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First-principle study of the Electronic and Magnetic Properties of Fe_2MnAl, Fe_2MnSi, Fe_2MnGa

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ABSTRACT

The electronic and magnetic properties of heusler alloys compounds Fe2MnAl, Fe2MnSi and Fe2MnGa are described in this article. We have applied the full-potential linearized augmented plane waves plus local orbitals (FP-L/APW) method based on the density functional theory (DFT). Generalized-gradient approximation (GGA) is used for the exchange and correlation potential. The calculated atomic resolved densities of states of Fe2MnAl, Fe2MnSi indicate half-metallic behavior with vanishing electronic density of states for minority spin at the Fermi level, which yields perfect spin polarization while for Fe2MnGa the full electron energy of ferromagnetic metallic fcc phase (μ_{fcc} =6.11μ_Bf.u.) is lower by about 0.06 meV (0.69 K) than that of ferrimagnetic half-metallic phase with L_{21} structure (μ_{L21} = 2.036μ_Bf.u.).

1. INTRODUCTION

In 19TH century a german mining engineer and chemist Fritz Heusler discovered some alloys with strong and interesting behavior. These alloys are named Heusler alloys. In this paper we are going to discuss the heusler alloys with general chemical formula X_2YZ. Our main objective of this research work is to study of the electronic and magnetic properties of fe_2MnZ (Z= Al, Si, Ga) heusler alloys.

These materials are characterized with small bandgap and high structural stability. Therefore these are frequently used as thermoelectrics. Heusler compounds containing Co and Mn have attracted attention during the last two decades due to their possible applications in spintronics [1]. Besides ternary Heusler X_2YZ compounds, there exist a large range of substitutional quaternary alloys of the type $X_2Y_{1-x}Y_xZ$, $X_2YZ_{1-x}Z_x$ and $(X_{1-x}X_x)_2YZ$ [6]. We have studied the electronic structure of $Co_2FeSi_{1-x}Al_x$. The series of $Co_2FeSi_{1-x}Al_x$ are found to exhibit half-metallic

ferromagnetism and show that the electron-doping stabilizes the gap in the minority states for x ¼0.5. we also examined the effect of the local environment on the formation of local magnetic moments for Fe_3xMnxAl alloys in the concentration range 0oxo0.5.

Main objective of the current research work is the study of the electronic and magnetic properties of Fe_2MnAl, Fe_2MnSi and Fe_2MnGa Heusler alloys. This article is organized as follows: In Section 2, the computational techniques used in this work is briefly described. Results and discussion of this study are presented in Section 3. Finally, a summary of the work is provided in Section 4.

2. COMPUTATIONAL DETAILS

The full heusler alloys generally crystallize in two possible structure: the Hg_2CuTi-type L21 structure and the Cu_2MnAl-type L21 structure. The structural formula is X_2Y_2 where X and Y denote transition metal elements and 2 is S-P elements. The structure is composed of four 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). In this study In this study the first principles calculations are performed using the all-electron full potential linearized augmented plane wave plus local orbitals (FPL/APW) method within the frame work of the density functional theory (DFT) [12,13] as implemented in the Wien2k code [14]. The exchange correlation term has been considered within the generalized gradient approximation (GGA) Using the energy eigen values and eigenvectors at these points, the DOS was determined by the tetrahedral integration method.

3. RESULTS AND DISCUSSION

a. Electronic Properties

The electronic properties are a set of parameters and representations that fully describe the state and behavior of electrons in the material. For example, the electronic band structure[1], which describes the states of the electrons in terms of their energy,E< and momentum,k, is such a representation.

