Electronic and Magnetic Properties of Transition-Metal-Doped ScN for Spintronics Applications

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Motivated by the ongoing interest in nitrides as materials for spintronics applications, the effects of doping with magnetic transition-metal elements \((T = \text{Cr, Mn, Fe, Co, and Ni})\) on the electronic properties of semiconducting scandium nitride (ScN) are studied. Using density functional theory together with the generalized gradient approximation (GGA) and PBE0r hybrid functional (with different mixing of the exact exchange), two different doping amounts of 25% \((\text{Sc}_{0.75} \text{T}_{0.25} \text{N})\) and 10% \((\text{Sc}_{0.9} \text{T}_{0.1} \text{N})\) are investigated. This is done in comparison to the reference compound ScN with a strong focus on identifying candidates for half-metallic or semiconducting ferromagnetic ground states. Within GGA, only \(\text{Sc}_{0.75} \text{Fe(Co,Ni)}_{0.25} \text{N}\) becomes the half-metal and \(\text{Sc}_{0.75} \text{Cr(Mn)}_{0.25} \text{N}\) the semiconductor. However, additional calculations assuming antiferromagnetic ordering reveal that \(\text{Sc}_{0.75} \text{T}_{0.25} \text{N}\) is the only compound of this series, which prefers an antiferromagnetic (and semiconducting) ground state. For the lower concentration, \(\text{Sc}_{0.9} \text{T}_{0.1} \text{N}\), similar results are predicted, and all the doped nitrides are found to prefer ferromagnetic ground state over an antiferromagnetic one.

1. Introduction

The simultaneous exploitation of the charge and spin degrees of freedom of electronic materials is at the heart of the rapidly emerging field of spintronics. Of particular interest in this field are especially two types of materials classes, namely, dilute magnetic semiconductors (DMS) and half-metallic ferromagnets (HMF), with the latter being regarded as good candidates for spin injection in magnetoelectronic devices. [13]

Specifically, Mn-doped III–V semiconducting nitrides and arsenides such as (Ga,Al,In)(N,As) have been extensively investigated. [4,5] However, their use in practical applications is hampered by their rather low Curie temperatures. So far, the highest Curie temperature of about 173 K was reported for Mn-doped GaN. [6,7] Yet, it has been argued that ferromagnetism even above 300 K could be possible in N-rich growth of Ga(Mn)N. [8] Further obstacles to applications are the known low solubilities of the magnetic ions in the semiconductor matrix due to the different crystal structures assumed by the metallic dopants. Finally, spin injection is often affected by the resistivity mismatches at semiconductor–ferromagnet interfaces. [9,10]

In contrast, transition-metal (TM) nitride semiconductors and their alloys recommend themselves due to their exceptional optical, electromechanical, and magnetic properties, which make them promising candidates for applications in optoelectronic devices. [9,11–14]

Scandium nitride (ScN) crystallizes in the rocksalt structure with a lattice parameter of 4.50 Å. [15,16] It has an indirect bandgap of \(\approx 0.9\) eV. [17–20] ScN has been experimentally investigated by a variety of techniques. [21–24] In addition, ab initio calculations have been carried out to investigate its electronic structure, [25–32] confirming the experimental results as the rocksalt crystal structure and lattice constant. While some density functional theory (DFT)-based calculations using the local density approximation found ScN as a semimetal, [25–29] more elaborated calculations using the framework of the GW approximation succeeded to reproduce the experimental bandgap of \(\approx 0.9\) eV. [30–33]

Considerable effort was devoted to tailoring the physical properties of ScN through nonmagnetic doping. [38] However, only few experimental studies have been reported on dilute ferromagnetism in doped ScN. [34–37] Al-Brithen et al. incorporated Mn atoms to obtain Sc\(_{1-x}\)Mn\(_x\)N-type alloys with \(0 \leq x \leq 0.25\), crystallizing in a tetragonal structure. [34] Electronic and optical properties of Sc(Mn)N thin films were also investigated, with up to 11% doping. [15] The authors suggested that dilute manganese doping compensates for the high n-type carrier concentrations, and an n-type to p-type carrier type transition could be observed. However, the magnetic properties of these films were not studied. Insertion of a low amount of iron (Fe) atoms in ScN has been achieved by Constantin et al., [36] who gave a magnetic moment of \(\approx 0.037\) \(\mu_B/\text{Fe atom}\) at the experimental volume of the pristine system.

