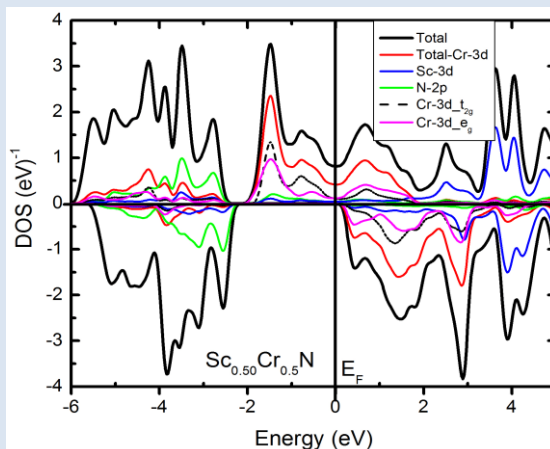


THEORETICAL STUDY OF THE STRUCTURAL AND ELECTRONIC PROPERTIES OF THE $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ COMPOUNDMiguel J. Espitia ^{R1}, John H. Díaz ^{F1}, César Ortega López^{2*}

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ABSTRACT

First principles calculations based on density functional theory were employed to investigate the structural, electronic, and magnetic properties of the $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.0, 0.25, 0.50, 0.75$, and 1.0) compound, in the wurtzite structure. We applied the full-potential linearized augmented plane wave (FP-LAPW) method as implemented in the Wien2k code. The analysis of the structural properties revealed that the lattice constant increases linearly with the increment of the Sc atoms in the structure, in accord with Vegard's law, whereas the bulk modulus decreases. The studies of the electronic density showed that the ternary compounds of $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) exhibit a half-metallic behavior with magnetic spin polarization of 100% and a magnetic moment of $3 \mu_B/\text{Cr-atom}$. The ferromagnetic behavior comes from a double exchange mechanism and hybridization of the Cr-d and N-p states that cross the Fermi level. These compounds are good candidates for applications in spintronics.

Keywords: DFT, structural properties, half-metallic ferromagnetism.

ESTUDIO TEORICO DE LAS PROPIEDADES ESTRUCTURALES Y ELECTRONICAS DE LOS COMPUESTOS $\text{Sc}_x\text{Cr}_{1-x}\text{N}$

RESUMEN

En este trabajo se realizaron cálculos por primeros principios para investigar las propiedades estructurales, electrónicas y magnéticas de los compuestos $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.0, 0.25, 0.50, 0.75$ y 1.0) en la estructura wurtzita. Se utilizó el método Ondas Plana Aumentadas y Linealizadas Potencial Completo (FP-LAPW), tal como está implementado en el código Wien2k. El análisis de las propiedades estructurales muestra que la constante de red aumenta linealmente acorde a la ley de Vegard's, con el incremento de la concentración de escandio Sc en la estructura, mientras que el módulo de volumen disminuye. Los estudios de la densidad electrónica muestran que los compuestos $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$ y 0.75) poseen un comportamiento semimetálicos con polarización de espín magnético del 100%, y un momento magnético de $3 \mu_B/\text{atomo-Cr}$, el estado ferromagnético proviene de un mecanismo de doble intercambio y de la hibridación de los estados Cr-d y N-p que atraviesan el nivel de Fermi. Estos compuestos son buenos candidatos para aplicaciones en espintrónica.

Palabras Claves: DFT, propiedades estructurales, ferromagnetismo semimetálico.

1. INTRODUCTION

Spintronics is a new branch of microelectronics in which essentially the spin of the charge carriers is used [1]. The expected advantages of spintronic devices over conventional electronic ones are nonvolatility, increased data processing speed, increased transistor density, and decreased power consumption [2]. The study of half-metallic ferromagnetism in semiconductors doped with transition metals is a topic of much current research, because of the promising applications of these materials in the field of spintronics [1, 3, 4] and spin injectors [5]. In recent years, the indirect gap semiconductor ScN [6] has begun to be studied for possible applications in diluted magnetic semiconductors, spintronic devices, and spin injectors. Al-Brithen et al. [7] grew $\text{Sc}_{1-x}\text{Mn}_x\text{N}$ via the molecular beam epitaxial technique, while A. Alsaad et al. [8] carried out studies of the structural and magnetic properties of the diluted magnetic $\text{Mn}_x\text{Sc}_{1-x}\text{N}$ semiconductors using density functional theory (DFT). Additionally, Birch J. et al. [9] grew ScN/CrN multilayers epitaxially via the magnetron sputtering technique.

