

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 is calculated within mean field and random phase approximations. The difference between two estimated values is related to the properties of the exchange interactions. The predicted Curie temperatures of all four systems are considerably above room temperature. The relation between 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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I. INTRODUCTION

An important current problem on the way to the practical use of spin transport in semiconductor devices is the fabrication of materials that make possible the injection of spin-polarized electrons into a semiconductor at room temperature.¹ One of the classes of systems promising to supply materials with the necessary combination of properties is the class of half-metallic ferromagnets, i.e., ferromagnetic systems where one spin channel is metallic and the other is semiconducting. The half-metallicity leads to 100% spin polarization of the electron states at the Fermi level E_F .^{2,3} The half-metallic ferromagnetism was discovered by de Groot *et al.* when studying the band structure of the semi-Heusler compound NiMnSb.⁴ Ishida *et al.* proposed that full-Heusler alloys of the type Co_2MnZ (Z=Si, Ge) are, as well, half-metals.⁵ Since then a number of further systems were predicted to be half-metallic. Among them are binary magnetic oxides (CrO_2 and Fe_3O_4), colossal magnetoresistance materials ($\text{Sr}_2\text{FeMoO}_6$, and $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$),⁶ diluted magnetic semiconductors ($\text{Ga}_{1-x}\text{Mn}_x\text{As}$), and zinc-blende compounds MnAs and CrAs.⁷⁻⁹

Heusler alloys form a particularly interesting class of materials since they are characterized by high Curie temperature and good crystallographic compatibility with the lattices of semiconductors used industrially.¹⁰⁻¹² Previous first-principles studies mainly focused on investigating the properties of the semiconducting gap in the minority-spin channel. Galanakis *et al.* have shown that the half-metallic gap in the electron structure of NiMnSb is caused by the interaction between the d orbitals of Ni and Mn atoms, leading to the formation of bonding and antibonding states separated by a hybridizational gap.¹³ Chioncel *et al.* have demonstrated by the example of NiMnSb that the electron-magnon interaction can lead to the formation of nonquasiparticle states in the half-metallic gap.¹⁴

For a number of Heusler alloys it was shown that half-metallicity is preserved under tetragonalization of the crystal

lattice¹⁵ and the application of hydrostatic pressure.¹⁶ Mavropoulos *et al.* studied the influence of spin-orbit coupling on the electron spin polarization at the Fermi level and found the effect to be very small,¹⁷ which corresponds to a small orbital moment calculated by Galanakis.¹⁸ Orgassa and collaborators have shown that the half-metallic gap decreases with increasing disorder.¹⁹ Picozzi and collaborators and Miura *et al.* demonstrated that different types of structural defects have a different influence on the half-metallicity.¹⁹⁻²¹

An important part of the theoretical efforts is a first-principles design of new half-metallic Heusler alloys. Galanakis studied the formation of half-metallic ferromagnetism in quaternary Heusler alloys.²² Xing *et al.* have predicted the half-metallic ferromagnetism in NiCrZ (Z=P, Se, Te) and NiVAs semi-Heusler compounds.^{23,24}

Despite very strong experimental and theoretical interest to the half-metallic ferromagnetism in Heusler alloys, the number of 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.*,²⁵ 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 interatomic exchange interactions in several Heusler compounds were reported by the present authors and Kurtulus *et al.*²⁶⁻²⁹

The purpose of the given work is a first-principles study of the exchange interactions and the temperature of the 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 a strong dependence of the effective exchange interaction between $3d$ atoms on the sp element (Z constituent).

TABLE I. Lattice parameters and magnetic moments (in μ_B) for NiVAs, NiCrZ (Z=P, Se, Te), and NiMnSb.

	a (Å)	Ni	V, Cr, Mn	Void	Z	Cell
NiVAs	5.85	-0.02	2.05	0.06	-0.09	2.0
	5.87 (InP)	-0.03	2.06	0.06	-0.09	2.0
NiCrP	5.59	-0.01	3.08	0.07	-0.15	3.0
	5.65 (GaAs)	-0.06	3.16	0.06	-0.16	3.0
NiMnSb ^a	5.93	0.19	3.86	0.04	-0.10	4.0
NiCrSe	5.64	0.24	3.64	0.12	-0.01	4.0
	5.65 (GaAs)	0.23	3.65	0.12	-0.01	4.0
NiCrTe	5.84	0.24	3.68	0.11	-0.03	4.0
	5.87 (InP)	0.23	3.70	0.11	-0.03	4.0

^aRef. 28.

