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Citation: *J. Appl. Phys.* **109**, 113912 (2011); doi: 10.1063/1.3592168

View online: <http://dx.doi.org/10.1063/1.3592168>

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Stability of ferromagnetism against doping in half-metallic alloys

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(Received 7 February 2011; accepted 12 April 2011; published online 7 June 2011)

We use a rigid band model to simulate doping in half-metallic NiMnSb and CoMnSb semi-Heusler alloys. Using first-principles calculations we calculate the intrasublattice exchange constants and the Curie temperature for these alloys as a function of the shift of the Fermi level and compare them also with the case of half-metallic CrAs and CrSe zinc-blende alloys. We show for all four compounds that the interactions between Cr-Cr(Mn-Mn) nearest neighbors are sufficient to explain the behavior of the Curie temperature. The interplay between the ferromagnetic RKKY-like and the antiferromagnetic superexchange interactions depends strongly on the details of the density of states around the minority-spin gap and thus it is found to be alloy-dependent. © 2011 American Institute of Physics. [doi:10.1063/1.3592168]

I. INTRODUCTION

Half-metallic ferromagnets are a special class of materials since they present metallic behavior for the majority-spin electrons while the minority-spin band exhibits a gap and thus a semiconducting character.¹ Due to this unique characteristic they have attracted a lot of attention due to their potential application in spintronic devices,²⁻⁴ e.g., in principle when employed in spin-valves they can exhibit an extremely high magnetoresistance ratio. Among these materials, Heusler compounds play a key role since they are intermetallic alloys with very high Curie temperatures approaching 1000 K and structure similar to the zinc-blende binary semiconductors.⁵ The prototype Heusler alloy is NiMnSb which crystallizes in the $C1_b$ structure (these alloys are called in the literature semi- or half-Heuslers). The latter consists of four interpenetrating fcc sublattices where the first one is occupied by Ni atoms, the second by Mn atoms, the third is empty and the fourth by Sb atoms⁵ (for the structure, see Fig. 1 in Ref. 6). The zinc-blende structure can be also described as consisting of four fcc sublattices, where the first two are occupied by the two chemical species of the binary semiconductor and the next two are empty. Moreover, NiMnSb was the first alloy where half-metallicity was predicted by de Groot and collaborators in 1983 using first-principles calculations.¹ Experimentally, the half-metallicity seems to be well-established in the case of single crystals.^{7,8} The origin of half-metallicity was elucidated in 2002 thanks to the work of Galanakis *et al.* who have shown that the minority-spin gap is created between the occupied bonding Ni-d - Mn-d hybrid orbitals and the empty antibonding ones while the role of Sb is to provide bands deep in energy accommodating part of the d-charge of the 3d transition metal atoms.⁶ As a result of the origin of the gap, the total spin magnetic moment exhibits a Slater-Pauling-like behavior.⁶

Although several calculations have confirmed the half-metallic character of NiMnSb (for a review, see Refs. 9 and 10), the stability of ferromagnetism has attracted much less attention. Şaşıoğlu and collaborators have calculated the exchange constants using a classical Heisenberg model and have shown that in half-metallic alloys like NiMnSb and CoMnSb the dominating interaction is the one between Mn atoms.¹¹ The latter one is indirect since Mn atoms are separated by large distance with respect to the nearest-neighbors distance and as shown in Ref. 12 can be separated in two contributions: (i) a ferromagnetic Ruderman-Kittel-Kasuya-Yoshida (RKKY)-type one due to the induced negative polarization of the s and p conduction electrons, and (ii) a superexchange antiferromagnetic interaction. The latter one corresponds to the excitations of the electrons occupying local orbitals toward unoccupied states and depends strongly on the unoccupied orbitals just above the Fermi level. In NiMnSb and CoMnSb the RKKY ferromagnetic interaction is the dominating one with respect to the superexchange one. The direct Ni(Co)-Mn nearest neighbors interaction contributes also to the ferromagnetic order but since each Mn atom has only 4 nearest-neighboring Ni(Co) atoms and 12 Mn ones, the Mn-Mn RKKY interaction is the dominant one and Ni(Co)-Mn direct exchange accounts by less than 10% of the Curie temperature.¹¹

