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MAGNETIC AND ELECTRONIC PROPERTIES OF TRANSITION METAL-DOPED AlN NANOSHEETS: A FIRST-PRINCIPLES STUDY FOR SPINTRONIC APPLICATIONS

We present here a Density Functional Theory-based ab initio study of the structural, electronic, magnetic and optical properties of a transition metal-doped AlN nanosheet. From the total energy difference, the stable ferromagnetic or antiferromagnetic configuration is determined. We find that the pure AlN nanosheet is a nonmagnetic, wide-bandgap (3.28 eV) semiconductor, while transition metal atoms induce magnetic moments, leading to structural changes around the dopant and neighboring atoms. The calculated partial DOS shows that d orbitals of transition metal atoms are strongly hybridized with the p orbitals of N near the Fermi level, resulting in a transition from semiconducting to half-metallic behavior. Cr- and Cu-doped AlN nanosheets, which exhibit 100% spin polarization, are promising candidates for spintronic devices due to their strong half-metallic ferromagnetic properties. These findings suggest that TM-doped AlN nanosheets are promising for applications in nanodevices and spintronic devices based on low-dimensional nanostructures.

Keywords: transition metal atoms, spin polarization, nanosheets, magnetic moments.

1. Introduction

In recent years, nanostructures of semiconducting materials have attracted significant interest due to their potential role in the development of future nanoscale technologies [1–3]. Among these, nanowires exhibit fascinating properties that offer advantages for advanced electronic devices, particularly when compared to quantum dots and bulk materials [4, 5].

AlN with a wurtzite structure is an important wide-bandgap semiconductor that has great potential for applications in electronic and light-emitting devices [6]. The AlN nanotube has been successfully synthesized [7] and widely investigated. AlN nanowires (NWs) stand out as a particularly appealing choice due to their low electron affinity [8] and polar N–Al bonds, which suggest that the AlN nanowires can be used in semiconductor-based chemical sensors.

It is known that diluted magnetic semiconductors (DMSs) are a promising class of materials for novel spintronic devices [9, 10]. Significant efforts have been made to study AlN-based DMSs [11, 13]. In recent years, various theoretical and experimental studies have been performed to study the electronic and magnetic properties of transition metal-doped AlN [14–

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22]. First-principles calculations showed that Mg doping in AlN nanosheets lowers transition energy levels and favors Al substitution under N-rich conditions, improving p-type doping efficiency [17]. Studies of AlN nanosheets doped with nonmagnetic atoms (Li, Na and K) revealed out-of-plane dopant positioning, deep *p*-type acceptor levels, and induced magnetism, with K-doped systems exhibiting room-temperature ferromagnetism at low concentrations [18]. The authors of Ref. [19] report that V-doped AlN nanosheets prefer Al-site substitution and exhibit *p*-*d* hybridization-driven ferromagnetism that is stabilized under tensile biaxial strain, indicating strong potential for spintronic applications. Recent first-principles studies have shown that transition metal-doped AlN systems, such as Co@AlN-V_{Al} and Pd@AlN-V_{Al}, exhibit excellent bifunctional catalytic activity for the hydrogen evolution, oxygen evolution, and oxygen reduction reactions, providing guidance for designing efficient single-atom catalysts [20]. Yang *et al.* [21] synthesized Mn-doped AlN NWs via chemical vapor deposition, which exhibited ferromagnetic properties. The authors of Ref. [22] conclude that the degree of surface passivation of dangling bonds in the Mn-doped AlN NW is an important factor affecting the magnetic properties of doped nanowires. Recent DFT studies have shown that Au-decorated AlN nanosheets can strongly adsorb theophylline and significantly enhance the sensing response, suggesting their potential as efficient biosensors [23]. The optical properties of AlN nanosheets have been investigated in several studies [24, 25], revealing isotropic spectra with semiconducting behavior [24], while *ab initio* simulations [25] further show that applied electric fields can modulate the band gap, dielectric response, and absorption peaks, leading to a semiconductor-metal transition with promising optoelectronic applications.

In general, the electronic, structural, and magnetic properties of TM-doped AlN nanosheets are systematically investigated. Our findings reveal the fundamental role of 3*d* transition-metal dopants in tuning the orbital hybridization and exchange interactions within the AlN lattice. These insights not only deepen the physical understanding of spin polarization and magnetism in low-dimensional AlN systems but also provide a theoretical basis for engineering AlN-based semiconductors with controllable functionalities. Such tunability makes TM-doped AlN na-

nosheets promising candidates for next-generation spintronic and optoelectronic applications, where precise control over electronic and magnetic behavior is crucial.

