*Full Length Research Paper*

# Theoretical calculation of half-metallic ferromagnetism in $Al_{1-x}V_xN$ compound

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Using the first-principles in the framework of density functional theory, the structural properties, electronic structure, and magnetism of V-doped aluminum nitride (AlN) were investigated. The calculations were carried out using the method based on pseudopotential, employed exactly as implemented in Quantum ESPRESSO code. For (x = 6.25%) $Al_{0.9375}V_{0.0625}N$ and (x = 12.5%) $Al_{0.875}V_{0.125}N$ concentrations, a half-metallic behavior with 100% carrier spin polarization of the conduction carriers in the ground state was found. The calculations showed that the substitution of a V atom at the Al site ($Al_{0.9375}V_{0.0625}N$ compound) introduces a magnetic moment of 2.0 $\mu_B$, while two V atom substitutions ($Al_{0.875}V_{0.125}N$ compound) introduce a magnetic moment of 4.0 $\mu_B$. These magnetic properties came from hybridization and polarization of states V-3d and their first neighboring Al-2p and first neighboring N-2p atoms. The calculated magnetic properties indicate that V-doped AlN compound can potentially be used in diluted magnetic semiconductors or as spin injectors.

**Key words:** Aluminum nitride (AlN), first-principles calculations, magnetic ordering.

## INTRODUCTION

Aluminum nitride (AlN) normally crystallizes in the wurtzite structure (Beloufa et al., 2009). This material has recently attracted the attention of researchers due to their excellent properties, has been widely used in: design Light-Emitting Diodes (LEDs) and Laser Diodes (LDs) (Taniyasu and Kasu, 2008), in electronic packaging material and applied to optical disk as well as lithographic photo masks (Jonnard et al., 2004; Carcia et al., 1996; Carcia et al., 1997). Due to its stability, high temperature, considerable thermal conductivity, low thermal expansion and high resistance to gases and chemicals (Beheshtian et al., 2012) has been used in many electronic devices

which must work in high temperature, high power, and corrosive ambients. In last years, AlN has received extensive attention, because of its possible use as a diluted magnetic semiconductor (DMS) with potential applications in the field of spintronics. For these applications, ferromagnetism at room temperature is a requirement. Recently, high-temperature ferromagnetism has been reported by many researchers in several types of transition-metal (TM)-doped semiconducting oxides and nitrides (Gonzalez et al., 2011; Vargas-Hernadez et al., 2015; Frazier et al., 2003). In particular, many theoretical and experimental works performed on the
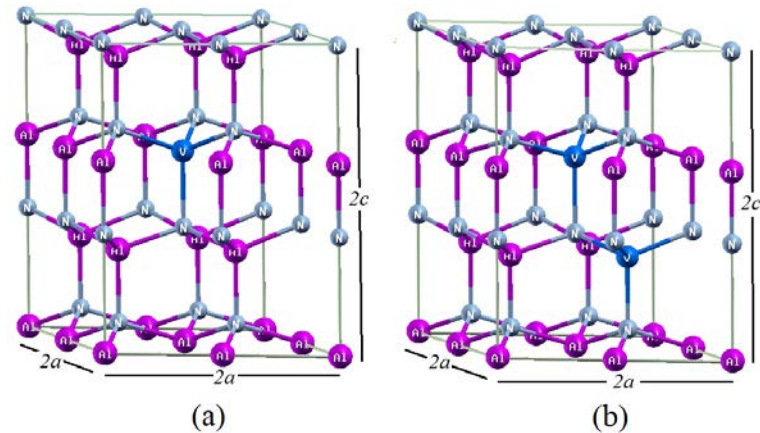
**Figure 1.** Unit cell of the ternary compound: (a) $Al_{0.9375}V_{0.0625}N$, (b) $Al_{0.875}V_{0.125}N$ after structural relaxation.