On the theoretical side, structural and optical properties of Cr\(_{1-x}\)Sc\(_x\)N alloys have been studied together with Cr-doped GaN. [18] However, with respect to the magnetic properties, focus was on the latter material. Supercell calculations on Mn-doped ScN have been carried out to study trends of the magnetic
properties.\textsuperscript{[9,39–41]} It was found that the exchange interactions are long range and affected by disorder and carrier concentrations.\textsuperscript{[10,40]} Furthermore, a structural phase transition has been predicted in Mn\textsubscript{0.75}Sc\textsubscript{0.25}N from a zinc-blende phase to a hexagonal phase.\textsuperscript{[49]} For iron doping, Fe\textsubscript{0.25}Sc\textsubscript{0.75}N has been investigated by means of DFT calculations, which predicted a magnetic semiconductor.\textsuperscript{[37]} The study, however, has focused more on the transport and thermoelectric properties.

Recently, a DFT-based study using the generalized gradient approximation (GGA) + U method has been reported on a large series of TM-doped [T,Sc]N (with T = Ti, V, Cr, Mn, Fe, Co, and Ni).\textsuperscript{[42]} The occurrence of half-metallicity was predicted for V, Cr, and Mn doping, whereas metallic behavior was expected for doping with late TM atoms.

Extending a previous study on pure ScN and Sc\textsubscript{0.75}Mn\textsubscript{0.25}N as based on the GGA,\textsuperscript{[41]} we investigate in the present investigation ScN doped with a larger variety of TM, including Cr, Mn, Fe, Co, and Ni. In doing so, we go beyond previous studies by applying a hybrid functional approach in addition to GGA calculations.

2. Theory and Computational Method

The first-principles calculations of the current work are based on DFT.\textsuperscript{[43,44]} In a first step, exchange–correlation effects are accounted for by the GGA.\textsuperscript{[45]} In addition, we applied a hybrid functional approach, which as well known replaces part of the exchange functional of the GGA by the exact exchange term provided by the Hartree–Fock method.\textsuperscript{[46,47]} Within this general approach, several implementations are in use. While the PBE0 method includes the exact exchange with a fraction of 25\% in all space,\textsuperscript{[48]} the HSE06 method uses this fraction only for the short-range part while keeping the long-range part of the exchange interaction at the GGA level.\textsuperscript{[49]} This idea is put to its extreme by the PBE0\textsubscript{r} functional, which restricts the exact exchange interaction to onsite matrix elements in a local orbital basis.\textsuperscript{[50,51]} The accuracy of the PBE0\textsubscript{r} functional, with respect to experiment, has been demonstrated in a study of TM oxides.\textsuperscript{[52]} Furthermore, a very recent extensive benchmark investigation using HSE06 and PBE0\textsubscript{r} functionals has been reported,\textsuperscript{[53]} where the latter is found to have an accuracy in the same range of the former. The PBE0\textsubscript{r} method is also used in the current study, where the exact exchange contribution is considered with different fractions (see Section 3.2). Note that a small value of 5\% suffices to reproduce the experimentally reported ScN bandgap of 0.9 eV.

The electronic and magnetic properties were calculated using the CP-PAW code, which is the original implementation of the projector-augmented wave (PAW) method.\textsuperscript{[54]} It uses the Car-Parrinello ab initio molecular dynamics (AIMD) framework to simultaneously calculate the atomic structure and the electronic wave functions.\textsuperscript{[55]} The Mermin functional\textsuperscript{[56]} was used to simultaneously calculate the atomic structure and the electronic wave functions.\textsuperscript{[55]} The Mermin functional\textsuperscript{[56]} was used to simultaneously calculate the atomic structure and the electronic wave functions.\textsuperscript{[55]}

3. Results and Discussion

3.1. Electronic Structure of Pure ScN

As the electronic properties of ScN are well established both experimentally and theoretically, this section just serves as a reference for the subsequent discussion. More thorough description can be found in the literature, as mentioned earlier in the introduction. The equilibrium structure of pure ScN has been determined by minimization of the total energy versus unit cell volume using both the GGA and hybrid functionals. From this, lattice constants of 4.58 and 4.52 Å were obtained from the GGA and the hybrid functional calculations, respectively. While the former as expected is somewhat larger than the experimental value of 4.50 Å, the latter shows better agreement.