II. MOTIVATION AND COMPUTATIONAL DETAILS

Recently, first-principles calculations have confirmed experimental findings¹³ that in both NiMnSb and CoMnSb the doping of the Ni(Co) by Cu atoms leads to a transition from a ferromagnetic to an antiferromagnetic state.^{14,15} The same phenomenon has been found to occur also in AuMnSn Heusler alloy when the Sn site is doped with Sb which has one valence electron more.^{16,17} The common feature of these transitions is that doping either the 3d or the sp site results in a shift of the bands as in a rigid band model (see Fig. 2 in Ref. 14 and Fig. 2 in Ref. 17). The Fermi level shifts higher

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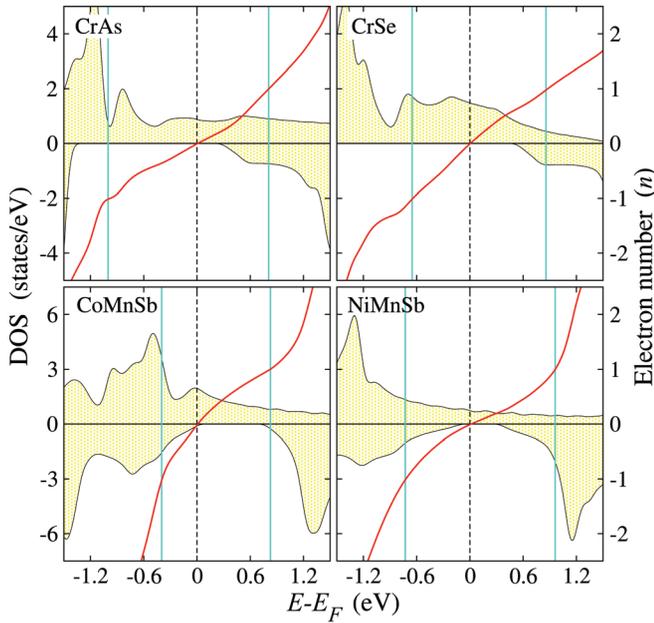


FIG. 1. (Color online) Calculated total density of states (DOS) and electron number counted from the Fermi level. Positive values of the DOS correspond to the majority (spin-up) electrons and negative values to the minority (spin-down) electrons. The zero of the energy has been chosen as the Fermi energy. The light vertical lines denote the position of the Fermi level with one electron added or removed.

in energy without disturbing the shape of the density of states (DOS) and the extra charge is accommodated in the states between the old and new position of the Fermi level. This behavior is also present if we substitute Sb atom in NiMnSb with another sp atom (see Fig. 7 in Ref. 6) Thus, if we shift the Fermi level in a rigid band model we can safely assume that we model the effect of doping at either the site occupied by the high-valent 3d transition metal atom (Ni in NiMnSb) or the sp atom (Sb in NiMnSb). Doping is very usual in Heusler compounds and several experimental data exist.^{5,18} The aim of the present report is to investigate using NiMnSb and CoMnSb as prototypes how this shift of the Fermi level influences the stability of ferromagnetism in these alloys and when does the antiferromagnetic superexchange interaction overcomes the ferromagnetic indirect RKKY one. These results are crucial for applications in devices since for the later ones, one would like ferromagnetism to be stable against small percentage of doping which can occur during growth of the alloys.

We compare our results on NiMnSb and CoMnSb compounds with results obtained for CrAs and CrSe in the zinc-blende structure which have been also shown to be half-metallic ferromagnets^{19,20} (for a review of these systems, see Ref. 21). CrAs has been fabricated by Akinaga and collaborators in 2000 in the form of very thin multilayers with GaAs and was argued to crystallize in the zinc-blende structure,²² although evidence exists both experimentally²³ and theoretically²⁴ against this structure. The reason why we have chosen CrAs and CrSe is that they present large width of the bandgap and comparable total spin magnetic moments to the two semi-Heusler compounds under investigation. To study the different exchange interactions we follow the same methodology as in Ref. 11. We use the augmented spherical waves ab-initio

