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Ab initio study of the structural, electronic, and magnetic properties of Co_2FeGa and Co_2FeSi and their future contribution to the building of quantum devices

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Abstract: How small can an electronic device be and still function? How many atoms are needed for such device? At what point will the semiconductor fabrication technology be unable to construct anything smaller? These are common questions asked by researchers, and the answers indicate the short-term limitations on the use of semiconductor technology. When we reach these limitations, we can propose two methods to solve these problems: first, we could continue using semiconductor technology, alongside the development of new theories and techniques to counter quantum effects caused by the miniaturization of electronic devices like transistors and microprocessors. Second, we could exploit these quantum effects to invent a new generation of electronic devices. Doing that, we propose spintronics or the use of spin properties. Heusler compounds as cobalt base alloys (Co_2YZ) present particular interest for spin electronics applications. In this paper, we present properties and results for two cobalt base alloys, Co_2FeGa and Co_2FeSi. These properties are interesting for the field of quantum computation. In the first part of this paper we introduce Moore's law, which explains the major limits of semiconductor technology. Then we discuss the results of our calculations based on the use of density functional theory and the WIEN2K program. This is for the purpose of making new quantum devices.

Key words: Heusler alloys, Co_2FeGa, Co_2FeSi, spin polarization, quantum devices

1. Introduction

To date, semiconductor technology has been the preferred method for the construction of circuits, chips, and computers. However, it is unclear how much longer we can continue to develop semiconductors before quantum effects become problematic. This was predicted by semiconductor industry experts in their National Technology Roadmap for Semiconductors [1], Gordon Moore [2], and other researchers [3–10]. It has been suggested that a solution may be found in the use of quantum computation techniques based on other kinds of materials such as Heusler alloys. The structural, electronic, and magnetic characteristics of ferromagnetic alloys like high-speed polarization and magnetic moment help to construct a new generation of quantum devices. The field of quantum computers had its first steps in the early 1980s, in the work of Paul Benioff [11] and Richard Feynman [12,13]. Subsequent attempts at the design of quantum algorithms included work by Deutsch and Jozsa [14], Simon [15], and Shor [16,17]. After that, the first 2-qubit quantum computer was built [18]. There are a number of additional textbook examples that demonstrate the power of quantum computation over semiconductor

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technology using classical computation methods [19–29]. Among the various half metallic materials proposed to date, such as double perovskite, spinel, or zinc-blende structured materials, Heusler alloys have recently attracted much attention for their relatively high spin polarization and large magnetic moment. On the base of an ab initio study on the structural, electronic, and magnetic properties of the two alloys Co_2FeGa and Co_2FeSi, we want to improve how quantum computation will be possible in the near future. Besides the construction of a quantum bit (Qubit), the use of the high spin polarization of the Heusler compounds offers an opportunity for the construction of a set of universal quantum gates such as QNOT, Hadamard, Y-Pauli, and Z-Pauli gates [30–36]. These are based on the use of the quantum superposition of electron orbits and spin polarization [37]. As a result of using developed techniques to obtain the electron superposition, the fabrication and the characterization of quantum dots and gates are possible [38]. The characteristic of quantum superposition of states in the quantum gates offers extensions in memory and speed. However, this is not the case in the classical gates (Not, AND, OR, NAND, XOR) and circuits based on semiconductor materials [39]. This needs more transistors in a chip to extend memory and accelerate computation. Based on density functional theory (DFT) and the WIEN2K program, we study if the properties of Heusler compounds respond to the needs of quantum device construction. Besides the use of generalized gradient approximation (GGA) to determine the partial and total magnetic moment, we study the spin polarization of the two materials, Co_2FeGa and Co_2FeSi.

2. Moore's law and the limits of semiconductor technology

How will quantum computing techniques end the power of the use of semiconductor technology? This is a big question for the contemporary electronic devices industry. After the invention of the transistor in 1947, technology rapidly progressed over the next six decades. This has led to progressively more sophisticated generations of microprocessors and computers. However, according to Moore's law and other researchers, it is possible that this progress may one day end.

From his experience in the employment of Intel, Gordon Moore forecasted the rapid development of semiconductor technology. Moore's law stated that the transistor density on integrated circuits doubles about every 2 years. As a result, we have obtained powerful computers with high functionality and performance, as shown in Table 1.

