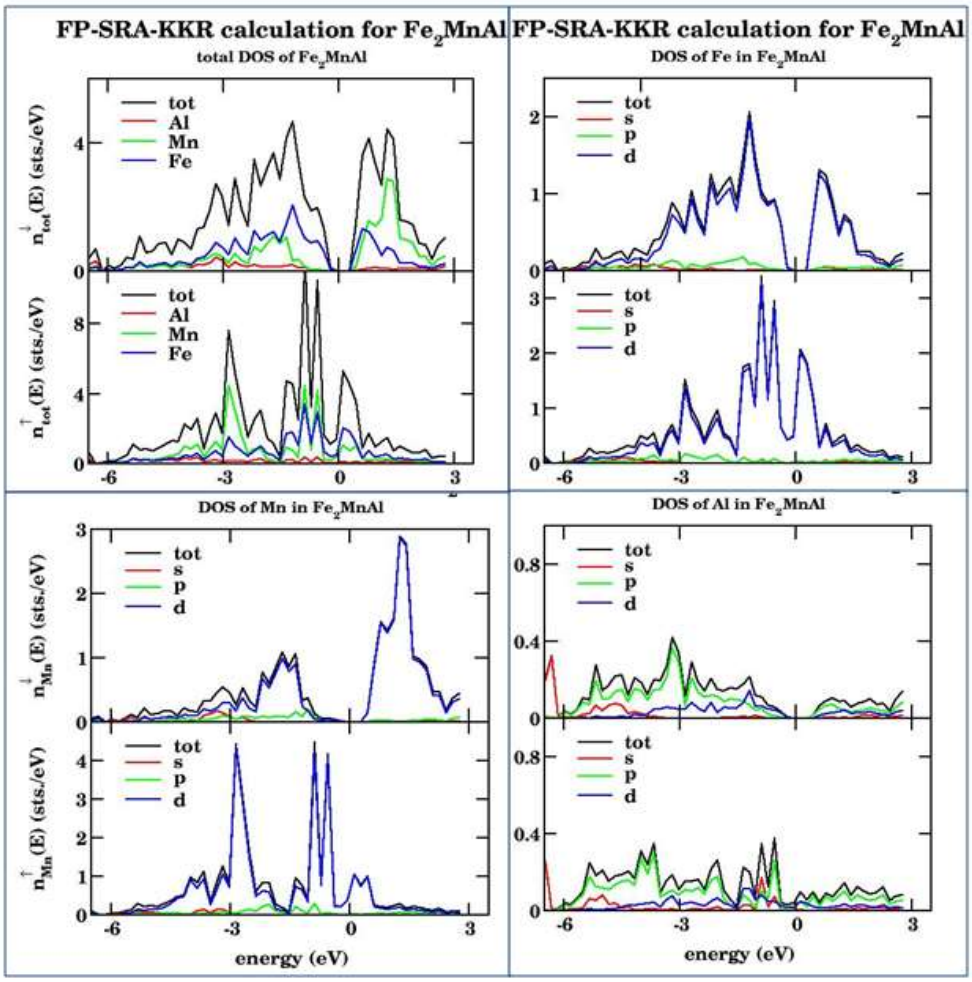

Fig. 3(c): Total and partial density of states of Fe_2MnAl

Table 2: Obtained Magnetic Parameters and Observed Band Gap at Gamma point Fermi energy

Sample	Magnetic moments (M)				Behavior	Band Gap (eV)
	M-Fe_2 (μ_B)	M-Y(μ_B)	M-Al (μ_B)	M-Total (μ_B)		
Fe_2TiAl						
Calculated	0.88	-0.12	-0.034	0.64	Metallic	----
Prev. Rep. Theo.	----	----	----	0.95[a]	Metallic	----
Prev. Rep. Exp.	----	----	----	0.10[a]	Metallic	----
Fe_2CrAl						
Calculated	-0.15	1.49	-0.03	1.31	Half Metallic	0.40
Prev. Rep. Theo.	----	----	----	0.94[a]	Half Metallic	0.48[a]
Prev. Rep. Exp.	----	----	----	1.67[a]	Half Metallic	----
Fe_2MnAl						
Calculated	-0.08	2.17	-0.001	2.09	Half Metallic	0.42
Prev. Rep. Theo.	-0.06	2.06	-0.006	2.00[b]	Half Metallic	0.49[b]
Prev. Rep. Exp.	----	----	----	1.80[c]	Half Metallic	----
Fe_2CuAl						
Calculated	4.5528	0.0537	-0.153	4.45	Metallic	----
Prev. Rep. Theo.	3.9[d]	0.00[d]	0.00[d]	3.80[d]	Metallic	----
Prev. Rep. Exp.	----	---	----	4.02[d]	Metallic	---

