THEORETICAL STUDY OF THE ELECTRONIC PROPERTIES OF X_2YZ ($X = \text{Fe, Co}$; $Y = \text{Zr, Mo}$; $Z = \text{Ge, Sb}$) TERNARY HEUSLER: AB- INITIO STUDY

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Article Info	Abstract
<p>Received: 16.01.2020 Accepted: 22.02.2020</p> <p>Keywords: Heusler alloys, 3d and 4d elements, Electronic properties, half metallic zone, Magnetic properties</p>	<p>In the purpose of exploring new Heusler alloys with different magnetic applications, we have employed first principles calculations method within density functional theory. After checking the structural stability of X_2YZ Heusler alloys ($X = \text{Fe, Co}$; $Y = \text{Zr, Mo}$ and $Z = \text{Ge, Sb}$), we found that Cu_2MnAl type structure is more favorable for most compounds except for X_2MoGe and Co_2MoSb, were the Hg_2CuTi structure is energetically more stable. The trends in magnetic and electronic structures can be predicted by the structure types as well as the different kinds of hybridizations between the constituents. Among the two series only two compounds were identified to be true half metals with potential applications in spintronic devices. While one compound was classified as a nonmagnetic semiconductor with a small band gap. For the rest of materials, we found that the metallic behavior is dominant. These materials show possible interesting features in technical applications as well. The effect of distortion on the magnetic properties of Co_2ZrGe and Fe_2ZrSb showed that the half metallic character was preserved within a moderate range of volume changes, which makes it possible to grow these materials as thin films with modern techniques.</p>

1. Introduction

Due to their exciting physical properties and promising applications especially in spintronic field [1,2], Heusler alloys [3] have been extensively studied, particularly compounds for which one spin direction presents a gap at the Fermi level (E_F) while the other exhibits a metallic character leading to 100% spin polarization. Special efforts have been dedicated to full Heuslers composed by a main group element with s-p valence electrons and two transition metals. The deficiency in electrons in the d shell of these transition metals makes them very useful for generating interesting magnetic and electronic aspects, primarily,

the half metallic character. Thanks to this feature [4, 5], the curiosity over Heusler materials have been awakened again, since from their discovery and till the seventies, the study of these alloys have witnessed a major disregarding and reports on new Heusler compounds were rarely published [6,7]. The search for half metallic materials has led to many theoretical and experimental investigations on Heusler compounds; ab-initio therefore, provides great opportunity for researchers in this area.

Continuous studies were performed on ternary Heuslers showing high Curie temperature [8,9], which makes them excellent candidates in spintronic domain and magnetic applications [10]. As a result, Co_2 , Mn_2 and Fe_2 based materials have been the essential topic of several investigations [11,12]. Still there is a certain lack in half metallic materials composed, besides the X atoms, by a 4d Y element instead of a 3d. Actually, many Co_2 based Heuslers are characterized by a semiconducting behavior in one spin channel. On the other hand, only few Fe_2 based compounds were found to exhibit half metallic aspect. And since the s-p elements conduce unexpected changes on the half metallic properties, we therefore have combined eight compounds permuting Fe with Co, Zr with Mo, and Ge with Sb elements, for the development of new materials with promising magnetic features. Trying to understand the effect of different hybridizations on the electronic and magnetic properties as these systems change composites was one of our main objectives. Besides we wish to clarify the origin of diversity in physical properties of these ternary alloys when replacing an sp^2 element by an sp^3 .

2. Computational details

Using ab initio simulation package (wien2k) [13], we have studied the electronic structure and magnetic properties with generalized gradient approximation (GGA-PBE) proposed by Perdew, Burke, and Ernzerhof [14]. Details of the calculation method are described in [15].

14^3 k-mesh were used for Brillouin zone integration and 104 special k-points in the symmetry irreducible BZ. The muffin tin radii for Fe ($4s^2 3d^6$), Co ($4s^2 3d^7$), Zr ($5s^2 4d^2$) and Mo ($5s^1 4d^5$) transition metals, and for s-p elements Ge ($4s^2 4p^2$) and Sb ($5s^2 5p^3$) atoms were in the range of 2.2. The density plane-wave cutoff is $Rk_{\text{max}} = 9.0$. The cutoff energy separating the valence and core states was chosen as -6.0 Ry.