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

II. 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 fourth 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 method³⁰ within the atomic-sphere approximation (ASA).³¹ The exchange-correlation potential is chosen in the generalized gradient approximation.³² A dense Brillouin zone sampling $30 \times 30 \times 30$ is used.

For each compound we performed calculations for two values of the lattice parameter (Table I): the theoretical equilibrium parameter^{23,24} and the lattice parameter of a binary semiconductor 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 to be equal.

To calculate the interatomic exchange interactions we use the frozen-magnon technique³³ and map the results of the calculation of the total energy of the helical magnetic configurations,³⁴

$$s_n = [\cos(\mathbf{q}\mathbf{R}_n)\sin\theta, \sin(\mathbf{q}\mathbf{R}_n)\sin\theta, \cos\theta] \quad (1)$$

onto a classical Heisenberg Hamiltonian,

$$H_{\text{eff}} = - \sum_{i \neq j} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j, \quad (2)$$

where J_{ij} is an exchange interaction between two Cr (V) sites and \mathbf{s}_i is the unit vector pointing in the direction of the magnetic moment at site i , \mathbf{R}_n are the lattice vectors, \mathbf{q} is the wave vector of the helix, and θ is the polar angle giving the deviation of the moments from the z axis. Within the Heisenberg model (2), the energy of frozen-magnon configurations can be represented in the form

$$E(\theta, \mathbf{q}) = E_0(\theta) + \sin^2\theta J(\mathbf{q}), \quad (3)$$

where E_0 does not depend on \mathbf{q} and $J(\mathbf{q})$ is the Fourier transform of the parameters of interatomic exchange interactions:

$$J(\mathbf{q}) = \sum_{\mathbf{R}} J_{0\mathbf{R}} \exp(i\mathbf{q} \cdot \mathbf{R}). \quad (4)$$

Calculating $E(\theta, \mathbf{q})$ for a regular \mathbf{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),

$$k_B T_C^{\text{MFA}} = \frac{2}{3} \sum_{j \neq 0} J_{0j} = \frac{M}{6\mu_B N} \sum_{\mathbf{q}} \omega(\mathbf{q}) \quad (5)$$

and random phase approximation (RPA),^{38,39}

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

where $\omega(\mathbf{q}) = 4/M[J(0) - J(\mathbf{q})]$ is the energy of spin-wave excitations, μ_B is the Bohr magneton, N is the number of \mathbf{q} points in the first Brillouin zone, and M is the atomic magnetic moment.

III. RESULTS AND DISCUSSION

A. 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 I and II). Therefore most of the results will be

TABLE II. MFA and RPA estimations of the Curie temperatures of NiVAs, NiCrZ (Z=P, Se, Te) and NiMnSb. The third column represents the relative difference of the MFA and RPA estimations.

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

^aLattice constant of GaAs.^bLattice constant of InP.^cRef. 28.

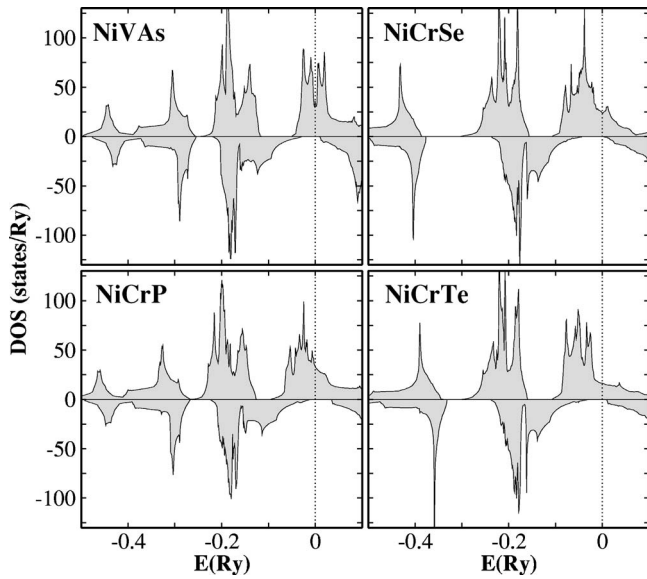


FIG. 1. Spin-projected density of states of NiVAs and NiCrZ ($Z=P, Se, Te$).

presented for one lattice constant. The entire discussion in this section is valid for both lattice spacings.

