Above-room-temperature ferromagnetism in half-metallic Heusler compounds NiCrP, NiCrSe, NiCrTe and NiVAs: A first–principles study

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We study the interatomic exchange interactions and Curie temperatures in half-metallic semi Heusler compounds NiCrZ (Z=P, Se, Te) and NiVAs. The study is performed within the framework of density functional theory. The calculation of exchange parameters is based on the frozen–magnon approach. It is shown that the exchange interactions in NiCrZ vary strongly depending on the Z constituent. The Curie temperature, \( T_C \), is calculated within the mean field and random phase approximations. The difference between two estimations is related to the properties of the exchange interactions. The predicted Curie temperatures of all four systems are considerably higher than room temperature. The relation between the half-metallicity and the value of the Curie temperature is discussed. The combination of a high spin-polarization of charge carriers and a high Curie temperature makes these Heusler alloys interesting candidates for spintronics applications.

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INTRODUCTION

An important current problem on the way to the practical use of the spin-transport in semiconductor devices is the fabrication of the materials that make possible the injection of spin-polarized electrons into a semiconductor at room temperature \( T \). One of the classes of systems promising to supply materials with necessary combination of properties is the half–metallic ferromagnets, i.e., ferromagnetic systems where one spin channel is metallic and other is semiconducting. The half-metallicity leads to the 100% spin-polarization of the electron states at the Fermi level \( E_F \). The half–metallic ferromagnetism (HMF) was discovered by de Groot et al. when studying the band structure of semi Heusler compound NiMnSb \( \text{[2, 3]} \). Ishida et al. have proposed that also the full-Heusler alloys of the type Co\(_2\)MnZ, \( Z=\text{Si,Ge} \), are half-metals \( \text{[4]} \). Since then a number of further systems were predicted to be half-metallic. Among them binary magnetic oxides (CrO\(_2\) and Fe\(_2\)O\(_4\)), colossal magnetoresistance materials (Sr\(_2\)FeMoO\(_6\) and La\(_{0.7}\)Sr\(_{0.3}\)MnO\(_3\)) \( \text{[5]} \), diluted magnetic semiconductors (Ga\(_1-x\)Mn\(_x\)As) and zinc-blende compounds MnAs and CrAs \( \text{[6]} \).

The Heusler alloys form a particularly interesting class of materials since they are characterized by a high Curie temperature and good crystallographic compatibility with the lattices of semiconductors used industrially \( \text{[7]} \). The main body of previous first-principles studies was focused on the investigation of the properties of the semiconducting gap in the minority-spin channel. Galanakis et al. considering NiMnSb have shown that the gap arises from the interaction between the \( d \)-orbitals of the Ni and Mn atoms leading to the formation of bonding and antibonding states separated by a hybridization gap \( \text{[8]} \). Chioncel et al. have demonstrated by the example of NiMnSb that the electron-magnon interaction can lead to the appearance of nonquasiparticle states in the half-metallic gap \( \text{[9]} \).

For a number of Heusler alloys it was shown that half–metallicity is preserved under tetragonalization of the crystal lattice \( \text{[10]} \) and application of the hydrostatic pressure \( \text{[11]} \). Mavropoulos et al. studied the influence of the spin-orbit coupling on the spin-polarization at the Fermi level and found the effect to be very small \( \text{[12]} \) that corresponds to a small orbital moment calculated by Galanakis \( \text{[13]} \). Orgassa and collaborators have shown that the half-metallic gap decreases with increasing disorder \( \text{[14]} \). Picozzi and collaborators and Miura et al. demonstrated that different types of structural defects have different influence on the half-metallicity \( \text{[15]} \).

An important part of theoretical efforts is a first-principles design of new half–metallic Heusler alloys. Galanakis studied the appearance of half-metallic ferromagnetism in quaternary Heusler alloys \( \text{[16]} \). Xing et al. have predicted the half-metallic ferromagnetism in NiCrZ \( Z=\text{P, Se, Te} \) and NiVAs semi Heusler compounds \( \text{[17]} \).

Despite a very strong experimental and theoretical interest to the half-metallic ferromagnetism in Heusler alloys the number of the studies of the exchange interactions in Heusler alloys is still very small. The first contribution to the density functional theory of the exchange interactions in these systems was made in an early paper by Kübler et al. \( \text{[18]} \) where the microscopic mechanisms of the magnetism of Heusler alloys were discussed on the basis of the comparison of the ferromagnetic and antiferromagnetic configurations of the Mn moments. Recently, the studies of the inter-atomic exchange interactions in several Heusler compounds were reported by the present authors and Kurtulmuş et al. \( \text{[19]} \).