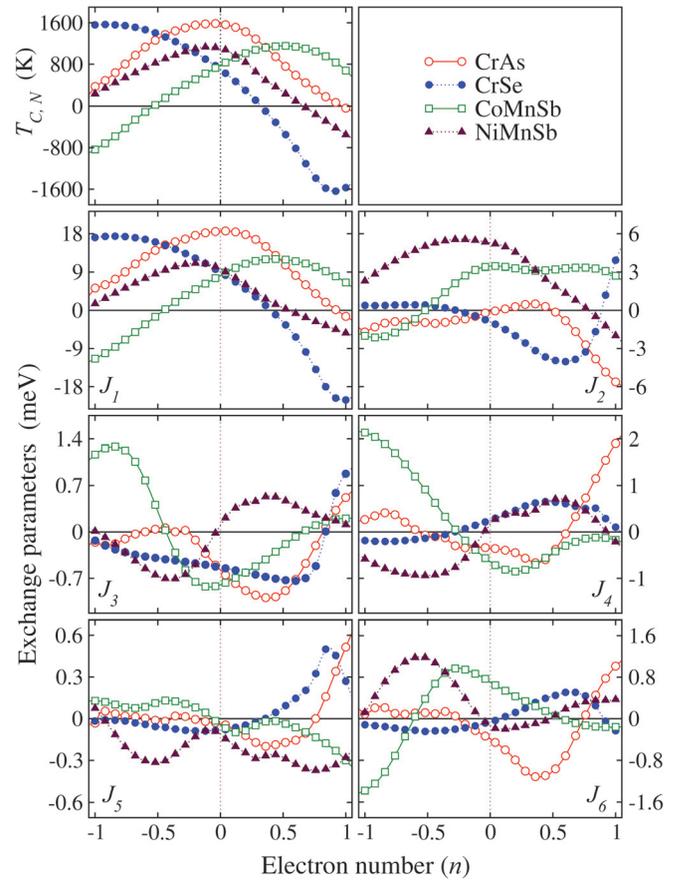


FIG. 2. (Color online) Curie temperature in the mean-field approximation (negative values mean an antiferromagnet) and first six nearest Cr-Cr(Mn-Mn) neighborhood exchange parameters as a function of electron number. Zero corresponds to the perfect undoped compounds. Note the different scaling of the vertical axis.

method²⁵ within the atomic-sphere approximation²⁶ to calculate the electronic structure in the ferromagnetic state. The exchange-correlation potential is chosen in the generalized gradient approximation.²⁷ A dense Brillouin zone sampling $30 \times 30 \times 30$ is used. The radii of all atomic spheres are chosen equal and we consider empty spheres to account for the unoccupied sites in both $C1_b$ and zinc-blende structures. We employ the frozen-magnon approach to calculate interatomic intrasublattice Heisenberg exchange parameters and then these are used to calculate the Curie temperature in the mean-field approximation as discussed in Ref. 11. Calculations have been performed for the experimental lattice constants of NiMnSb (5.93Å) and CoMnSb (5.87Å)⁵ while for CrAs and CrSe we used the experimental lattice parameters of GaAs (5.65 Å) and CdS (5.82 Å), respectively.

III. RESULTS AND DISCUSSION

In Table I we have gathered the calculated spin-magnetic moments for NiMnSb and CoMnSb Heusler alloys together with the spin-moments of the CrAs and CrSe zinc-blende alloys. For the two Heusler compounds the total spin magnetic moment follows as expected the Slater-Pauling behavior being in μ_B the total number of valence electrons in the unit cell minus 18.⁶ The magnetism stems mainly from the Mn atoms while Ni(Co) atoms present small values of their magnetic

TABLE I. Lattice constants, atom-resolved and total spin magnetic moments (in μ_B), and width of the half-metallic gap (Δ) for CrAs, CrSe, CoMnSb, and NiMnSb. For CrAs and CrSe, we have used the experimental lattice constants of the zinc-blende GaAs and CdS semiconductors, respectively, while for CoMnSb and NiMnSb, their own experimental lattice constants (Ref. 5).

	CrAs	CrSe	CoMnSb	NiMnSb
$a(\text{\AA})$	5.65 [GaAs]	5.82 [CdS]	5.87	5.93
$m_{[Cr,Mn]}$	3.24	3.92	3.41	3.85
$m_{[Co,Ni]}$			-0.32	0.20
$m_{[As,Se,Sb]}$	-0.31	-0.10	-0.11	-0.09
$m_{[Total]}$	3.00	4.00	3.00	4.00
Δ (eV)	1.68	3.38	0.78	0.47