The site- and orbital-projected densities of states (DOS) as calculated using the GGA, within the experimental lattice, are shown in Figure 1.

They confirm the semiconducting state with a bandgap of about 0.35 eV, which is much smaller than the measured experimental one (≈0.9 eV). This is due to the well-known failure of the local and semilocal approximations to reproduce experimental bandgaps. As many previous local-density approximation (LDA) and GGA calculations have predicted vanishing gap, as pointed out in the introduction,\textsuperscript{[28,29]} we have performed additional complementary GGA with a another method based on a different wavefunction basis set. Using the full-potential augmented spherical wave method (FP-ASW),\textsuperscript{[61,62]} with a carefully

![Figure 1](image-url)
converged calculation, a bandgap of 0.38 eV has been computed. Still being far from the experimental one, this result is close to our first one.

While the nitrogen 2p states are more prevailing in the valence band, the conduction band is dominated by the TM d states. The latter fall into nonbonding t$_{2g}$ subbands in the lower part (with a large peak around 5 eV), whereas the e$_g$ states due to stronger overlap with the N-2p and, therefore, larger splitting into bonding and antibonding manifolds are found at higher energies. As already reported, the trivalent character of Sc is almost complete, i.e., ScN can be written as Sc$^{+\delta}N^{-\delta}$ with $\delta \approx 3$, making the compound almost ionic.$^{[41]}$

In a second step, hybrid functional calculations were performed with a 5% admixture of the exact exchange interaction as mentioned earlier, which allowed to reproduce the experimentally observed bandgap of 0.9 eV.

### 3.2. Trends of Electronic Structure and Magnetic Properties of Sc$_{1-x}$T$_x$N (T = Cr, Mn, Fe, Co, and Ni)

This section is devoted to study the effect of the substitution of scandium by several TM atoms, i.e., Sc$_{1-x}$T$_x$N, where T = Cr, Mn, Fe, Co, and Ni, with two different concentrations $x = 0.25$ and $x = 0.10$.

In the first case, the simulations are performed using a simple-cubic supercell of the fcc-rocksalt structure of the form Sc$_3$T$_1$N$_4$. The calculated theoretical equilibrium lattice parameters are found very close to each other in the whole series. With hybrid functional framework, we computed the following values: 4.423 Å (T = Cr), 4.439 Å (T = Mn), 4.457 Å (T = Fe), 4.430 Å (T = Co), and 4.445 Å (T = Ni), whereas those calculated by GGA are about 3% larger. Thus, the substitution leads to a slightly smaller lattice constants compared with pure ScN.

We mention, however, that neither experimental nor theoretical data are available in the literature, to which our results could be compared.

We have first considered a ferromagnetic alignment of the TM atoms. The ferromagnetic state is found more stable than the spin-degenerate situation for all five dopants considered here. The electronic DOS of the five compounds as described within the GGA framework are shown in Figure 2.

Obviously, all types of substitution lead to loss of the semiconducting character of pure ScN. While Mn, Fe, Co, and Ni insertion induce metallic behavior, Sc$_{0.75}$Cr$_{0.25}$N is found to be a half-metal. In the latter case, an energy bandgap of $\approx 0.9$ eV is opened in the spin-down states, whereas a small contribution to the density of states at the Fermi level can be seen in the spin-up states. Therefore, the compound is at the verge of being a semiconductor. Similarly, Sc$_{0.75}$Mn$_{0.25}$N is close to being half-metallic.

In all the compounds, the distribution of the scandium d states remains almost unchanged to that in pure ScN, indicating only weak hybridization with the d states of the dopant. In contrast, the d states of the substitutional alloying elements can be regarded as in-gap states between N-p and Sc-d states of ScN.