The purpose of the present work is a first–principles study of the exchange interactions and the temperature of magnetic phase transition for four semi Heusler
compounds NiCrZ (Z=P, Se, Te) and NiVAs that were recently predicted to be half-metals \(^{23, 24}\). For all four systems we find the Curie temperature substantially exceeding room temperature. We discuss the relation between the value of the Curie temperature and half-metallicity. We demonstrate strong dependence of the effective exchange interaction between 3d atoms on the sp element (Z constituent).

The paper is organized as follows. In Sec. II we present the calculational approach. Section III contains the results of the calculations and discussion. Section IV gives the conclusions.

### COMPUTATIONAL METHOD

The semi Heusler compounds crystallize in the \(C1_b\)-type structure. The lattice consists of three interpenetrating fcc atomic sublattices. Compared with full Heusler alloys the forth atomic sublattice is vacant. In the calculations, the atomic positions of the fourth sublattice are occupied by empty spheres.

The calculations are carried out with the augmented spherical waves method \(^{30}\) within the atomic–sphere approximation (ASA) \(^{31}\). The exchange–correlation potential is chosen in the generalized gradient approximation \(^{32}\). A dense Brillouin zone (BZ) sampling \(30 \times 30 \times 30\) is used.

For each compound we performed calculations for two values of the lattice parameter: the theoretical equilibrium parameter \(^{23, 24}\) and the lattice parameter of a binary semiconductor (Table I) that can be considered as a possible substrate for growing the corresponding Heusler alloy: GaAs for NiCrP and NiCrSe and InP for NiVAs and NiCrTe. The radii of all atomic spheres are chosen equal.

To calculate the interatomic exchange interactions we use the frozen-magnon technique \(^{33}\) and map the results of the calculation of the total energy of the helical magnetic configurations

\[
s_n = (\cos(qR_n) \sin \theta, \sin(qR_n) \sin \theta, \cos \theta)
\]

onto a classical Heisenberg Hamiltonian

\[
H_{\text{eff}} = - \sum_{i \neq j} J_{ij} s_i s_j
\]

where \(J_{ij}\) is an exchange interaction between two Cr (V) sites and \(s_i\) is the unit vector pointing in the direction of the magnetic moment at site \(i\). \(R_n\) are the lattice vectors, \(q\) is the wave vector of the helix, \(\theta\) polar angle giving the deviation of the moments from the z axis. Within the Heisenberg model \(^{24}\), the energy of frozen-magnon configurations can be represented in the form

\[
E(\theta, q) = E_0(\theta) + \sin^2 \theta J(q)
\]

where \(E_0\) does not depend on \(q\) and \(J(q)\) is the Fourier transform of the parameters of exchange interaction between pairs of Cr(V) atoms:

\[
J(q) = \sum_{\mathbf{R}} J_{0\mathbf{R}} \exp(iq \cdot \mathbf{R}).
\]

Calculating \(E(\theta, q)\) for a regular \(q\)-mesh in the Brillouin zone of the crystal and performing back Fourier transformation one gets exchange parameters \(J_{0\mathbf{R}}\) between pairs of Cr(V) atoms.

The Curie temperature is estimated in the mean-field approximation (MFA)

\[
k_B T_C^{\text{MFA}} = \frac{2}{3} \sum_{j \neq 0} J_{0j} = \frac{M}{6 \mu_B} \frac{1}{N} \sum_{\mathbf{q}} \omega(\mathbf{q})
\]

and random phase approximation (RPA)

\[
k_B T_C^{\text{RPA}} = \frac{6 \mu_B}{M} \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{\omega(\mathbf{q})}
\]

where \(\omega(\mathbf{q}) = \frac{1}{M} [J(0) - J(\mathbf{q})]\) is the energy of spin–wave excitations.

### RESULTS AND DISCUSSION

#### DOS and magnetic moments

The two lattice parameters used in the calculations resulted for all systems in very similar physical properties (see, e.g., Tables III). Therefore the most of the results will be presented for one lattice constant. All the discussion in this section is valid for both lattice spacings.