3. Results and discussion

Full Heusler compounds crystallize in two prototype structures. The regular Heusler (here named TI) crystallizes in a cubic structure Cu_2MnAl prototype with the space group $\text{Fm}\bar{3}\text{m}$ (space group number 225, L_{21}), and the inverse Heusler, with prototype Hg_2CuTi (here named TII) (space group $\text{F}\bar{4}3\text{m}$: number 216) structure.

In L_{21} structure, the most and least electronegative elements form a Rock-salt (NaCl) type lattice. These elements occupy the atomic positions (0, 0, 0) and (1/2, 1/2, 1/2). X atoms having electronegativity in between those of Y and Z elements are in symmetric positions and occupy (1/4, 1/4, 1/4).

In inverse Heusler structure, the X atoms are placed on (1/2, 1/2, 1/2) and (3/4, 3/4, 3/4) positions while Y and Z atoms occupy (1/4, 1/4, 1/4) and (0, 0, 0) positions.

For the full Heuslers X_2ZrGe , X_2ZrSb and Fe_2MoSb we find that L_{21} structure with AlCu_2Mn as prototype is more favorable than the inverse one. However, X_2MoGe and Co_2MoSb are predicted to crystallize in CuHg_2Ti type structure. This is confirmed by the fit plot of total energy as function of volume for the nonmagnetic and ferromagnetic states of both types of structures for the two series (Figure 1 and 2). Moreover, we note that except for Fe_2ZrGe , the ferromagnetic phase is lower in energy as compared to the paramagnetic state for all studied

Table 1. Calculated lattice constants, structure type, magnetic moments; the minority spins gap ($E_{g_{\text{min}}}$) and the half metallic gap ($E_{g_{\text{HM}}}$) of X_2YZ compounds.

System	Lattice constant (Å)	Structure type	Magnetic moment (μ_B)	$E_{g_{\text{min}}}$ (eV)	$E_{g_{\text{HM}}}$ (eV)
Fe_2ZrGe	6,01 (5.93 for Fe_2ZrSi)	TI	0	0.135	/
Fe_2ZrSb	6,24	TI	0.99	0.73	0
Fe_2MoGe	5,95 (5.78 for Fe_2MoSi)	TII	3.54	/	/
Fe_2MoSb	6,10	TI	2.81	/	/
Co_2ZrGe	6,08 (6.08)[12](6.06)[11]	TI	1.96	0.59 (0.58[12] (0.43)[11]	0.32 (0.31)[12]
Co_2ZrSb	6,28	TI	1.69	0.59	/
Co_2MoGe	5,88 (5.78 for Co_2MoSi)	TII	0.16	/	/
Co_2MoSb	6,12	TII	0.20	/	/

systems. Also the obtained lattice constants of the lowest energy Heusler phases increase when replacing Fe atoms by Co atoms except for $X_2\text{MoGe}$ that crystallizes in TII structure, it is observed that the lattice constant decreases when the Fe atoms are replaced by Co atoms. $X_2\text{MoSb}$ compound that changes its structure type when changing X atom shows an almost equal lattice constant's value. In case of Fe_2ZrZ and Co_2ZrZ ($Z = \text{Ge}, \text{Sb}$), the increased lattice constants can be explained on the basis of relative sizes of the X and Z elements atomic radii. In Table I we present the structural properties (the crystal structure type and the equilibrium lattice constant).

Figure 1. Total energy as function of volume for Co_2YZ compounds for the normal Heusler structure in the ferromagnetic states (NFM), nonmagnetic states (NNM) and for the inverse structures in the ferromagnetic states (IFM), nonmagnetic states (INM)

Figure 2. Total energy as function of volume for Fe2YZ compounds for the normal Heusler structure in the ferromagnetic states (NFM), nonmagnetic states (NNM) and for the inverse structures in the ferromagnetic states (IFM), nonmagnetic states (INM)

Figure 3. Spin-polarized band structures of Co2YZ ternary alloys at their predicted equilibrium lattice constants. The dashed lines correspond to minority spin channel and the solid lines correspond to majority spin channel.

Figure 4. Spin-polarized band structures of Fe_2YZ ternary alloys at their predicted equilibrium lattice constants. The dashed lines correspond to minority spin channel and the solid lines correspond to majority spin channel.

The band structures of ternary compounds presented in Figure. 3 and 4 were calculated at equilibrium lattice constants along their high symmetry directions in the Brillouin zone. These band plots in addition to the Slater Pauling rule are very useful for the prediction of the half metallic properties.

