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Electronic structure of diluted magnetic semiconductors $\text{Ga}_{1-x}\text{Mn}_x\text{N}$ and $\text{Ga}_{1-x}\text{Cr}_x\text{N}$

Nandan Tandon¹, G P Das² and Anjali Kshirsagar^{1,3}

¹ Department of Physics, University of Pune, Pune 411 007, India

² Department of Material Science, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, India

E-mail: anjali@physics.unipune.ernet.in

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Abstract

We have undertaken a study of the diluted magnetic semiconductors $\text{Ga}_{1-x}\text{Mn}_x\text{N}$ and $\text{Ga}_{1-x}\text{Cr}_x\text{N}$ with $x = 0.0625, 0.125$, using the all-electron linearized augmented plane wave method (LAPW) for different configurations of Mn as well as Cr. We study four possible geometries of the impurity atoms in the wurtzite GaN structure to predict the energetically most favourable structure within a 32-atom supercell and conclude that the near-neighbour geometry has the lowest energy. The on-site magnetic moment at the transition metal site shows insignificant variation with distance. We have also analysed two configurations in which the local moments on the impurity atoms are parallel and anti-parallel. The density of states as well as band structure indicate a half-metallic state for all the systems. T_c has also been estimated for these systems and shows that for near-neighbour substitution of dopants T_c is above room temperature.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Gallium nitride doped with transition metals (TMs), is one of the most promising diluted magnetic semiconductor (DMS) materials for application in spintronics. By doping TM atoms, Mn or Cr, local magnetic moments are introduced in the semiconductor which mediate ferromagnetically. The Cr-doped GaN-based DMS is predicted to show high T_c [1] for high enough concentration of Cr. Hashimoto *et al* [2] further observed that (Ga, Cr)N-based DMS grown by electron cyclotron resonance (ECR) molecular beam epitaxy showed T_c above 400 K. Cr^+ -implanted GaN, studied by photoluminescence and superconducting quantum interference device (SQUID), reveal that the implanted Cr^+ incorporates substitutionally at the Ga site and

³ Author to whom any correspondence should be addressed.

the ferromagnetic order is retained up to 300 K [3]. Takeuchi *et al* [4] have reported a systematic study of changes in the occupied and unoccupied N-partial density of states (DOS) and confirm the wurtzite N 2p DOS and substitutional doping of Cr into Ga sites using soft x-ray emission spectroscopy (SXES) and x-ray absorption spectroscopy (XAS). Recently, ferromagnetism above 900 K was reported in Cr–GaN thin films [5]. Theoretically it was predicted that the ferromagnetic (FM) interaction in (Ga, Mn)N may be retained up to room temperature [6]. The initial reports of high T_c in (Ga, Mn)N were followed by controversial results where the reported T_c varied between 20 and 940 K [7–10]. Zajac and co-workers observed that Mn ions in $\text{Ga}_{1-x}\text{Mn}_x\text{N}$ ($x < 0.1$) crystals coupled in an anti-ferromagnetic (AFM) manner [11]. The electronic structure and magnetic properties of zinc blende $\text{Ga}_{1-x}\text{Mn}_x\text{N}$ for several values of x with varied spatial distribution of dopant atoms are discussed by Uspenskii *et al* [12] to understand the magnetic interactions for an explanation of FM–AFM competition. These calculations were done using the tight binding LMTO method within the local spin density approximation. Sanyal and Mirbt [13] have studied Mn-doped GaAs and GaN DMS using the *ab initio* plane wave code (VASP) within density functional theory (DFT). They have determined the interatomic exchange interactions by substituting Mn in various positions in the unit cell and have attributed the origin of ferromagnetism in (Ga, Mn)N to a double-exchange mechanism involving the hopping of Mn d electrons. Ferromagnetism in the metallic phase of (Ga, Mn)N thin layers has been studied by Boselli and co-workers [14], using the Monte Carlo technique. They have assumed indirect exchange of the RKKY type via the spin-polarized hole system and have obtained transition temperatures one order of magnitude higher than in similar (Ga, Mn)As nanostructures. A detailed review of the ferromagnetism in doped GaN is given by Liu *et al* [15]. Raebiger *et al* [16] used the full potential linearized augmented plane wave (FP-LAPW) method to investigate the interplay between clustering and exchange coupling in the magnetic semiconductor $\text{Ga}_{1-x}\text{Mn}_x\text{As}$. They have studied all possible arrangements of the two Mn atoms on the Ga sublattice for $x \sim 6\%$ and found that clustering of Mn atoms at near-neighbour Ga sites is energetically preferred. Our analysis of the wurtzite GaN doped with Mn or Cr is motivated by the latter study.