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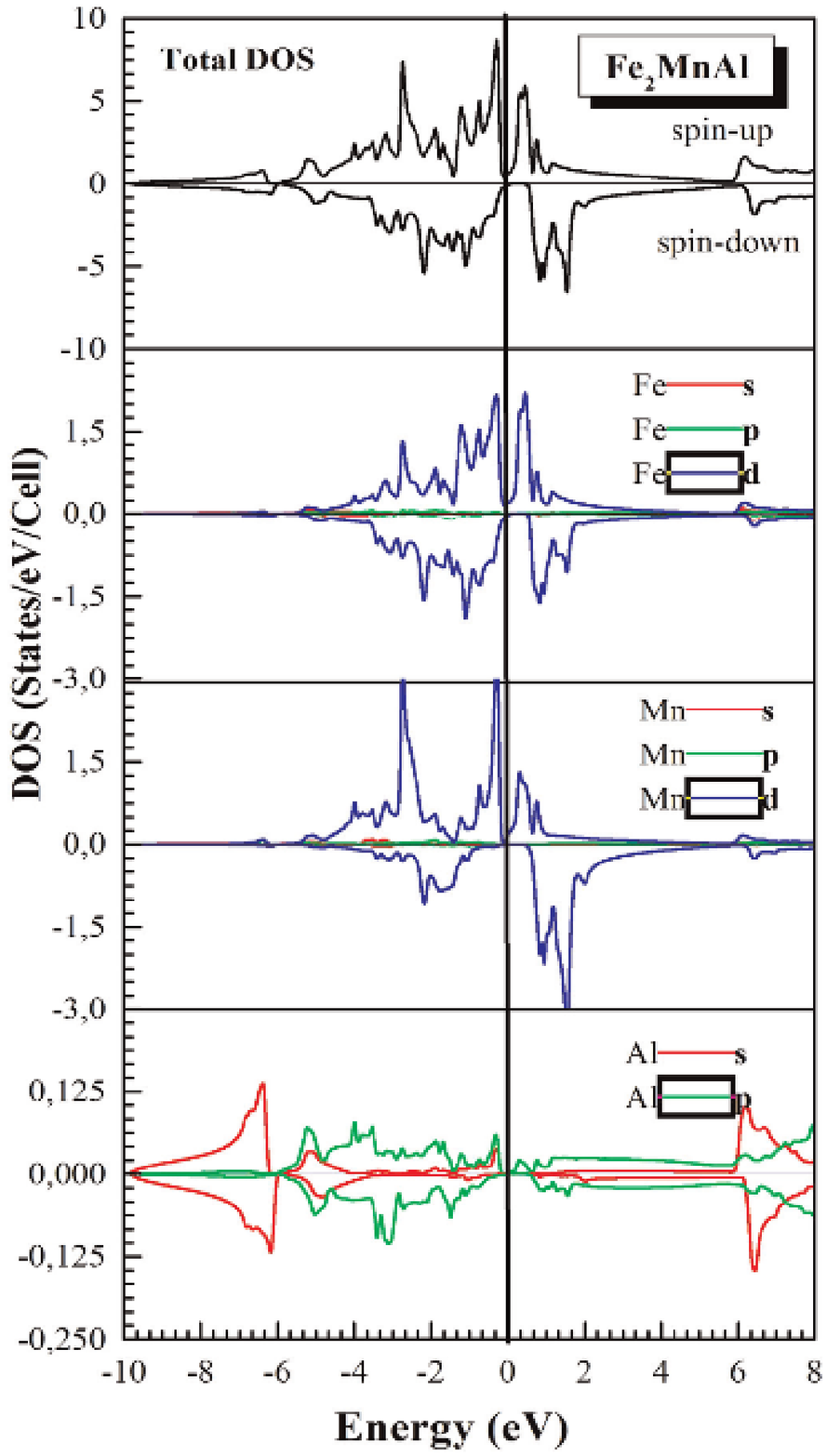
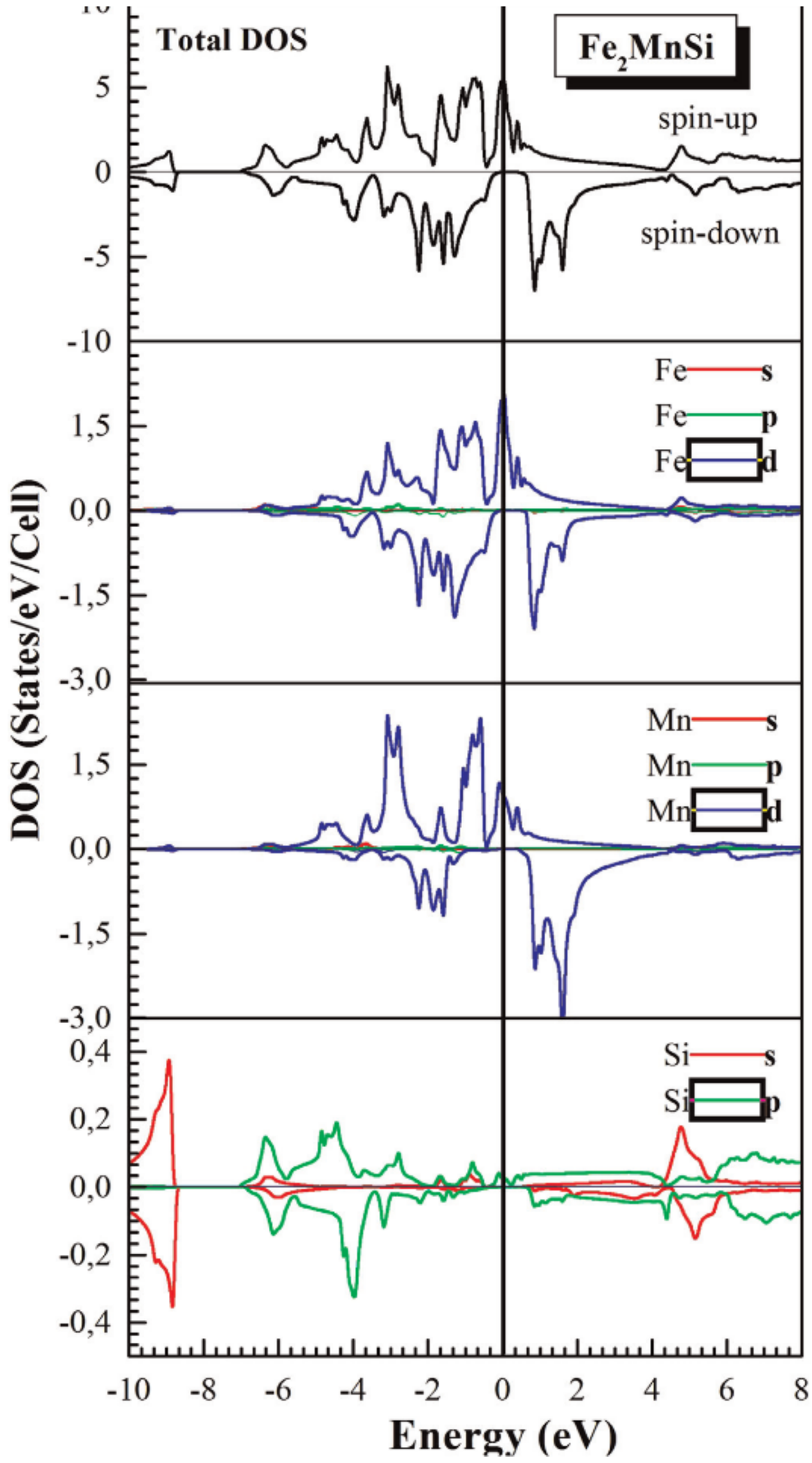


