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# First Principles Study of Fe based Full Heusler Alloy

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**ABSTRACT**

The electronic structure of Fe-based quaternary Heusler compounds $Fe_2CoZ$ (Z=Ga, Ge) is calculated by first-principles density functional theory. Structural optimization is performed for two possible structures: $Hg_2CuTi$-type and $Cu_2MnAl$-type structures of $Fe_2CoZ$. We found that $Hg_2CuTi$-type structure is energetically more favorable than $Cu_2MnAl$-type structure. The calculated equilibrium lattice constant is 5.812Å and 5.75Å respectively for Ga and Ge based alloy. The calculations reveal that $Fe_2CoGa$ material exhibit 100% spin-polarization whereas $Fe_2CoGe$ has 62% spin-polarization. The value of magnetic moment for $Fe_2CoGa$ and $Fe_2CoGe$ is 5.72$\mu_B$, 4.96$\mu_B$ respectively.

*Keywords: Density Functional Theory, Electronic Structure, Half-metallic, Heusler Alloy*

## Introduction

Half-metallic (HM) ferromagnets, which have complete (100%) spin polarization at the Fermi level, have attracted much attention for their useful applications in spin dependent devices, such as spin injection devices and non-volatile magnetic random access memories (MRAM). Among the various half metallic materials proposed until now, such as double perovskite, spinel, zinc-blende structured materials, Heusler alloys etc., full-Heusler alloys have recently attracted much attention for their relatively high Curie temperature and large magnetic moment.[1,2] Heusler alloys were discovered by de Groot et. al. during a computational study of magnetic compounds.[3] Heusler alloys offers the possibility of studying in the same family of alloys a series of interesting diverse magnetic phenomena, ranging from half-metallic ferromagnets over completely compensated ferromagnets to nonmagnetic semiconductors and even superconductors.[4-7] Recently, their application as shape-memory alloys has also been intensively discussed.[8] In this paper, we report the structure and magnetic properties of iron based Heusler alloys $Fe_2CoGa$, $Fe_2CoGe$.

## Methodology

The spin-polarized electronic structure calculations are performed using DFT as implemented in the Spanish Initiative for Electronic Simulations with Thousands of Atoms code[9] using Generalized Gradient Approximation with exchange-correlation potential of Perdew-Burke-Ernzerhof.[10] The core electrons are described by norm-conserving scalar relativistic pseudo-potentials constructed using the Troullier–Martins parameterization[11] including nonlinear core corrections for transition-metal atoms. The atomic positions as well as lattice parameters are allowed to relax until the forces are smaller than 0.0016 Ryd/Bohr. For band-structure calculations the Brillouin zone is sampled by a 20×20×20 Monkhorst-Pack grid.

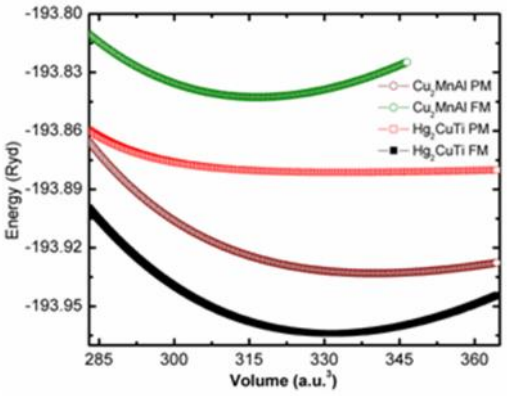


**Figure 1.** Variation of total energy vs. volume for $Fe_2CoGa$

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The full-Heusler compounds, $X_2YZ$, where X and Y are transition metal elements and Z is a group III or IV element, generally crystallize in two possible structures: $Hg_2CuTi$-type structure (space group *F43m*) and $Cu_2MnAl$-type structure (space group *Fm3m*). The Wyckoff coordinates are 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 the $Cu_2MnAl$-type structure, *X* atoms occupy the *A* and *C* sites, while in the $Hg_2CuTi$-type structure, the *A* and *B* sites are occupied by *X* atoms. According to Luo et.al.[12] site preference of the X and Y atoms is strongly influenced by the number of their 3d electrons. The real structure is determined by the energetic preference in the crystallization process.