moments. Thus, as shown in Ref. 11, taking into consideration also the small number of Ni(Co)-Mn nearest-neighbors, the Ni(Co)-Mn direct exchange interactions account only 5–10% of the calculated Curie temperature and can be neglected when compared to the Mn-Mn nearest-neighbors interactions. In the case of CrAs and CrSe, the total spin magnetic moment follows again a Slater-Pauling-like behavior for the zinc-blende transition-metal chalcogenides and pnictides being in μ_B the total number of valence electrons in the unit cell minus 8.¹⁹ CrAs has a total spin moment of 3 μ_B same as CoMnSb and CrSe a total spin moment of 4 μ_B same as NiMnSb. Magnetism is located almost exclusively at the Cr atoms and As(Se) atoms show a small induced negative spin magnetic moment. Note that the sum of the atom-resolved spin moments is not equal to the total spin magnetic moment in the cell since we do not present the spin moments associated to the empty spheres. These features have been already shown in several calculations,²¹ thus, we will concentrate on the gap properties. Zinc-blende CrAs and CrSe present minority-spin gaps with very large width with respect to the Heusler alloys. CrAs presents a gap width of 1.68 eV and CrSe of 3.38 eV, while for NiMnSb and CoMnSb the gap width is 0.47 and 0.78 eV, respectively. In CrAs and CrSe, the gap is created between the occupied minority-spin Cr-d - As(Se)-p bonding hybrid states which have their weight mainly at the As(Se) atom and the unoccupied antibonding Cr-d - As(Se)-p orbitals with their weight mainly on the Cr atom.¹⁹ Thus, the gap is large due to the large exchange splitting between the occupied majority-spin Cr d-states and the unoccupied minority-spin Cr d-states and in the case of CrSe the gap is larger than CrAs due to the larger electronegativity of the Se atom with respect to the As.¹⁹ In the case of the Heusler alloys, the exchange-splitting between the Mn majority-spin d-states and the unoccupied minority-spin Mn d-states is smaller due to the effect of the Co and Ni atoms which have a large fraction of both their majority- and minority-spin states occupied, and the gap is smaller for NiMnSb since we have one valence electron more than CoMnSb occupying exclusively majority-spin states and reducing the exchange-splitting.⁶

In Fig. 1, we present the total density of states (DOS) for all four compounds and we have focused on the gap region. For CrAs and CrSe the Fermi level (defined as the zero of the energy axis) is close to the upper edge of the gap while for CoMnSb and NiMnSb it is exactly at the lower edge of

the gap. We also present in Fig. 1 the electron number counted from the Fermi level. If we use the Fermi energy for the perfect compounds as the starting point and we add electronic charge in a rigid band model, which occurs, e.g., when we dope NiMnSb with Cu at the sites occupied by Ni atoms, the Fermi level shifts to higher energy values and the electron number counted from the initial Fermi level is positive. The opposite occurs when we remove electronic charge; the Fermi level moves to lower energy values and the electron number counted is negative. In the case of CrAs and CrSe, the lines representing the electron numbers counted from the initial Fermi level are almost straight while for CoMnSb and NiMnSb the lines have a much larger gradient. Relevant to the superexchange interaction is the position of the unoccupied minority-spin d-states of Mn(Cr) atoms. Since for CrAs and CrSe the exchange splitting between occupied majority-spin and unoccupied minority-spin states is much stronger than for the two Heusler alloys the unoccupied states for CrAs and CrSe have a broader peak structure with the center of the peak located at higher energy than for the two Heusler compounds. But except the shape and position of the unoccupied minority-spin d-states, we should also discuss the imbalance of the DOS for the two spin directions as we move away from the Fermi level since this is relevant to the strength of the RKKY-interaction due to the coupling between the local d-states and the s and p conduction electrons. In CrAs and CrSe, as we go to lower values of the energy with respect to the Fermi level, we are still within the gap and we have only majority-spin states, but the two compounds show an opposite behavior as we move to higher energies with respect to the Fermi level. CrAs shows an almost constant value of the majority-spin DOS for energy values higher than the Fermi level while for CrSe the majority-spin DOS decays very fast. In the case of the Heusler alloys the Fermi level for the perfect compounds is located at the left edge of the gap, and when we subtract electronic charge and move to lower energies we enter immediately the area where minority-spin DOS exhibits large values with respect to the majority-spin one. When we move toward higher energies CoMnSb presents larger values of the majority-spin DOS with respect to NiMnSb.