The total and partial densities of states (DOS and PDOS) for Heusler compounds Fe_2MnSi, Fe_2MnAl and Fe_2MnGa are illustrated in Figs. 1,2 and 3. From the spin-resolved bands, it is seen that the majority bands cross the Fermi level in almost all directions of high symmetry, whereas the minority bands exhibit a band gap of Eg¼0.58 eV for Fe_2MnSi and 0.49 eV for Fe_2MnAl and 0. 36 for Fe_2MnGa. Hence they have half metallic character. The origin of energy gap in the low spin channel can be discussed on the basis of electron splitting.



The d-d hybridization between the transition metal atoms play an very important role in the origin of energy gap in minority spin states. The origin of the gaps in case of heusler alloys (full-heusler alloys) is due to the hybridization between the nearest neighbors of the Mn – Mn 3D orbitals. It is known that covalent hybridization between low valent and high valent atoms, such as Fe, while the unoccupied antibonding states are mainly at the low valent transition metal, such as Mn. It is clear that the Fe and Mn - 3D states behave quite differently, the Fe – 3D states are atmost completely occupied and show no exchange splitting. Therefore, the Fe atoms only have small moments and contribute very little to the magnetism. The Mn – 3D states extend from – 4 to +2ev with a clear exchange splitting appeared between clear exchange splitting appeared between the majority and minotity spin states