In Sc$_{0.75}$Cr$_{0.25}$N and Sc$_{0.75}$Mn$_{0.25}$N, the nonbonding d-$t_{2g}$ states of chromium and manganese experience a strong exchange splitting. As a result, spin-majority states are completely filled leading to a high-spin configuration of the Cr and Mn d$_{3z^2-r^2}$ shells. However, the two compounds differ with respect to the d-e$_g$ states. Like in ScN, the dopant d-e$_g$ states hybridize strongly with the N-p states and are split into bonding and antibonding manifolds below and above the Fermi energy, respectively. While in the case of Cr, the latter are empty for both spin populations, the Mn-d-e$_g$ states are only half-filled. As a result, magnetic moments per Cr and Mn atom of 2.9 and 3.8 $\mu_B$, respectively, were obtained in the doped compounds.

![Figure 2](https://www.advancedsciencenews.com/physical-solid-state)
Beyond Cr and Mn, the exchange splitting of the $t_{2g}$ states decreases progressively due to the filling of the corresponding minority spin states, which are shifted below the Fermi level. Finally, for $\text{Sc}_{0.75}\text{Ni}_{0.25}\text{N}$ the exchange splitting is almost vanishing and both the majority and minority spin channels of the Ni-$t_{2g}$ states are completely filled. The calculated magnetic moments per dopant atom are 2.8, 1.7, and 0.2 $\mu_B$ for the Fe-, Co-, and Ni-doped compounds, respectively.

As the main purpose of this investigation is the search for ferromagnetic half-metals and semiconductors, a correct evaluation of the bandgap is of great importance. As mentioned earlier, use of the hybrid functional allowed to reproduce the experimentally reported bandgap for ScN. To explore the effect of the main ingredient of the hybrid functional scheme which is the inclusion of the exact exchange, we have performed calculations with three different mixing parameters (i.e., the weight of the Fock term, noted $\alpha$). The PBE0 functional allows

![Figure 3](image-url)

**Figure 3.** Site-, orbital-, and spin-projected DOS of $\text{Sc}_{0.75}\text{T}_{0.25}\text{N}$ with $\text{T} = \text{Cr, Mn, Fe, Co, and Ni}$ from hybrid functional calculations with three mixing parameters (admixture in %) of the exact exchange: (a) $\alpha = 0.05$ (5%), (b) $\alpha = 0.1$ (10%), and (c) $\alpha = 0.2$ (20%). The $\text{Sc-d, T-d-t}_{2g}$, $\text{d-e}_{g}$, and $\text{N-p}$ contributions (color and lines) are the same as in Figure 2.
to specify this mixing parameter on each site. So, we kept the one on Sc and N atoms fixed to 5% (α = 0.05, like in pure ScN), while increasing the one on the TM element gradually: 5% (α = 0.05), 10% (α = 0.10), and finally 20% (α = 0.20). The corresponding results of the site- orbital-, and spin-projected DOS for the five doped compounds are shown in Figure 3.

In Figure 3a corresponding to the lowest value of the mixing parameter (α = 0.05), the electronic structure of Sc0.75(Fe,Co, Ni)0.25N-doped nitrides remains almost unchanged, with respect to GGA, and still shows metallic character. The situation is different for the doping with Cr and Mn. Specifically, for Sc0.75Cr0.25N a ferromagnetic semiconducting is found with a bandgap of ≈0.5 eV, whereas Sc0.75Mn0.25N turns out to be a ferromagnetic half-metal with a finite DOS in the majority spin channel and a bandgap of ≈0.8 eV in the minority spin channel.

When increasing the the mixing parameter to α = 0.1, the picture starts to change noticeably, as shown in Figure 3b. Here, while the electronic character of two first Sc0.75Cr(Mn)0.25N compounds remains the same as for α = 0.05 (just with a slightly enhanced gap to the Cr-doped nitride ≈0.7 eV), we note that Sc0.75Fe(Fe,Co)0.25N turns to be half-metallic ferromagnets with a small minority spin bandgap. Moreover, Ni-doped nitride Sc0.75Ni0.25N is found at the verge of being a half-metal too, where a tiny gap starts to open in the minority spin channel. This situation becomes completely resolved with the highest mixing parameter value α = 0.2, leading to a clear semiconducting ferromagnetism in the first two compounds Sc0.75Cr(Mn)0.25N (with bandgap values of ≈0.85 and ≈0.45, for Cr and Mn doping, respectively). In the other Fe-, Co-, and Ni-doped nitrides, a very net half-metallic character is stabilized. Of course, both physical states are of high interest for spintronics applications.