In Table 1 we see how the number of transistors increases with each new generation of microprocessors. The first microprocessor 4004 included 2300 transistors on a relatively large chip. However, in the latest generations of microprocessors such as Intel Itanium and Intel Itanium 2 there are more than 100 million transistors contained on a very small chip. Thus, we can extrapolate to a future microprocessor generation with more than 100 billion transistors on a micrometer chip. Furthermore, Moore's predictions point towards a future limit on semiconductor technology. According to Moore, semiconductor technology will approach the atomic scale. Thus, we have many difficulties in the development of exponential trends such as functionality and performance. Thinking about other material is a necessity. Ferromagnetic materials have different characteristics than semiconductor materials. Heusler alloys, a kind of ferromagnetic material, have high spin polarization and magnetic moment, which will be proven in the next parts of this work. This allows electrons to occupy more states than their original states. The superposition of electrons states can extend the performance and the speed of electronic devices. For the two Heusler compounds Co_2FeGa and Co_2FeSi spin (up and down) polarization represents the superposition of electrons. This is the representation of the quantum bit, which is the smallest unit of quantum information. With the use of the quantum computation, we can assure a doubling of speed and performance every 18 months or less. Thus, Moore's law returns to play a great role in the determination of the future generation of computers and microprocessors.

Table 1. The integration rate of transistors in microprocessor generations [1].

Microprocessor	Year of introduction	Transistors
4004	1971	2300
8008	1872	2500
8080	1974	4500
8086	1978	29,000
Intel286	1982	134,000
Intel386TM processor	1985	275,000
Intel486TM processor	1989	1,200,000
Intel Pentium Processor	1993	3,100,000
Intel Pentium II Processor	1997	7,500,000
Intel pentium III Processor	1999	9,500,000
Intel Pentium 4 Processor	2000	42,000,000
Intel Itanium Processor	2001	25,000,000
Intel Itanium 2 Processor	2002	220,000,000
Intel Itanium 2 Processor (9 Mb cache)	2004	592,000,000

3. The DFT method and the WIEN2K program

3.1. The DFT theory

DFT is one of the most widely used methods in ab initio calculations of the structure of atoms, molecules, crystals, and surfaces. Furthermore, it is a standard method of calculation used for solving many-body quantum problems of the types encountered in the studies of correlated polyelectronic systems in general and crystalline solids in particular. A first approach was proposed by Thomas and Fermi in the 1920s. Then the theory was developed on the basis of the Hohenberg–Kohn theorems, which are relative to any electron (fermion) system in an external field such as that induced by the nuclei and going beyond the Hartree–Fock approximation through taking into account correlation effects in the studies of the ground state physical properties of correlated polyelectronic systems. In addition, the corrections introduced in terms of exchange-correlation contributions have revealed better precision of the polyelectronic systems' energies calculations [40].

The bodies in the crystal structure are atoms (nuclei, electrons). The Hamiltonian of the system composed of electrons and nuclei is written in the following form:

$$\hat{H} = \hat{T}_e + \hat{T}_n + \hat{U}_{e-e} + \hat{U}_{e-n} + \hat{U}_{n-n}, \tag{1}$$

where $\hat{T}_e$ and $\hat{T}_n$ refer to the kinetic energy operators of electrons and nuclei, and the three other terms $\hat{U}_{e-e}$, $\hat{U}_{e-n}\hat{U}_{n-n}$ represent the interaction between electrons and electrons, electrons and nuclei, and nuclei and nuclei, respectively.

3.2. The WIEN2K program

The simulation code WIEN was developed at the Institute of Materials Chemistry at the Technical University of Vienna and was published by Peter Blaha and Karlheinz Schwarz. This code has been continuously revised and has experienced several updates. Versions of the WIEN code have been developed, named according to the

year of their publication. such as WIEN93, WIEN95, and WIEN97. In our study we use the version WIEN2K. WIEN2K has powerful characteristics, particularly in terms of speed and universality (multiplatform). The WIEN2K package is written in FORTRAN90 and runs on a UNIX operating system. Moreover, it consists of several independent programs, which perform electronic structure calculations of solid bodies based on DFT. Several properties of materials can be calculated with this code such as energy bands, density of states, Fermi surface, electron density, spin density, X-ray structure factors, total energy, atomic forces, equilibrium geometries, optimizations of structure, electric field gradients, isometric offsets, hyperfine fields, polarization of spins (ferromagnetic, antiferromagnetic, or other structures), spin-orbit coupling, X-ray emission and adsorption spectra, and optical properties. In our paper we depend on WIEN2K to achieve the different characteristics of the two ferromagnetic Heusler alloys Co_2FeGa and Co_2FeSi.