In the present paper, a theoretical study of the structural, electronic, and magnetic properties of $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) was carried out, due to its potential applications in spintronic devices and spin injectors.

2. COMPUTATIONAL METHOD

The calculations were performed within the framework of density functional theory (DFT), and the full-potential linearized augmented plane wave (FP-LAPW) method was used as implemented in the Wien2k software package [10]. The exchange and correlation effects of the electrons were dealt with using the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) [11]. In the LAPW method, the cell is divided into two types of regions, namely spheres centered at the atomic nuclear sites and an interstitial region between non-overlapping areas. Within the atomic spheres, wave functions are replaced by atomic functions; whereas in the interstitial region, the function is expanded in the form of plane waves. The charge density and potential expand to form spherical harmonics up to $l_{\text{max}} = 10$ inside the atomic spheres, and the wave function in the interstitial region expands in the form of plane

waves with a cutoff parameter of $R_{\text{MT}} K_{\text{max}} = 8$, where R_{MT} is the smallest radius of the atomic level within the unit cell and K_{max} is the magnitude of the largest k vector of the reciprocal lattice. To ensure convergence in the integration of the first Brillouin zone, 1600 points were used, which corresponds to 140 k -points at the irreducible part of the first Brillouin. The integrals over the Brillouin zone were solved using the special approximation of k points provided by the Monkhorst-Pack method. Self-consistency was achieved by requiring that the convergence of the total energy be less than 10^{-4} Ry. To achieve expansion of the potential in the interstitial region, it was considered that $G_{\text{max}} = 12$. The corresponding muffin-tin radii were 1.6 bohr for N, 1.85 bohr for Sc, and 1.95 bohr for Cr. Calculations were performed considering the spin polarization caused by the presence of Cr in the compounds. To calculate the lattice constant, the minimum volume, the bulk modulus, and the cohesive energy of the two structures studied, calculations were fit to the Murnaghan equation of state [12] Eq (1)

$$E(V) = E_0 + \frac{B_0 V}{B'_0} \left[\frac{(V_0/V)^{B'_0}}{B'_0 - 1} + 1 \right] - \frac{B_0 V_0}{B'_0 - 1} \quad (1)$$

Where B_0 is the bulk modulus, its first derivative is B'_0 , V_0 is equilibrium volume of the cell, and E_0 represents the cohesive energy.

In order to study the relative stability of $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) compounds in concentration of x ScN molecules and $1-x$ CrN molecules, the energy of formation was calculated. For the ternary compound, the energy of formation is defined as the difference between the total energy of the ternary phase $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ and the total energy of the binary compounds in their ground state, GaN wurtzite and CrN zincblende, $E_{\text{GaN}}^{\text{wurtzite}}$ and $E_{\text{CrN}}^{\text{zincblende}}$, respectively. Therefore, the energy of formation is given by Eq. (1) [13, 14]

$$\Delta E_f = E_{\text{Sc}_x\text{Cr}_{1-x}\text{N}} - (1-x)E_{\text{CrN}}^{\text{zincblende}} - xE_{\text{GaN}}^{\text{wurtzite}} \quad (2)$$

3. RESULTS AND DISCUSSION

3.1 Structural properties

To determine the structural properties in the ground state, such as the lattice constant (a_0), the bulk

modulus (B_0), and the total energy (E_0) of ScN and CrN binary compounds and allowed ternary $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) compounds in the wurtzite structure, the variation of total energies and equilibrium volumes were fit to Murnaghan's equation of state, Equation (1). Additionally, in order to investigate the magnetic phase most favorable of compounds ($x = 0.25, 0.50$ and 0.75), the total energies of different compounds as functions of volume have been calculated in both ferromagnetic phase (FM) and antiferromagnetic phase (AFM) states. Figure 1 shows the energy-volume curves of $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ compounds for $x = 0.25, 0.50$ and 0.75 in the FM and AFM states.