2. Method and computational details

We have employed the spin-polarized linearized augmented plane wave method (FP-LAPW) as implemented in the WIEN2K package [17] within the generalized gradient approximation (GGA) for the exchange–correlation potential proposed by Perdew, Burke and Ernzerof (PBE96) [18]. This is a state-of-the-art electronic structure method, which does not use any shape approximation for the potential, to solve the Kohn–Sham type of equations self-consistently.

GaN normally occurs in the wurtzite structure with lattice constants $a = 3.19 \text{ \AA}$ and $c = 5.19 \text{ \AA}$, giving a c/a ratio of 1.62. Each Ga is tetrahedrally bonded to N atoms at an average distance of 1.95 \AA and each N in turn is surrounded by four Ga neighbours. The calculations for DMS were performed within a 32-atom supercell, constructed from the $2 \times 2 \times 2$ standard unit cell of the wurtzite structure wherein the dopant is substituted at various cation sites, since it has been shown that the formation energy for interstitial Mn doping is higher than that for substitutional doping [13]. The supercell approach is used to restrict the dopant concentration to a small value, which is of interest for studying the magnetic properties of the system, without altering the original underlying lattice structure. Our interest was in observing the changes in the electronic structure of the DMS with respect to different possible geometries of the dopants within the host semiconductor. Self-consistent electronic structure calculations were performed using the APW + local orbitals (lo) basis set for the valence and semi-core

electrons with $R_{\text{MT}} * K_{\text{max}} = 7$, $l_{\text{max}} = 10$ and total energy convergence of 0.000 01 Ryd. The muffin-tin radii for Ga, Mn and Cr were kept at 2.0 Å and that for N at 1.6 Å. Spin-polarized calculations were carried out to observe the effect of spin-splitting and to calculate the on-site magnetic moment at the TM site.

We have studied wurtzite GaN doped with one TM atom impurity, which is $\sim 6.25\%$ doping, and two identical TM atoms in the 32 atom unit cell amounting to $\sim 12.5\%$ doping. To simulate different surroundings for the TM atoms we have spanned certain geometries within the 32-atom unit cell wherein the distance between the dopants is varied. In the case of the single impurity substitution, the nearest distance between two TM atoms is 6.38 Å in-plane and 10.38 Å along the c -axis. To find out the effect on impurity–impurity coupling we have studied four different geometries of two TM atom substitutions at 3.19 Å, near-neighbour (nn), 4.5, 5.19 and 6.08 Å separations. When two near-neighbour (nn) Ga atoms are substituted by TM atoms the in-plane TM–TM atom distance is 3.19 Å and along the c -axis it is 10.38 Å. For the second case the out-of-plane distance is 4.5 Å and the in-plane distance between the dopants is 6.3 Å. In the third case, two Ga atoms, lying one above the other and separated by a distance of 5.19 Å along the c -axis, are substituted by TM atoms and the in-plane TM atoms are at a distance of 6.38 Å. The last case is such that the in-plane separation (6.38 Å) and out-of-plane separation (6.09 Å) between the TM atoms is comparable. For estimating the magnetically favourable configuration, we have studied two possible orientations of the local magnetic moments on the impurity atoms. This is a local arrangement of the spins and has no long-range order. When we have the spins of the dopants locally aligned parallel to each other, we refer to it as the ferromagnetic (FM) arrangement and when the spins are locally aligned anti-parallel to each other, we refer to it as the anti-ferromagnetic (AFM) arrangement. The self-consistency was achieved on a mesh of $5 \times 5 \times 2$ k -points.

Structural relaxation for the TM site and the nn N sites was carried out to observe changes in the bond lengths between the TM and the first shell of N atoms. A very small change ($\sim 3\text{--}4\%$) was observed in the bond lengths and no significant changes were seen in the band structure, in agreement with the earlier reported results [19]. Thus the calculations reported here are for systems without allowing any relaxation.