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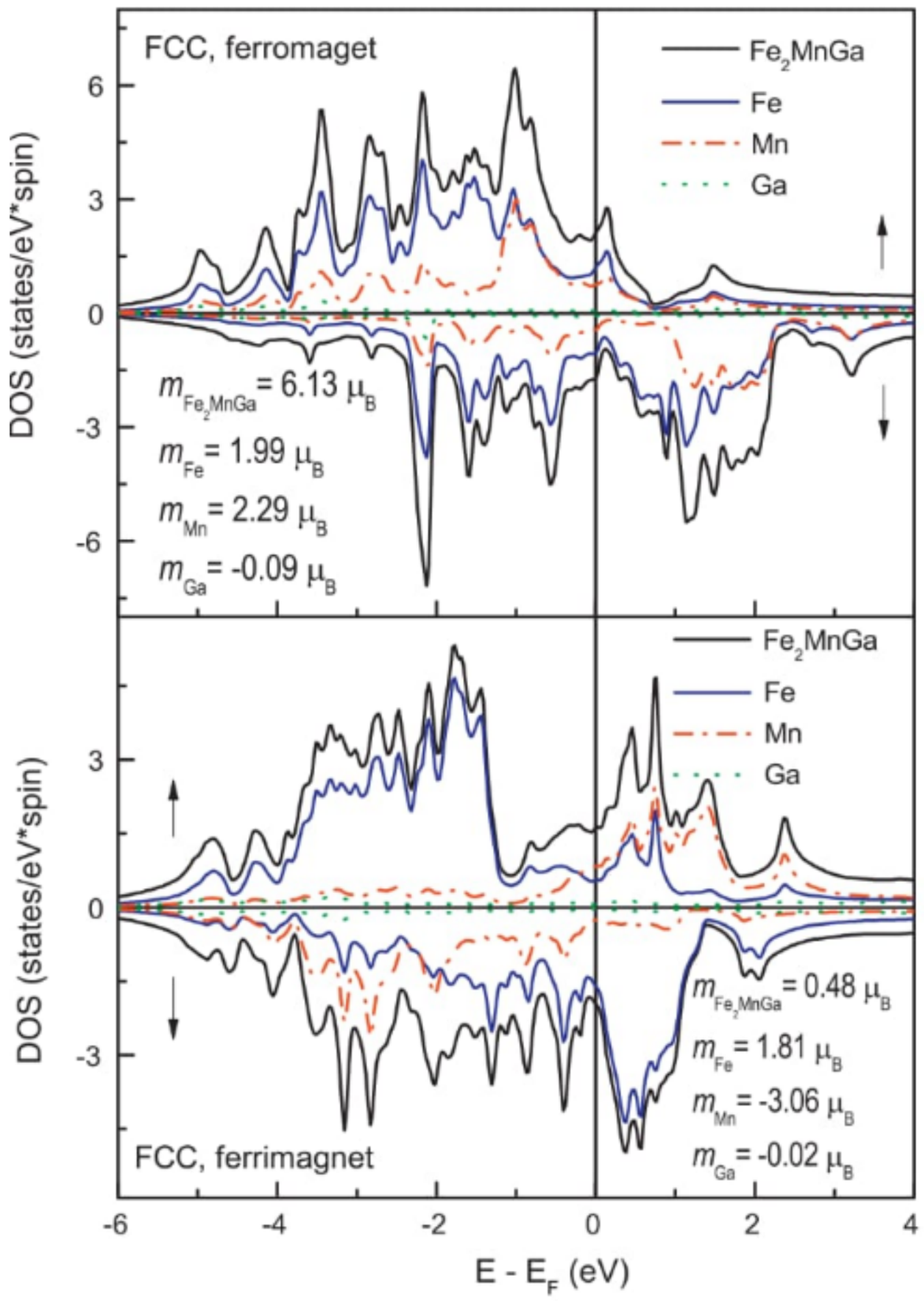

Magnetic Properties

The magnetic properties of a substance originate from the electron present in the atoms or molecules. Every electron in an atom behaves like a small magnet. Electron can also be referred to as small loops of current which retain their magnetic moment or we can also say that, The magnetic property of a material is the atomic or subatomic response a material to an applied magnetic field wherein the electron spin and charge create a dipole moment and a magnetic field.

In task (2), The magnetic moments of Fe_2MnSi, Fe_2MnAl, Fe_2MnGa are listed. We find that the total magnetic moment per formula units is an integer value 2 μB/f.u for Fe2MnAl and 3 μB/f.u for Fe2MnSi. The results show that the total magnetic moments come from the Mn, while the Si and Al atoms have a very small magnetic moment including Ga. Our calculated values are matching with other theoretical values. For task(2) do not give integer numbers for the total moment. We note that the total spin magnetic moments of quaternary alloy is calculated by integer over the entire call. Therefore, it is just the combination of the moments at X (2 times), Y and 2 sites but also include the moment of the interstitial between the steps.

The Gacontibution to the total DOS is small, i.e. Ga atoms form basically ionic bonds with surrounding atoms. The resulting magnetic moment ofFe_2MnGa in L_{21} phase agree well with the

results of ZAYAK et al. (2.15μgf.U) and HUANG cell et al. (2.041μgf.U)

Table 2 Calculated total and local magnetic moments (in μ_B) for Fe_2MnSi, Fe_2MnAl and Fe2MnGa Experimental and previous theoretical data are also quoted for comparison.

	Tot	**Fe**	**Mn**	**Si**	**Ga**	**Al**
Fe_2MnAl	2.00	-0.06	2.06	_		-0.006
	2.00	-0.15	2.32			-0.015
	2.00	-0.31	2.62			
Fe_2MnSi	3.00	0.01	2.41	0.06		
	3.00	0.27	2.46	-0.016		
	3.00	0.20	2.63			
Fe_2MnGa	6.13 μ_B	1 .99 μ_B	2.29 μ_B		-0.09 μ_B	
	0.48μ_B	1.81μ_B	-3.06μ_B		-0.02 μ_B	

4. CONCLUSION

The full potential linearized augmented plane wave plus local orbitals (FP-L/APW) based on the density functional theory, within generalized-gradient approximation we have studied structural, electronic and magnetic properties of Fe_2MnAl, Fe_2MnSi, Fe_2MnGa. Our calculated lattice constants and spin magnetic moments are in good agreement with the available theoretical and experimental data. Our data indicates thatFe_2MnZ (Si,Al,Ga have half metallic behavior with small spin down electronic densities of stats at Fermi level.

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