2. Method of Calculation

We carried out our calculations using density functional theory (DFT) [26] and the APW method as implemented in the AtomistixToolKit quantumwise (ATK) package [27]. The generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof scheme for solids (PBEsol) was used to calculate the exchange–correlation energy. The Pseudo-Dojo pseudopotential was used to represent the valence electrons and ionic cores. A plane-wave cutoff energy of 400 eV was chosen. Brillouin zone (BZ) sampling was conducted using the Monkhorst–Pack scheme with a mesh size of $1 \times 1 \times 15$. A maximum force criterion of 0.01 eV/Å was applied during optimization. A vacuum layer larger than 20 Å was introduced along the *z*-direction to prevent interactions between periodic images. The optimized lattice parameters for the bulk material and the nanosheet are $a = b = 3.113$ Å, $c = 4.981$ Å and $a = b = 3.128$ Å, $c = 21.565$ Å, respectively.

A $1 \times 3 \times 5$ supercell of the AlN nanosheet (AlNNS), comprising 120 atoms (60 Al and 60 N in the undoped configuration), was employed in the calculations. This nanosheet size provided sufficient separation between periodic images of dopants and allowed the investigation of a wide range of doping concentrations while maintaining computational feasibility. Transition metal dopants (TM = Cr, Mn, Fe, Co, V, Cu) were introduced by substituting 2, 4 and 6 Al atoms, corresponding to doping concentrations of approximately 2.08%, 4.16% and 6.25%, respectively.

3. Results and Discussions

In the first step, the band structures and DOS of bulk AlN and AlN NSs were calculated. Fig. 1, *a* and *b* show the band structures of the AlN bulk and NS, respectively.

For bulk AlN, the calculated band gap is 5.57 eV, which is in good agreement with theoretical and experimental values of 5.6 eV [28] and 6.02 eV [29].

The spin-polarized electronic band structure of the pure AlNNS, illustrated in Fig. 2, reveals its non-magnetic nature, as evidenced by the symmetry observed in both spin-up and spin-down states in the

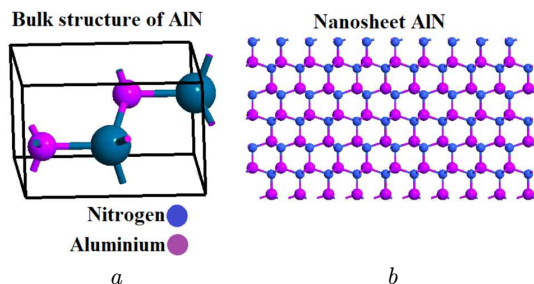


Fig. 1. Bulk (a) and nanosheet (b) structure model of undoped AlN

Table 1. The binding energy, bond lengths and magnetic moments of TM-doped AlNNS

TM atom	E_b , (eV)	Bond length (Å)	Concentration (%)	Magnetic moment (μ_B)
V	-2.96	1.89	2.08	3.47
			4.16	3.59
			6.25	3.62
Cr	-3.74	1.81	2.08	4.34
			4.16	4.30
			6.25	4.29
Mn	-3.21	1.87	2.08	4.99
			4.16	5.08
			6.25	5.14
Fe	-3.07	1.84	2.08	4.36
			4.16	4.75
			6.25	4.81
Co	-2.62	1.81	2.08	3.28
			4.16	3.25
			6.25	3.16
Cu	-3.11	1.82	2.08	0.73
			4.16	0.75
			6.25	0.81

valence band (VB) and conduction band (CB). The calculated band gap (4.05 eV) is in good agreement with the value of 3.74 eV reported in Ref. [30] for an AlN nanotube.

In a theoretical study [17], the band gap for an AlN nanosheet was reported as 2.93 eV using GGA with the PBE functional. The difference originates from the use of different pseudopotentials: while the earlier work employed standard GGA-PBE, we used the PseudoDojo pseudopotentials within the GGA framework, which are known to provide improved accuracy for structural and electronic properties.

