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# Appearance of half-metallicity in the quaternary Heusler alloys

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## Abstract

I report systematic first-principles calculations of the quaternary Heusler alloys, e.g.  $\text{Co}_2[\text{Cr}_{1-x}\text{Mn}_x]\text{Al}$ ,  $\text{Co}_2\text{Mn}[\text{Al}_{1-x}\text{Sn}_x]$  and  $[\text{Fe}_{1-x}\text{Co}_x]_2\text{MnAl}$ . I show that these alloys are also half-ferromagnets when the normal Heusler compounds corresponding to concentration values of zero and unity are half-metals. Moreover, the total spin moment  $M_t$  in  $\mu_B$  scales linearly with the total number of valence electrons  $Z_t$  (and thus with the concentration  $x$ ) following the relation  $M_t = Z_t - 24$ , independently of the origin of the extra valence electrons, confirming the Slater–Pauling behaviour of the normal Heusler alloys. These results pave the way for experimentalists searching for new half-metallic alloys.

## 1. Introduction

Heusler alloys consist of a large family of intermetallic compounds which attract regularly considerable attention due to the variety of magnetic phenomena which they present. Lately the interest has been focused on the ones that are half-metals<sup>1</sup> (HMs) such as NiMnSb [1, 2] or  $\text{Co}_2\text{MnSn}$  [3]. These compounds are ferromagnets for which the minority spin-band presents a gap and the Fermi level falls within this gap. Thus the spin polarization at the Fermi level is 100% and these materials are of special interest for spintronic applications [4, 5]; the spin of the electron and not the charge is used as the property to control the device. In contrast to other HM systems such as the diluted magnetic semiconductors or the manganites and some oxides [5], the half- and full-Heusler alloys (e.g. NiMnSb and  $\text{Co}_2\text{MnSn}$ , respectively) [6] and the zinc-blende compounds such as CrAs [7–9] present very high Curie temperatures, making them attractive for industrial applications.

In [11] it was shown from first-principles calculations in the case of the ordered half-Heusler alloys such as NiMnSb that the gap is formed between the occupied bonding d states

<sup>1</sup> I will use the abbreviation HM to denote both 'half-metal' and 'half-metallic'.

resulting from the interaction between the higher- and the lower-valent transition metal atoms and the corresponding antibonding states [10]. For the full-Heusler alloys such as  $\text{Co}_2\text{MnSn}$  the situation is more complicated since there are also states located only at the Co sites and the resulting gap is tiny [11]. The total spin moment for the latter compounds is given by the relation  $M_t = Z_t - 24$ , where  $M_t$  is the total spin moment in  $\mu_B$  and  $Z_t$  the total number of valence electrons. This is the so-called Slater–Pauling (SP) behaviour.

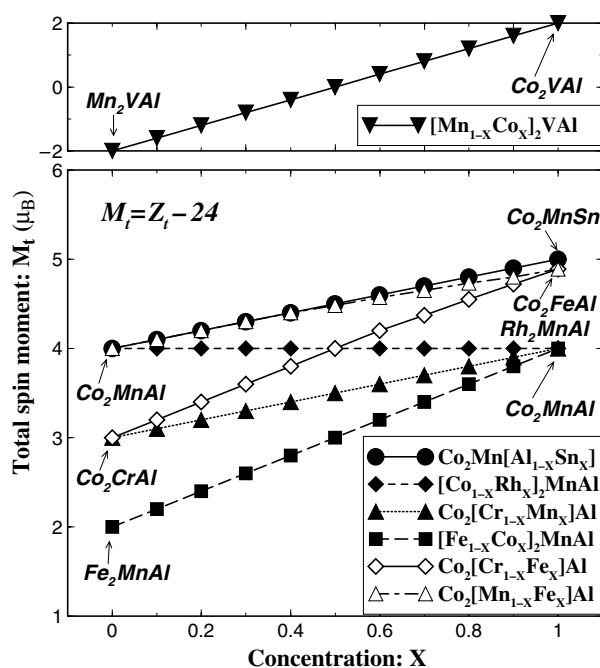
The scope of this paper is to expand the previous study on the normal full-Heusler alloys [11] to also include the quaternary Heusler alloys and provide a guide for experimentalists working in this field and trying to grow new half-metallic systems with predefined electronic and magnetic properties. These new materials could possibly be more suitable for industrial applications and recently experiments on  $\text{Co}_2\text{Cr}_{0.6}\text{Fe}_{0.4}\text{Al}$  have been performed [12]. In the quaternary compounds, one of the four sites is occupied by two different kinds of neighbouring element as in  $\text{Co}_2[\text{Cr}_{1-x}\text{Mn}_x]\text{Al}$  where the Y site is occupied by Cr or Mn atoms (see figure 1 in [11] for the definition of the structure). I will firstly focus my study on the behaviour of the total spin moment for several cases and show that it follows the Slater–Pauling behaviour when the limiting cases are half-metals. Afterwards I will study the case where the Y site is occupied by two different elements as in  $\text{Co}_2[\text{Cr}_{1-x}\text{Mn}_x]\text{Al}$ , followed by the case when there are two different types of sp atom as in  $\text{Co}_2\text{Mn}[\text{Al}_{1-x}\text{Sn}_x]$ . The final case is when the X sites are disordered as in  $[\text{Fe}_{1-x}\text{Co}_x]_2\text{MnAl}$ . In the final section I summarize and conclude.