3.3. Heusler alloys

The full Heusler alloys crystallize in the structure $L2_1$, and they have a stoichiometric composition of type X_2YZ, where X and Y are transition metals and Z represents the nonmagnetic element of the groups III, IV, or V in the periodic table. In general, the Heusler alloys crystallize in cubic structures of the face-centered cubic (fcc) Bravais lattice, which show centered faces (space group Fm-3, No. 255), where the X atoms occupy sites A (1/4, 1/4, 1/4) and C (3/4, 3/4, 3/4), the Y atom occupies site B (0, 0, 0), and the Z atom occupies site D (1/2, 1/2, 1/2). Figure 1 shows the full Heusler alloys of type X_2YZ structural characterization.

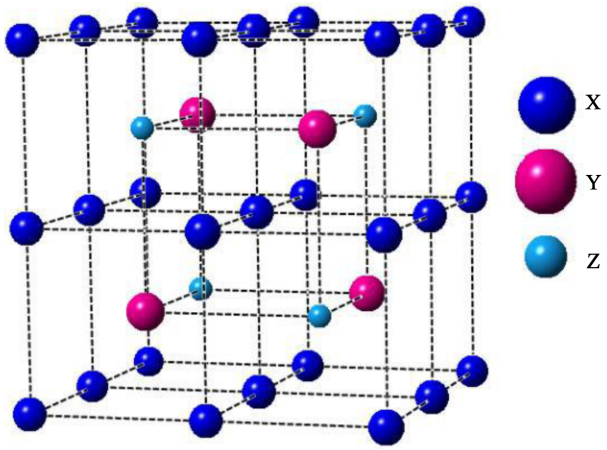

Figure 1. Schematic representation of the $L2_1$ structure for full Heusler alloys of type X_2YZ.

Cobalt-based alloys (Co_2YZ) [41] are theoretically predicted to have a semimetallic character at room temperature. Therefore, they present particular interest for tspin electronics applications. In addition, these materials have a Curie temperature much higher than room temperature [42], with values up to 1120 K in Co_2FeSi [43]. Moreover, they present a good lattice mismatch (epitaxy) with that of the MgO substrate. This good epitaxy between the layer and the substrate leads to a significant improvement in magnetic properties of these systems [44].

4. Calculation details

The calculations have been carried out based on DFT [45] and with the use of the WIEN2K program [46,47], which is an implementation of the FP-LAPW method [48,49]. The exchange and correlation potential is treated with GGA as presented by Perdew et al. [50–53].

The first step is to make a precise choice of important parameter values such as muffin-tin radius R_{mt} and the Brillouin zone of the various atoms constituting the compounds studied. R_{mt} is an approximation proposed by John C Slater and it is a form approximation of the potential field in an atomistic environment. Moreover, the Brillouin zone was developed by Leon Brillouin, and it is the set of points enclosed by the Bragg planes. We also call it the Wigner–Seitz cell.

We choose our R_{mt} values as follow: for the cobalt atom 2.2 UA, for the iron atom 2.0 UA, and for the silicon and the gallium a value of 1.9 UA has been chosen.

The sampling of the Brillouin zone must be done with care using the special point's technique of the Monkhorst and Pack lattice [54]. In our case, we use 10 special points, which are able to ensure the convergence of total energy by the mismatch of crystal.

These choices permit us to ensure the integration of the majority of core electrons in the sphere and to avoid overlapping spheres (muffin-tin).

5. Results and discussion

We calculate the total magnetic moment, and in each atomic sphere we use GGA for the two compounds. Moreover, we calculate the spin polarization of the two alloys Co_2FeGa and Co_2FeSi at an energy E (in particular at the Fermi level E_F, and in relation to the electronic spin-dependent densities of state (DOSs)).