[a](Shreder et al, 2005), [b](Azar et al, 2012), [c](Vinesh et al, 2009), [d](Gilleßen & Dronskowski, 2010)

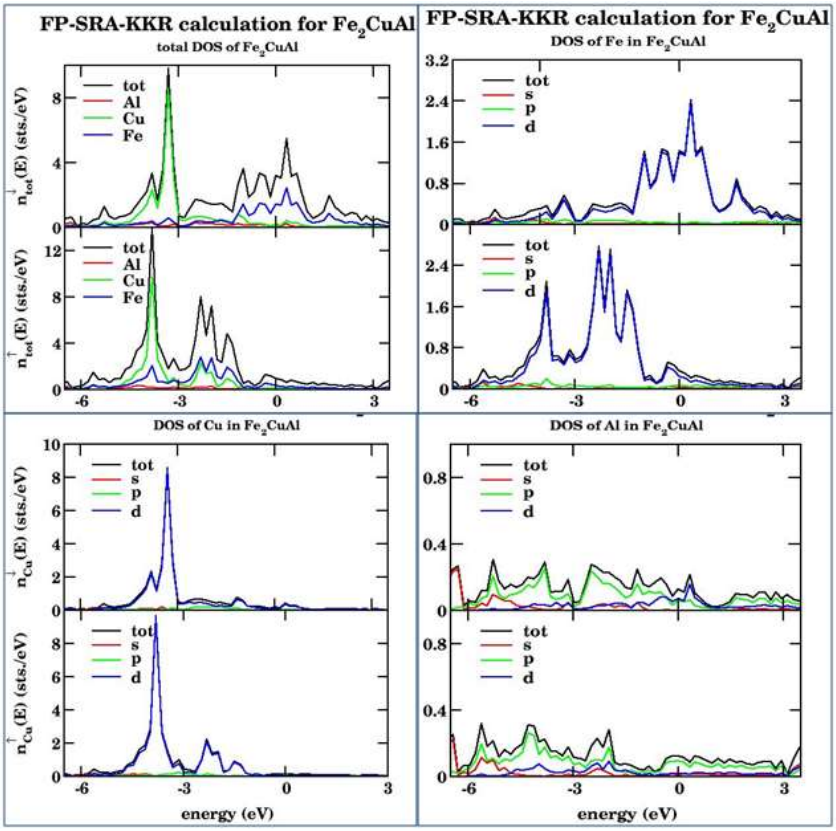

Fig. 3(d): Total and partial density of states of Fe_2CuAl

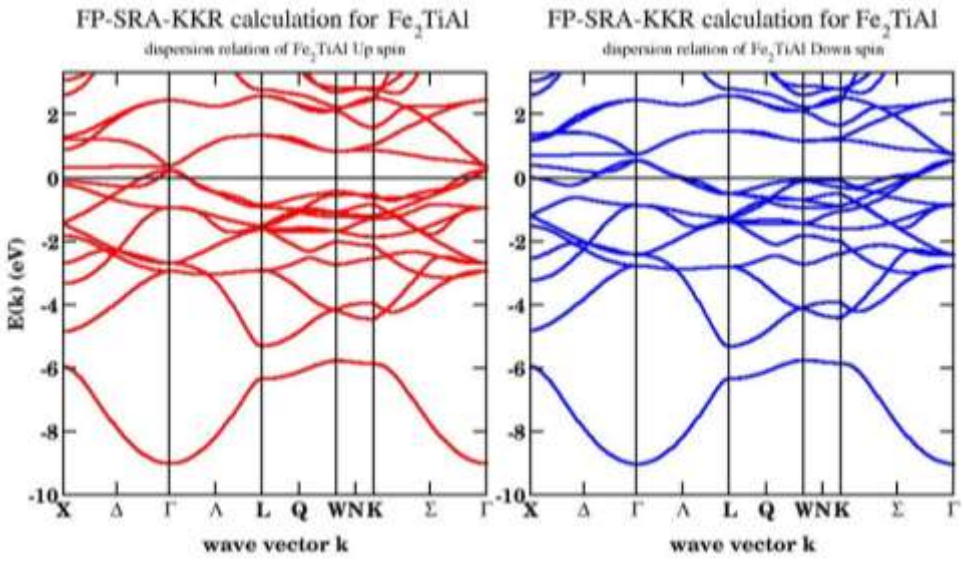

Fig. 4(a):E(k) curve of Fe_2TiAl

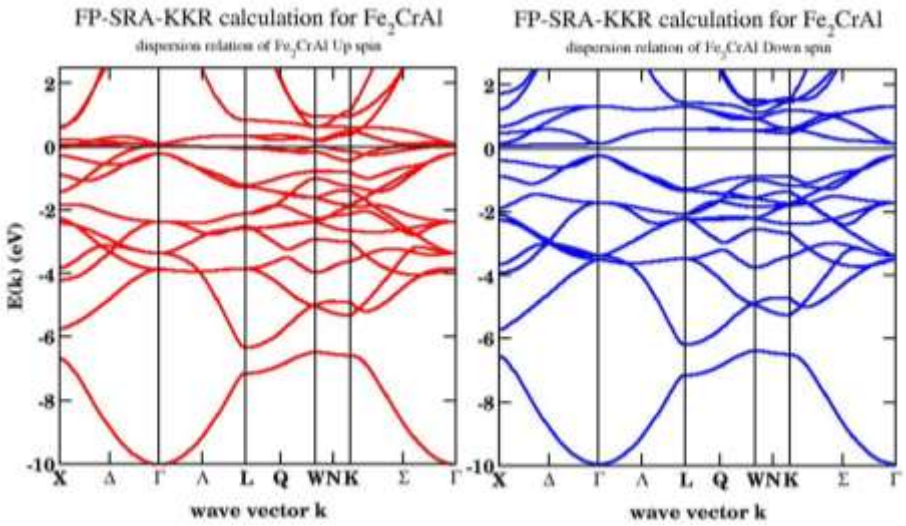

Fig. 4(b):E(k) curve of Fe_2CrAl

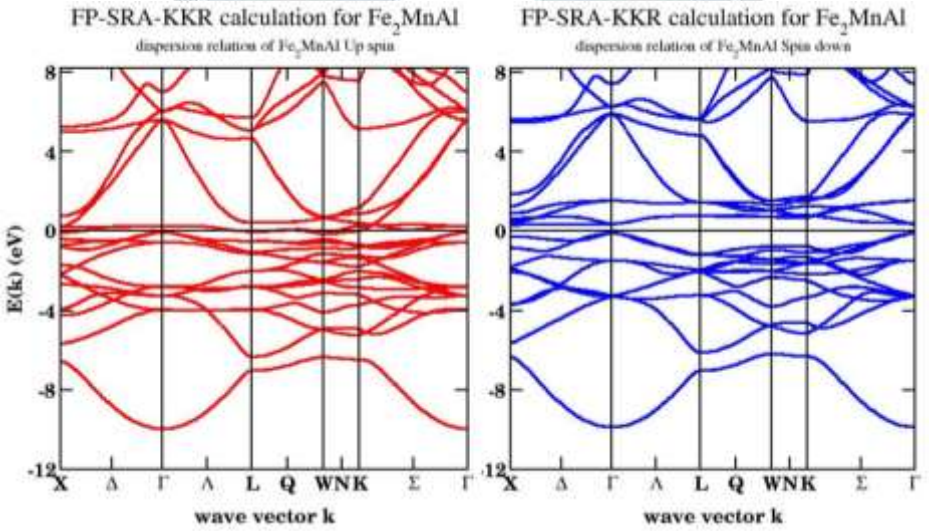

Fig. 4(c):E(k) curve of Fe_2MnAl

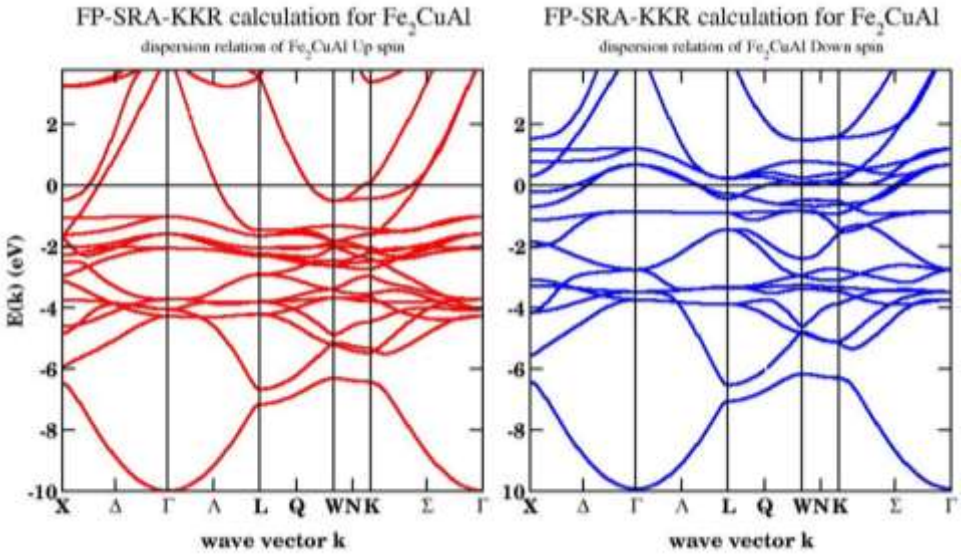

Fig. 4(d):E(k) curve of Fe_2CuAl

IV. CONCLUSION

The aim of this work is to study the electronic structure properties of Fe_2YAl (Y=Ti, V, Cr, Cu). The lattice parameter, magnetic moment, half metallicity,band gap and spin polarization have been investigated. It is confirmed that full-Heusler alloy Fe_2CrAl, Fe_2MnAl exhibits Half metallic behavior and Fe_2TiAl, Fe_2CuAl exhibits metallic behavior. The calculated magnetic moment underestimates from experimental studies and Slater Pauling curve behavior.