## 2. Computational details

To perform this study I used the Korringa–Kohn–Rostoker (KKR) method [13] within the local density spin approximation (LSDA) to the exchange–correlation potential [14] as implemented in [15]. The coherent potential approximation (CPA) is used to simulate the disorder in the crystal [15]. This method has already been applied with success to study another class of disordered materials: the diluted magnetic semiconductors [15]. The space within this method is divided into non-overlapping muffin-tin spheres and the vanishing charge in the interstitial region is considered to be constant and charge neutrality is imposed. Such an approximation is reasonable to describe a close-packed structure such as the one of the Heusler alloys. To check the validity of this description I compared the total spin moment with the full-potential calculations performed in [11]. For all the compounds with the exception of  $\text{Co}_2\text{VAl}$  both methods produced similar magnetic properties for the experimental lattice constants [16, 17]. V 3d wavefunctions have a large extent and the muffin-tin approximation is not adequate to describe the V magnetism; thus I had to use a lattice constant 4% larger than the experimental one to get a half-metallic compound, as predicted by the full-potential KKR for the experimental lattice constant. I assumed that the lattice constant varies linearly with the concentration  $x$  which has been verified for several quaternary alloys [16]. Finally I should mention that the total spin moment is not exactly an integer due to numerical inaccuracies. To decide whether an alloy is half-metallic or not I used the total DOS as a criterion, as was also the case in the previous studies [9–11].

## 3. Results and discussion

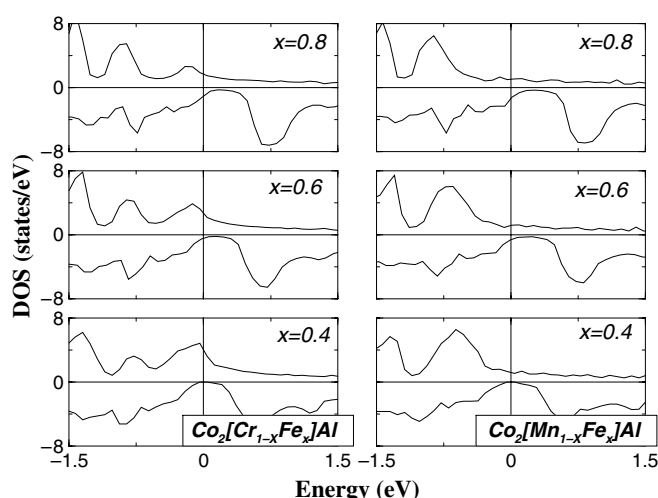
As shown in [11] the total spin moment in the case of the half-metallic full-Heusler alloys obeys the rule  $M_t = Z_t - 24$ , where  $M_t$  is the total spin moment in  $\mu_B$  and  $Z_t$  the total number of valence electrons. The 24 arises from the fact that there are in total 12 occupied minority states; e.g. in the case of  $\text{Co}_2\text{MnAl}$  Al provides one minority s band very low in energy and three minority p bands which accommodate also transition metal d electrons. There are also five occupied bonding d bands created from the interaction between the Mn and the Co atoms.