magnetic properties of AlN via TM doping (Fan and He, 2010; Wu et al., 2003; Li et al., 2008; Yang 2002) showed that it may be a promising candidate for spintronics. However, it was found out that the magnetic TM dopants in TM-doped DMS segregate to form ferromagnetic clusters, precipitate, or secondary phases (Park et al., 2004; Kaspar et al., 2008; Zhou et al., 2008). This represents a big obstacle for practical applications of diluted magnetic semiconductors. It is at this point that the theoretical calculations play a key role, because theoretical methods are able to reliably predict the relative stability, the atomic and electronic properties of increasingly complex structures, for example, theoretically it can calculate the energy formation parameter which is important for obtaining sufficient magnetization at room temperature. On the other hand, it has been reported that MT = Sc-, Cr-, Co-, Mn-, Er-, Mg-, Ca- and Cu MT-doped AlN are ferromagnetic (FM) (Lei et al., 2009; Wu et al., 2006, 2007; Yang et al., 2007; Dridi et al., 2011; Zhang et al., 2008). But the investigation of AlN:V system is rare, either theoretically or experimentally. For these reasons, this paper presents a systematic theoretical study of the electronic and magnetic properties of V-doped AlN.

## COMPUTATIONAL METHODS

The theoretical calculations were performed using the Quantum ESPRESSO package (Giannozzi et al., 2009). Within the density functional theory (DFT) framework, the DFT is an extremely successful approach for the description of the ground-state properties of metals, semiconductors, and insulators. The correlation and exchange effects of the electrons were treated using the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) (Perdew et al., 1997). Electron–ion interactions were treated with the pseudopotential method (Vanderbilt, 1990; Laasonen et al., 1993). Electron wave functions were expanded into plane waves with a kinetic-energy cutoff of 40 Ry. For the charge density, a kinetic energy cutoff of 400 Ry was

used. A 6×6×4 Monkhorst-Pack mesh (Monkhorst et al., 1976) was used to generate the k-points in the unit cell. The calculations were performed taking into account the spin polarization. All the crystal structures were fully relaxed via geometrical optimization by displacement of the atoms in the z axis. Structural optimizations are finished when the total energy converged to less than $10^{-7}$ eV/atom and the magnitude of the force acting on each ion is less than 10 meV/Å. To calculate the structural, electronic, and magnetic properties of pure AlN, a 32-atom $2a \times 2b \times 2c$ wurtzite supercell was considered. The concentrations $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ were obtained by substituting one and two Al-atoms in the supercell. Pure AlN and $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds were modeled according to the special quasirandom structures approach and the disorder aspects were ignored (Zunger et al., 1990). Figure 1 shows the supercell of the $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds obtained after of the structural relaxation.

## RESULTS AND DISCUSSION

### Structural parameters

To determine the structural properties in the ground state, such as the lattice constant ($a_0$), the bulk modulus ($B_0$), the c/a ratio, the total energy ($E_0$) and the magnetic moment ($\mu$) per supercell of pure AlN, $Al_{0.9375}V_{0.0625}N$, and $Al_{0.875}V_{0.125}N$ concentrations in the wurtzite structure, the total energy was calculated as a function of the volume and the results were fit to the Murnaghan equation of state (Murnaghan, 1944). Additionally, for the $Al_{0.9375}V_{0.0625}N$ compound, the total energy variation was calculated as a function of the volume for the FM and non-magnetic phases, while $Al_{0.875}V_{0.125}N$ compound allows the calculation of the relative energies of FM and antiferromagnetic (AFM) phases, in order to find the most favorable magnetic ordering. Figure 2 shows the energy-volume curves.