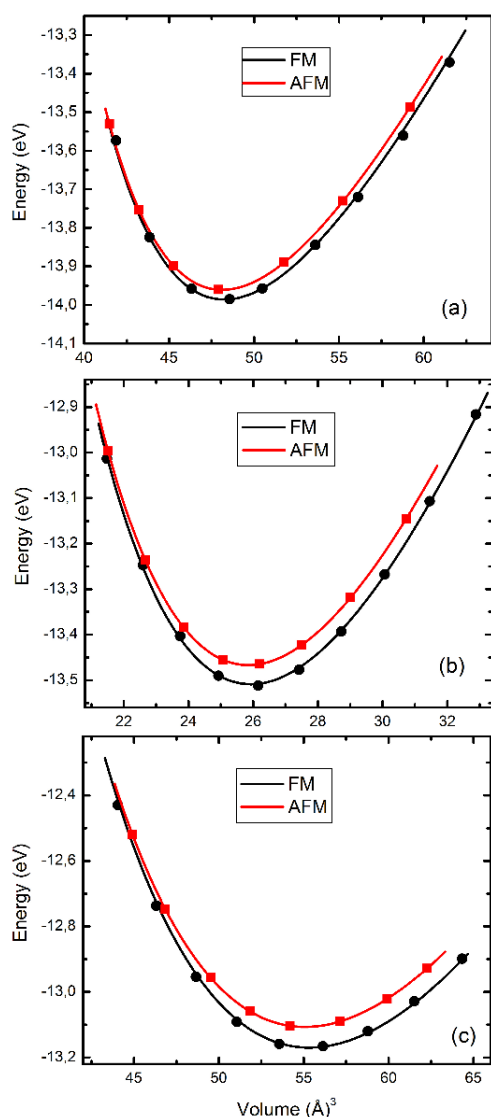


Figure 1. Total energy as a function of volume for the allowed ternary compounds of $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ (a) $x = 0.25$ (b) $x = 0.50$ and (c) $x = 0.75$ in both FM and AFM states.

The calculated total energy differences between the FM and AFM states are about -0.025 , -0.042 and -0.063 eV for $x = 0.25, 0.5$ and 0.75 , respectively. For all cases, FM states are more favorable in energy than AFM states, so the FM phase is a stable ground state for $\text{Sc}_x\text{Cr}_{1-x}\text{N}$. Our results and various theoretical data are listed in Table 1

Table 1. Structural parameters

Compound	Crystal system		In this work	Other calculation
CrN	Hexagonal P6 ₃ mc N° 186	a_0 (Å)	3,21	3,142 ^a
		B_0 (GPa)	192,80	-
		E_0 (eV)	-14,85	-
		$\mu_B/\text{Cr-atom}$		
ScN	Hexagonal P6 ₃ mc N° 186	a_0 (Å)	3,52	3,49 ^b -3,58 ^c
		B_0 (GPa)	156,06	156 ^b -148,3 ^c
		E_0 (eV)	-13,56	-13,35 ^b /-13,75 ^c
		$\mu_B/\text{Cr-atom}$	0	
$\text{Sc}_{0.25}\text{Cr}_{0.75}\text{N}$	Trigonal P3m1 N° 156	a_0 (Å)	3,217	
		B_0 (GPa)	183,90	-
		E_0 (eV)	-13,98	
		$\mu_B/\text{Cr-atom}$	3,0	
$\text{Sc}_{0.50}\text{Cr}_{0.50}\text{N}$	Trigonal P3m1 N° 156	a_0 (Å)	3,32	
		B_0 (GPa)	175,0	-
		E_0 (eV)	-13,81	
		$\mu_B/\text{Cr-atom}$	3,0	
$\text{Sc}_{0.75}\text{Cr}_{0.25}\text{N}$	Trigonal P3m1 N° 156	a_0 (Å)	4.408	
		B_0 (GPa)	165,40	-
		E_0 (eV)	-13,17	
		$\mu_B/\text{Cr-atom}$	3,0	

a [15] Theoretical GGA

b [16] Theoretical GGA

c [17] Theoretical GGA

The ground state structural properties (a_0 , B_0 , E_0) for the wurtzite structure of the binary compounds ScN and CrN are very close to the theoretical results [15-17]. For the allowed ternary $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25$,

0.50, and 0.75) compounds, structures are obtained by replacing Cr atoms with Sc atoms in the supercell. For $x = 0.25$ and $x = 0.50$, a Cr atom is replaced by a Sc atom in a supercell of 8 and 4 atoms, respectively. For $x = 0.75$, three Cr atoms are replaced by three Sc atoms in the supercell of 8 atoms. The figure 2 shows the crystal structure of the allowed ternary $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) compound obtained after structural relaxation. In all cases, the space group obtained is the same, the tetragonal structure $P3m1$ ($N^\circ 156$). As we can see in Table 1, the values of the bulk modulus of the allowed ternary $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) compounds are larger, and therefore they are quite rigid, making them good candidates for possible applications in devices that must operate at high temperatures and high power, and in hard coatings.