**Results and Discussion**

We have done structural optimization for both possible structures: $Hg_2CuTi$-type structure and $Cu_2MnAl$-type structure. It is clear from figure 1 that $Hg_2CuTi$-type structure is energetically more favorable than $Cu_2MnAl$-type structure. Our result is in agreement with rule given by Luo et.al.[12] Also FM (magnetic) state is favorable in energy than the corresponding PM (non-magnetic) state. The structural parameters for $Hg_2CuTi$-type structure are then calculated by fitting total energies versus volume values to the Birch equation of state.[13] The obtained structural parameters are listed in table 1.

**Table 1:** Calculated lattice constant ($a_o$) and bulk modulus (BM) for $Fe_2CoZ$ (Z=Ga, Ge)

| | **$Fe_2CoGa$** | | **$Fe_2CoGe$** | |
|---|---|---|---|---|
| | $a_o$ (Å) | BM (GPa) | $a_o$ (Å) | BM (GPa) |
| Present Work | 5.812 | 204 | 5.731 | 225 |
| Exp. | 5.767 [14] | - | 5.78 [16] | - |
| Other work | 5.781 [15] | - | 5. 764 [17] | - |

We have studied the electronic structure of alloys at equilibrium lattice constant. The spin-dependent density of states (DOS) of $Fe_2CoGa$ and $Fe_2CoGe$ is shown in figure 2. It is evident from the figure 2a that minority spin states cut the Fermi level ($E_F$) whereas for majority spin states an energy gap exist which indicates that $Fe_2CoGa$ is a half-metallic material. The spin-polarization ratio (*P*) for Heusler alloys is calculated by using formula, $P=D_{\uparrow}-D_{\downarrow}/D_{\uparrow}+D_{\downarrow}$, where $D_{\uparrow}$ and $D_{\downarrow}$ are majority-spin and minority-spin DOS at $E_F$ respectively. The material is said to be fully spin polarized if either spin-up or spin-down electrons take part in electron transport properties. The value of P is 100% for $Fe_2CoGa$ which show usefulness of this material for spin-dependent devices[1]. For $Fe_2CoGe$, spin polarization is 62% (figure 2b).

To consider electronic properties in detail we analyze orbital projected density of states (PDOS) for $Fe_2CoZ$. The PDOS for Fe-*3d*, Co-*3d* and Z atom-*s*, *p* states are shown in figure 3. The valence band split up into two parts: the lower part of valence band (energy below -6eV for Ga based compound and energy below -8eV for Ge based compound) is due to *s*-states of Z-atom which are well separated from upper valence band states which consist of *p*-states of Z-atom and *d*-states of two transition metal atoms. Hybridization between Z *p*-states and transition metal *d*-states leads to small spin-polarization on Z atom and it acquires a small induced magnetic moment. Fe and Co-*d* states are dominant in the vicinity of Fermi level. The exchange splitting of Co-*d* and Fe-*d* states leads to asymmetry of DOS of majority-spin and minority-spin states and is responsible for the creation of energy gap as well as magnetic moment. The calculated local and total magnetic moment, energy gap and the majority spin energy gap values with other available results are shown in table 2. The majority spin energy gap is calculated by taking minimum of $E_v$ and $E_c$ where $E_v$ is maximum energy of valence band and $E_c$ is minimum energy of conduction band.

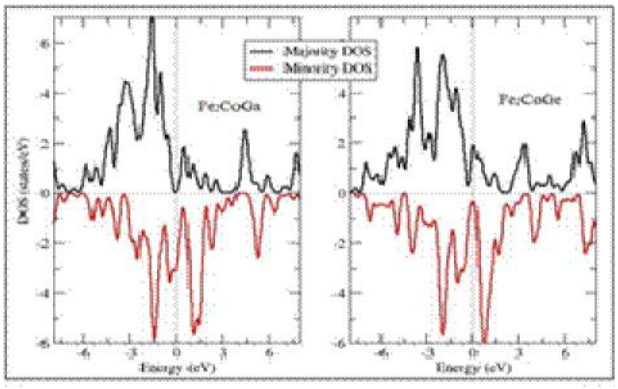


**Figure 2.** Density of States (DOS) for $Fe_2CoZ$ (Z=Ga, Ge) at equilibrium lattice constant. Fermi level is set to 0eV.