Table 1 shows the lattice constant ($a_0$), the c/a value, the bulk modulus ($B_0$), the total energy ($E_0$), and the magnetic moment ($\mu_\beta$) per supercell. The solid line is
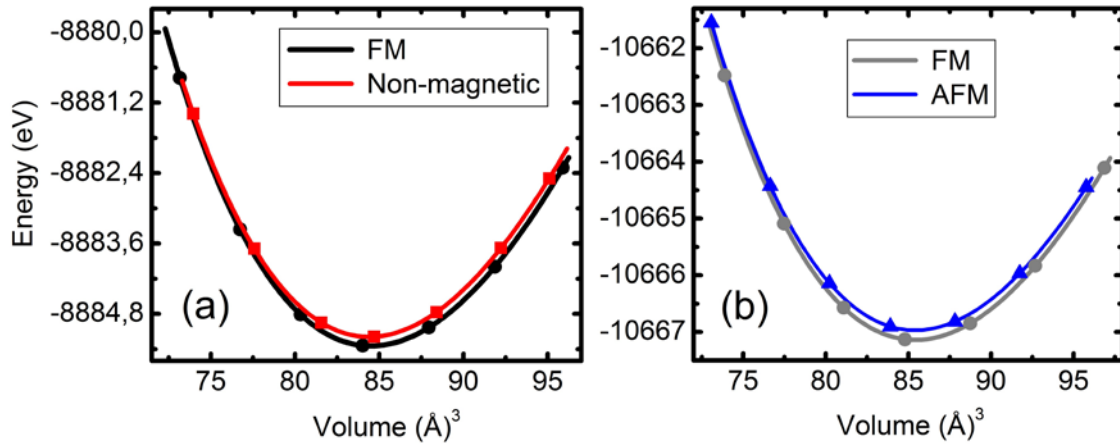
**Figure 2.** Total energy as a function of volume for (a) $Al_{0.9375}V_{0.0625}N$, (b) $Al_{0.875}V_{0.125}N$.

**Table 1.** Lattice constant, c/a ratio, bulk modulus, total energy, and magnetic moment per supercell of pure AlN, $Al_{0.9375}V_{0.0625}N$, and $Al_{0.875}V_{0.125}N$.

| Compound | $a_0$(Å) | c/a | $B_0$ (GPa) | $E_0$ (eV) | $\mu$ ($\mu_\beta$/cell) |
|---|---|---|---|---|---|
| AlN | 3.121 | 1.603 | 192.93 | - 7101.912 | 0.0 |
| | 3.110[a] | 1.601[a] | 192[b] | - | - |
| | | | | | |
| | 3.117 | 1.604 | 191.86 | - 8885.344 | 2.0 |
| $Al_{0.9375}V_{0.0625}N$ | 3.125[c] | 1.602[c] | - | - | 2.0[c] |
| | 3.112[d] | 1.600[d] | - | - | 2.0[d] |
| | | | | | |
| $Al_{0.875}V_{0.125}N$ | 3.114 | 1.608 | 191.11 | - 10667.056 | 4.0 |

[a]Experimental reference (Schulz and Thieman, 1977), [b]Theoretical reference (Peng et al., 2008), [c]Theoretical reference (Yao et al., 2013), [d]Theoretical reference (Dihn et al., 2005).

the fit to the Murnaghan equation of state.

The lattice constant *a* and c/a ratio value calculated for the pure AlN agree well with values reported experimentally, since it differs by less than 1%. The values of the bulk modules of the pure AlN, $Al_{0.9375}V_{0.0625}N$, and $Al_{0.875}V_{0.125}N$ concentrations are higher, which confirms that they are quite rigid, making them good candidates for possible application in devices operated at high temperature and high power, as well as in hard coatings.

For $Al_{0.9375}V_{0.0625}N$ compound, the values calculated for lattice constant *a*, c/a ratio and magnetic moment are in good agreements with that reported theoretically by Yao et al. (2013) and Dihn and Katayma-Yoshida (2005). However, for $Al_{0.875}V_{0.125}N$ compound, Yao et al., (2013) and Dihn and Katayma-Yoshida (2005) did not give the structural parameter value and the magnetic moment value; these values are given for the first time as shown in Table 1.