Overall, the trend of the DOS of all the compounds is very similar to the one observed for the GGA calculations, for the three mixing parameters, especially concerning the Sc and N electronic DOS. In particular, the projected DOS shown in Figure 2 and 3 have almost the same shape and distribution and the general discussion of the GGA results applies also to the hybrid functional calculations apart from the relative shifts of the groups of bands. There is, however, a noticeable difference concerning the exchange splitting of t2g and eg shells in the TM ions, when increasing the weight of the Fock term α. This can be seen from the computed values of the magnetic moments for the different cases, as shown in Table 1. A saturated magnetic moment for all the compounds is obtained with the two last fractions of the exact exchange (i.e., α = 0.1 to α = 0.2), where semiconducting or half-metallic behavior is obtained.
To finalize the investigation of Sc<sub>0.75</sub>T<sub>0.25</sub>N compounds, the calculations of the ferromagnetic states were complemented by investigations regarding possible antiferromagnetic alignment of the magnetic moments of the dopant atoms. To this end, supercells (formed by doubled simple-cubic cell) were considered to simulate a simple type I antiferromagnetic alignment (AFM(001)). The latter consists on a ferromagnetic plans alternating along the z-axis direction. To the best of our knowledge, the study of AFM ordering in doped-ScN has not been reported elsewhere.

As a result, except for chromium-doped ScN antiferromagnetic order was found to be less stable than the ferromagnetic state discussed earlier. Specifically, in Sc<sub>0.75</sub>Cr<sub>0.25</sub>N the Cr atoms prefer to antiferromagnetic over ferromagnetic one, which is by ≈8 and ≈10 mHa per formula unit higher in energy, in GGA and hybrid functional, respectively. The site-, orbital-, and spin-projected DOS of antiferromagnetic Sc<sub>0.75</sub>Cr<sub>0.25</sub>N are shown in Figure 4.

The GGA calculations lead to a metallic state with an almost vanishing density at Fermi level and magnetic moments of

![Figure 4](image_url)

**Figure 4.** Site-, orbital-, and spin-projected DOS of Sc<sub>0.9T0.1</sub>N with T = Cr, Mn, Fe, Co, and Ni obtained from a) GGA and from hybrid functional with b) α = 0.1 and c) α = 0.2. The contributions of the atomic species (lines and colors) are the same as in Figure 3.
±2.75 $\mu_B$ located at the Cr ions. In contrast, use of the hybrid functional gives rise to a semiconducting state with a bandgap of ≈0.8 eV, and a slightly enhanced Cr magnetic moment of ±2.8 $\mu_B$.

The second part of our study consists to investigate the electronic structure and magnetic properties of the doped ScN nitride with a lower substitution concentration, that is, Sc$_{0.9}$T$_{0.1}$N-ordered compounds (T = Cr, Mn, Fe, Co, and Ni). Like in the previous case, we started first by considering a ferromagnetic alignment of the TM ions. The obtained DOS within GGA are shown along side with those obtained with hybrid functional frameworks in Figure 5. Here, we show the results of moderate ($\alpha = 0.1$) and highest ($\alpha = 0.2$) mixing parameters, and we omit the lowest one ($\alpha = 0.05$) because it does not bring noticeable changes to the GGA findings.

