Review on Structural and Electronics properties of Rh-based Full-Heusler compounds

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Abstract

The structural and electronic properties of Rh_2FeZ (Z=Ga, In) and Rh_2YIn (Y=Nd, Sm) have been calculated by using ab-intio method of FP-LAPW+lo and FP-LAPW respectively. All four compounds are stable in ferromagnetic phase and both spins behaved in a different way for both former compounds. Indirect band gap showed semiconducting nature in spin-down and crossed electronic states showed metallic nature in spin-up states, which demonstrated the half-metallic nature of Rh_2FeZ (Z=Ga, In) compounds. On the other hand both spins behaved in a same way for Rh_2YIn (Y=Nd, Sm) compounds and demonstrated their metallic nature.

Keywords: Full heusler compounds, Electronic structure, Density functional theory, Band structure

1. Introduction

Friedrich Heusler introduced the concept of Heusler Compounds in 1903 after the investigation of Cu_2MnAl full- Heusler compound, which turned out to be ferromagnetic material without the presence of any magnetic element [1, 2]. These compounds generally have two types known as half-Heusler compounds, whose structure type is $C1_b$ and full-Heusler compounds with $L2_1$ structure. Fm-3m (225) and F-43m (216) are two space groups either of which can be stable for $L2_1$ structure. XYZ composition represents half-Heusler and X_2YZ represents full- Heusler compounds [3, 4], where X and Y stand for transition metals and Z signifies main group elements [5]. The researchers are investigating these materials due to their useful applications in memory devices, thermoelectric materials, spintonics, spin value generators and magnetoresistive materials [6-9]. The useful property called half-metallicity that made these materials applicable for these applications was first examined in NiMnSb by de Groot et al. [10] in 1983. For investigating Rhodium based compounds first principles-based Density functional approach [11] has been used for calculating electronic and structural properties of Heusler compounds. FP-LAPW [12] method has been worked on compounds Rh_2SmIn and Rh_2NdIn while for compounds Rh_2FeGa and Rh_2FeIn FP-LAPW+lo [13, 14] has been used where lo stands for local orbital as included in Wien2k computer code [15]. The Exchange correlation potential were estimated by using generalized gradient approximation GGA, GGA+U (Hubbard approximation) and local density approximation LDA [16-18] through convergence parameter Kmax*Rmt= 8 to 9, where Rmt is radius of muffin tin spheres and Kmax is plane wave cut off energy. In the present review paper four Rh-

based full-Heusler compounds have been studied and their structural and electronic properties have been taken into account. Monir et al. [19] in 2017 investigated Rh_2FeZ (Z=Ga, In) and Rh_2YIn (Y=Nd, Sm) were investigated by Brahmi et al. [20] in 2018.

2. Structural and Electronic properties

The lattice parameter, minimum energy and stable magnetic phase shown in Table 2 of Rhodium based compounds were calculated by considering paramagnetic and ferromagnetic phase in Fm-3m (225) space group. The structural parameters of Rh_2FeZ (Z=Ga, In) were calculated by GGA approximation, whereas for Rh_2YIn (Y=Nd, Sm) results of LDA and GGA approximations were compared. All four of above compounds represent found to be stable in ferromagnetic phase. The structural parameters at equilibrium were specified by fitting the total energies to Birch Murnaghan's equation of state [21]. The atomic positions of these compounds are shown in Table 1.

Table 1: Atomic coordinates and Wyckoff positions.

Compound	8c (0.25, 0.25, 0.25)	4b (0.5, 0.5, 0.5)	4a (0, 0, 0)
Rh_2SmIn	Rh	Sm	In
Rh_2NdIn	Rh	Nd	In
Rh_2FeGa	Rh	Fe	Ga
Rh_2FeIn	Rh	Fe	In

Table 2: Lattice parameters and Equilibrium energies.