For 6.25% concentration of V doping, the lattice constant in the $Al_{0.9375}V_{0.0625}N$ compound changes only slightly with respect to pure AlN. There is a reduction of 0.128% for *a*, which resulted from the minor difference in atomic radius between V (1.34 Å) and Al (1.43 Å). For 12.5%, the reduction on the lattice constant is 0.224%.

Figure 2a shows that for the $Al_{0.9375}V_{0.0625}N$ compound, the calculated total energy of spin polarized state (FM phase) is lower than that of the non-spin polarized state (non-magnetic phase) by about 55.4 meV, while that for the $Al_{0.875}V_{0.125}N$ compound (Figure 2b), in the ground state (FM state) is lower than the AFM state by about $\Delta E$ = 21.2 meV. This indicates that the ground state of V-doped AlN is ferromagnetic.

The spin polarization calculations for $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds result in a magnetic moment of 2.0 and 4.0 $\mu_\beta$ per supercell, respectively. The magnetization for $Al_{0.9375}V_{0.0625}N$ is the same magnitude than that of $Ga_{0.9375}V_{0.0625}N$ compound (Guangrui et al., 2012). This demonstrates that it is very likely for V to order ferromagnetically in AlN.

In order to verify the relative stability of the $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds, the

**Table 2.** Formation energy.

| Compound | $E_f$ (eV) |
|---|---|
| $Al_{0.9375}V_{0.0625}N$ | 2.66 |
| $Al_{0.875}V_{0.125}N$ | 3.04 |

corresponding formation energy is calculated, which is expressed as:

$$E_f = E_{V:AlN} - E_{AlN} - nE_V + nE_{Al}$$

where $E_{V:AlN}$, $E_{AlN}$, $E_V$ and $E_{Al}$ are the energies in the ground state of V-doped AlN, pure wurtzite AlN, bcc V, and fcc Al, respectively (Murillo et al., 2015). The integer $n$ is the number of V atoms that substitute for Al. The total energy $E_V$ and $E_{Al}$ in their ground states was calculated. The energy values are -1955.656 eV and -169.564 eV, respectively. Additionally, to ensure the results are accurate, a formation enthalpy of -3.31 eV for AlN wurtzite was obtained, which is in good agreement with the experimental value of -3.28 eV and the theoretical value of -3.33 eV (Shi et al., 2008; Thapa et al., 2010). Table 2 shows the calculated values of formation energy $E_f$.

The value of the formation energy of $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds are positive. Therefore, the compounds are metastable and the moderate formation energy values indicate that the compounds can easily be grown experimentally. Additionally, it was found out that the value of formation energy for $Al_{0.9375}V_{0.0625}N$ is significantly lesser than the Cr-doped AlN ($E_f$ = 4.41 eV) (Cui et al., 2004), Mg-doped AlN ($E_f$ = 3.80 eV) (Sandhya et al., 2014). This indicates that V-doped AlN is energetically preferred and therefore this proves that is most likely to obtain sufficient magnetization, a room temperature in V-doped AlN. Additionally, the heat energy $K_BT$ (where $K_B$ is constant Boltzmann and T is the temperature) was calculated. In this case $K_BT$ = 26.55 eV. It was found out that the heat energy $K_BT$ (26.55 meV) is greater than the energy difference $\Delta E$ (21.2 meV). This result confirms that it is possible to obtain sufficient magnetization, a room temperature in V-doped AlN

## Electronic and magnetic properties

The theoretical lattice constants and c/a ratio of the AlN and the $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds shown in Table 1 were used to calculate the band structure and the spin-polarized density of states (DOS) along the high-symmetry direction in the first Brillouin zone.

The band structure for pure AlN and $Al_{0.9375}V_{0.0625}N$ and

$Al_{0.875}V_{0.125}N$ compounds are shown in Figure 3. Figure 3a shows the band structure of pure AlN. This confirms the direct semiconductor behavior, with the top of the valence band and the bottom of the conduction band located at the point of the Brillouin zone. A direct band gap of about 4.3 eV was found. The magnitude of this gap is smaller than the value reported experimentally (6.2 eV) for AlN in the wurtzite structure (Vurgaftman et al, 2001). This occurs because the GGA approximation underestimates the forbidden energy gap in semiconductors. The valence band is mainly determined by Al-2p states and N-2p makes a minor contribution.