While GGA describes all the compounds as metals, the hybrid functional predicts both semiconducting and half-metallic ferromagnetic characters. Let us first note that the densities of N and Sc atoms are nearly not affected with respect to pure ScN, where the states of the former dominate the valence band and those of the latter are prevailing in the conduction band. In GGA (Figure 5a), the TM t$_{2g}$ states experience an exchange splitting of the two spin populations due to the weak bonding with nitrogen, which decreases in intensity going from Cr to Ni. In contrast, the e$_g$ states with a strong hybridization with N states show similar spin-up and spin-down distributions. The hybrid functional with a mixing parameter of $\alpha = 0.1$ leads to a half-metallicity in Cr-, Mn-, Fe-, and Ni-doped nitrides, whereas the Co-doped one still behaves as a metal. When increasing the parameter to $\alpha = 0.2$, some changes occur and we find a similar situation to the high concentration ($\alpha = 0.25$) compounds. Thus, Cr and Mn doping lead to semiconducting nitrides, whereas Sc$_{0.9}$Fe(Co,Ni)$_{0.1}$N one becomes half-metals. We note that the overall trends of the TM DOS and the contribution to the magnetic moments are also similar to the high concentration case.

Finally, we complemented this second part of the study by a check on the possible stability of antiferromagnetic alignment of the TM ions (AFM(001), as in the first case of high concentration). Here, and in contrast to the former case, all the Sc$_{0.9}$T$_{0.1}$N-doped nitrides are found energetically more stable in the ferromagnetic configuration.

4. Conclusion

To conclude, first-principles calculations as based on DFT were used to explore the change in electronic and magnetic behavior of ScN upon substitution with TM ions T = Cr, Mn, Fe, Co, and Ni, i.e., Sc$_{1-x}$Cr$_x$N, with two concentrations $x = 0.25$ and $x = 0.1$. In particular, the influence of exchange effects beyond the semilocal approximation as captured by the generalized gradient approximation was investigated.

In a first step, the electronic structure of ScN was studied by both GGA and hybrid functional calculations to establish a reference for the doped compounds. With a fraction as small as 5% of the exact exchange functional, the experimental bandgap of ScN of 0.9 eV could be reproduced.

Within GGA approximation, and initially focusing on the ferromagnetic state, we found Sc$_{0.75}$T$_{0.25}$N to be ferromagnetic metals for T = Mn, Fe, Co, and Ni, whereas Sc$_{0.75}$T$_{0.25}$N is a half-metal. Decreasing the substitution concentration to 10%, all Sc$_{0.9}$T$_{0.1}$N compounds are found metallic. Using hybrid functional framework, with increasing exact exchange mixing parameter, the electronic behavior of the compounds changes progressively. As a consequence, Sc$_{0.75}$T$_{0.25}$N is established as ferromagnetic half-metals for T = Fe, Co, and Ni, whereas Sc$_{0.75}$Cr(Mn)$_{0.25}$N is turned out to be semiconducting ferromagnets. Similar findings have been obtained in second substitution concentration Sc$_{0.9}$T$_{0.1}$N.

Considering antiferromagnetic ordering, it was found unstable for all Sc$_{0.75}$T$_{0.25}$N compounds except Sc$_{0.75}$T$_{0.25}$N, leading to a semiconducting antiferromagnetic ground state of this compound. In the lower concentration, however, all Sc$_{0.9}$T$_{0.1}$N compounds are found to prefer a ferromagnetic ground state.

We conclude that in the two limits of substitution concentrations, the predicted physical properties could be interesting for practical applications in spintronics.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords

chemical bonding, computational physics, density functional theory, Hartree-Fock, magnetic semiconductors, spintronics