3. Results

Pure GaN is a direct band gap semiconductor with the top of the valence band consisting of N p states and the bottom of the conduction band having Ga sp character. The Ga d levels are deep and do not take part in the bonding. Thus they are treated as semi-core states. The band gap of GaN, which is underestimated by density functional theory within the approximation used for the exchange correlation energy functional, is ~ 2 eV. The experimentally determined band gap of undoped GaN is ~ 3.4 eV. Das *et al* [20] have shown that, for Mn atoms to couple ferromagnetically, they need to be kept apart by more than the critical distance of 2.5 Å. Similar calculations on clusters of (GaN)Cr indicate that the critical Cr–Cr distance is 2.7 Å [21]. In all our calculations the distance between the dopants was greater than the corresponding critical distances.

3.1. Mn-doped systems

Localized magnetic moments are introduced within the GaN system by substituting the cations with TM impurity atom(s). The Mn atom, with $4s^2$ and $3d^5$ electrons in the valence region, replaces the Ga atom with valency $4s^2 4p^1$. On substitution, Mn atoms contribute five d levels per atom which are thus expected to contribute to the observed magnetic moment. Since three

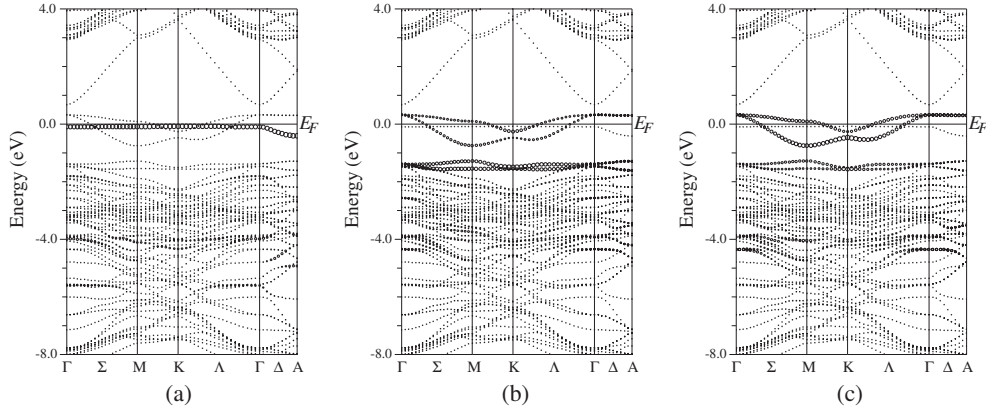


Figure 1. Mn-projected majority spin (a) $a_{1\uparrow}(d_{3z^2-r^2})$ (b) $e_{1\uparrow}(d_{xz} + d_{yz})$ and (c) $e_{2\uparrow}(d_{x^2-y^2} + d_{xy})$ bands in $\text{Ga}_{15}\text{MnN}_{16}$.

of the valence electrons from Mn go into compensating the three electron states of substituted Ga, one hole per Mn is introduced into the system. Figure 1 shows the Mn-projected majority spin d levels in the electronic structure for $\text{Ga}_{15}\text{MnN}_{16}$. The Mn d states lie at the top of the valence band and cross the Fermi level (ϵ_F) in some places. These are split into one singlet $a_{1\uparrow}(d_{3z^2-r^2})$ and two doublets $e_{1\uparrow}(d_{yz}, d_{xz})$ and $e_{2\uparrow}(d_{x^2-y^2}, d_{xy})$, out of which the $a_{1\uparrow}$ and $e_{1\uparrow}$ are filled, and $e_{2\uparrow}$ is half-filled. $a_{1\uparrow}$ and $e_{2\uparrow}$ lie close to ϵ_F , well above the valence band of GaN due to strong interaction with the N p states. Such interaction is not present for the Mn $e_{1\uparrow}$ level, rendering its position insensitive with respect to the valence band maxima (VBM) of GaN. The actual position depends on whether Ga(3d) electrons are treated as valence electrons or as core electrons [22]. All electron calculations performed with FP-LAPW method treat these electrons as semi-core and therefore are able to predict the position of the $e_{1\uparrow}$ level correctly. It lies about 1.4 eV below ϵ_F . The minority spin levels are empty and lie above ϵ_F , indicating 100% spin-polarized states. The Mn-induced states lie in the gap region of GaN. The top of the valence band in GaN is composed of the N p levels and the unique properties, particularly the half-metallic state of DMS, thus arise from the TM d and host p interactions that couple the two subsystems.