The electronic band structures of the studied X_2YZ compounds show remarkable differences when going from Fe to Co or even in the same series when the number of valence electrons increases or decreases by one simple electron. Across the two series under investigation, we identify three compounds, Fe_2MoGe , Co_2ZrSb and Co_2MoSb having much deviated moments than those predicted by the Slater Pauling rule [16]-[17]. In both series, the s-p atoms as well as the interstitial region carry a negligible magnetic moment which does not contribute much to the overall moment. These small moments are caused by the effect of polarization of the surrounding X and Y magnetic atoms [18]. We also notice that except for Fe_2MoSb , the partial moment of the Y element is antiparallel to X moment. This means that the X-X and X-Y interactions play a crucial role for the determination of the half metallic ferromagnetism. In Table II we present the total and partial magnetic moments along with the spin polarizations for all the compounds considered here.

Table II. The unit cell total magnetic moment M_{tot} and the atomic magnetic moments M_i of constituent i for X_2YZ compounds N_v is the number of valence electrons of the systems.

Systems	N_v	M_x	$M_{x'}$	M_y	M_z	M_{int}	M_{tot}
Fe₂ZrGe (TI)	24	0.00	0.00	0.00	0.00	0.00	0.00
Fe₂ZrSb (TI)	25	0.65745	0.65745	-0.15185	-0.01979	-0.14675	0.99651
Fe₂MoGe (TII)	26	1.78877	2.22991	-0.36676	0.00748	-0.11187	3.54752
Fe₂MoSb (TI)	27	1.31352	1.31352	0.19772	-0.01415	0.00049	2.81110
Co₂ZrGe (TI)	26	1.08258	1.08258	-0.09574	0.02929	-0.13373	1.96470
Co₂ZrSb (TI)	27	0.90737	0.90737	-0.05440	0.02690	-0.09288	1.69436
Co₂MoGe (TII)	28	0.23990	-0.02800	-0.02460	-0.00783	-0.01630	0.16316
Co₂MoSb (TII)	29	0.33771	0.14250	-0.18359	-0.01259	-0.08020	0.20383

In case of Fe₂YZ series (Y = Zr, Mo and Z = Ge, Sb), the number of valence electrons is greater than or equal to 24, and according to Slater Pauling rule ($M = N_v - 24$) [19], the magnetic moments are 0, 1, 2 and 3, respectively. Overall our results coincide with the predicted ones and show that Fe₂ZrGe having 24 valence electrons is a non-magnetic semiconductor and is in excellent agreement with the Slater Pauling rule. Fe₂MoSb in spite of having a moderate moment of 2.81 μ_B , it can only be considered as a metal. Both Fe atoms in this compound carry a moment of almost 2.6 and are ferromagnetically coupled to the Y elements. The Fe-Mo interactions might have reduced the magnetic moment of Fe atoms thus destroying the half metallic gap. Fe₂ZrSb with an almost integer moment is a half metallic compound with a large band gap of 0.73 eV. The Fermi level in this compound is a top of the highest minority spin valence band. Both Fe atoms are ferromagnetically coupled and contribute with a magnetic moment of about 1.31 μ_B , while the interactions between the 3d and 4d magnetic atoms are antiparallel. This antiparallel alignment is beneficial to the Fe atoms leading to a total magnetic moment of 0.99 μ_B . Whereas the only compound with TII structure in this series, Fe₂MoGe, having a magnetic moment of almost 3.55 μ_B , absolutely differs from the Slater Pauling predictions (2 μ_B). Obviously there is a huge difference between the properties of Co₂ZrGe (which will be discussed in the next paragraph) and Fe₂MoGe both having 26 valence electrons, this might be originated from the different types of structures that each compound prefers. The reduction in the magnetic moment of Fe_I in comparison to Fe_{II} is caused by the interactions between both Fe atoms in addition to the

antiferromagnetic interactions between Fe_I and Mo, which leaves little chance for a half metallic aspect.