The spin polarization that measures the spin asymmetry is given by the following expression [55]:

$$P(E_F) = \frac{n\uparrow(E_F) - n\downarrow(E_F)}{n\uparrow(E_F) + n\downarrow(E_F)} \tag{2}$$

where $n\uparrow(E_F)$ and $n\downarrow(E_F)$ are the majority and the minority densities of states at the Fermi level.

The values of total and partial magnetic moments of the two compounds as well as the polarization are shown in Table 2. We notice that the major part of these magnetic moments is strongly localized in the site of the element (Co) with a low contribution of Fe and the atoms of Si and Ga. The calculated magnetic moments are in a good agreement with the available results.

Table 2. The calculated value of the total magnetic moment, the partial magnetic moment in μ_B, and the spin polarization of the Heusler alloys Co_2FeSi and Co_2FeGa.

Compound	$m_{total}(\mu_B)$	$m_{Co}(\mu_B)$	$m_{Fe}(\mu_B)$	$m_{Si}(\mu_B)$	$m_{Ga}(\mu_B)$	P (%)
Co_2FeSi	5.42035	1.36471	2.74021	–0.00054	-	63.22
	6^c					
	5.08^d					
Co_2FeGa	5.00434	1.19597	2.76564	-	–0.02673	96.89
	5.08^a					
	5.02^b	1.22^b	2.76^b	-	$–0.028^b$	

^{a,b,c}Ref [56,57]. ^{d}Ref [58].

We can see that for the studied alloys, the spin polarization at the Fermi level is greater than 95% and can reach up to 100% for a slight variation of the lattice parameter, which is the case for the Co_2FeGa alloy. That said, the value of the spin polarization for the alloy can be explained by the gap absence in the majority spin band at the Fermi level (in this study, the majority spin band is the spin-up part), as can be seen clearly

in Figure 2a. Figure 2b represents the electronic DOS of the different energy level of the Co_2FeSi alloy. It is easy to see that the electronic structures for both alloys are approximately similar. They all have a forbidden bandwidth in one spin direction. Also, it is clear from these figures that we have the presence of some peaks around the Fermi level. Thus, we can assume that the DOS at the Fermi level is essentially linked to the Co atom. Furthermore, the gap width is 0.45 eV for Co_2FeGa and 0.49 eV for Co_2FeSi. It has been found that in Co_2FeZ (Z = Si, Ga) the width of the band gap decreases with the increase of the atomic number of element Z. Thus, the decrease in gap width can be explained in two ways. The first is the hybridization of p-d states. The second is the change of the lattice parameter. The width of the gap is very sensitive to the change of the lattice parameter and it decreases with the expansion of this parameter. In addition, we can note that, for the two materials in our study, the magnetic moments of the Z elements are very small (less than 0.086 μB) at 0.086 for Ga and 0.050 for Si. They have the same sign as the element Fe, and they are antiparallel to the magnetic moment of Co. Therefore, there is a double effect of the Z element in Co_2FeZ. First, it determines the lattice parameter of the alloy, and therefore the degree of localization of the electrons. Second, the total magnetic moment is determined by the number of electrons supplied.