**Figure 1.** Calculated total spin moment  $M_t$  in  $\mu_B$  for a variety of compounds as a function of the concentration  $x$  ( $x = 0, 0.1, 0.2, \dots, 0.9, 1$ ). I assumed that the lattice constant varies linearly with the concentration  $x$ . With filled geometrical objects the cases obey the rule  $M_t = Z_t - 24$  where  $Z_t$  is the total number of valence electrons; this is the so-called Slater–Pauling behaviour.

The Fermi level falls within the gap created by the occupied triply degenerate d states and the unoccupied doubly degenerate d states which are exclusively located at the Co sites and are permitted by the symmetry of the crystal. The moments' behaviour is the Slater–Pauling behaviour well known from the binary alloys. In the latter compounds the spin moment decreases with  $Z_t$  since the spin-up states are completely occupied and the extra electrons occupy spin-down states reducing the total spin moment. In the case of the full Heusler alloys the Fermi level is fixed within the minority bandgap, the extra electrons, as I change the chemical elements, occupy exclusively spin-up states and the total spin moment increases.

Using the KKR-CPA method I calculated the total spin moment for several quaternary alloys taking into account several possible combinations of chemical elements and assuming in all case a concentration increment of 0.1. I summarize my results in figure 1. The first possible case is when I have two different low-valent transition metal atoms at the Y site such as  $\text{Co}_2[\text{Cr}_{1-x}\text{Mn}_x]\text{Al}$ . The total spin moment varies linearly between the  $3 \mu_B$  of  $\text{Co}_2\text{CrAl}$  and the  $4 \mu_B$  of  $\text{Co}_2\text{MnAl}$ . In the case of the  $\text{Co}_2[\text{Cr}_{1-x}\text{Fe}_x]\text{Al}$  and  $\text{Co}_2[\text{Mn}_{1-x}\text{Fe}_x]\text{Al}$  compounds and up to around  $x = 0.6$  the total spin moment shows the SP behaviour but for larger concentrations it slightly deviates to account for the non-integer value of  $\text{Co}_2\text{FeAl}$  [11]. This behaviour can also be found in the DOSs (see figure 2). As the concentration of Fe increases the Fermi level moves lower in energy with respect to the energy position of the gap and for  $x = 0.6$  it is just below the gap and half-metallicity is lost (note that  $\text{Co}_2\text{FeAl}$  is not half-metallic). The second case is when one mixes the sp elements as in  $\text{Co}_2\text{Mn}[\text{Al}_{1-x}\text{Sn}_x]$ ; these compounds also obey the rule for the total spin moments. The third and final case is to mix the higher-valent transition metal atoms as in  $[\text{Fe}_{1-x}\text{Co}_x]_2\text{MnAl}$  and  $[\text{Rh}_{1-x}\text{Co}_x]_2\text{MnAl}$  alloys. In the first case the total spin moment varies linearly between the  $2$  and  $4 \mu_B$  of  $\text{Fe}_2\text{MnAl}$  and

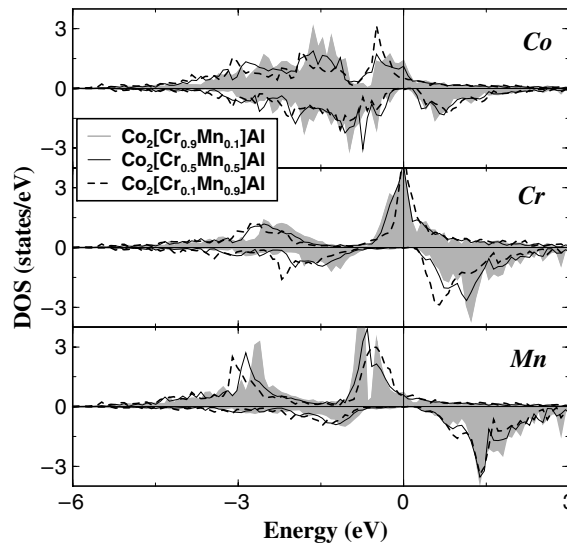


**Figure 2.** Total DOS of  $\text{Co}_2[\text{Cr}_{1-x}\text{Fe}_x]\text{Al}$  and  $\text{Co}_2[\text{Mn}_{1-x}\text{Fe}_x]\text{Al}$  compounds for three different values of the concentration  $x$ : 0.4, 0.6, 0.8. For  $x = 0.6$  half-metallicity is lost since the Fermi level is slightly under the minority gap.