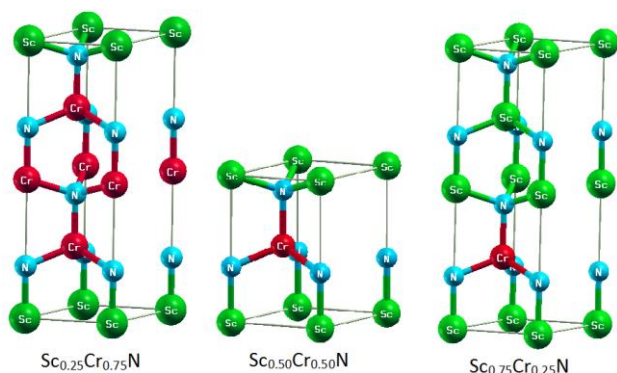


Figure 2. Unit cell of the allowed ternary $\text{Sc}_{0.25}\text{Cr}_{0.75}\text{N}$, $\text{Sc}_{0.50}\text{Cr}_{0.50}\text{N}$ and $\text{Sc}_{0.75}\text{Cr}_{0.25}\text{N}$ compound after structural relaxation.

Figure 3 shows the variation of the lattice constant as a function of the concentration of Sc. It can be observed that the lattice constant equilibrium increases with increasing concentration (x) of Sc atoms. This can be attributed to the fact that the atomic radius of Sc $r_{\text{Sc}} = 1.62 \text{ \AA}$ is much larger than the atomic radius of Cr $r_{\text{Cr}} = 1.27 \text{ \AA}$. On the other hand, Figure 4 shows that the modulus decreases with an increasing amount (x) of the concentration of Sc atoms in all compounds. A similar result obtained was by López W. et al. [17] in their study of the structural properties of the $\text{Sc}_{1-x}\text{In}_x\text{N}$ compound in the wurtzite structure.

Figure 3 shows that the lattice constant increases linearly with the concentration of Sc atoms. Conventionally, the lattice constant $a(x)$ of the ternary $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ compound is described by

Vegard's law [18], which expresses the lattice constant of each ternary compound $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) as a linear combination of the lattice constants of the two binary compounds, as follows: $a(x) = xa_{\text{ScN}} + (1-x)a_{\text{CrN}}$. However, there is a small upward deviation of the linear behavior of the lattice constant of the allowed $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ compounds with respect to Vegard's law. We calculated the value of the deviation λ_a , with the equation $a(x) = xa_{\text{ScN}} + (1-x)a_{\text{CrN}} + \lambda_a x(1-x)$ [19]. We found a small value, $\lambda_a = -0.0405 \text{ \AA}$, for the lattice constant deviation of allowed $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ compounds in the wurtzite structure. The small value of the deviation can be attributed to the fact that the lattice constants of ScN and CrN compounds are similar. The lattice constant of ScN is 11.3% larger than the lattice constant of CrN. In this case, the ternary compound $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) satisfies Vegard's law because interactions between inoes (Sc, Cr and N) which form the ternary compounds are weak.

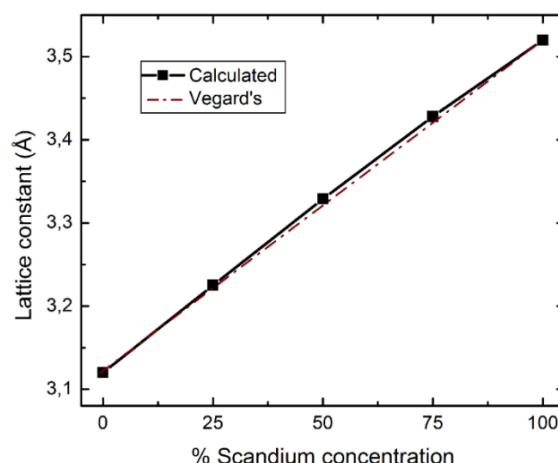


Figure 3. Lattice constant as a function of the scandium concentration for the allowed $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ compounds in the wurtzite phase. The calculations (square dots) are compared with the linear trend of Vegard's law.