To study the electronic, magnetic, and optical properties of TM-doped AlNNSs (TM = Cr, Mn, Fe, Co, and V) at concentrations of 2.08%, 4.16% and 6.25% (Fig. 3), the structural stability of the doped nanosheets was first investigated by calculating their binding energies using the following relation:

$$E_b = E_{\text{TMAIN}} - (E_{\text{AIN}} + E_{\text{TM}}),$$

where E_b represents the binding energy of the TM-doped AlNNS; the total energies of the doped and pure nanosheet structures are denoted by E_{TMAIN} and E_{AIN} , respectively; and E_{TM} denotes the total energy of the dopant TM atom. The TM atoms are substituted at Al sites. As is known from previous investigations of AlN, TM atoms substitute for Al atoms [31–33].

The calculated binding energy values are summarized in Table 1, where the E_b values for the doped nanosheets range from -2.62 to -3.74 eV. All the doped structures considered have negative E_b values, which confirms that they are energetically more stable than the pure AlNNS. Additionally, the atomic bond lengths between the transition metal atoms and their nearest-neighbor N atoms in the optimized structure are also provided in Table 1. The average bond lengths between the V, Cr, Mn, Fe, Co, and Cu atoms and their nearest N neighbors are 1.89, 1.81, 1.87, 1.84, 1.81, and 1.82 Å, respectively. The observed distortion, compared to the pure nanosheet structure (where the Al–N bond length is 1.80 Å), is mainly due to the differences in atomic radii between the dopant atoms and the Al atom.

Fig. 4 to 6 present the calculated projected DOS for TM-doped AlNNSs. As illustrated in these figures, all TM-doped nanosheets exhibit spin splitting around the Fermi energy (EF), indicating the presence of magnetic moments. For certain TM atoms, the electronic states cross the Fermi level for only one spin channel, suggesting half-metallic behavior. Additionally, strong hybridization occurs between the TM dopant and its neighboring N atoms, as evidenced by the overlap of the TM-*d* and N-*p* states in the PDOS.

The strong hybridization between TM-*d* and N-*p* orbitals is confirmed by the overlapping peaks in the PDOS. Specifically, the TM-*d* states and the N-*p* states show significant intensity over the same energy ranges (both below and near the Fermi level), which indicates orbital mixing and strong covalent interaction.

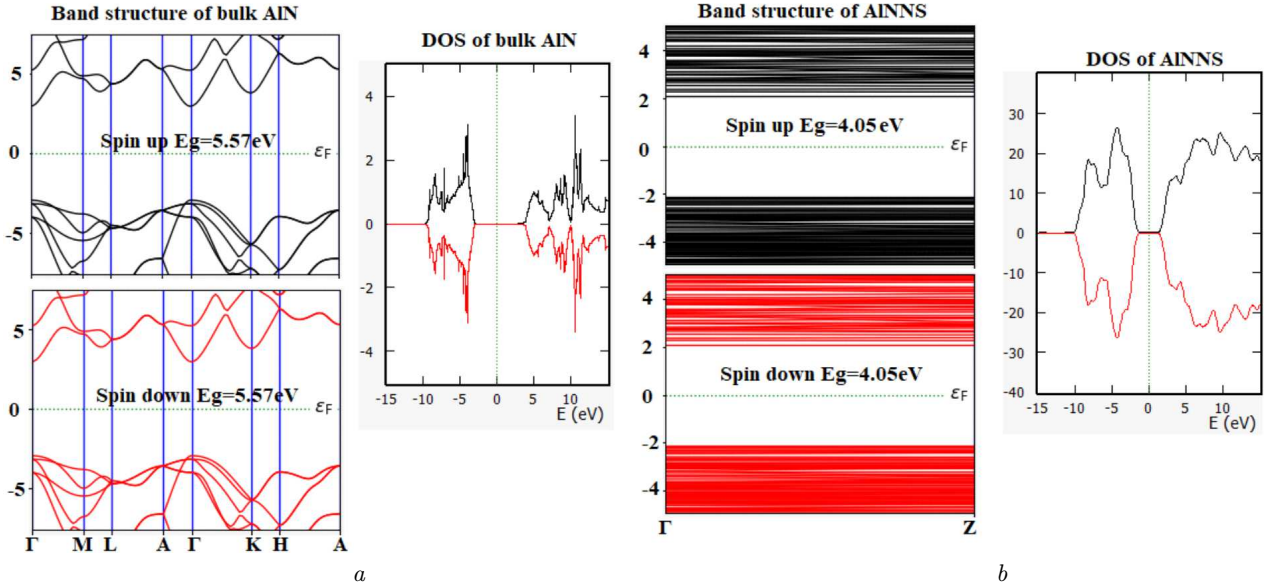


Fig. 2. Band structure and DOS for bulk (a) and AlNNS (b) structure, respectively