Figure 3b and c shows the band structure of the ternary $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds, respectively. It can be observed that the minority spin (down) states preserve a band gap (with an energy gap larger than 4.4 eV), but in the majority spin (up) states being metallic, because there is a penetration towards the prohibited energy zone of the states 3d-V in greater proportion and states N-2p and Al-2p in lesser proportion. Therefore, due to the introduction of one and two V atoms into the structure of AlN, it loses its semiconductor nature. The allowed ternary $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds exhibit half-metallic behavior. It can be seen that the spin up orientation of $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds is partially filled, because they exhibit dispersed bands above the Fermi level. High polarization of the conduction carriers is confirmed by the fact that the V atom dopants couple ferromagnetically and that there is a high presence of conduction carriers in the majority spin channel. These compounds exhibit a spin polarization of 100% of the conduction carriers in the ground state, and they are responsible for the conduction in V-doped AlN. This is a requirement for spin injectors (Díaz et al., 2015). This finding suggests that these ternary compounds can be efficiently used in spintronics.

In order to fully understand the mechanism by which the FM state in $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds is stabilized and at the same time identify the contribution of each atom to the ferromagnetism, the total density of states (TDOS) and partial density of states (PDOS) for the $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds were calculated. Figure 4a and b shows the TDOS and PDOS: 3d states of V atom, 2p states of the first neighboring Al atom, and the first neighboring N atom of $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds, respectively. The total density of states confirms that due to the V substitution at the Al site, the compound has a half-metallic character. This behavior occurs because in the valence band near the Fermi level, majority of the spins are metallic and the minority spins are semiconductors. According to the energy scale, Figure 4a shows that in the valence band near the Fermi level, the spin-up density is mainly dominated by the V-3d states and to a lesser extent by the Al-2p and N-2p states, which cross the Fermi level. This indicates the magnetic moment comes from 3d-V orbitals mainly and the Al-2p and N-2p states in minor
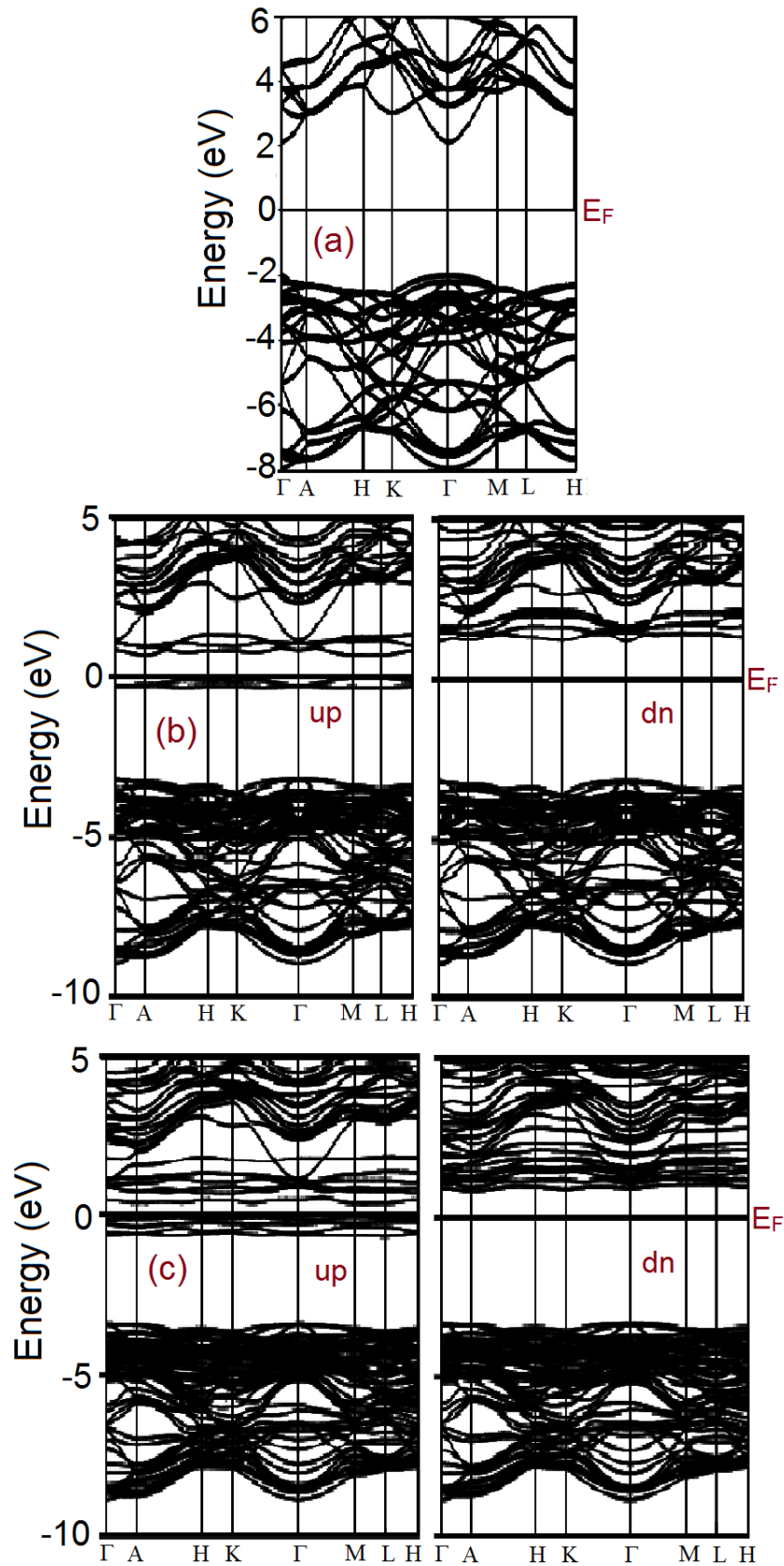
**Figure 3.** Electronic energy bands for: (a) pure AlN, (b) $Al_{0.9375}V_{0.0625}N$, (c) $Al_{0.875}V_{0.125}N$.