In Fig. I we present the calculated electron densities of states (DOS) of the ferromagnetic states of the four Heusler compounds. All systems are found to be half-metallic with the Fermi level lying in the semiconducting gap of the minority-spin channel. Our DOS are in good agreement with the DOS presented in Refs. \(^{23, 24}\).

| Element | Ni | V, Cr, Mn | Void | Z | Cell |
|---------|----|----------|------|---|-----|
| NiVAs   | 5.85 | -0.02 | 2.05 | 0.06 | -0.09 | 2.0 |
| NiCrP   | 5.59 | -0.01 | 3.08 | 0.07 | -0.15 | 3.0 |
| NiCrTe  | 5.84 | 0.24  | 3.68 | 0.11 | -0.03 | 4.0 |
| NiCrSe  | 5.64 | 0.19  | 3.86 | 0.04 | -0.10 | 4.0 |
| NiCrP   | 5.65 | 0.23  | 3.65 | 0.12 | -0.01 | 4.0 |
| NiCrSe  | 5.65 | 0.23  | 3.65 | 0.12 | -0.01 | 4.0 |
| NiCrTe  | 5.87 | 0.23  | 3.70 | 0.11 | -0.03 | 4.0 |

(a) Ref. 25
In Table I, the calculated magnetic moments are collected. Since the systems are half-metallic, the magnetic moments per formula unit are integer: 2\(\mu_B\) for NiVAs, 3\(\mu_B\) for NiCrP and 4\(\mu_B\) for NiCrSe and NiCrTe. The major part of the magnetic moment comes from the second formula atom (V, Cr). Small induced magnetic moments are found on Ni and \(sp\) atoms.

**Exchange constants and Curie temperature**

Figure 2a presents the frozen-magnon dispersion for one direction in the reciprocal space. Additionally to NiCrZ (\(Z=P, Se, Te\)) and NiVAs we present for comparison the results for NiMnSb \([28]\). The five systems can be subdivided into two groups. One group contains NiVAs, NiCrP and NiMnSb. Here the frozen-magnon dispersions are monotonous and resemble, visually, a simple cosinusoid. The second group contains NiCrSe and NiCrTe and is characterized by nonmonotonous dispersions with a maximum close to the center of the \(q\)-interval (Fig. 2a). Note, that the \(sp\) elements (the third chemical-formula constituents) within each of the group belong to the same column of the Mendeleev’s table whereas for different groups these columns are different. The importance of the valency of the \(sp\) element for magnetic properties of Heusler alloys has been already observed in our earlier studies \([26]\).

The calculated exchange parameters are given in Fig. 2b. Since the inter-atomic exchange parameters are the Fourier transforms of the frozen-magnon dispersions they reflect the properties of the dispersions: The exchange parameters belonging to the same group show similar qualitative behavior. On the other hand, there is strong difference between the systems belonging to different groups (Fig. 2b). In the first group (Fig. 2b, left panel), the strongest exchange interaction takes place between nearest magnetic \(3d\) atoms. This strongest interaction determines the cosinusoidal form of the corresponding magnon dispersion. The sizable interaction between the second-nearest magnetic \(3d\) atoms describes the deviation of the dispersion from a simple cosinusoid.

In the second group of compounds (Fig. 2b, right panel), the strongest interaction is between the second-nearest magnetic atoms. Because of the decreased period of the Fourier component corresponding to the second exchange parameter the dispersions are nonmonotonous and have the maximum not at the boundary of the Brillouin zone but inside of it.

A remarkable feature of the exchange interactions is their short range character: the leading contribution into the Curie temperature of all systems is provided by the interactions within the first two coordination spheres. The interactions with further coordination spheres are very weak and can be neglected in the calculation of the Curie temperature. The interaction between Ni atoms and the interaction of Ni with V and Cr are very weak and are not presented.

The calculated exchange parameters are used to evaluate the Curie temperature (Table II). It is important to note that the similarity of the form of the magnon dispersions within one group of compounds is not accompanied by a quantitative closeness of the curves (Fig. 2a). Therefore the Curie temperature can differ strongly for compounds belonging to the same group.

The Curie temperatures are estimated within two different schemes: MFA and RPA. For all systems and for both theoretical schemes the calculated Curie temperatures are substantially higher than room temperature. The MFA always gives the value of \(T_c\) that is larger than the corresponding RPA value and usually overestimates the experimental Curie temperature \([37, 38]\). The reason for the difference of the MFA and RPA estimations is a different weighting of the spin-wave excitations within two calculational approaches: The MFA takes all excitations with the same weight whereas the RPA gives a larger weight to the excitations with lower energy. The RPA weighting is better grounded from the viewpoint of statistical mechanics.