In Fig. 2, we present the calculated Curie temperature, T_C , in the mean-field approximation and the exchange parameters for the intrasublattice Cr-Cr(Mn-Mn) interactions going up to the sixth neighbors as a function of the electron number. Note that negative values of T_C correspond to the antiferromagnetic alignment of the spin moments and do not have a physical meaning.¹² The zero of the electron number means the perfect undoped compounds while positive values correspond to doping increasing the number of valence electrons and negative values correspond to doping resulting in a reduction of the number of valence electrons. Since the scope of the present report is not the discussion of the T_C values already presented in Refs. 11 and 20 for the perfect compounds, we will concentrate our discussion on the behavior of the exchange constants and their relation to the behavior of the T_C . The number of neighbors changes with the coordination sphere; each Cr(Mn) atom has 12 Cr(Mn) atoms as nearest neighbors in the first coordination sphere, 6 Cr(Mn)

atoms as next-nearest neighbors in the second coordination sphere, 24 in the third sphere, 12 in the fourth, 24 in the fifth, and finally 8 in the sixth coordination sphere. But the strength of the exchange constants as shown from the different scaling of the vertical axis decays fast with the coordination number. As a result, the lines connecting the calculated T_C values as a function of the electron number follow exactly the behavior of the lines for the calculated exchange constants between nearest Cr-Cr(Mn-Mn) neighbors, J_1 . The other exchange constants although present more complex behavior are not relevant for our discussion. Also, as we discussed above for the Heusler compounds the direct Co(Ni)-Mn ferromagnetic interaction can be neglected with respect to the indirect Mn-Mn interactions.¹¹

Let us now discuss the behavior of each alloy separately. In CrAs, ferromagnetism is always stable, but as we move away from the Fermi level, the strength of the ferromagnetic order is weakening, and when we reduce or increase the electronic charge by one electron, the ferromagnetic and antiferromagnetic interaction annihilate each other. When moving toward higher energy values, the superexchange interaction becomes important since we approach the unoccupied minority-spin Cr d-states, while when moving toward lower values of the energy, the ferromagnetic RKKY interaction becomes less important since the population of the p-states, mainly responsible for the coupling of the conduction electrons to the local d-states, decreases. In CrSe, the gap is much larger in width than CrAs, and the extra electron occupies mainly p-like states. Thus, as we move to lower energy values, the ferromagnetic RKKY interaction is further enhanced, but when we move to higher energies the available p-states are less than for CrAs, and antiferromagnetism dominates for more than about 0.3 extra electron. For CoMnSb, as we add charge up to one electron, the Fermi level does not cross the minority-spin unoccupied states and the ferromagnetism remains stable while as we move to lower, than the Fermi level for the perfect compound, energy values at some point, the population of the minority-spin states is such that antiferromagnetism is stabilized. In NiMnSb, the gap is much smaller in width than CoMnSb. Thus, as we add electronic charge for a value of about 0.5, we cross the minority-spin d-states, and superexchange antiferromagnetic interaction dominates while when we subtract electronic charge up to one electron, the RKKY interaction is still overcoming the superexchange one. These results explain also why upon Cu doping NiMnSb shows a transition to antiferromagnetism for a smaller value of Cu concentration than CoMnSb.^{13,14} Note that Cu has one more valence electron than Ni and two than Co and thus corresponds to positive electron numbers in Fig. 2.

Before concluding, we should also discuss the effect of the chosen approximation to the exchange-correlation functional on our results. In our work, we have used the Generalized Gradient Approximation (GGA) functional²⁷ which takes into account also the gradient of the charge density contrary to Local Density Approximation (LDA).²⁸ GGA is well known to perform well for metallic systems but with respect to usual ferromagnets the compounds under study in this paper have the peculiarity of presenting an energy gap in the minority-spin band. In the case of semiconductors, both