$\text{Co}_2\text{MnAl}$  compounds, respectively. Rh is isoelectronic to Co and for the second family of compounds I find a constant integer value of  $4 \mu_B$  for all the concentrations. A special case is  $\text{Mn}_2\text{VAl}$  which has 22 electrons and the total spin moment is  $-2 \mu_B$ , while  $\text{Co}_2\text{VAl}$  with 26 valence electrons has a total spin moment of  $2 \mu_B$ . If now I mix Mn and Co I get a family of compounds where the total spin moment varies linearly between  $-2 \mu_B$  and  $2 \mu_B$ . For  $x = 0.5$  there are on average 24 electrons per unit cell and from the SP rule  $[\text{Mn}_{0.5}\text{Co}_{0.5}]_2\text{VAl}$  should have a zero total spin moment, which is verified by my *ab initio* results in figure 1. Thus all the compounds obey the rule  $M_t = Z_t - 24$ , showing the Slater–Pauling behaviour regardless of the origin of the extra charge. In the next paragraphs I will analyse every case in detail.

### 3.1. $X_2(Y_{1-x}Y_x^*)Z$ compounds

The first large family of quaternary alloys which are susceptible to being HMs are the ones where there are two kinds, Y and  $Y^*$ , of low-valent transition metal atom:  $X_2(Y_{1-x}Y_x^*)Z$ , where X stands for the high-valent transition metal atom and Z for the sp atom. I will concentrate my analysis on  $\text{Co}_2[\text{Cr}_{1-x}\text{Mn}_x]\text{Al}$ . Already in [11] it has been shown that both  $\text{Co}_2\text{CrAl}$  and  $\text{Co}_2\text{MnAl}$  are HMs with a total spin moment of  $3 \mu_B$  and  $4 \mu_B$ , respectively. In figure 3, I present the atom-projected DOS and in table 1 the spin moments scaled to one atom for several concentrations. For all concentrations, one gets an HM system since the Fermi level falls within the minority gap. The width of the gap is the same for all compounds since the gap is formed between states located exclusively at the Co sites and which are little affected by the lower-valent transition metal atoms such as Mn and Cr [11]. This is clearly seen in figure 3 where the gap in the case of the Cr and Mn atoms is much larger than for the Co atoms. The total spin moment scales linearly between the two extremes, reflecting the half-metallicity. For low Mn concentrations, the Mn atom acts like an impurity and the  $e_g$  and  $t_{2g}$  electrons are well separated. This is clearly seen in the Mn DOS, where for small Mn concentration there is a double peak in the majority band just below the Fermi level. The lower peak is the  $e_g$  electrons and the higher peak the  $t_{2g}$  electrons of Mn. When the Mn concentration increases these states overlap and cannot be distinguished any longer and Mn shows a more itinerant-like magnetism. The states lower in energy around  $-3$  eV are  $t_{2g}$ -like states which couple to the



**Figure 3.** Atom-projected DOS of  $\text{Co}_2[\text{Cr}_{1-x}\text{Mn}_x]\text{Al}$  for three different values of the concentration  $x$ : 0.1, 0.5, 0.9. The DOSs have been scaled to one atom.

**Table 1.** Spin moments for  $\text{Co}_2[\text{Cr}_{1-x}\text{Mn}_x]\text{Al}$  with  $x = 0, 0.1, 0.2, \dots, 0.9, 1$ . The spin moments have been scaled to one atom. The total moment is given by the relation  $m^{\text{total}} = 2m^{\text{Co}} + (1-x)m^{\text{Cr}} + xm^{\text{Mn}} + m^{\text{Al}} + m^{\text{int}}$ , where int stands for the interstitial region.