The analysis of the calculational data allows to make a number of important conclusions. First, there is a strong influence of the \(sp\) atom on the value of \(T_c\). Indeed, the comparison of NiCrSe and NiCrTe that differ by the \(sp\) atom shows that the Curie temperature changes from about 500 K in NiCrSe to about 800 K in NiCrTe. This strong dependence reveals the sensitivity of the exchange interactions and the Curie temperature to the details of
the electron structure.

An interesting feature of the calculated Curie temperatures (Table III) is a large difference between the MFA and RPA estimations for the first group of compounds in contrast to a small difference for the second group. Characterizing the relative difference of the MFA and RPA values of the Curie temperature by the relation

\[ \frac{T_{c\text{MFA}} - T_{c\text{RPA}}}{T_{c\text{RPA}}} \]

we get for the first group of compounds a large value of 20-24% compared to a small value of 5-8% in the second group. This feature reflects the properties of the corresponding frozen-magnon spectra.

In MFA, the Curie temperature is determined by an arithmetic average of the magnon energies while in RPA \( T_{c\text{RPA}} \) is determined by the harmonic average of the same quantities (the first average is always larger than the second). In terms of magnon energies, \( T_{c\text{MFA}} \) is equal to \( T_{c\text{RPA}} \) in the case that the magnon spectrum is dispersion-less: the magnon energy does not depend on the wave vector \( q \).

From Fig. 2 we see that the frozen–magnon curves of the second group of compounds are flat in the second half of the \( q \) interval demonstrating a very weak dispersion. On the other hand, the first group of compounds have considerable dispersion in this part of the \( q \) interval. Comparing now the low-\( q \) parts of the curves we notice that the curves of the second group of compounds lie higher than the first group. Therefore, the relative contribution of the low-energy magnons to the RPA value of the Curie temperature is smaller in the second group of compounds.

This combination of features of the wave-vector dependencies of the frozen-magnon energies is responsible for a larger (smaller) difference between the RPA and MFA estimations of the Curie temperature of the first group (second group) of compounds in the two cases.

**Curie temperature and half-metallicity**

An important question concerning the magnetism of the half-metallic systems is the relation between half-metallicity and Curie temperature. Indeed, a number of studies has shown that the half-metallicity can stimulate an increase of the Curie temperature [39, 40, 41]. The analysis of Fig. 3 allows us to establish a correlation between the value of the Curie temperature and the energy distance \( \delta \) between the Fermi level and the upper edge of the semiconducting gap. This quantity determines the spacing between the highest occupied spin-up state and the lowest empty spin-down state. For very small \( \delta \) of 0.03 eV in NiCrSe we obtained the lowest Curie temperature of 508 K. On the other hand, for large \( \delta \) in NiCrP and NiMnSb we obtained the Curie temperature substantially above 800 K.

Since the value of the Curie temperature is determined by the magnetic excitations to interpret the \( \delta - T_c \) correlation we need to understand the origin of the influence of the \( \delta \) value on the spin-wave energies.
The magnon energies reflect the energy prize for the deviations of the atomic moments from parallel directions. In the ground-state ferromagnetic configuration the spin-projection is a good quantum number and the electron states with opposite spin projections do not interact. The deviation of the atomic moments from parallel directions leads to the mixing of the majority-spin and minority-spin states. The hybridization of a pair of the states leads to their repulsion. As a result, the energy of the lower state decreases (bonding state) and the energy of the upper state increases (antibonding state). If the lower state is occupied and the upper state is empty this process leads to the decrease of the energy making ferromagnetic state energetically less favorable. The smaller is the energy distance between interacting states the stronger is the effect.

Coming back to the half-metallic compounds considered in the paper we note that the hybridizational interaction of this type takes place between the occupied majority-spin states below the Fermi level and the empty spin-down states at the bottom of the conduction band. The distance between these states is given by parameter $\delta$. Therefore this process provides a mechanism for the correlation between $\delta$ and Curie temperature.

Since the strength of the hybridizational repulsion increases with decreasing energy distance between interacting states the negative contribution to the spin-wave energies is larger in the case of smaller $\delta$. However, the correlation between parameter $\delta$ and $T_c$ or, more general, between the half-metallicity and $T_c$ should not be considered as a universal rule. The hybridizational repulsion considered above is only one of numerous processes arising in a complex multi-band system with the deviation of the atomic moments from the parallel directions. The combined result of these processes cannot be predicted without the direct calculation of the excitation energies. Such a calculation must take into account the complexity of the electron structure of a real system. Indeed, the comparison of NiVAs and NiCrTe shows that both systems have the same $\delta$ of 0.14eV. However, their Curie temperatures differ strongly.