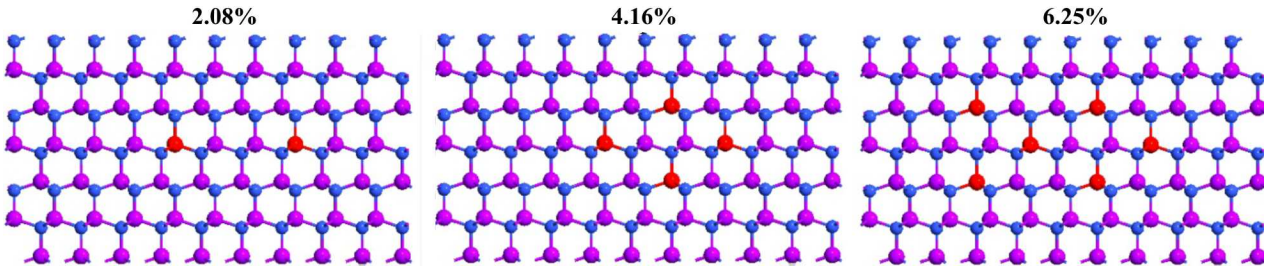


Fig. 3. The TM atoms are substituted at Al sites at various concentrations (TM atoms are shown in black color)

The magnetic coupling strength was evaluated from the total energy difference between the ferromagnetic (FM) and antiferromagnetic (AFM) states, defined as $\Delta E = E_{\text{FM}} - E_{\text{AFM}}$. A negative value of E indicates that the FM configuration is energetically more favorable. According to our calculated energy differences (see Table 2), ΔE is negative for Fe-, Co-, Cu-, V-, and Cr-doped AlN nanosheets, confirming that their ground state is ferromagnetic. In contrast, ΔE is positive for Mn-doped AlNNS, indicating that the AFM configuration is the ground state. Qiushi Wang *et al.* in their study [34] indicate that AlN:Mn nanosheets exhibit room temperature ferromagnetism, which is due to the unpaired electrons in the 3d shell of Mn^{2+} ions.

The results of the half-metallic gap and band gap calculations are shown in Table 3. The spin-polarized partial density of states (PDOS) of the transition

Table 2. The spin-dependent band gap for the TM-doped AlNNSs

TM atom	Energy band gap (eV)					
	2.08%		4.16%		6.25%	
	Spin					
	up	down	up	down	up	down
V	2.47	3.91	1.64	3.75	1.61	3.52
Cr	2.64	2.85	1.21	4.21	0.0	3.68
Mn	2.05	3.92	2.27	3.85	1.63	3.61
Fe	4.26	2.75	4.03	2.67	3.02	1.54
Co	4.21	1.63	4.55	2.05	4.32	1.52
Cu	4.28	1.26	4.53	0.53	4.59	0.0

metal (TM) doped AlNNSs was analyzed to understand the electronic and magnetic properties of the systems. The PDOS provides the distribution of elec-