$\text{Co}_2[\text{Cr}_{1-x}\text{Mn}_x]\text{Al}$	$m^{\text{Co}}$	$m^{\text{Cr}}$	$m^{\text{Mn}}$	$m^{\text{Al}}$	$m^{\text{total}}$
$\text{Co}_2\text{CrAl}$	0.698	1.686	—	-0.060	3.007
$\text{Co}_2[\text{Cr}_{0.9}\text{Mn}_{0.1}]\text{Al}$	0.709	1.615	3.116	-0.060	3.106
$\text{Co}_2[\text{Cr}_{0.8}\text{Mn}_{0.2}]\text{Al}$	0.718	1.547	3.068	-0.061	3.206
$\text{Co}_2[\text{Cr}_{0.7}\text{Mn}_{0.3}]\text{Al}$	0.722	1.483	3.020	-0.061	3.305
$\text{Co}_2[\text{Cr}_{0.6}\text{Mn}_{0.4}]\text{Al}$	0.726	1.416	2.971	-0.061	3.405
$\text{Co}_2[\text{Cr}_{0.5}\text{Mn}_{0.5}]\text{Al}$	0.731	1.342	2.920	-0.062	3.505
$\text{Co}_2[\text{Cr}_{0.4}\text{Mn}_{0.6}]\text{Al}$	0.729	1.317	2.864	-0.063	3.605
$\text{Co}_2[\text{Cr}_{0.3}\text{Mn}_{0.7}]\text{Al}$	0.738	1.220	2.806	-0.063	3.706
$\text{Co}_2[\text{Cr}_{0.2}\text{Mn}_{0.8}]\text{Al}$	0.746	1.093	2.744	-0.064	3.806
$\text{Co}_2[\text{Cr}_{0.1}\text{Mn}_{0.9}]\text{Al}$	0.752	0.834	2.682	-0.064	3.907
$\text{Co}_2\text{MnAl}$	0.755	—	2.603	-0.064	4.020

p states of Al and fill the bands created by the latter. In the case of Cr the behaviour is the inverse. This is for the case of high Cr concentrations, where the  $e_g$  and  $t_{2g}$  are distinguished. For low Cr concentrations the population of the occupied minority states is larger and they are lower in energy than for high concentrations, also attracting the unoccupied states lower in energy and resulting in a smaller spin moment. The differences in the Co DOS mainly arise from the different positions of the Cr and Mn majority bands through the Coulomb interaction, and the Co spin moment only changes slightly with the concentration. Finally, in the case of  $\text{Co}_2[\text{Cr}_{1-x}\text{Fe}_x]\text{Al}$  and  $\text{Co}_2[\text{Mn}_{1-x}\text{Fe}_x]\text{Al}$  compounds the situation is similar but the Co moments show more important changes since Fe cannot account by itself for the extra electron and the Co moment has also to reach a higher value. This was discussed in detail in [11].

### 3.2. $X_2Y[Z_{1-x}Z_x^*]$ compounds

Now I will go on with the case of the  $X_2Y[Z_{1-x}Z_x^*]$  compounds, where I change the charge at the Z site. I studied both  $\text{Co}_2\text{Mn}[\text{Al}_{1-x}\text{Si}_x]$  and  $\text{Co}_2\text{Mn}[\text{Al}_{1-x}\text{Sn}_x]$ . Si and Sn are isoelectronic

**Table 2.** The same as table 1 for the  $\text{Co}_2\text{Mn}[\text{Al}_{1-x}\text{Sn}_x]$  compounds.

$\text{Co}_2\text{Mn}[\text{Al}_{1-x}\text{Sn}_x]$	$m^{\text{Co}}$	$m^{\text{Mn}}$	$m^{\text{Al}}$	$m^{\text{Sn}}$	$m^{\text{Total}}$
$\text{Co}_2\text{MnAl}$	0.755	2.603	-0.064	—	4.020
$\text{Co}_2\text{Mn}[\text{Al}_{0.9}\text{Sn}_{0.1}]$	0.766	2.673	-0.065	-0.047	4.113
$\text{Co}_2\text{Mn}[\text{Al}_{0.8}\text{Sn}_{0.2}]$	0.789	2.744	-0.067	-0.048	4.223
$\text{Co}_2\text{Mn}[\text{Al}_{0.7}\text{Sn}_{0.3}]$	0.800	2.821	-0.068	-0.049	4.324
$\text{Co}_2\text{Mn}[\text{Al}_{0.6}\text{Sn}_{0.4}]$	0.820	2.889	-0.069	-0.050	4.434
$\text{Co}_2\text{Mn}[\text{Al}_{0.5}\text{Sn}_{0.5}]$	0.841	2.951	-0.069	-0.051	4.541
$\text{Co}_2\text{Mn}[\text{Al}_{0.4}\text{Sn}_{0.6}]$	0.863	3.010	-0.070	-0.051	4.644
$\text{Co}_2\text{Mn}[\text{Al}_{0.3}\text{Sn}_{0.7}]$	0.882	3.069	-0.070	-0.052	4.743
$\text{Co}_2\text{Mn}[\text{Al}_{0.2}\text{Sn}_{0.8}]$	0.902	3.125	-0.070	-0.052	4.843
$\text{Co}_2\text{Mn}[\text{Al}_{0.1}\text{Sn}_{0.9}]$	0.925	3.180	-0.071	-0.052	4.946
$\text{Co}_2\text{MnSn}$	0.944	3.235	—	-0.052	5.043