In order to understand the variation of exchange interaction among the TM impurity atoms with the distance between them, the concentration of Mn atoms was increased to 12.5%, equivalent to introducing 2 Mn atoms in the supercell. Self-consistent calculations were carried out for two different magnetic configurations of Mn electrons in which the spins of electrons on two atoms are parallel or antiparallel corresponding to the FM or AFM configuration. For all the geometries of the dopants, as described in section 2, the FM configurations of Mn atoms were found to have lower energy. Since the Mn d levels are responsible for the observed half-metallic behaviour, a comparison of Mn d DOS in various geometries is shown in figure 2, (a) for separations 3.19 and 5.2 Å and (b) for 6.0 and 6.3 Å. Here the half-metallic state is evident in all the cases. The TM–TM distance of 6.3 Å corresponds to single TM doping (6.25%).

The Mn d DOS is broad for substitution at nn distance. In all the other cases the band is split, indicating that the majority spin d bands, of the two Mn atoms at nn distance, overlap. On increasing the Mn–Mn distance, d-band splitting takes place, implying a reduction in the interaction between the TM atoms. It may be noted that the minority spin conduction band overlaps with the majority spin band for nn substitution. A gap of ~ 0.5 eV is present between the minority spin and majority spin conduction bands for Mn–Mn distance greater than nn. The

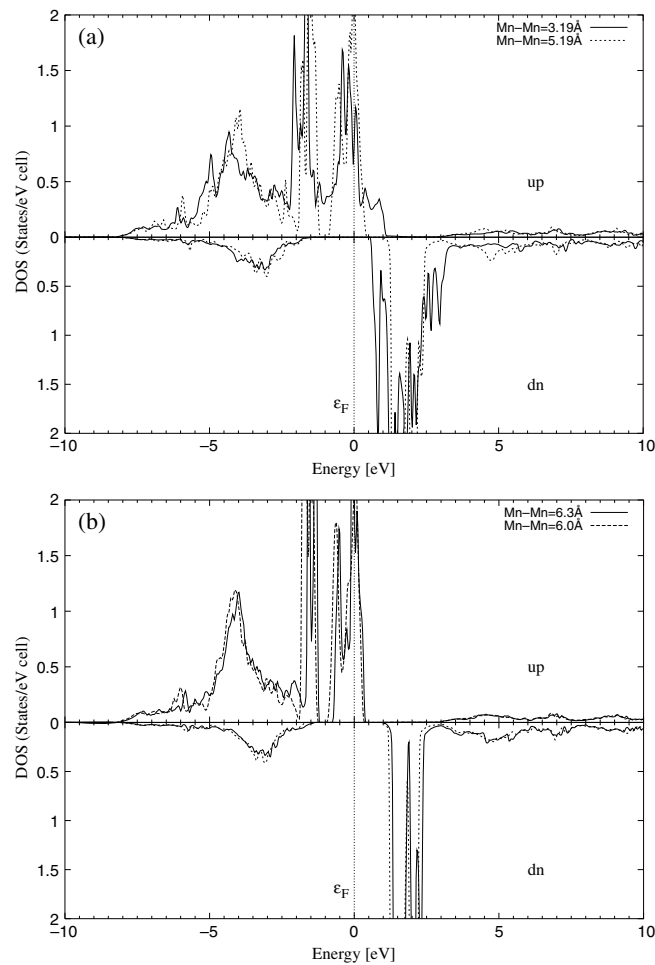


Figure 2. Mn-projected d DOS in $\text{Ga}_{14}\text{Mn}_2\text{N}_{16}$ (a) with Mn–Mn distance equal to 3.19 and 5.19 Å and (b) 6.0 and 6.3 Å. The upper and lower panels represent the majority and minority spin DOS respectively.

minority spin valence band as well as the conduction band is far apart from ϵ_F , thus retaining the highly spin polarized state, also seen in the single Mn-doped $\text{Ga}_{14}\text{MnN}_{16}$ system. The down-spin gap is 2 eV for the nn geometry and increases to 2.5 eV at larger separations. On increasing the distance between the Mn atoms, splitting of the d level increases. This is consistent with the observation that in single-impurity doping, the TM–TM atom distance is 6.3 Å and splitting of the Mn d band is larger, as seen in figure 2(b). The magnetic moment at the Mn site does not depend on the distance between the dopant atoms and has a value $3.34 \mu_B$ for all the geometries as indicated in table 1. The total magnetic moment per unit cell per Mn atom is $4 \mu_B$.