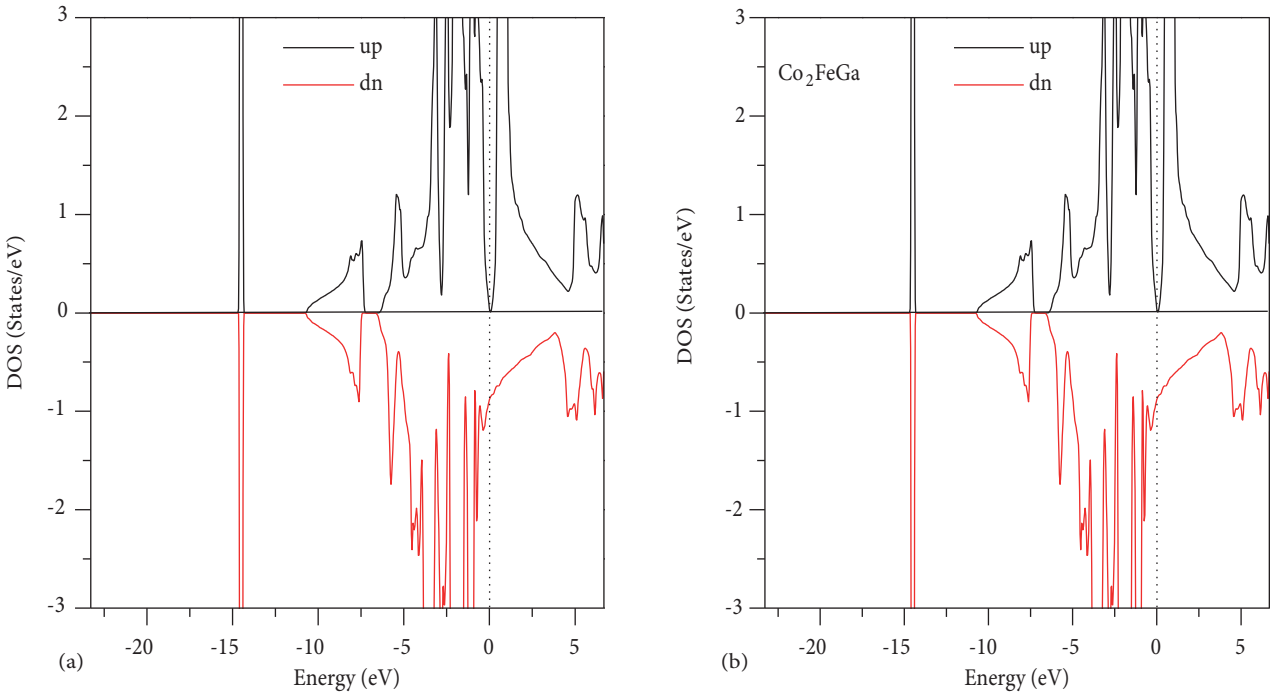

Figure 2. Electronic density of state for the alloys Co_2FeGa (a) and Co_2FeSi (b) at the Fermi level region.

Interesting properties of these materials result from exchange interactions between electrons and holes near bands. In a tetrahedral crystal field, the d states divide into two states, t_{2g} and e_g, while the p states have a symmetry t_{2g}. States with the same symmetry form strong p-d hybridization. This hybridization reduces the magnetic moment.

According to Galanakis et al. [59], the total magnetic moment in Heusler alloys follows the rule of Slater and Pauling, $m_t = N_v - 24$, where N_v is the total number of valence band electrons, even for compounds containing more than 24 electrons such as the alloys studied in our case, Co_2FeGa ($N_v = 29$) and Co_2FeSi ($N_v = 30$).

As we can see in Figure 3, which represents the total magnetic moment in function of the number of valance band electrons (Slater–Pauling behavior), our calculations show a small deviation from this rule, indicating that some compounds are not perfectly semimetals. Heusler cobalt-based alloys are also intermetallic compounds based on 3d transition metals and they present a localized magnetism relative to a route character. The explanation of the magnetism origin of these alloys is very complicated; however, their magnetic moments vary regularly according to the number of valence band electrons and the crystalline structure. This behavior is called Slater–Pauling behavior [60,61]. Those two physicists discovered that the magnetic moment m of 3d elements can be estimated on the basis of the average number of valence electrons (N_v) per atom.