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[1] M. Bowen, M. Bibes, M. A. Barthélémy, J. P. Contour, A. Anane, Y. Lemaitre, A. Fert, Appl. Phys. Lett. 2003, 82, 233.
[2] S. A. Wolf, D. D. Awschalom, R. A. Buhrman, J. M. Daughton, S. von Molnar, M. L. Roukes, A. Y. Chichkalanova, D. M. Treger, Science 2001, 294, 1488.
[3] C. M. Fang, G. A. De Wijs, R. A. De Groot, J. Appl. Phys. 2002, 91, 8340.
[4] S. Sonoda, S. Shimizu, T. Sasaki, Y. Yamamoto, H. Hori, J. Cryst. Growth 2002, 237, 1358.
[5] K. M. Yu, W. Walukiewicz, T. Wojtowicz, W. L. Lim, X. Liu, Y. Sasaki, M. Dobrowolska, J. K. Furdyna, Appl. Phys. Lett. 2002, 81, 844.
[6] K. Y. Wang, R. P. Champion, K. W. Edmonds, M. Sawicki, T. Dietl, C. T. Foxon, B. L. Gallagher, AIP Conf. Proc. 2005, 772, 333.
[7] T. Jungwirth, K. Y. Wang, J. Masek, K. W. Edmonds, J. Konig, J. Sinova, M. Polini, N. A. Goncharuk, A. H. MacDonald, M. Sawicki, A. W. Rushforth, R. P. Campion, L. X. Zhao, C. T. Foxon, B. L. Gallagher, Phys. Rev. B 2005, 72, 165204.
[8] M. B. Haider, C. Constantin, H. Al-Brithen, G. Caruntu, C. J. O'Connor, A. R. Smith, Phys. Status Solidi A 2005, 202, 1135.
[9] A. Herwadkar, W. R. L. Lambrecht, Phys. Rev. B 2005, 72, 235207.
[10] G. Schmidt, D. Ferrand, L. W. Molenkamp, A. T. Filipe, B. J. Van Wess, Phys. Rev. B 2000, 62, R4790.
[11] A. Houari, S. F. Matar, M. A. Belkhir, M. Nakhla, Phys. Rev. B 2007, 75, 064420.
[12] A. Houari, S. F. Matar, M. A. Belkhir, J. Magn. Magn. Mater. 2008, 322, 392.
[13] A. Houari, S. F. Matar, V. Eyert, Phys. Rev. B 2010, 82, 241201(R).
[14] V. Rajan, L. Bélaich, E. J. Walter, Phys. Rev. Lett. 2003, 90, 257602.
[15] D. Gall, I. Petrov, N. Hellgren, L. Hultman, J. E. Sundgren, J. E. Greene, J. Appl. Phys. 1998, 84, 6034.
[16] T. D. Mostakas, R. J. Moinar, J. P. Dismukes, Electrochem. Soc. Proc. 1996, 96, 197.
[17] H. A. Al-Brithen, A. R. Smith, Appl. Phys. Lett. 2000, 77, 2485.
[18] H. A. Al-Brithen, A. R. Smith, D. Gall, Phys. Rev. B 2004, 70, 045303.
[19] P. Burmistrova, J. Maassen, T. Favaloro, B. Saha, S. Salamat, Phys. Rev. B 2010, 82, 045204(R).
[20] D. Gall, I. Petrov, N. Hellgren, L. Hultman, J. E. Sundgren, J. E. Greene, J. Appl. Phys. 1998, 84, 6034.
[21] G. Conibeer, Mater. Today 2007, 10, 42.
[22] G. V. Naik, B. Saha, T. D. Sands, A. Boltasseva, in 4th Int. Topical Meeting on Nanophotonics and Metamaterials (NANOMETA 2013), Seefeld, Austria, 2013.
[23] H. A. Al-Brithen, E. M. Trifan, D. C. Ingram, A. R. Smith, D. Gall, J. Cryst. Growth 2002, 242, 345.
[24] D. Gall, I. Petrov, L. D. Madsen, J. E. Sundgren, J. E. Greene, J. Vac. Sci. Technol. A 1998, 16, 2411.
[25] N. Takeuchi, Phys. Rev. B 2002, 65, 045204.
[26] R. Monnier, J. Rhyner, T. M. Rice, D. K. Koelling, Phys. Rev. B 1985, 31, 5554.
[27] A. Neckel, P. Rastl, R. Eibler, P. Weinberger, K. Schwarzer, J. Phys. C 1976, 9, 579.
[28] R. Eibler, M. Dorrer, A. Neckel, Theor. Chim. Acta 1983, 63, 133.
[29] M. S. Abu-Jafara, A. M. Abu-Labdeh, M. El-Hasana, Comput. Mater. Sci. 2010, 50, 269.
[30] F. Tran, P. Blaha, J. Phys. Chem. A 2017, 121, 3318.
[31] C. Stampfı, R. Asahi, A. J. Freeman, Phys. Rev. B 2002, 65, R161204.
[32] A. Qteish, P. Rinke, M. Scheffler, J. Neugebauer, Phys. Rev. B 2006, 74, 245208.
[33] W. R. L. Lambrecht, Phys. Rev. B 2000, 62, 13538.

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