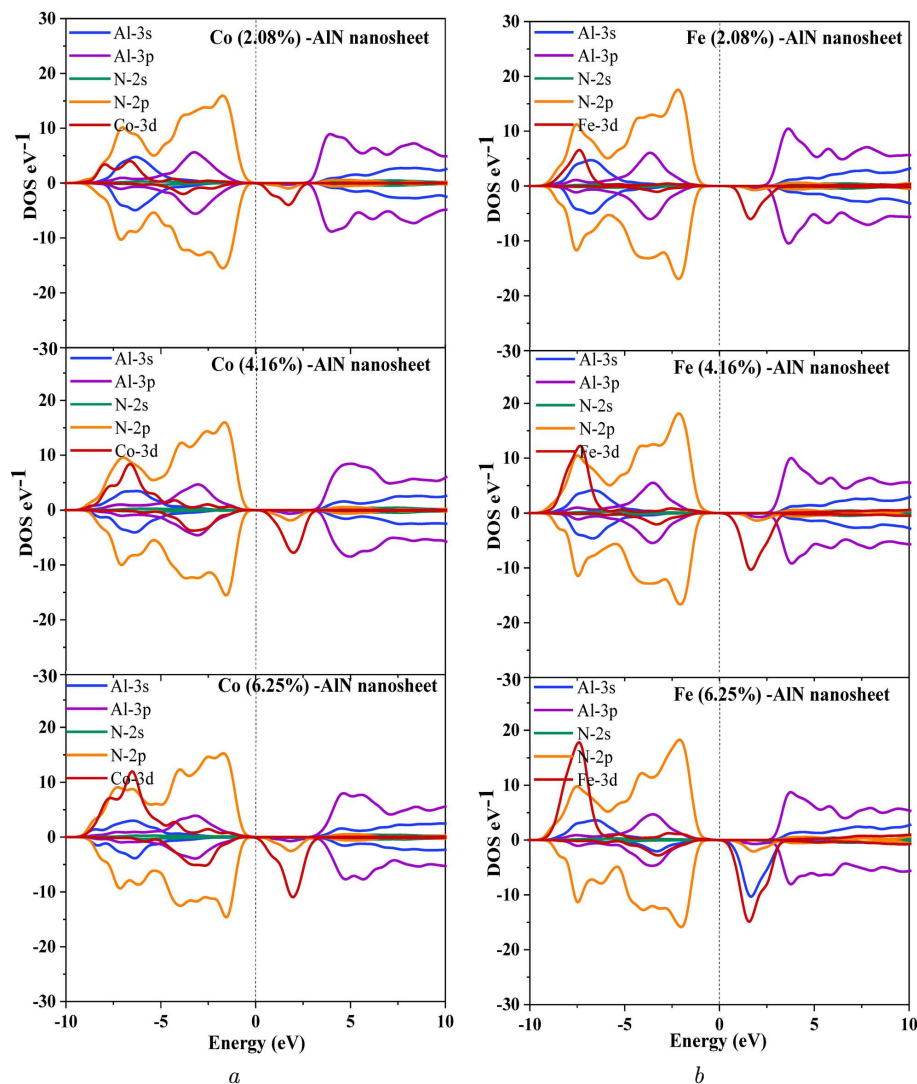


Fig. 4. Calculated spin-polarized partial DOS for Co- and Fe-doped AlNNS

Table 3. Calculated total energies for ferromagnetic and antiferromagnetic phases of TM-doped AlN

TM doped AlNNS	Concentration (%)	E_{FM}	E_{AFM}	$\Delta E(E_{\text{FM}} - E_{\text{AFM}})$	TM doped AlNNS	Concentration (%)	E_{FM}	E_{AFM}	$\Delta E(E_{\text{FM}} - E_{\text{AFM}})$
AlN-Mn	2.08	-17503.81750	-17503.81883	0.00134	AlN-Fe	2.08	-18487.01395	-18487.01275	-0.00126
AlN-Mn	4.16	-23218.05875	-23218.06076	0.00196	AlN-Fe	4.16	-25183.35809	-25183.35731	-0.00083
AlN-Mn	6.25	-28935.69074	-28935.69284	0.00201	AlN-Fe	6.25	-31880.32859	-31880.32768	-0.00102
AlN-Co	2.08	-21902.96795	-21902.96452	-0.00345	AlN-V	2.08	-15640.73500	-15640.73436	-0.00067
AlN-Co	4.16	-27842.49897	-27842.49543	-0.00352	AlN-V	4.16	-19502.24163	-19502.24163	-0.00092
AlN-Co	6.25	-35868.31423	-35868.31065	-0.00367	AlN-V	6.25	-23356.59142	-23356.588891	-0.00148
AlN-Cr	2.08	-16549.64501	-16549.64418	-0.00095	AlN-Cu	2.08	-28314.96547	-28314.96492	-0.00057
AlN-Cr	4.16	-21316.07609	-21316.07495	-0.00116	AlN-Cu	4.16	-32017.46004	-32017.45746	-0.00264
AlN-Cr	6.25	-26084.47903	-26084.47667	-0.00239	AlN-Cu	6.25	-42136.36467	-42136.36184	-0.00291