Also our numerical experiments with varying the lattice parameter in half-metallic systems have shown that in some systems the loss of the half-metallicity caused by this variation does not lead to the decrease of the Curie temperature.

**CONCLUSION**

We have systematically studied exchange interactions and Curie temperature in predicted half-metallic semi Heusler compounds NiVAs and NiCrZ ($Z=\text{P, Se, Te}$). The calculations are performed within the parameter–free density functional theory. The RPA and MFA are used to estimate the Curie temperatures. We show that the behavior of exchange interactions in these systems vary strongly depending on the $Z$ constituent.

The exchange interactions are short range with the leading contribution to the Curie temperature provided by the interactions within the first two coordination spheres.

**TABLE II:** MFA and RPA estimations of the Curie temperatures in NiVAs, NiCrZ ($Z=\text{P, Se, Te}$) and NiMnSb. The third column represent the relative difference of the MFA and RPA estimations.

| Compound          | $T_c^{\text{MFA}}$ (K) | $T_c^{\text{RPA}}$ (K) | $T_c^{\text{MFA-RPA}}$ (%) |
|-------------------|------------------------|------------------------|-----------------------------|
| NiVAs             | 723                    | 603                    | 20                          |
| NiVAs$^{(a)}$     | 715                    | 595                    | 20                          |
| NiCrP             | 1030                   | 848                    | 21                          |
| NiCrP$^{(b)}$     | 938                    | 770                    | 22                          |
| NiMnSb$^{(c)}$    | 1096                   | 880                    | 24                          |
| NiCrSe$^{(a)}$    | 537                    | 508                    | 6                           |
| NiCrSe$^{(b)}$    | 543                    | 515                    | 5                           |
| NiCrTe$^{(a)}$    | 868                    | 805                    | 8                           |
| NiCrTe$^{(a)}$    | 874                    | 812                    | 8                           |

$^{(a)}$ lattice constant of GaAs

$^{(b)}$ lattice constant of InP

$^{(c)}$ Ref.28
spheres of the magnetic 3d atoms. The predicted Curie temperatures of all four systems are considerably higher than room temperature. The relation between the half-metallicity and the value of the Curie temperature is discussed. The combination of a high spin-polarization of charge carriers and a high Curie temperature makes these Heusler alloys interesting candidates for spintronics applications. We hope that the present study will provide a guideline for experimental work stimulating the fabrication of these materials.