In Fig. 1, we present the calculated electron densities of states (DOS) of the ferromagnetic phases 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 obtained in Refs. 23 and 24.

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.

B. Exchange constants and Curie temperature

Figure 2(a) presents the frozen-magnon dispersion for NiCrZ ($Z=P, Se, Te$) and NiVAs. To compare we show the results for NiMnSb as well.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. 2(a)]. Note that the sp elements (the third chemical-formula constituents) within each of the groups 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. 2(b). Since the interatomic 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 a similar qualitative behavior. On the other hand, there is a strong difference between the systems belonging to different groups [Fig. 2(b)]. In the first group [Fig. 2(b), 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

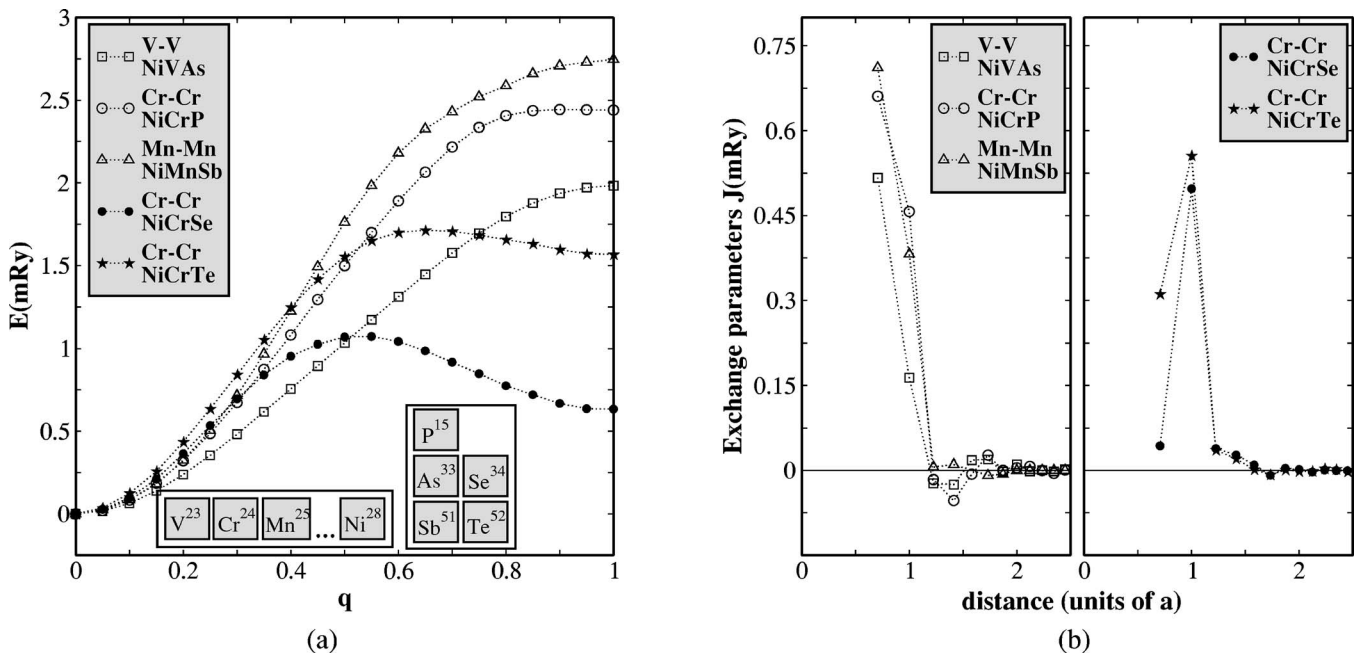


FIG. 2. (a) Frozen-magnon dispersions for NiVAs, NiMnSb, and NiCrZ ($Z=P, Se, Te$). The spectrum is shown for the $[00q]$ direction in the reciprocal space. The wave vector is given in units of $2\pi/a$. In the calculations only the V-V, Cr-Cr, and Mn-Mn interactions were taken into account. (b) Interatomic exchange interactions. The calculational data for NiVAs and NiCrZ are presented for the theoretical equilibrium lattice constant. The data for NiMnSb are taken from Ref. 28.