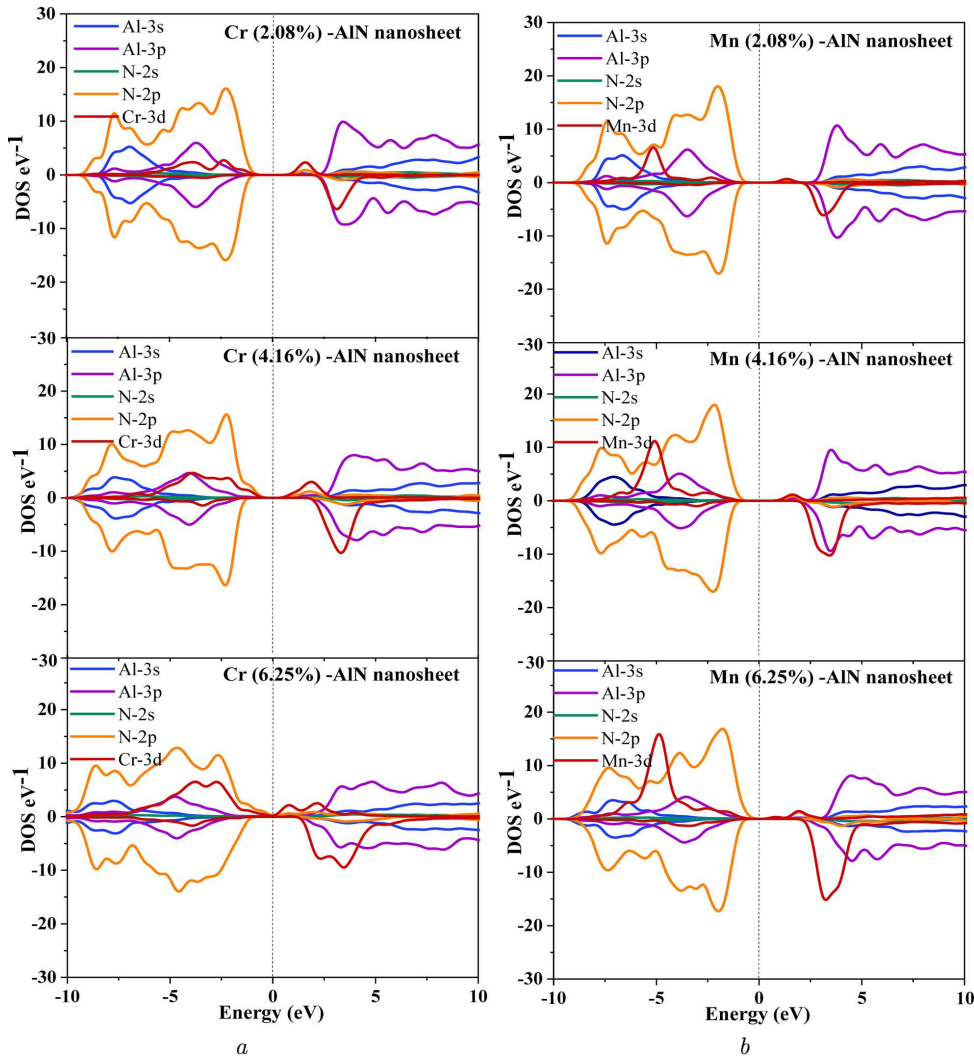


Fig. 5. Calculated spin-polarized partial DOS for Cr- and Mn-doped AlNNSs

tronic states for each spin channel (up and down) near the Fermi level (E_F). For Cr- and Cu-doped AlNNSs, the PDOS shows that in one spin channel (spin-up and spin-down, respectively), there is a finite density of states at the Fermi level, indicating metallic behavior, while in the opposite spin channel (spin-down and spin-up, respectively), there is a band gap at E_F , indicating semiconductor behavior. This asymmetry between spin channels is the defining feature of a half-metal (Fig. 4, Fig. 5). The 3d and N-2p hybridization states of TM and N atoms close to the Fermi level are responsible for this. The very minor energy differences (ΔE) (Table 3) indicate that V- and Fe-doped AlNNSs are all weakly FM semiconductors.

For Mn-doped nanosheet evidently, there is not much variation in DOS (in contrast to other dopants, which induce noticeable changes in the DOS, Mn-doping results in only a shift by less than 0.7 eV for all different concentrations in peak positions and negligible changes near the Fermi level, maintaining the overall semiconducting character) (Fig. 4) with the substitution of Mn and even at the highest concentration of TM atoms the spin-up and spin-down channel retain their semiconductor nature with a different band gap value (Table 2).