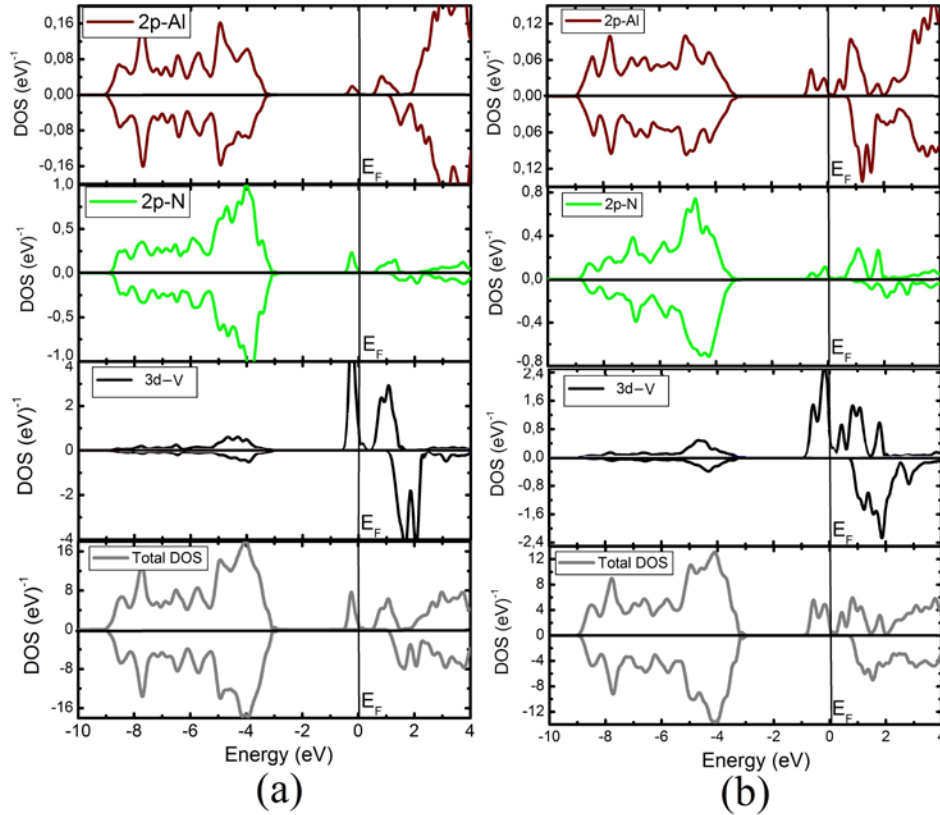**Figure 4.** Partial and total density of states for the allowed ternary (a) $Al_{0.9375}V_{0.0625}N$ and (b) $Al_{0.875}V_{0.125}N$ compounds.