LDA and GGA strongly underestimate the gap, and it was shown that the use of hybrid functionals can improve the obtained energy gaps. For example, in Ref. 29, the Heyd-Scuseria-Ernzerhof (HSE)³⁰ hybrid functional was used to study the Mn impurities in GaN, and it was shown that HSE predicts an energy gap much larger than the LDA and GGA ones in agreement with experiments. Moreover, it was also shown in Ref. 29, concerning the Mn impurities, that HSE describes in a more accurate way the localized character of the Mn d-states. These results cannot be simply extrapolated to compounds like NiMnSb, CoMnSb, CrAs, and CrSe, since (i) contrary to Mn impurities the d-states of transition-metal atoms in these alloys are not so localized presenting strong hybridization with the d- and p-states of the surrounding atoms⁶, and (ii) they are metallic and not semiconducting and thus the energy gap in the minority-spin band is determined by the exchange-splitting between the occupied majority-spin d-states of Mn(Cr) and the unoccupied minority-spin d-states of these atoms.^{6,19} Thus, GGA is expected to give a good estimation of the width of the gap and this is confirmed for NiMnSb where the theoretical gap in our calculations is about 0.47 eV in perfect agreement with the experimental findings of Kirillova *et al.*⁷ The suitability of GGA to study the gap-related properties of the alloys under study in this paper is further enhanced by the theoretical results presented by Guo and Liu.³¹ Authors have used the hybrid modified Becke-Johnson exchange³² plus LDA correlation potential (mBJLDA) to study the properties of half-metallic pnictides and chalcogenides in the zinc-blende structure. The mBJLDA functional has been proved to produce accurate gaps for wide-band semiconductors, *sp* semiconductors and 3d transition-metal oxides.³³ Guo and Liu found that the mBJLDA functional leads to a lower energy position of the occupied p-states and a shift of the unoccupied e_g states to higher energy values with respect to the GGA results. The broad t_{2g} d-states of the transition metal atoms were not affected by the use of mBJLDA instead of GGA. p-states do not affect the gap while the shift of the unoccupied e_g states leads to an increase of the minority-spin gap by about 20% with respect to the GGA results and not to a gap 2 or 3 times larger as in semiconductors.²⁹ This larger gap had in practice effect only in the case of MnAs where the Fermi level was within the conduction minority-spin band while for CrAs and CrSe studied also here the picture of their electronic and magnetic properties was almost unaltered. We believe that for NiMnSb and CoMnSb, the effect would be even smaller since the gap is considerably smaller with respect to CrAs and CrSe and as shown in the band-structure presented in Fig. 1 in Ref. 34 and discussed in Ref. 6 the minority-spin gap is created between the occupied t_{2g} and the unoccupied e_g states but the latter ones strongly overlap with the unoccupied t_{2g} states. Thus the shift of the e_g states caused by the use of the mBJLDA functional should only marginally affect the width of the gap.

IV. SUMMARY

Since doping in the half-metallic semi-Heusler compounds can be simulated from the shift of the Fermi level in

a rigid band model, we have used NiMnSb and CoMnSb as prototypes and have calculated how the Curie temperature and the exchange constants vary when we shift the Fermi level with respect to the perfect alloys. We also compare our results to the case of CrAs and CrSe alloys in the zinc-blende lattice structure. In all four compounds, the interactions between Cr-Cr(Mn-Mn) nearest neighbors are sufficient to explain the behavior of the Curie temperature. We have shown that there are two competing interactions: (i) a ferromagnetic RKKY-like one and (ii) an antiferromagnetic superexchange one. As we move away from the Fermi level of the perfect compounds, the details of the density of states around the gap play a decisive role on the interplay between these two magnetic interactions and behavior is different for each compound under study. Our results explain why antiferromagnetism appears in NiMnSb for a larger degree of Cu-doping with respect to CoMnSb, observed both experimentally (Ref. 13) and theoretically (Ref. 14).

Fruitful discussions with L. M. Sandratskii are gratefully acknowledged.

¹R. A. de Groot, F. M. Mueller, P. G. van Engen, and K. H. J. Buschow, *Phys. Rev. Lett.* **50**, 2024 (1983).

²H. Zabel, *Materials Today* **9**, 42 (2006).

³I. Zutić, J. Fabian, and S. Das Sarma, *Rev. Mod. Phys.* **76**, 323 (2004).

⁴C. Felser, G. H. Fecher, and B. Balke, *Angew. Chem. Int. Ed.* **46**, 668 (2007).

⁵P. J. Webster and K. R. A. Ziebeck, in *Alloys and Compounds of d-Elements with Main Group Elements. Part 2*, edited by H. R. J. Wijn, Landolt-Boörnstein, New Series, Group III, Vol. 19, Pt.c (Springer-Verlag, Berlin, 1988), pp. 75–184.

⁶I. Galanakis, P. H. Dederichs, and N. Papanikolaou, *Phys. Rev. B* **66**, 134428 (2002).

⁷M. N. Kirillova, A. A. Makhnev, E. I. Shreder, V. P. Dyakina, and N. B. Gorina, *Phys. Stat. Sol. (b)* **187**, 231 (1995).