Table 2 shows the energy formation values of the allowed ternary $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) compounds, which we calculated using Equation 2. We can see in Table 1 that the energy of binary compounds in their ground state is negative, whereas, according to the results of Table 2, the value of the energy of formation of each ternary compound is positive; therefore, the $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) compounds are metastable.

This implies that a ternary compound can't grow under equilibrium conditions, so to grow them it is necessary to supply power to the system [12, 13]. The result that we found for the energy of formation is very important, because these values will improve the growth conditions and will therefore produce $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) compounds of excellent quality.

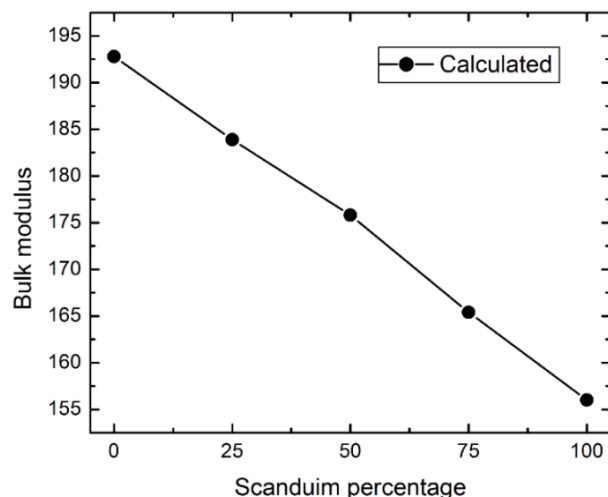


Figure 4. Bulk modulus as a function of the concentration of Sc atoms for the $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ compound in the wurtzite phase.

Table 2. Energy of formation of the allowed ternary $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) compound.

Compound	ΔE_0 (eV)
$\text{Sc}_{0.25}\text{Cr}_{0.75}\text{N}$	0.225
$\text{Sc}_{0.50}\text{Cr}_{0.50}\text{N}$	0.395
$\text{Sc}_{0.75}\text{Cr}_{0.25}\text{N}$	1.035

According to Table 2, the $\text{Sc}_{0.25}\text{Cr}_{0.75}\text{N}$ compound has the smallest value by far of the energy of formation, and therefore it is the most energetically stable.

3.2 Electronic properties

The theoretical lattice constants of the allowed $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) compounds shown in Table 1 were used to calculate the spin-polarized density of states (DOS) and the band

structure along the high symmetry direction in the first Brillouin zone.