Compound	Approximation	State	Lattice parameter a (Å)	Equilibrium Energy E_o(Ry)
Rh_2FeIn	GGA	PM	6.1992	-33453.132600
		FM	6.2447	-33453.166900
Rh_2FeGa	GGA	PM	5.9870	-25574.943900
		FM	6.0411	-25575.046400
Rh_2NdIn	LDA	PM	6.5250	-50125.569279
		FM	6.5490	-50125.650496
	GGA	PM	6.5964	-50162.133429
		FM	6.6317	-50162.229662
Rh_2SmIn	LDA	PM	6.4861	51734.08810600
		FM	6.5389	−51734.3748110
	GGA	PM	6.5597	−51771.2518390
		FM	6.6198	−51771.5472600

The electronic properties of Rh_2FeZ (Z=Ga, In) were calculated by using GGA+U approximation, which showed semiconducting nature with indirect band gap from Γ to X point in minority spin and confirmed metallic nature in majority spin for both compounds. The different behavior of both spins illustrates half-metallic nature of both compounds. For Rh_2YIn (Y=Nd, Sm) LDA approximation were used for calculating the band structure. Both these compounds showed same behavior in both spins with no band gap which illustrates the metallic nature of these compounds.

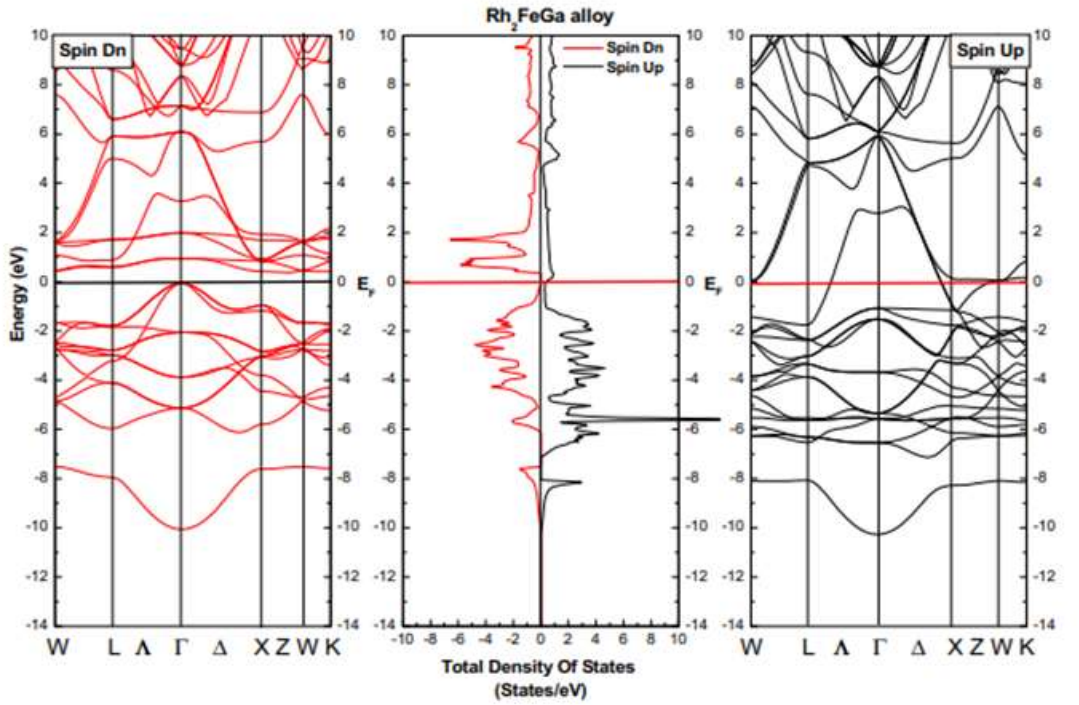

Fig 1: Band structure and total DoS of Rh_2FeGa with GGA+U approximation

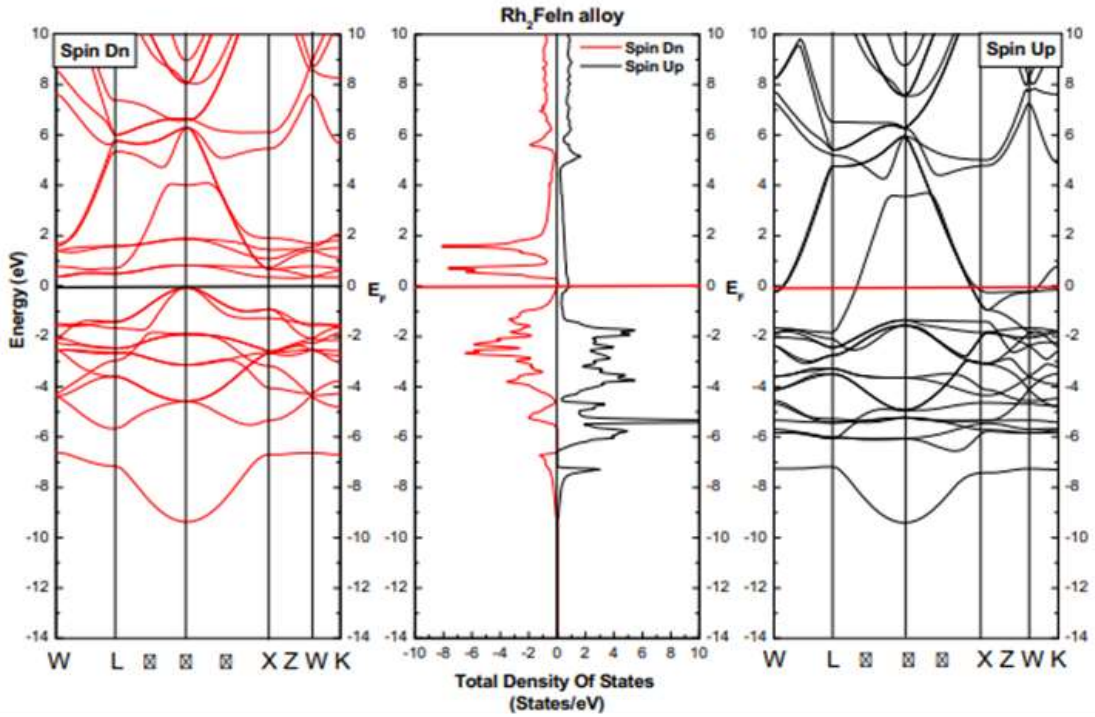

Fig 2: Band structure and total DoS of Rh_2FeIn with GGA+U approximation

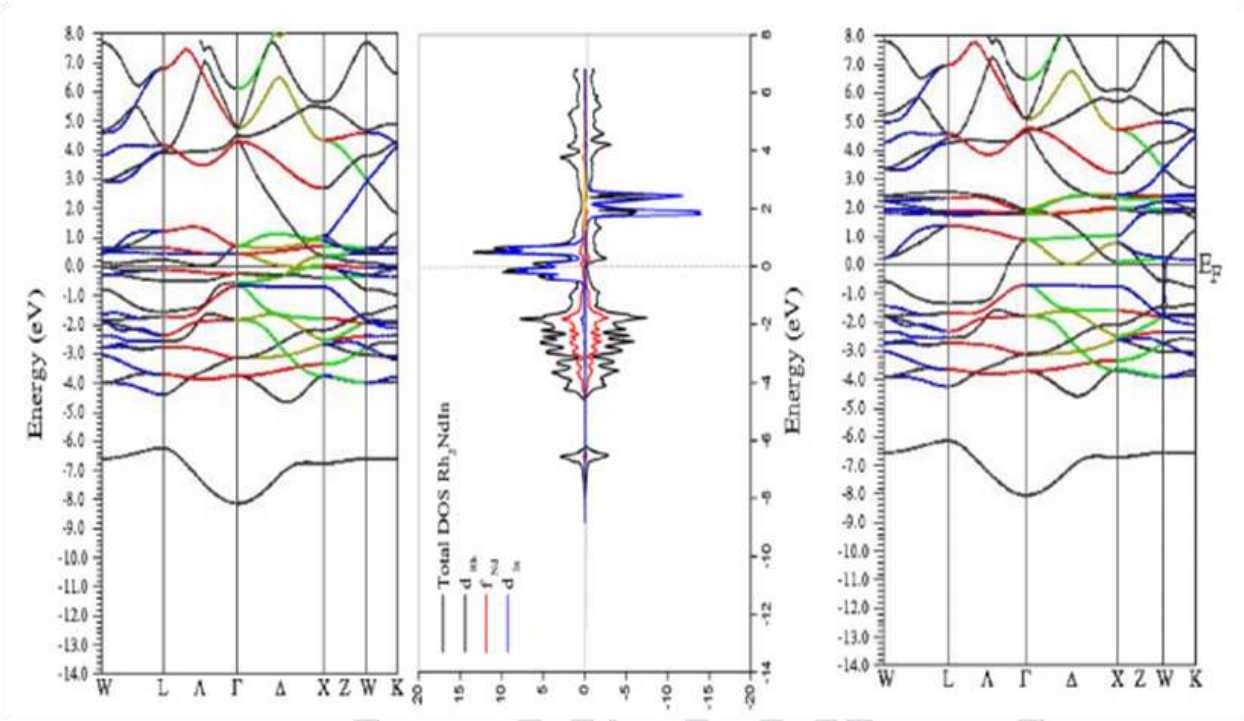