The presence of a localized moment influences the near-neighbour N atoms within the GaN system, such that the DOS of the nn N atoms around the impurity atom becomes as shown in figure 3(a). Due to the p–d interaction, induced states are seen on N atoms. The magnitude of the induced states is maximum at nn N atoms and decreases as the distance from the TM atom increases. This again indicates localized nature of the TM states. Figure 3(b) shows the spin charge density (SCD) in a plane containing three nn N atoms for single Mn doping. The plot

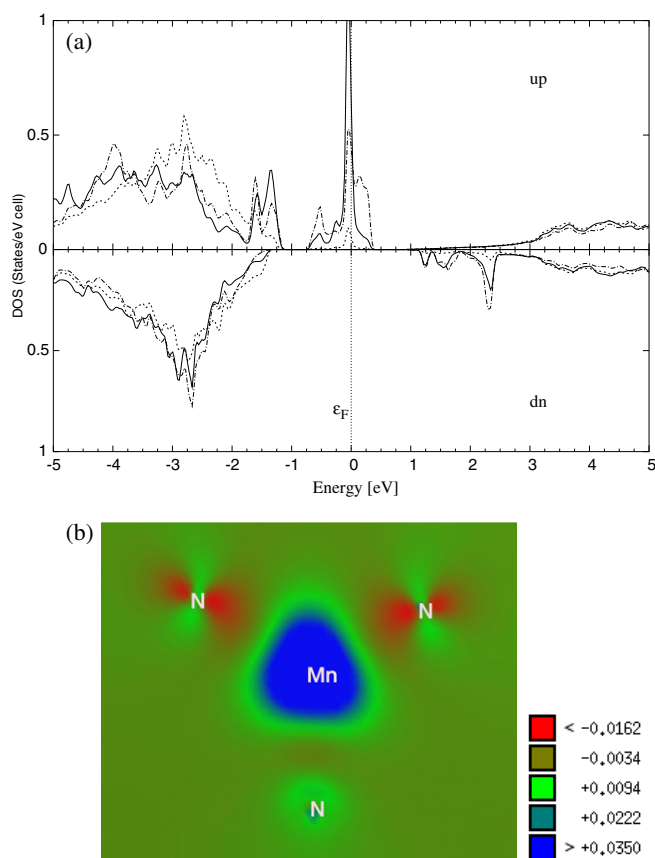


Figure 3. (a) Variation in partial DOS at three N-sites in $\text{Ga}_{15}\text{MnN}_{16}$. The solid lines: nn N along the c -axis. Dotted lines: nn N in plane. Dashed-dotted lines: next-nn N. (b) SCD plot in a plane of three nn N atoms.

Table 1. Magnetic moment (μ_B) in various Mn-doped systems. $\text{Total}_{\text{mom}}$ indicates mag. mom./unit cell, $\text{dopant}_{\text{mom}}$ is the magnetic moment at the dopant site and N_{mom} is the average magnetic moment at nn N sites.

System	$\text{Total}_{\text{mom}}$	$\text{Dopant}_{\text{mom}}$	N_{mom}
$\text{Ga}_{15}\text{MnN}_{16}$	4.00	3.33	0.001
$\text{Ga}_{14}\text{Mn}_2\text{N}_{16}$ Mn–Mn = 3.19 Å	8.00	3.34	0.001
$\text{Ga}_{14}\text{Mn}_2\text{N}_{16}$ Mn–Mn = 4.5 Å	8.00	3.34	0.005
$\text{Ga}_{14}\text{Mn}_2\text{N}_{16}$ Mn–Mn = 5.19 Å	8.00	3.33	0.006
$\text{Ga}_{14}\text{Mn}_2\text{N}_{16}$ Mn–Mn = 6.0 Å	8.00	3.34	0.005

shows that the SCD on the N atoms lying above the Mn atom is negative whereas it is positive for the N atom lying below the Mn atom. The average magnetic moment on the nn N atoms is positive as shown in table 1 for all the different geometries.