⁸K. E. H. M. Hanssen and P. E. Mijnders, *Phys. Rev. B* **34**, 5009 (1986); K. E. H. M. Hanssen, P. E. Mijnders, L. P. L. M. Rabou, and K. H. J. Buschow, *ibid.* **42**, 1533 (1990).

⁹I. Galanakis, Ph. Mavropoulos, and P. H. Dederichs, *J. Phys. D: Appl. Phys.* **39**, 765 (2006); I. Galanakis and Ph. Mavropoulos, *J. Phys.: Condens. Matter* **19**, 315213 (2007).

¹⁰M. I. Katsnelson, V. Yu. Irkhin, L. Chioncel, A.I. Lichtenstein, and R. A. de Groot, *Rev. Mod. Phys.* **80**, 315 (2008).

¹¹E. Şaşıoğlu, L. M. Sandratskii, P. Bruno, and I. Galanakis, *Phys. Rev. B* **72**, 184415 (2005).

¹²E. Şaşıoğlu, L. M. Sandratskii, and P. Bruno, *Phys. Rev. B* **77**, 064417 (2008).

¹³N. P. Duong, L. T. Hung, T. D. Hien, N. P. Thuy, N. T. Trung, and E. Brück, *J. Magn. Magn. Mater.* **311**, 605 (2007); S. K. Ren, W. Q. Zou, J. Gao, X. L. Jiang, F. M. Zhang, and Y. W. Du, *ibid.* **288**, 276 (2005).

¹⁴I. Galanakis, E. Şaşıoğlu, and K. Özdoğan, *Phys. Rev. B* **77**, 214417 (2008).

¹⁵J. Kudrnovský, V. Drchal, I. Turek, and P. Weinberger, *Phys. Rev. B* **78**, 054441 (2008).

¹⁶C. Walle, L. Offernes, and A. Kjekshus, *J. Alloys and Comp.* **349**, 105 (2003).

¹⁷K. Özdoğan, E. Şaşıoğlu, and I. Galanakis, *J. Phys. D: Appl. Phys.* **42**, 085003 (2009).

¹⁸K. R. A. Ziebeck and K.-U. Neumann, in *Magnetic Properties of Metals*, edited by H. R. J. Wijn, Landolt-Börnstein, New Series, Group III, Vol. 32/c (Springer, Berlin, 2001), pp. 64–414.

¹⁹I. Galanakis and Ph. Mavropoulos, *Phys. Rev. B* **67**, 104417 (2003).

²⁰E. Şaşıoğlu, I. Galanakis, L. M. Sandratskii, and P. Bruno, *J. Phys.: Condens. Matter* **17**, 3915 (2005).

²¹Ph. Mavropoulos and I. Galanakis, *J. Phys.: Condens. Matter* **19**, 315221 (2007).

²²H. Akinaga, T. Manago, and M. Shirai, *Jpn. J. Appl. Phys.* **39**, L1118 (2000).

²³V. H. Etgens, P. C. de Camargo, M. Eddrief, R. Mattana, J. M. George, and Y. Garreau, *Phys. Rev. Lett.* **92**, 167205 (2004).

²⁴S. J. Hashemifar, P. Kratzer, and M. Scheffler, *Phys. Rev. B* **82**, 214417 (2010).

²⁵A. R. Williams, J. Kler, and C. D. Gelatt, *Phys. Rev. B* **19**, 6094 (1979).

²⁶O. K. Andersen, *Phys. Rev. B* **12**, 3060 (1975).

²⁷J. P. Perdew and Y. Wang, *Phys. Rev. B* **45**, 13244 (1992).

²⁸S. H. Vosko, L. Wilk, and N. Nusair, *Can. J. Phys.* **58**, 1200 (1980).

²⁹A. Stroppa and G. Kresse, *Phys. Rev. N* **79**, 201201(R) (2009).

³⁰J. Heyd, G. E. Scuseria, and M. Ernzerhof, *J. Chem. Phys.* **118**, 8207 (2003); **124**, 219906(E) (2006).

³¹S.-D. Guo and B.-G. Liu, *Europhys. Lett.* **93**, 47006 (2011).

³²A. D. Becke and E. R. Johnson, *J. Chem. Phys.* **124**, 221101 (2006).

³³F. Tran and P. Blaha, *Phys. Rev. Lett.* **102**, 226401 (2009).

³⁴M. Ležaić, I. Galanakis, G. Bihlmayer, and S. Blügel, *J. Phys.: Condens. Matter* **17**, 3121 (2005).