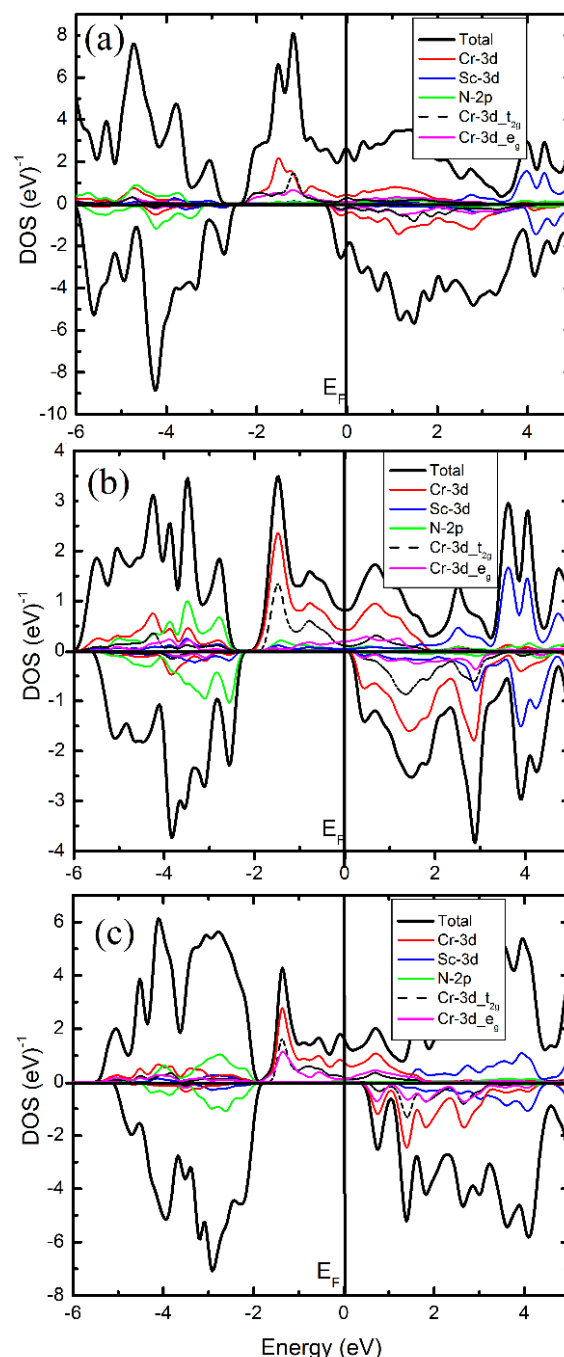


Figure 5. Partial and total density of states for the allowed ternary compounds of $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ (a) $x = 0.25$ (b) $x = 0.50$ and (c) $x = 0.75$

The total spin-polarized density of states (TDOS) and partial spin-polarized density of states (PDOS)

for $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) are shown in Figure 5. It is clear that $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25$) does not exhibit half-metallicity (i.e., valence and conduction bands cross the Fermi level). However, the TDOS for $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.50$ and 0.75) are half-metallic and ferromagnetic, since in the valence band near the Fermi level the majority spin (spin-up) is metallic, and the minority spin (spin-down) is semiconducting. The $\text{Sc}_{0.50}\text{Cr}_{0.50}\text{N}$ and $\text{Sc}_{0.75}\text{Cr}_{0.25}\text{N}$ compounds exhibit 100% polarization of the conduction carriers in the ground state, which is required in spin injection [20]. This suggests that it can be used efficiently for injection of spin polarized charge carriers. Figure 5 shows that above the valence band the density of the up spin and below the conduction band the minority spins are mainly dominated by the hybrid state Cr-3d, and N-2p makes a smaller contribution. Additionally, based on crystal field theory, when a Cr atom replaces an atom of Sc, the tetrahedral crystal field formed by the N ion at the cationic site splits the five-fold degenerate 3d states of the Cr ion into three degenerate states of high energy, t_{2g} (d_{xy} , d_{xz} , and d_{yz}) and two degenerate states of low energy e_g (d_{z^2} and $d_{x^2-y^2}$) [21]. The electron configuration of the Cr atom in the $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) compounds can be attributed to the Cr^{3+} [22]. The figure 6 shows the Cr-3d level split in minority and majority spin due to the exchange and show the splitting into doubly degenerate e_g and triply degenerate t_{2g} levels, when put Cr^{3+} atom in a tetrahedral environment, in this case there is not contribution of spin down, according to the density of states figure 5. We explain better the configuration of Cr^{3+} atom, we know that Cr atoms have six valence electrons $\{[\text{Ar}]3d^5 4s^1\}$. When Cr occupies the site of Sc, it donates three electrons. Of the remaining three electrons, two electrons occupy the doubly degenerate e_g states and one electron and two holes the triply degenerate t_{2g} state. Therefore, the major spin states of Cr-3d are not filled, because although the doubly degenerate state is completely filled, the triply degenerate state is only one-third full. As a result, the three electrons produce a total magnetic moment of $3 \mu_B/\text{atom-Cr}$. Therefore the compounds exhibit a half-metallic ferromagnetic behavior.

Additionally, according to the theory by Jhi et al. [23], the hybridization of the metallic Cr-3d states and the nonmetallic N- 2p electrons that cross the

Fermi level results in a strong covalent bond, which is responsible for the high rigidity of the ternary compounds.

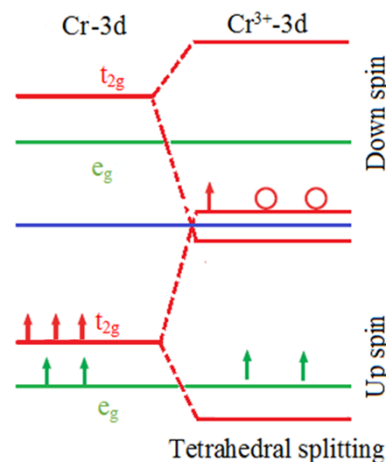


Figure 6. Schematic mechanisms of the Cr 3d level split in minority and majority spin due to the exchange and the splitting into doubly degenerate e_g and triply degenerate t_{2g} levels, when put Cr^{3+} atom in a tetrahedral environment. The formation of the local moment (given by the contribution of the majority represented by up arrows) as well as the two holes represented by empty circles is clearly shown.