When replacing Fe by Co atoms, and by adding one electron in d shell, the magnetic moments start to deviate from the predicted ones. Co_2YZ compounds have valence electrons from 26 to 29, so according to Slater Pauling rule; the magnetic moments should be 2, 3, 0 and 1, respectively. However, the resulting moments show a major decrease with increasing the number of valence electrons N_v . Excluding Co_2MoSb ; the Y elements (Mo and Zr) in this series contribute with a small antiparallel moment as compared to the ones found in Fe based series. The Co moment decreases significantly from Co_2ZrGe to Co_2MoSb . We found that Co_2ZrSb with a magnetic moment of $1.69 \mu_B$ which is far less from the one predicted by Slater Pauling rule ($3\mu_B$) shows magnetic character. Co_2ZrGe has a total magnetic moment of $1.96 \mu_B$ and exhibits half metallic character. Concerning this compound, our results are supported by previous theoretical works. Actually it was found that Co_2ZrGe has a perfect magnetic moment of $2.00 \mu_B$. Our calculations show a slightly smaller moment than the ones found in [20,21]. This might be due to the different atomic positions chosen for L_{21} structure, as well as the different methods used in calculations [12-23]. Moving to compounds with TII structure, Co_2MoGe with 28 valence electrons is an ordinary metal, and it has a small magnetic moment of $0.16 \mu_B$, which disobeys the Slater Pauling rule. Co_2MoSb having the same ground state structure (TII), shows identical electronic features around the Fermi level in both spin directions. The Co_I and Co_{II} atoms have small contributions that are less than $0.5 \mu_B$ and the hybridizations of Co_{II} with Mo reduce its moment in comparison to Co_I , leading to a total moment of $0.20 \mu_B$. Co_2MoSb is then an ordinary metal.

The electronic structure plays an important role for the determination of magnetic properties and the prediction of half-metallic ferromagnets. Furthermore it allows us to better understand the hybridizations between the constituents of the compounds [15]. Generally, the hybridization between the d orbitals of transition metals is mainly responsible for the existence of the minority gap, while the s-p elements are very important for structural stability of Heusler alloys. In order to determine the types of atomic hybrids and confirm the origin of the half metallic gap, we have calculated the total and partial densities of states (DOS) of the two series as shown in Figs. 5 and 6. We note that for the studied compounds, all obtained gaps are indirect with the maximum valence band at Γ point and the minimum of the conduction band along X direction.

Figure 5. Spin polarized total and atom projected densities of states for Co₂YZ compounds at their ground states

Figure 6. Spin polarized total and atom projected densities of states for Fe₂YZ compounds at their ground states

In the minority and majority spin channels, the Sb-p orbitals contribute significantly to the density of states of X₂YSb compounds. The s bands of Sb and Ge atoms are very low in energy, and are located in an isolated range of -12.5 eV to -10.5 eV, and -11 eV to -9 eV, respectively. Like Sb-p bands, Ge-p bands contribute to the density of states in an energy

region between ~ -7 eV and -3 eV. These s and p states show almost identical band structures for the two spin directions in both series and are hybridized with X and Y d electrons, which explains the small negative moments of these s-p elements.

In Fe_2 based compounds, the electronic structures show few similar features in all of these systems. We notice that the d states of both Fe atoms, in Fe_2MoGe compound with type II structure, contribute the most to the density of states below Fermi level, while the Mo-d states extend into the unoccupied part of the majority spin channel. The minority spin channel is characterized by a pseudo gap below Fermi level. The Fe_I d states are localized around E_F and are coupled to Fe_II d states as well as Mo d orbitals below Fermi level, which explains the reduction in the moment of Fe_I atoms. The Mo d states show much larger contributions for Fe_2MoSb compound with type I structure as compared to Fe_2MoGe in both spin directions. The main contributions of Fe and Mo atoms in this compound are centralized below Fermi level in majority spin channel. In spin down channel, the bonding states exist at the higher valence transition metal element. These states are strongly mixed to the d states of Mo atoms reducing the magnetic moment of Fe atoms in comparison to that in Fe_2MoGe compound and destroying the half metallicity of the system. Fe_2ZrGe which has 24 valence electrons is a semiconductor with a narrow band gap. The Fe d states dominate the higher valence band of Fe_2ZrGe , while they are located at about 0.14 eV above the conduction band. Whereas the Zr d states are splitted into occupied states lying around -2 eV below Fermi level and unoccupied states in the lowest conduction band above Fermi level. Basically the electronic structure of Fe_2ZrGe compound show the same behavior as the majority channel of Fe_2ZrSb , except that in the latter, the Fermi level is located closer to the valence band. The spin up channel of Fe_2ZrSb Heusler alloy is also manifested by Fe d states surrounding the Fermi level, whereas the Zr d states are located in the unoccupied part of this channel. The minority spin channel presents significant band gaps in the partial DOS, these gaps are larger for Y and Z atoms as compared to X atoms. The Fe d states surrounding the half metallic gap hybridize with Zr-d orbitals, opening a large indirect gap of 0.73 eV above Fermi level.