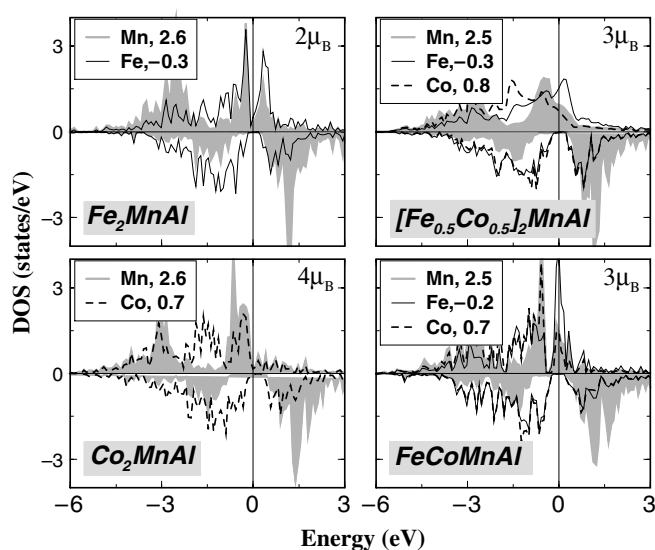
and both families present the same behaviour, thus I will restrict my presentation to the second family. The moment changes from 4 up to 5  $\mu_{\text{B}}$  linearly and thus all the intermediate cases are HMs. In table 2, I have gathered the atom-resolved spin moments. The sp atoms show a practically constant moment and the extra charge is taken into account by the transition metal atoms. If I look carefully at the Mn majority spin band (not presented here), there are unoccupied states at the vicinity of the Fermi level which pass under the Fermi level and become occupied as the concentration of Sn increases. Thus the Mn spin moment increases practically linearly from 2.6 to 3.2  $\mu_{\text{B}}$ . The higher polarization of the Mn d states also polarizes the Co bands since they form a common majority band and the Co moment increases by 0.2  $\mu_{\text{B}}$ .

### 3.3. $[\text{X}_{1-x}\text{X}_x]_2\text{YZ}$ compounds

The last case, which will be discussed in this section, is the one when the high-valent transition metal atoms are mixed. The first family is the  $[\text{Fe}_{1-x}\text{Co}_x]_2\text{MnAl}$ , where the total spin moment increases from 2 to 4  $\mu_{\text{B}}$  with the concentration. The Al moment stays small and is negligible while the Mn moment is 2.6  $\mu_{\text{B}}$  for all concentrations. The Fe moment varies from -0.32 to -0.26  $\mu_{\text{B}}$  and the Co one from 0.63 to 0.75  $\mu_{\text{B}}$ . Thus the atomic spin moments change little and the increase in the total spin moment arises exclusively from the substitution of Fe by Co. It is also interesting to compare  $[\text{Fe}_{0.5}\text{Co}_{0.5}]_2\text{MnAl}$  with  $\text{FeCoMnAl}$ . In the latter compound one of the sublattices is occupied exclusively by Fe atoms and the other sublattice by Co atoms. Both systems are HMs as can be seen in figure 4 and the total spin moment is 3  $\mu_{\text{B}}$ . Both compounds show similar atomic spin moments, thus the exact position of the Fe and Co atoms is not so relevant for the magnetic properties, which are controlled mainly by the concentration of the chemical elements. If I compare the DOSs presented in figure 4, I see that the atom-projected ones have the same characteristics although the ones for  $\text{FeCoMnAl}$  are more spiky. The main difference is a small majority gap just below the Fermi level in  $\text{FeCoMnAl}$  which is washed out for  $[\text{Fe}_{0.5}\text{Co}_{0.5}]_2\text{MnAl}$ . This gap is the signature of the order.