contributions.

Figure 4b shows that in the $Al_{0.875}V_{0.125}N$ compound, the magnetic moment induced by two V dopant and the corresponding moment distribution are nearly consistent with those in the cases of a single V atom substitution in a supercell.

Figure 4a and b shows that in the majority spin, the partial density of states belonging to the V-3d orbital exhibits a high peak near the Fermi level, about -0.5 eV for $Al_{0.9375}V_{0.0625}N$ and -0.65 eV for $Al_{0.875}V_{0.125}N$, thus indicating localized states in that region. In the valence band around the Fermi level, the V-3d states overlap with another two peaks of smaller amplitude belonging to N-2p and Al-2p. Therefore, there is hybridization between the V-3d, N-2p, and Al-2p orbitals. Additionally, the TDOS confirms the presence of some unoccupied bands above the Fermi level, because there is no contribution of spin down and the majority spin exhibits a hybridization and polarization between the V-3d, N-2p, and Al-2p states, resulting in a magnetic moment of 2.0 $\mu_\beta$/Cell for $Al_{0.9375}V_{0.0625}N$ and 4.0 $\mu_\beta$/Cell for $Al_{0.875}V_{0.125}N$. The magnetic moment is due to the $V^{3+}$ configuration (with electronic configuration $[Ar]3d^2$). This implies that when the V atom occupies at the Al site in the AlN, it gives up three electrons and two valence electrons remain ($d^2$

configuration). These valence electrons couple ferromagnetically and as a result the two electrons produce a total magnetic moment of 2 $\mu_\beta$/atom-V. Touati et al., (2008)[41] reported a valence of $V^{3+}$ for infrared luminescence in V-doped GaN samples grown with MOVPE on a sapphire substrate. Finally, the magnetic moment of $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds are integers, therefore, this confirms that each compound is ferromagnetic and half-metallic.

## Conclusions

First-principles total energy calculations to determine the structural, electronic, and magnetic properties of $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds were carried out. The calculated values of the bulk modules were quite high; therefore, the ternary compounds are quite rigid, which makes them attractive for potential applications at high temperatures and for hard coatings. Also, the compounds were found to exhibit ferromagnetic and half-metallic behavior; due to polarization and hybridization, the orbitals V-3d, 2p-N, and 2p-Al cross the Fermi level. Finally, it was found that $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds exhibit magnetic properties with magnetic

moments 2 $\mu_\beta$ and 4 $\mu_\beta$ per supercell, respectively. These properties show that these compounds are good candidates for possible application in diluted magnetic semiconductors, spin injectors, and other spintronics applications.

## Conflict of Interests

The authors have not declared any conflict of interests.

## ACKNOWLEDGEMENTS

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