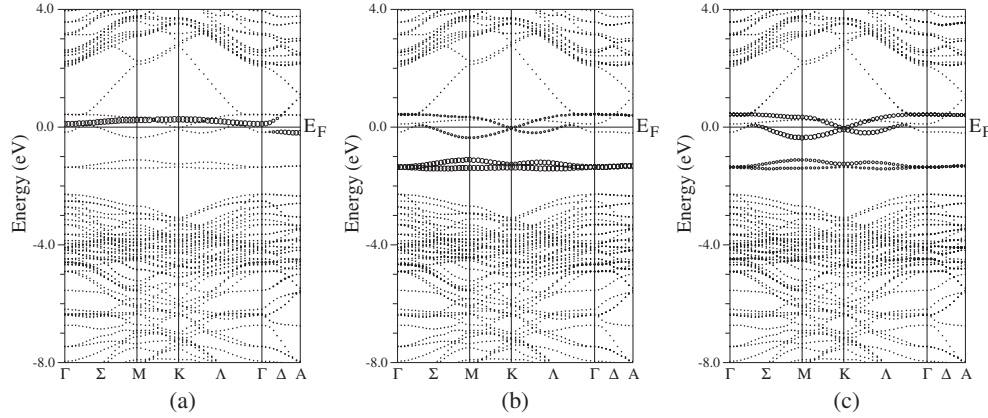


Figure 4. Cr-projected majority spin (a) $a_{1\uparrow}(d_{3z^2-r^2})$, (b) $e_{1\uparrow}(d_{xz} + d_{yz})$ and (c) $e_{2\uparrow}(d_{x^2} + d_{xy})$ bands in $\text{Ga}_{15}\text{CrN}_{16}$.

Table 2. Magnetic moment (μ_B) in Cr-doped systems. $\text{Total}_{\text{mom}}$ indicates mag.mom./unit cell, $\text{dopant}_{\text{mom}}$ is the magnetic moment at the dopant site and N_{mom} is the average magnetic moment at the nn N sites.

System	$\text{Total}_{\text{mom}}$	$\text{Dopant}_{\text{mom}}$	N_{mom}
$\text{Ga}_{15}\text{CrN}_{16}$	3.00	2.47	-0.025
$\text{Ga}_{15}\text{Cr}_2\text{N}_{16}$	6.00	2.48	-0.031
Cr-Cr = 3.19 Å			
$\text{Ga}_{15}\text{Cr}_2\text{N}_{16}$	6.00	2.47	-0.022
Cr-Cr = 4.5 Å			
$\text{Ga}_{15}\text{Cr}_2\text{N}_{16}$	6.00	2.48	-0.025
Cr-Cr = 5.19 Å			
$\text{Ga}_{15}\text{Cr}_2\text{N}_{16}$	6.00	2.48	-0.026
Cr-Cr = 6.0 Å			

3.2. Cr-doped systems

An electronic structure calculation for substitutional doping of Cr in the GaN system was also done, and it was analysed in a similar fashion. For each Cr doped in the 32-atom supercell, equivalent to 6.25% doping, there are five spin-up d states which are introduced in the GaN band gap. Since the Cr atom has $4s^23d^4$ valence electrons, only three of the electron states out of the five 3d levels are occupied, thus creating two hole states per Cr substitution. Single Cr doping into the 32-atom supercell at the cation site results in the Cr d levels appearing in the band gap of the semiconductor host as seen in figure 4. The Cr d states, like the Mn d states, split into one singlet $a_{1\uparrow}(d_{3z^2-r^2})$ and two doublets $e_{1\uparrow}(d_{yz}, d_{xz})$ and $e_{2\uparrow}(d_{x^2-y^2}, d_{xy})$. Out of these $e_{1\uparrow}$ lies below ϵ_F and is completely filled and other three levels are partially (1/3) filled. As in the case of Mn doping, the Cr minority spin d states are above ϵ_F and so the impurity states at ϵ_F are 100% spin polarized.

In the $\text{Ga}_{14}\text{Cr}_2\text{N}_{16}$ system, figure 5 shows that even though the Cr atoms are substituted at nn sites there is a gap seen between the split Cr majority d levels, unlike in the nn Mn-doped system. The minority spin conduction band overlaps with the majority spin conduction band for the nn Cr case, as in the nn Mn case. For all the geometries of the dopant atoms the system is half-metallic. The band gap for the minority spin, in the case of two Cr substitutions at 3.19 Å,