V. ACKNOWLEDGMENT

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REFERENCES

[1] Adebambo, P. O., Adetunji, B. I., Olowofela, J. A., Oguntuase, J. A., & Adebayo, G. A. 2016. Prediction of metallic and half-metallic structure and elastic properties of $Fe_2Ti_{1-x}Mn_xAl$ Heusler alloys. Physica B: Condensed Matter, 485, 103-109.

[2] Azar, S. M., Hamad, B. A., Khalifeh, J. M. 2012. Structural, electronic and magnetic properties of $Fe_{3-x}Mn_xZ$ (Z= Al, Ge, Sb) Heusler alloys. Journal of Magnetism and Magnetic Materials, 324(10), 1776-1785.

[3] Buchelnikov, V. D., Zagrebin, M. A., Sokolovskiy, V. V., Taranenko, I. A., Zayak, A. T. 2014, Investigation of structural and magnetic properties of Heusler $Fe_{2+x}Mn_{1-x}Al$ alloys by first principles method. Physica Status Solidi (c), 11(5 - 6), 979-983.

[4] Chandra, A. R., Jain, V., Lakshmi, N., Jain, V. K., Soni, K., Jain, R. 2018, Electronic structure properties of new equiatomic CoCuMnZ (Z= In, Sn, Sb) quaternary Heusler alloys: An ab-initio study. Journal of Alloys and Compounds, 748, 298-304.

[5] Chandra, A. R., Jain, V., Lakshmi, N., Jain, R., & Jain, V. K. (2018a, April). Study of the electronic structure properties in Co_2NbIn/Sn Heusler alloys. In AIP Conference Proceedings (Vol. 1942, No. 1, p. 090037). AIP Publishing.

[6] Ebert, H. 2012, The Munich SPR-KKR package, version 6.3 http://ebert. cup. uni-muenchen. de.

[7] Fujii, S., Ishida, S., & Asano, S. 1995, A half-metallic band structure and Fe_2MnZ (Z= Al, Si, P). Journal of the Physical Society of Japan, 64(1), 185-191.

[8] Gilleßen, M., & Dronskowski, R. 2010, A combinatorial study of inverse Heusler alloys by first principles computational methods. Journal of computational chemistry, 31(3), 612-619.

[9] Graf, T., Felser, C., &Parkin, S. S. 2016, Heusler Compounds: Applications in Spintronics. Handbook of Spintronics, 335-364.

[10] Jain, V. K., Jain, V., Lakshmi, N., &Venugopalan, K. (2014, April).Ab initio study of Fe_2MnZ (Al, Si, Ge) Heusler alloy using GGA approximation. In SOLID STATE PHYSICS: Proceedings of the 58th DAE Solid State Physics Symposium 2013 (Vol. 1591, No. 1, pp. 1130-1132). AIP Publishing.

[11] Jain, V. K., Lakshmi, N., Jain, R., Jain, V., Chandra, A. R., & Venugopalan, K. 2017, Electronic structure, magnetic and optical properties of quaternary Fe_{2-x} Co_xMnAl Heusler alloys. Journal of Materials Science, 52(11), 6800-6811.

[12] Paduani, C., Migliavacca, A., Pöttker, W. E., Schaf, J., Krause, J. C., Ardisson, J. D., & Yoshida, M. I. 2007, A study of $Fe_{2+x}Mn_{1-x}Al$ alloys: Structural and magnetic properties. Physica B: Condensed Matter, 398(1), 60-64.

[13] Sharma, V., & Pilania, G. 2013, Electronic, magnetic, optical and elastic properties of Fe_2YAl (Y= Ti, V and Cr) using first principles methods. Journal of Magnetism and Magnetic Materials, 339, 142-150.

[14] Shreder, E. I., Svyazhin, A. D., & Fomina, K. A. 2012, Optical properties of Fe_2NiAl and Fe_2MnAl Heusler alloys. The Physics of Metals and Metallography, 113(2), 146-152.

[15] Vinesh, A., Hina Bhargava, N. Lakshmi, and K. Venugopalan."Magnetic anisotropy induced by high energy ball milling of Fe_2MnAl." Journal of Applied Physics 105, no. 7 (2009): 7A309.