The magnetic moment value obtained by present calculation agrees well with experimental value and earlier calculation but contradict the SP rule[18] which gives value of total magnetic moment $4\mu_B$, $5\mu_B$ for $Fe_2CoZ$ (Z=Ga, Ge) respectively. The sign of atomic magnetic moments shows ferromagnetic coupling between Co and Fe atoms whereas antiferromagnetic coupling between Ga (Ge) and transition metal atoms.

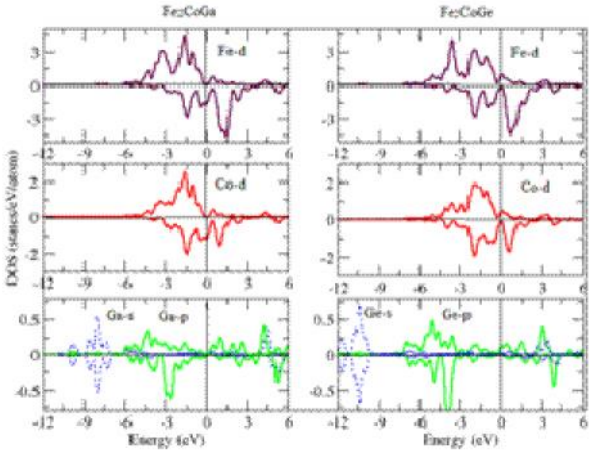


**Figure 3.** Partial Density of States (PDOS) for $Fe_2CoZ$ (Z=Ga, Ge) at equilibrium lattice constant. Fermi level is set to 0eV.

**Table 2:** Calculated total and atomic magnetic moments ($\mu_B$/formula unit), Minority-spin energy gap $E_b$ (eV), Half-metallic gap $E_g$ (eV)

| | | $M_{total}$ | $m_{Fe(A)}$ | $m_{Fe(B)}$ | $m_{Co}$ | $m_Z$ | $E_b$ | $E_g$ |
|---|---|---|---|---|---|---|---|---|
| $Fe_2CoGa$ | Present work | 5.72 | 2.135 | 2.277 | 1.18 | -0.23 | 0.03 | 0.13 |
| | Experiment [14] | 5.09 | - | - | - | - | - | - |
| | Other work [15] | 6.14 | 2.26 | - | 1.85 | -0.07 | - | - |
| $Fe_2CoGe$ | Present work | 4.96 | 1.49 | 2.24 | 0.89 | -0.16 | - | 0.06 |
| | Experiment [16] | 5.4 | 1.6 | 2.6 | 1.1 | - | - | - |
| | Other work[17] | 5.15 | 1.38 | 2.74 | 0.94 | -0.06 | - | - |

## Conclusion

We have studied the electronic and magnetic properties of $Fe_2CoGa$ and $Fe_2CoGe$. The spin polarization value is 100% for $Fe_2CoGa$ and 62% for $Fe_2CoGe$. The 100% value of spin polarization shows that $Fe_2CoGa$ is a potential half-metallic ferromagnet. The calculated density of states (DOS) for $Fe_2CoGa$ shows metallic nature of minority spin electrons and semiconducting nature of majority spin electrons with $E_g$ 0.13eV. The value of magnetic moment is $5.72\mu_B$ which agrees well with previous results. The magnetic moment and energy gap calculated for $Fe_2CoGe$ is $4.96\mu_B$ and 0.06eV.