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. 2(b), 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 interactions between Ni atoms and the interactions 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. 2(a)]. Therefore the Curie temperatures 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.^{39,40} The reason for the difference of the MFA and RPA estimations is 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 us 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 II) 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 $[T_C^{\text{MFA}} - T_C^{\text{RPA}}]/T_C^{\text{RPA}}$, we get for the first group of compounds a large value of 20–24% compared to a small value of 5–8% for 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 is determined by the harmonic average of the same quantities

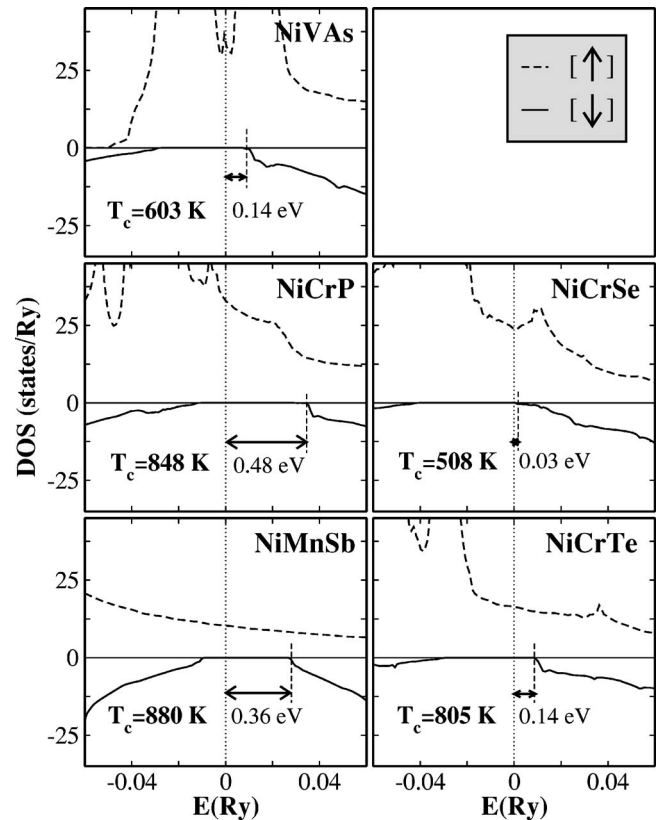


FIG. 3. Spin-projected density of states of NiVAs, NiCrP, NiMnSb, NiCrSe, and NiCrTe near the Fermi level. Also shown are the RPA estimations of the Curie temperature and the energy distances between the Fermi level and the bottom of the spin-down conduction band.

(the first average is always larger than the second): T_C^{MFA} is equal to T_C^{RPA} in the case of the dispersionless magnon spectrum.

From Fig. 2(a) we see that the frozen-magnon curves of the second group of compounds are flat in the second half of the \mathbf{q} interval, demonstrating here very weak dispersion. On the other hand, the first group of compounds has considerable dispersion in this part of the \mathbf{q} interval. In addition, the low- \mathbf{q} part of the curves for the second group of compounds lies higher than the corresponding part of the curves for 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 difference between the RPA and MFA estimations of the Curie temperature of the first group of compounds.

C. 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.^{41–43} The analysis of Fig. 3 allows us to establish a correlation between the value of the Curie temperature and the energy distance δ 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 δ of 0.03 eV in NiCrSe, we obtained the lowest Curie temperature of 508 K. On the other hand, for large δ 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 δ - T_C correlation we need to understand the origin of the influence of the δ value on the spin-wave energies.

The magnon energies reflect the energy prize for the deviations of the atomic moments from parallel directions.³⁵⁻³⁷ 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 of the magnon, making the 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 the parameter δ . Therefore this process provides a mechanism for the correlation between δ and the 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 δ . However, the correlation between parameter δ and T_C or, more generally, 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 δ of 0.14 eV. However, their Curie temperatures differ strongly.

Also, our numerical experiments with varying the lattice parameter in various 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.²⁸

IV. CONCLUSION

We have systematically studied exchange interactions and Curie temperature in half-metallic semi-Heusler compounds NiVAs and NiCrZ (Z=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 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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