In Co_2 based series, our results show that the magnetic moments of Co atoms in compounds with TII structure are considerably reduced as compared to those in TI structure. The density of states in Co_2MoGe is almost identical in majority and minority spin channels. The Co_I and Co_II d states are strongly mixed around the Fermi level, as well as the d states of Mo atoms extending along E_F . These interactions minimize the magnetic moment of Co_II atoms, leaving no possibility for half metallicity in this compound. Co_2MoSb that crystallizes in the same structure type shows common features as Co_2MoGe . The energy range between -

3.0 and 1.0 eV is relative to the d states of transition elements cutting through the Fermi level. Because of the strong interactions between Co_I - Co_II , and Co_II -Mo atoms, the magnetic moment of Co_II atom lowers significantly leaving no chance for any half metallic properties. For Co_2ZrZ compounds, the magnetic moment carried by Co atoms decreases with increasing valence electrons number. While the density of states of these two systems show almost the same features in both spin channels. The Fermi level in Co_2ZrGe alloy lies almost at the center of the minority band gap. This last one is limited by 0.32 eV below Fermi level and 0.27 eV above the Fermi level resulting in an equal band gap to that of Co_2ZrSb (0.59 eV). Whereas in Co_2ZrSb compound, the Fermi level is situated near the conduction band. Besides, the spin down gap occurred by Zr atoms, in both compounds, is broader than the one presented by Co atoms around E_F . The bonding states of Co_2ZrZ compounds mostly exist at the Co atom. While, the unoccupied antibonding bands mainly exist at Zr 4d orbitals. We also notice that the minority conduction band of Co_2ZrSb , unlike Co_2ZrGe , constitute a larger peak extending upon the Fermi level. It is evident that the hybridizations between the d states of Co atoms and the s-p states of Sb or Ge atoms have a huge impact when defining the material's properties. As a result, the magnetic moment in Co sites diminishes, which influences the half metallic properties of Co_2ZrSb system.

Regarding the importance of the half metallic character, and knowing that any shift in the lattice parameter especially during the growth of thin films may affect the robustness of materials, it is worthful studying the constancy of the magnetic moment with respect to variation of the lattice parameter. As can be seen in figure 7, we have performed a change of the lattice parameter within a range of 5.65 Å to 6.55 Å for Co_2ZrGe , and from 5.41 to 6.34 Å for Fe_2ZrSb compound, and found that half metallicity in both materials is sustainable against a reasonable range of changes of the lattice parameter. For Co_2ZrGe , the half metallic character exists when the lattice parameter reaches a value of 5.76 Å up to 6.46 Å. We point out that our result outperforms the previous investigations in [21]-[21]. While in Fe_2ZrSb , the half metallic gap exists only if the material is under compression. In fact it appears when the lattice constant is equal to 5.54 Å and disappears as soon as overreaching the equilibrium lattice parameter. Since the magnetic properties for these two systems are preserved in a moderate range of volume changes, an experimental study would be very useful in enriching our theoretical work.

Figure 7. The range of half mettalicity with respect to the lattice parameter

4. Conclusion

The general idea of this work was based on the development of new half metals with different properties by mixing both 3d and 4d elements, using the FP-LAPW method based on DFT within the generalized gradient approximation GGA. Only two compounds, Co_2ZrGe and Fe_2ZrSb , having indirect band gaps of 0.59 eV and 0.73 eV, respectively, in the minority spin channel were identified to be true half metals. We also found that Fe_2ZrGe that shows a narrow band gap above Fermi level is a nonmagnetic semiconductor. In case of compounds having the same valence electrons (Fe_2MoGe and Co_2ZrGe pair), we have concluded that as long as the ground structure types are different, there are no common features in the electronic properties of these compounds. While for Fe_2MoSb and Co_2ZrSb pair, the differences in their electronic structures might be correlated to the different kinds of hybridizations between the constituents. In general all studied compounds show very similar features in their electronic structures when Y element remains the same, except for Fe_2MoZ pair. Once again this might be correlated to the different atomic structures adopted by each of Fe_2MoGe and Fe_2MoSb Heusler alloys. Another interesting point in this work concerns the steadiness of the half metallic properties when changing the lattice constants. Actually it was found that both Fe_2ZrSb and Co_2ZrGe can keep their half metallic characteristics in a moderate range of lattice constant's changes, which make them promising materials for spintronic applications.