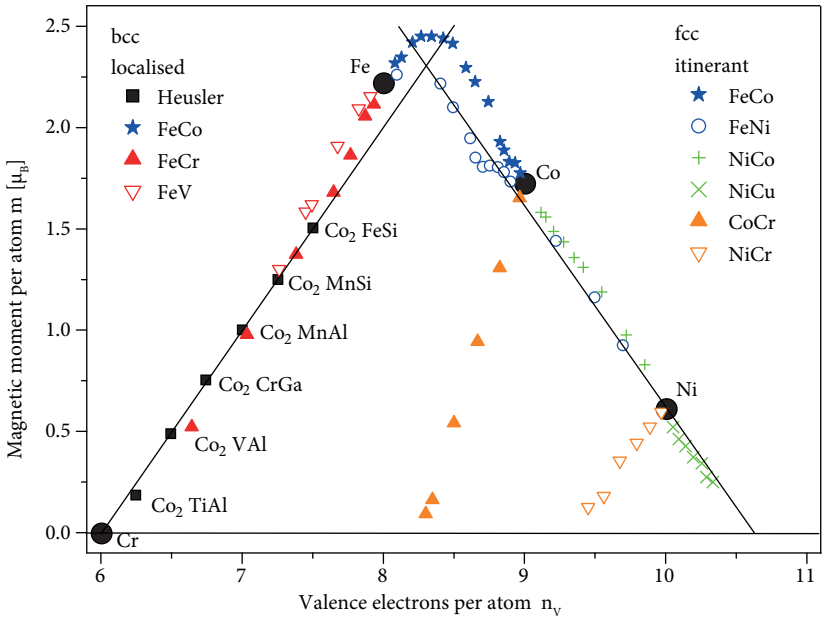

Figure 3. The Slater–Pauling curve for the 3d alloys in function of the number of valence band electrons.

The materials in Figure 3 are divided into two areas according to m (N_v): the first zone of the Slater–Pauling curve is the domain of low valence electron concentrations ($N_v \leq 8$) and localized magnetism. Here, the related structures mainly found are bcc. The second zone is the zone of high valence electron concentrations ($N_v \geq 8$) and itinerant magnetism. In this area, systems with closed structures are found such as fcc. Iron (Fe) is located on the border between localized and itinerant magnetism. However, Heusler alloys are located in the localized part of this curve. Therefore, we focus on this part of the curve. The magnetic moment per atom is given by the following relation:

$$m \approx N_v - 6, \tag{3}$$

where N_v is the number of valence band electrons.

As presented before, cobalt-based Heusler alloys show eight d minority states contained in the lattice. There is a doubly degenerate state of lower energy e_g, a triply degenerate state of lower energy t_{2g}, and a triply degenerate state of higher energy $t1u$ below the Fermi level. Besides the state d, there is a state s and three other p states, which are not counted in the gap structure. Finally, we have twelve minority occupied states per lattice. The total magnetic moment is given by the majority electron number in excess ($N_{\max}$) with relative to

minority electrons ($N_{\min}$):

$$m = N_{maj} - N_{min}. \tag{4}$$

The number of valence band electrons is determined by:

$$N_v = N_{maj} + N_{min}, \tag{5}$$

and the total magnetic moment becomes:

$$m = N_v - 24. \tag{6}$$

This relation is called the generalized Slater–Pauling rule, equivalent to the Slater–Pauling behavior for binary alloys of transition metals [62]. Since cobalt-base Heusler alloys have an integer number of valence, this rule is used to determine their magnetic moments. Figure 3 shows that the Heusler alloys magnetic moment is controlled by the atom Z. For example, the Si, which has four valence electrons, has a higher magnetic moment than an equivalent Heusler compound that contains Ga as the Z element. This effect is due to the increase of the d electron number associated with the Z atom. As indicated before, the structural changes of the Heusler alloys can have a significant effect on their magnetic properties. Also, all atomic exchanges can change the local hybridization of orbitals. The magnetic moment from valence electrons located at the orbital d level can be affected by this interatomic exchange. The change of the lattice parameter can be used to describe the structural disorder level. For instance, the alloy Co_2FeSi presents a magnetic moment of 6 μ_B/f.u. for the phase $L2_1$ [63]. In the case of the exchange between the atoms Co and Fe, the magnetic moment is reduced to 5.5 μ_B/f.u., whereas, during the exchange between Co and Si, the disorder leads to an increase in the magnetic moment at 6.05 μ_B/f.u.