Figure 7 shows the band structures of the $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) ternary compounds. For $x = 0.25$ and 0.50 ($\text{Sc}_{0.50}\text{Cr}_{0.50}\text{N}$ and $\text{Sc}_{0.75}\text{Cr}_{0.25}\text{N}$), Figures 4a and 4c confirm the half-metallic nature of both compounds. For $x = 0.75$ ($\text{Sc}_{0.25}\text{Cr}_{0.75}\text{N}$), Figure 5c shows the metallic behavior of the two spin channels. However, we can see that the minority spin has a gap while the majority spin has a metallic character, because strong hybridization appears between Cr-3d(t_{2g}) and N-2p, dominating both the DOS and the band structure at the Fermi level in the three compounds. Additionally, increasing value of the concentration of Cr atoms results in the broadening of the partially filled t_{2g} band, so DOS weight transfers from the Fermi level to lower energies, thereby leading to a gain in energy [24, 25]. Energy gain due to band broadening is known as Zener's double exchange, and is responsible for stabilizing the ferromagnetism [26].

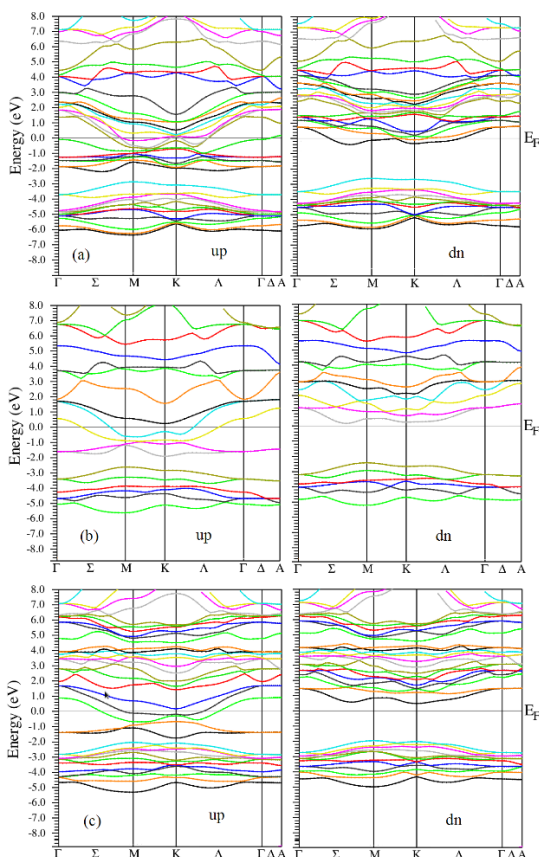


Figure 7. Band structure of allowed ternary compounds (a) $\text{Sc}_{0.25}\text{Cr}_{0.75}\text{N}$, (b) $\text{Sc}_{0.50}\text{Cr}_{0.50}\text{N}$ and (c) $\text{Sc}_{0.75}\text{Cr}_{0.25}\text{N}$.

4. CONCLUSIONS

We reported theoretical investigations of the structural and electronic properties of $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ compounds, with concentrations $x = 0.0, 0.25, 0.50, 0.75$, and 1.0 of Sc atoms, using first principles calculations with the full-potential linearized augmented plane wave (FP-LAPW) method within density functional theory and the generalized gradient approximation (GGA). We found that the variation of the lattice constant of $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ as a function of the concentration x Sc atoms is in agreement with Vegard's law, with a very small deviation, where the sizes of the lattices constant (ScN and CrN) of binary compounds are the determining factor for this deviation. Furthermore, we found that the bulk modulus diminishes with an increase of Sc atoms. However, the values of the bulk modulus of ternary $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$ and 0.75) compounds are high, and therefore the compounds are rigid, making them good candidates for possible applications in devices that must

operate at high temperatures and high power, and in hard coatings.

Additionally, we found that $\text{Sc}_x\text{Cr}_{1-x}\text{N}$ ($x = 0.25, 0.50$, and 0.75) compounds exhibit a half-metallic behavior with a magnetic moment of $3 \mu_B/\text{Cr-atom}$. The ferromagnetic behavior in the ground state comes from a double exchange mechanism and the hybridization of the Cr-3d and N-2p orbitals that cross the Fermi level. These compounds are good candidates for applications in spintronics.

5. ACKNOWLEDGEMENTS

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