The surrounding nitrogen atoms in Cr-doped AlNNS play a significant role in the formation of the magnetic moment, particularly in the spin-up channel (Fig. 3). This is evident from the projected DOS,

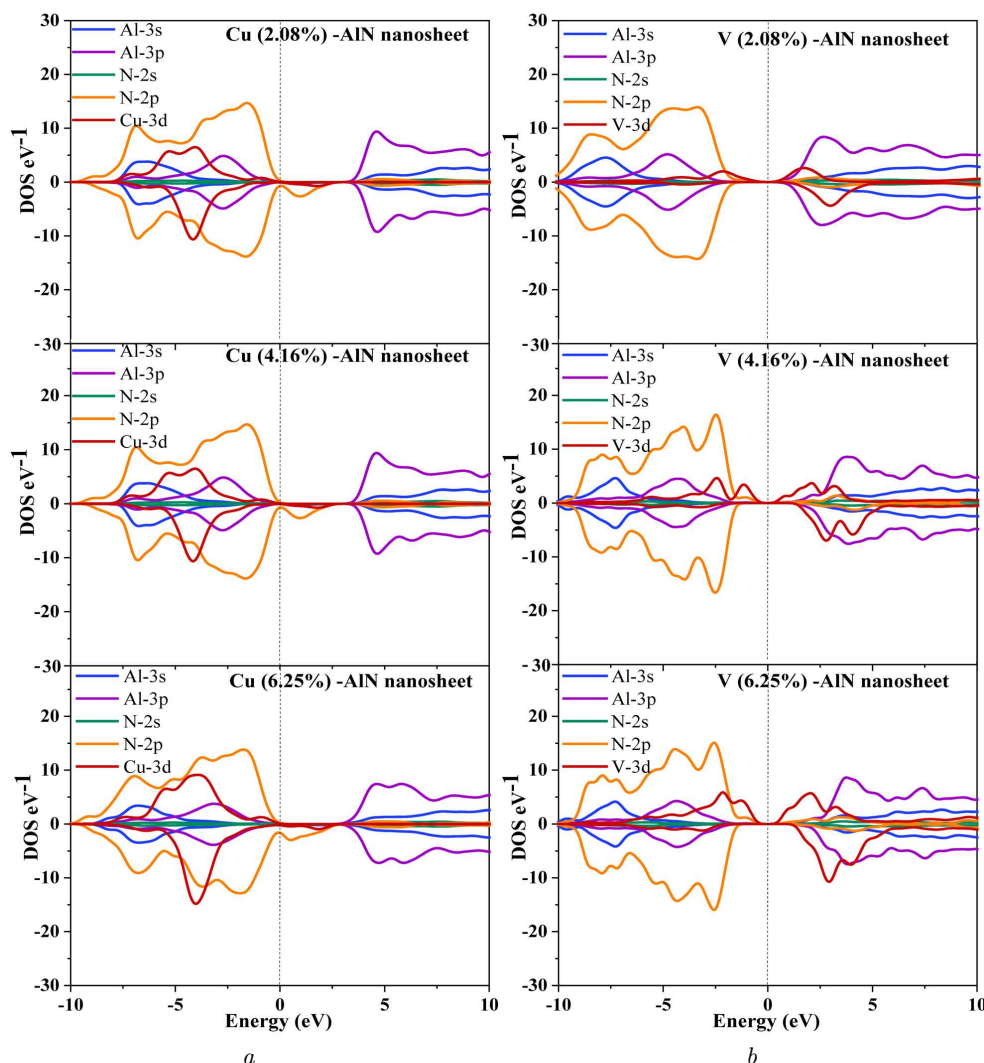


Fig. 6. Calculated spin-polarized partial DOS for Cu- and V-doped AlNNSs

where pronounced peaks of Cr-3d and N-2p states appear in the same energy region (from approximately -2 eV to 0 eV) in the spin-up channel. The overlapping energy range of these states demonstrates strong hybridization between the Cr-3d orbitals and the neighboring N-2p orbitals. Slight hybridization near the bottom of the conduction band causes partial charge transfer from the Cr atom to adjacent N atoms, leading to electronic charge redistribution within the Cr-N bonding environment.

In the spin-down channel, the N-2p states remain unoccupied, preserving a clear band gap, whereas in the spin-up channel, the Cr-3d states appear near the bottom of the conduction band and the top of

the valence band, crossing the Fermi level and leading to metallic behavior. This asymmetry between the spin-up and spin-down DOS indicates spin polarization and confirms that the net magnetic moment mainly originates from the localized spin-up electrons in the Cr-3d orbitals. As the hybridization strength increases with higher Cr concentration, the Cr-3d states broaden and shift closer to the Fermi level. Consequently, the spin-up band gap gradually narrows and eventually closes, indicating enhanced Cr-N orbital interaction and a transition from semiconducting to nearly metallic behavior in the spin-up channel. The spin-down channel remains semiconducting, but its band gap increases from 2.85 to

3.68 eV with increasing Cr concentration. Our results are consistent with the earlier research reported in Ref. [33]. According to that study, Cr-doped AlN is half-metallic.