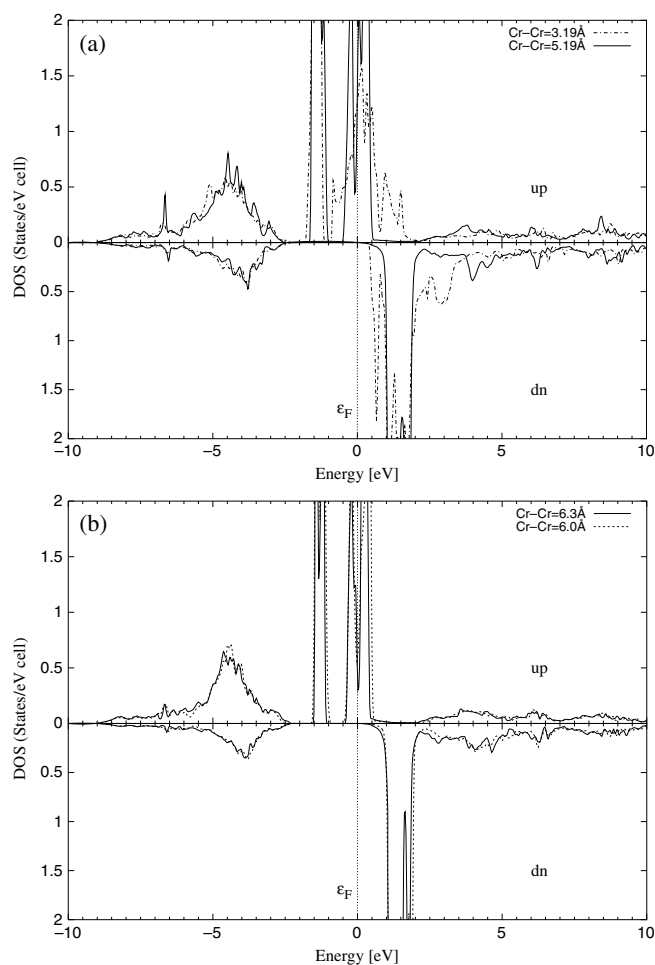


Figure 5. Cr-projected d DOS in $\text{Ga}_{14}\text{Cr}_2\text{N}_{16}$ for Cr–Cr separation of (a) 3.19 and 5.19 Å and (b) 6.0 and 6.3 Å.

is ~ 3 eV, which is larger than the corresponding Mn case which has a gap of ~ 2.0 eV. When the TM–TM distance is 5.19 Å, in the Cr case the gap is ~ 3.0 eV whereas for Mn substitution it is ~ 2.5 eV. The lowest energy configuration for Cr substitution occurs for a Cr–Cr distance of 3.19 Å and for all the geometries studied the FM configuration of TM atoms has lower energy compared to the AFM configuration. The magnetic moments at the Cr site in various geometries are as shown in table 2. Again it is seen that the magnetic moment does not show much variation depending on the distance, indicating that the direct interaction between the Cr atoms is minimal, as in the case of Mn doping.

The magnetic moment per unit cell per Cr atom is $3 \mu_B$. The average magnetic moment on the nn N atom is anti-parallel to the Cr moment. This may be contrasted with the average magnetic moment on the nn N atoms in the case of Mn doping which is parallel to the Mn moment. This can be understood as penetration of the spin-polarized Mn states to the neighbouring host which does not have any of its own states in the gap region. It may be mentioned that the difference in the orientation of the average magnetic moment on nn N atoms of Mn and Cr is due to the difference in the p DOS of the nn N along the z -axis

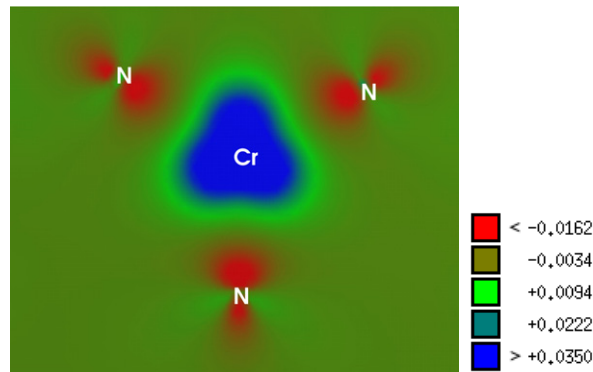


Figure 6. SCD plot in a plane of three nn N atoms around the TM atom in $\text{Ga}_{14}\text{CrN}_{16}$.