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[1] H. Ohno, Science 281, 951 (1998).
[2] I. ˇZuti´ c, J. Fabian, and S. Das Sarma, Rev. Mod. Phys. 76, 323 (2004).
[3] J. de Boeck, W. van Roy, J. Das, V. Motsnyi, Z. Liu, L. Lagae, H. Boeve, K. Dessein, and G. Borghs, Semicond. Sci. Tech. 17, 342 (2002).
[4] R. A. de Groot, F. M. Mueller, P. R. en van Engen, and K. H. J. Buschow, Phys. Rev. Lett. 50, 2024 (1983).
[5] S. Ishida, S. Akazawa, Y. Kubo, and J. Ishida, J. Phys. F: Met. Phys. 12, 1111 (1982); S. Ishida, S. Fujii, S. Kashihagi, and S. Asano, J. Phys. Soc. Jpn. 64, 2152 (1995).
[6] R. J. Soulen Jr., J. M. Byers, M. S. Osofsky, B. Nadgorny, T. Ambrose, S. F. Cheng, P. R. Broussard, C. T. Tanaka, J. Nowak, J. S. Moodera, A. Barry, and J. M. D. Coey, Science 282, 85 (1998).
[7] A. stroppa, S. Picozzi, A. Continenza, and A. J. Freeman, Phys. Rev. B 68, 152403 (2003).
[8] H. Akai, Phys. Rev. Lett. 81, 3002 (1998).
[9] H. Akinaga, T. Manago, and M. Shirai, Jpn. J. Appl. Phys. 39, L1118 (2000).
[10] P. 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-Bo¨ r nstein, New Series, Group III, Vol. 19, Pt.c (Springer-Verlag, Berlin 1988), pp. 75-184.
[11] J. Q. Xie, J. W. Dong, Lu J., C. J. Palmstrøm and S. McKernan, Appl. Phys. Lett. 79, 1903 (2001).
[12] M. Kurfiss and R. Anton, J. Alloy. Comp. 361, 36 (2003).
[13] I. Galanakis, P. H. Dederichs, and N. Papanikolaou, Phys. Rev. B 66, 134428 (2002).
[14] L. Chioncel, M. I. Katsnelson, R. A. de Groot, and A. I. Lichtenstein, Phys. Rev. B 68, 144425 (2003).
[15] T. Block, M. J. Carey, D. A. Gurney, and O. Jepsen, Phys. Rev. B 70, 205114 (2004).
[16] S. Picozzi, A. Continenza, and A. J. Freeman, Phys. Rev. B 66, 094421 (2002); I. Galanakis, S. Ostanin, M. Alouani, H. Dreyssé, and J. M. Wills, Phys. Rev. B 61, 4093 (2000).
[17] Ph. Mavropoulos, K. Sato, R. Zeller, P. H. Dederichs, V. Popescu, and H. Ebert, Phys. Rev. B 69, 054424 (2004); Ph. Mavropoulos, I. Galanakis, V. Popescu, and P. H. Dederichs, J. Phys.: Condens. Matter 16, S5759 (2004).
[18] I. Galanakis, Phys. Rev. B 71, 012413 (2005).
[19] D. Orgassa, H. Fujiwar, T. C. Schulthess, and W. H. Butler, Phys. Rev. B 60, 13 237 (1999).
[20] S. Picozzi, A. Continenza, and A. J. Freeman, Phys. Rev. B 69, 094423 (2004).
[21] Y. Miura, K. Nagao and M. Shirai, Phys. Rev. B 69, 144413(2004).
[22] I. Galanakis, J. Phys. Condens. Matter 16, 3089 (2004).
[23] Ming Zhang, Xuefang Dai, Haining Hu, Guodong Liu, Yuting Cui, Zhuhong Liu, Jinglan Chen, Jianli Wang and Guangheng Wu, J. Phys.: Condens. Matter 15, 7891 (2003).
[24] Ming Zhang, Zhu-Hong Liu, Hai-Ning Hu, Guo-Dong Liu, Yu-Ting Cui, Guang-Heng Wu, Ekkes Brueck, Frank R.de Boer, and Yang-Xian Li, J. Appl. Phys. 95, 7219 (2004).
[25] J. Kübler, A. R. Williams, and C. B. Sommers, Phys. Rev. B 28, 1745(1983).
[26] E. ˇSasha ´gilu, L. M. Sandratskii, and P. Bruno, Phys. Rev. B 70, 024427 (2004).
[27] E. ˇSasha ´gilu, L. M. Sandratskii, and P. Bruno, J. Phys.: Condens. Matter 17, 995 (2005).
[28] E. ˇSasha ´gilu, I. Galanakis, L. M. Sandratskii and P. Bruno, unpublished.
[29] Y. Kurtuluş, R. Dranskowski, G. D. Samolyuk, and V. P. Antropov, Phys. Rev. B 71, 014425 (2005).
[30] A. R. Williams, J. Kübler, and C. D. Gelatt, Phys. Rev. B 19, 6094(1979).
[31] O. K. Andersen, Phys. Rev. B 12, 3060 (1975).
[32] J. P. Perdew and Y. Wang, Phys. Rev. B 45, 13244 (1992).
[33] N. M. Rosengaard and B. Johansson, Phys. Rev. B 55, 14975 (1997); S. V. Halilov, H. Eschrig, A. Ya. Perlov, and P. M. Oppeneer, Phys. Rev. B 58, 293 (1998); L. M. Sandratskii and P. Bruno, Phys. Rev. B 66, 134435 (2002).
[34] L. M. Sandratskii, Adv. Phys. 47, 1 (1998).
[35] L. M. Sandratskii and P. Bruno, Phys. Rev. B 67, 214402 (2003).
[36] L. M. Sandratskii, P. Bruno and S. Mirbt, Phys. Rev. B 71, 045210 (2005).
[37] M. Pajda, J. Kudrnovsky, I. Turek, V. Drchal, and P. Bruno, Phys. Rev. B 64, 174402 (2001).
[38] G. Bouzerar, J. Kudrnovsky, L. Bergqvist, and P. Bruno, Phys. Rev. B 68, 081203(R) (2003).
[39] J. Kübler Phys. Rev. B 67, 220403, (2003).
[40] A. Sakuma, J. Phys. Soc. Jpn. 71, 2534 (2002).
[41] B. Sanyal, L. Bergqvist and O. Eriksson, Phys. Rev. B 68, 054417 (2003).