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## References


1. Galanakis I, Mavropoulos P, Dederichs P H, Electronic structure and Slater–Pauling behaviour in half-metallic Heusler alloys calculated from first principles, *J. Phys. D* **2006**, *39*, 765–775.
2. Kandpal H C, Fecher G H, and Felser C, Calculated electronic and magnetic properties of the half-metallic, transition metal based Heusler compounds, *J. Phys. D* 2007, *40* 1507 –1523.
3. DeGroot R A, Mueller F M, van Engen P G, and Buschow K H J, New Class of Materials: Half-Metallic Ferromagnets, *Phys. Rev. Lett*. **1983**, *50*, 2024- **2027.**
4. Kübler J, Williams A R, and Sommers C B, Formation and coupling of magnetic moments in Heusler alloys, *Phys. Rev. B* **1983**, *28*, 1745 – 1755.
5. Wurmehl S, Kandpal H C, Fecher G H, and Felser C, Valence electron rules for prediction of half-metallic compensated-ferrimagnetic behaviour of Heusler compounds with complete spin polarization, *J. Phys.: Condens. Matter* **2006**, *18*, 6171 –6181.
6. Jung D, Koo H J, and Whangbo M H, Study of the 18-electron band gap and ferromagnetism in semi-Heusler compounds by non-spin-polarized electronic band structure calculations, *J. Mol. Struct. (Theochem)* **2000**, *527*, 113-119.
7. Wernick J H, Hull G W, Geballe T H, Bernadini J E, and Waszczak J V, Superconductivity in ternary Heusler intermetallic compounds, *Mater. Lett.* **1983**, *2*, 90-92.
8. Zayak A T, Entel P, Enkovaara J, Ayuela A, and Nieminen R M, First-principles investigation of phonon softenings and lattice instabilities in the shape-memory system $Ni_2MnGa$, *Phys. Rev. B* **2003**, *68*, 132402-1 - 132402-4.
9. Soler J M, Artacho E, Julian D, Gale J D, Garc A, Junquera J, Ordejon P and Sanchez-Portal D, The SIESTA method for ab initio order-N materials simulation, *J. Phys.: Condens. Matter* **2002**, *14*, 2745–2779.
10. Perdew J P, Burke K, and Erzerhof M, Generalized Gradient Approximation Made Simple, *Phys. Rev. Lett.* **1996**, *77*, 3865-3868.
11. Troullier N, and Martins J L, Efficient pseudopotentials for plane-wave calculations, *Phys. Rev. B* **1991**, *43*, 1993-2006.
12. Luo H, Zhu Z, Liu G, Xu S, Wu G, Liu H, Qu J, Li Y, Prediction of half-metallic properties for the Heusler alloys $Mn_2CrZ$ (Z=Al, Ga, Si, Ge, Sb): A first-principles study, *J. Magn. Magn. Mater.* **1944**, *320*, 421.
13. Murnaghan F D, The Compressibility of Media under Extreme Pressures, *Proc. Natl. Acad. Sci. U. S. A.* **1944**, *30*, 244–247.
14. Webster P J and Ziebeck K. R. A., Magnetic and chemical order in Heusler alloys containing cobalt and titanium, *J. Phys. Chem. Solids.* **1973**, *34*, 1647-1656.
15. Kulkova S E, Sergey V. E., T. Kakeshita T. Kulkov S S and Rudenski G E, The Electronic Structure and Magnetic Properties of Full- and Half-Heusler Alloys**,** *Materials Transactions* **2006,** *47*, 599-606.
16. Gasi T, Ksenofontov V, Kiss J, Chadov S, Nayak A K, Nicklas M, Winterlik J, Schwall M, Klaer P, Adler P and Felser C, New iron-based Heusler compounds Fe2YZ: Comparison with theoretical predictions of the crystal structure and magnetic properties, arXiV 1301.1988
17. Ren Z, Li S T, and Lu H Z, Structure and magnetic properties of $Fe_2CoGe$ synthesized by ball-milling, *Physica B* **2010**, *405*, 2840-2843.
18. Galanakis I, Dederichs P H, and Papanikolaou N, Slater-Pauling behavior and origin of the half-metallicity of the full-Heusler alloys, *Phys. Rev. B* **2002**, *66*, 174429-1 - 174429-9.