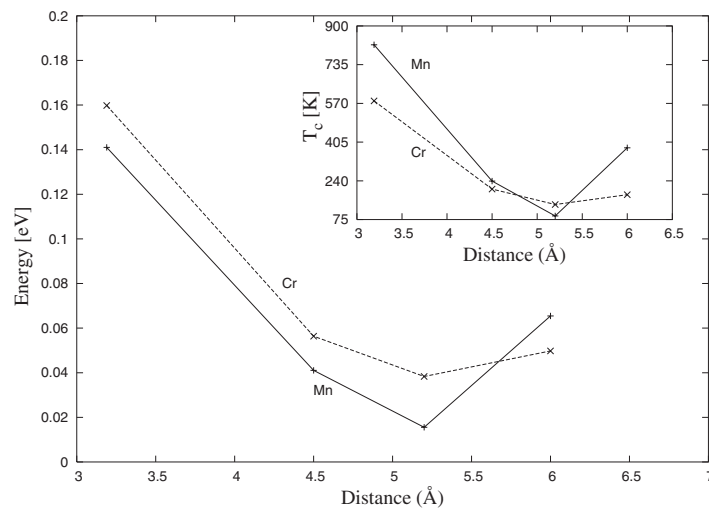


Figure 7. $\Delta E = E_{\text{AFM}} - E_{\text{FM}}$ for Mn and Cr doping. The inset shows the mean field T_c variation with distance between dopants.

(figure not shown here) compared to the nn N atoms lying in the xy plane above the TM atoms. The magnitude of the average nn N magnetic moment is greater in the case of Cr substitution, which contributes one less electron to the hybridized valence band. The SCD in figure 6 on all of the nn-N atoms of the single Cr (only three nn N atoms are shown in figure 6) doped system is negative, thus showing that the TM atom and the nn N are anti-ferromagnetically coupled.

3.3. Estimation of T_c

We have predicted T_c for the DMS based on $\text{Ga}_{16}\text{Mn}_2\text{N}_{16}$ and $\text{Ga}_{16}\text{Cr}_2\text{N}_{16}$ considering the mean field approximation. Figure 7 shows $\Delta E = E_{\text{AFM}} - E_{\text{FM}}$ for the Mn/Cr-doped systems, where E_{AFM} is the total energy for the antiferromagnetic (AFM) configuration and E_{FM} is the total energy for the ferromagnetic (FM) configuration. The variation of ΔE with distance between the dopants for Mn-substituted DMS agrees with the one reported by Sanyal [13]. ΔE is a measure of the exchange interaction in the system. The highest ΔE is seen for the case where the TM atoms are substituted as near neighbours, signifying larger overlap of the

magnetic impurity orbitals. For Mn doping at near neighbours, $\Delta E \sim 0.14$ eV compares well with the value calculated for dimer substitution by Uspenskii *et al* [12] and matches with the measured $T_c = 940$ K [9]. For the identical Cr case, $\Delta E \sim 0.16$ eV also compares well with the observed T_c but is lower than the 900 K observed by Liu and co-workers [15]. From figure 7 it also emerges that the exchange interaction decreases sharply as the distance between the TM atoms increases. Thus the exchange interaction is short ranged.

4. Summary and conclusions

The present work employed the all-electron full potential LAPW method to study the electronic structure and related properties of diluted magnetic semiconductors $\text{Ga}_{1-x}\text{Mn}_x\text{N}$ and $\text{Ga}_{1-x}\text{Cr}_x\text{N}$. The method is a state-of-the-art electronic structure method and treats the core electrons fully relativistically. It was therefore felt necessary to employ such a reliable method to study these systems to resolve a few issues related to (i) the positioning of impurity levels with respect to the host band, (ii) hybridization of TM states with the host states and (iii) the nature of charge density and spin charge density in these materials. We have analysed the electronic structure of GaN doped with TMs Mn and Cr with 6.25% and 12.5% doping for various possible geometries to replicate the situation where the TM atoms would appear either to cluster or be separated. Our calculations predict a half-metallic state for both 6.25% and 12.5% doping. Comparing the total energies of the FM and AFM configurations for 12.5% doping, the FM state is found to be lower in energy and is predicted to be the preferred state. The self-consistent FP-LAPW calculations give accurate total energies resulting in quite reliable exchange interaction. The on-site magnetic moment at the TM site shows insignificant variation with distance between the dopants. The nn N atoms contribute to the states in the energy gap of the semiconductor due to the influence of the TM atoms. The average magnetic moment at the nn N site is parallel to the Mn magnetic moment whereas it is anti-parallel to the Cr magnetic moments. We observe that both the systems with nn substitution of Mn/Cr atom would show high T_c . The energy gap between the minority spin band in Mn is ~ 1 eV lower than in the Cr-doped system. But the magnetic moment at the Mn site is higher than that at the Cr site. It would therefore be of interest to study mixed systems of Mn and Cr to incorporate the salient features of both TM atoms and to tailor a suitable system for DMS applications.

Acknowledgments

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