These characteristics of magnetic moment in the case of atom exchange and the behavior of spins in these two Heusler alloys lead to the appearance of new quantum states. Each spin state represents a quantum bit. In contrast to the classical bit, which is a fundamental concept of classical computation that occupies two states (0 and 1), the quantum bit (Qubit) exists in many different states according to the spin polarization and state shown before. The Qubit is a fundamental concept of quantum computation, which can be in a superposition of states $|0\rangle$ and $|1\rangle$, where $|0\rangle$ and $|1\rangle$ are known as computational basis states. In our case they represent the two spin up and down states of polarization. This is the Dirac representation of classical states 0 and 1, respectively. Thus, we can represent a Qubit state as a linear combination of states $|0\rangle$ and $|0\rangle$ as follows:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \tag{7}$$

This shows that a state $|\psi\rangle$ is in superposition of states $|0\rangle$ and $|1\rangle$, where α and β are complex numbers representing the probability of states spin up and spin down: $|\alpha|^2 + |\beta|^2 = 1$. Therefore, we cannot precisely determine the final Qubit state. However, quantum mechanics can measure a Qubit state. This gives either $|0\rangle$ with probability $|\alpha|^2$ or $|1\rangle$ with probability $|\beta|^2$. Controlling the spin behavior of the two Heusler compounds Co_2FeGa and Co_2FeSi leads to total control over Qubits. As a result, we can construct quantum gates. Similar to the way a classical computer is built from an electrical circuit containing logic gates (AND, OR, NOT... etc.) and wires, a quantum computer is built from a quantum circuit containing quantum gates (QNOT, Hadamard, Pauli-Y, Pauli-Z, etc.) and wires to perform quantum computation and information.

6. Conclusion

In this work we focus on the study of a very precise class of ferromagnetic Heusler alloys of the type Co_2FeZ, where Z is either Ga or Si. Our calculations are based on DFT with the help of WIEN2K code, which is an

implementation of the FP-LAPW method. The exchange and the correlation potential is treated with GGA as presented by Perdew et al. [50–53]. Due to their magnetic and electronic properties, these materials seem to be much more practical than other classes of ferromagnetic alloys for quantum computation applications.

The results showed that the total magnetic moment for these alloys is between 5.5 μ_B/f.u. and 6.5 μ_B/f.u., which is in perfect agreement with Slater and Pauling's rule $m_t = N_v - 24$. The spin polarization at the Fermi level is high, and it can reach up to 100%. Moreover, the structural properties such as DOS clearly show the metallic character of these alloys given by the absence of a gap at the Fermi level.

The structural changes in Heusler alloys can have a significant effect on their magnetic properties. All these atomic exchanges can change the local hybridization of orbitals. The magnetic moments from the valence electrons that localize in the level of orbitals d can be affected by this interatomic exchange. The lattice parameter change can serve to describe the structural disorder. For example, the Co_2FeSi alloy presents a magnetic moment of 6 μ_B/f.u. for the $L2_1$ phase. In the case of the exchange between the Co and Fe atoms, the magnetic moment is reduced to 5.5 μ_B/f.u. However, in the case of the exchange between Co and Si atoms, the disorder increases the magnetic moment to 6.05 μ_B/f.u. The calculations prove that Co_2FeSi and Co_2FeGa are semimetallic.

With regard to the two compounds, we remark that the metallic characteristic is dominant in both directions of the spin, i.e. there is no band gap at the Fermi level whether it is in the direction of majority spins or that of minority spins. This confirms that it is not quite half-metallic. However, this compound does not have perfect half metallic characteristics; a small change of the lattice parameter can restore the half metallicity and can give a full magnetic moment. Indeed, the variation of the lattice constant modifies the hybridization between the electrons of the different atoms. This variation causes the change of the gap width and position and the electrons become more localized, which results in a shift of the majority and the minority bands relative to the Fermi level. The bandwidth of the minority bands in both compounds consists essentially of covalent hybridization between the d states of Co and Fe, leading to the binding and antibinding band formations with a gap between the two.

Due to the lattice parameter variation, the two Heusler compounds (Co_2FeGa and Co_2FeSi) have approximately a complete (100%) spin polarization at the Fermi level. These properties widely serve the spintronics and quantum computation fields. Furthermore, they attracted much attention for their useful applications in spin-dependent devices. In quantum computation we start to invest in these structural and electronic properties to make a new generation of quantum devices such as spin injection devices, nonvolatile magnetic random access memories, and magnetic Qubits. Doing that, we depend on the two spin states (spin up and spin down) to determine the basic element for quantum computation, which is the Qubit. Full control over the spin states will contribute to the construction of a set of universal quantum gates and circuits totally different than the classical one based on semiconductor technology. As a final result, the fabrication of a future quantum computer will be possible.

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