The second family of compounds is  $[\text{Rh}_{1-x}\text{Co}_x]_2\text{MnAl}$ . Rh and Co are isoelectronic elements and the total spin moment is 4  $\mu_{\text{B}}$  for all concentrations. Also  $\text{RhCoMnAl}$  is an HM with magnetic properties similar to  $[\text{Rh}_{0.5}\text{Co}_{0.5}]_2\text{MnAl}$  as was the case for the compounds containing Fe. Since the Rh moment is much smaller than the Co one, the Mn moment has to increase considerably, from 2.6 to 3.4  $\mu_{\text{B}}$ , with the increase of Rh concentration to keep the total spin moment constant.

A special case under study is the  $[\text{Mn}_{1-x}\text{Co}_x]_2\text{VAl}$  family. For these compounds the spin moment changes from -2 to 2  $\mu_{\text{B}}$  with the concentration  $x$ . As shown in [11] the Mn and V atoms in  $\text{Mn}_2\text{VAl}$  are antiferromagnetically coupled and V carries a large spin moment, while



**Figure 4.** Atom-projected DOS in the case where both X sites are occupied by Co and Fe with 50% probability (the system is denoted by  $[\text{Fe}_{0.5}\text{Co}_{0.5}]_2\text{MnAl}$ ) and when one sublattice is occupied exclusively by Fe and the other by Co atoms (the system is denoted by  $\text{FeCoMnAl}$ ). All compounds are half-metals. The numbers in the legends are the atomic spin moments in  $\mu_B$  and the larger ones are the total spin moments.

in  $\text{Co}_2\text{VAl}$  the Co and V atoms are ferromagnetically coupled and the moment is mainly carried by the Co atoms. For  $x = 0.5$  there is the case of a compound with zero total spin moment but with magnetic constituents:  $m^{\text{Mn}} = -0.47 \mu_B$ ,  $m^{\text{Co}} = 0.20 \mu_B$  and  $m^{\text{V}} = 0.23 \mu_B$ . It seems that for this compound it is energetically more favourable to have magnetic constituents than the case of zero atomic spin moments. The Mn spin moment decreases from  $-1.45 \mu_B$  to  $-0.35$  with the concentration  $x$  while the Co spin moment increases from 0.2 to  $0.95 \mu_B$  and the V one decreases from 0.8 to  $0.16 \mu_B$ .

#### 4. Summary and conclusions

In this contribution I expanded the study already performed for the ordered Heusler alloys to also cover the quaternary Heusler compounds such as  $\text{Co}_2[\text{Cr}_{1-x}\text{Mn}_x]\text{Al}$ ,  $\text{Co}_2\text{Mn}[\text{Al}_{1-x}\text{Sn}_x]$  and  $[\text{Fe}_{1-x}\text{Co}_x]_2\text{MnAl}$ . Using the Korringa–Kohn–Rostoker method in the coherent potential approximation I have shown that, independently from which site is disordered, all compounds are half-metals and the total spin moment  $M_t$  scales linearly with the total number of valence electrons  $Z_t$  following the rule  $M_t = Z_t - 24$ , thus  $M_t$  also scales linearly with the concentration  $x$ . Depending on the family under study the atomic spin moments change in such a way that the above rule, known also as the Slater–Pauling behaviour, is obeyed. Finally, an interesting case is  $[\text{Mn}_{1-x}\text{Co}_x]_2\text{VAl}$ , where the moment scales linearly from  $-2 \mu_B$  to  $2 \mu_B$  and for  $x = 0.5$  the total spin moment vanishes but the constituents are magnetic. These results are of particular interest to experimentalists searching for new half-metallic materials for spintronic devices.

#### Acknowledgment

Financial support from the RT Network of Computational Magnetoelectronics (contract RTN1-1999-00145) of the European Commission is gratefully acknowledged.



*Note added in proof.* After acceptance I became aware of a paper by Y Miura and collaborators [18] in which they study the  $\text{Co}_2[\text{Cr}_{1-x}\text{Fe}_x]\text{Al}$  compounds also using a KKR-CPA code.

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