At the end, we highlight that all of these compounds are worth further studies and hope this work would be advantageous and inspiring to researchers working in this domain.

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References

- [1] A.Prinz, Science 282 (1998)1660.
- [2] J. de Boeck, W. van Roy, J. Das, V. Motsnyi, Z. Liu, L. Lagae, H. Boeve, K. Dessen and G. Borghs, Semicond. Sci. Technol. 17 (2002) 342.
- [3] H. P. J. Wijn. Heusler alloys. In: H. P. J. Wijn (eds), *Magnetic Properties of Metals. Data in Science and Technology* (Springer, Berlin, Heidelberg, 1991), pp. 168-173.
- [4] R. A. de Groot, F. M. Mueller, P. G. van Engen and K. H. J. Buschow, Phys. Rev. Lett. 50 (1983) 2024.
- [5] J. Kübler, A. R. Williams and C. B. Sommers, Phys. Rev. B 28 (1983) 1745.
- [6] P. J. Webster, J. Phys. Chem. Solids 32 (1971) 1221.
- [7] S. Brooks, J. M. Williams, Phys. Stat. Sol. A 32 (1975) 413.
- [8] S. Wurmehl, G. H. Fecher, H. C. Kandpal, V. Ksenofontov, C. Felser and H.-J. Lin, Appl. Phys. Lett. 88 (2006) 032503.
- [9] T. Graf, C. Felser and S. S. Parkin, Prog. Solid State. Chem. 39 (2011) 1.
- [10] T. Gasi, V. Ksenofontov, J. Kiss, S. Chadov, A. K. Nayak, M. Nicklas, J. Winterlik, M. Schwall, P. Klaer, P. Adler and C. Felser, Physical Review B 87 (2013) 064411.
- [11] N. I. Kourov, V. V. Marchenkov, K. A. Belozerova and H. W. Weber, Journal of Experimental and Theoretical Physics 121 (2015) 844–852.
- [12] N. Arıkan, A. İyigör, A. Candan, Ş. Uğur, Z. Charifi, H. Baaziz and G. Uğur, Journal of Materials Science 49 (2014) 4180–4190.
- [13] P. Blaha, K. Schwarz, G.K.H. Madsen, D. Kvasnicka and J. Luitz, WIEN2k: An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties, Karlheinz Schwarz, Techn. Universitat Wien, Wien, Austria, 2001, ISBN: 3-9501031-1-2.
- [14] J. P. Perdew, K. Burke and M. Ernzerhof, Phys. Rev. Lett. 77 (1996) 3865.
- [15] P. Hohenberg and W. Kohn, Phys. Rev. 136 (1964) B864; W. Kohn and L. J. Sham, Phys. Rev. 140 (1965) A1133.

- [16] J. C. Slater, Phys. Rev. 49 (1936) 537
- [17] I. Galanakis, Theory of Heusler and Full-Heusler Compounds, pp. 3-36, Springer International Publishing, Cham (2016).
- [18] H.C. Kandpal, G. H. Fecher, and C. Felser, J. Phys. D: Appl. Phys. 40 (2007) 1507.
- [19] I. Galanakis, P. H. Dederichs and N. Papanikolaou, Phys. Rev. B 66 (2002) 174429.
- [20] S. Li, Y. Liu, Z. Ren, X. Zhang, and G. Liu, J. Korean. Phys. Soc. 65 (2014) 1059.
- [21] Abada Ahmed; Hiadsi Said; Ouahrani Tarik; Amrani Bouhalouane; Amara Kadda. International Journal of Environmental, Chemical, Ecological, Geological and Geophysical Engineering 9 (2015) 349.
- [22] M. C. Payne, M. P. Teter, D. C. Allan, T. A. Arias and J. D. Joannopoulos, Rev. Mod. Phys. 64 (1992) 1065.
- [23] M. D. Segall, P. L. D. Lindan, M. J. Probert, C. J. Pickard, P. J. Hasnip, S. J. Clark and M. C. Payne, J. Phys.: Condens. Matter 14 (2002) 2717.