Fig 3: Band structure and total DoS of Rh_2NdIn with GGA+U approximation

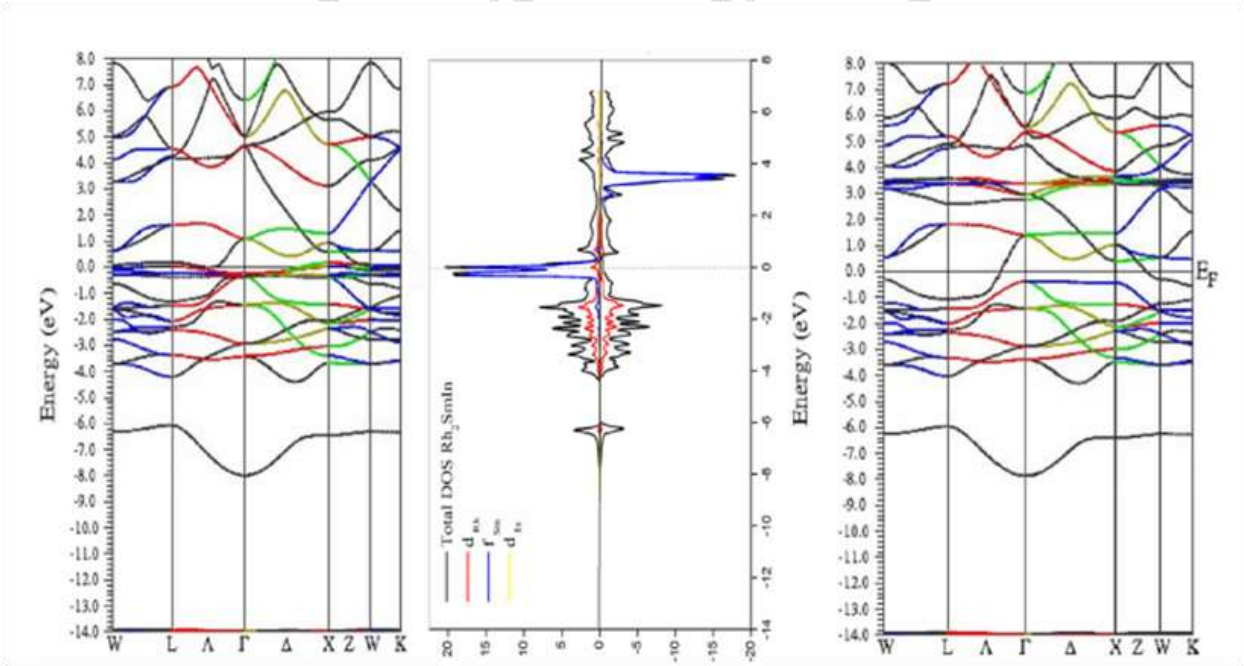

Fig 4: Band structure and total DoS of Rh_2SmIn with GGA+U approximation

3. Conclusion

This paper deals with calculation of structural and electronic properties of Rhodium based compound using FP-LAPW and DFT. We concluded here that all compounds are found to be energetically stable in their ferromagnetic phase. Rh_2FeIn and Rh_2FeGa are found to be half metallic material while Rh_2NdIn and Rh_2SmIn are metallic material. These compounds fulfill the criteria to be good ferromagnetic material.

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