Our calculated partial DOS (Fig. 5) demonstrates that Cu doping mainly contributes to the valence band in the low-energy range of -2 to -4 eV and has minimal effect on the conduction band in the energy range of $1 \div 2$ eV. However, as shown in Fig. 4, additional energy levels appear near the top of the valence band and the bottom of the conduction band within the energy range of -2 eV to 2.5 eV, originating from the N- $2p$ orbitals. The shift of the Fermi level toward the valence band can be directly observed in our calculated DOS, as shown in Fig. 5. The Fermi level lies very close to the top of the valence band, clearly indicating this shift with Cu doping. This finding is also in good agreement with previous studies on Cu-doped AlN bulk structures [33–35].

This electronic behavior is characteristic of a p -type metallic conductor [36]. The hybridization between the $3d$ orbitals of Cu and the $2p$ orbitals of the nearest N atoms around the Fermi level is important because it results in ferromagnetism.

Fig. 5 shows the partial DOS of V-doped AlNNS near the Fermi level. As shown in Fig. 5, the spin-up states differ noticeably from the spin-down states, leading to considerable spin splitting. This results in a reduction of the band gap from 2.47 eV to 1.61 eV in the spin-up channel and from 3.91 eV to 3.62 eV in the spin-down channel, indicating semiconducting behavior. At a V concentration of 6.25% , the increased atomic interactions and correlations maximize the contribution of $3d$ -orbital electrons near the Fermi level and enhance the possibility of hybridization between the $2p$ and $3d$ orbitals.

A clear overlap between the V $3d$ and N $2p$ orbitals near EF is observed in the spin-up DOS, suggesting a double-exchange mechanism for the FM coupling. In contrast to the results obtained in Ref. [37], which show half-metallic behavior with increasing V concentration, our results indicate that the system retains its semiconducting properties even at the highest V concentration.

As can be seen from Fig. 3, at an Fe concentration of 2.08% , the spin-up band gap increases slightly to 4.26 eV, while the band gap of the spin-down channel decreases to 2.75 eV. As the Fe concentration is further increased to 4.17% , the band gap of the spin-

down channel decreases to 2.67 eV, while that of the spin-up channel decreases slightly to 4.03 eV. At an Fe concentration of 6.25% , the band gaps are 3.02 eV for the spin-down channel and 1.54 eV for the spin-up channel. A new impurity level appears mainly at the bottom of the conduction band and, to a lesser extent, at the top of the VBM for the spin-down channel, as clearly seen in the calculated partial DOS. The peaks associated with the Fe- $3d$ electronic-state density are strongest and show pronounced localization at a doping ratio of 6.25% , thus making the greatest contribution to the conduction-band electrons. Our result is in good agreement with the previously reported result [38].

The magnetic properties of the TM-doped nanosheets were analyzed using Mulliken population analysis [39–51] within the Atomistix ToolKit (ATK) package. The local magnetic moment of each atom represents the net spin associated with that atom and is calculated as the difference between the number of spin-up and spin-down electrons:

$$\mu_i = n_i \uparrow - n_i \downarrow,$$

where $n_i \uparrow$, $n_i \downarrow$ are the spin-up and spin-down electron populations on atom i . The local moments of the $3d$ transition metal (TM) dopants and their nearest-neighbor N atoms were specifically examined to reveal the distribution of magnetism in the nanosheet.

The total magnetic moment of the nanosheet is obtained by summing the contributions of all atoms, reflecting the net magnetic polarization of the system:

$$\mu_{\text{total}} = \sum_i (\mu_i) = \sum_i (n_i \uparrow - n_i \downarrow).$$

This approach provides a clear and physically meaningful description of both the local and overall magnetic behavior of the TM-doped nanosheets.

The comparison reveals that, except for the Cu-doped AlNNS, the total magnetic moments of all other nanosheets predominantly arise from the TM atoms, with minimal contributions from the nearest-neighbor N atoms. Specifically, the local magnetic moment of copper is approximately $0.735 \mu_B$, which is lower than the corresponding moments of the other TM atoms, suggesting that copper atoms are less favorable for spin polarization. In the case of the Cu-doped AlNNS, the local magnetic moment of the nearest-neighbor N atoms was $0.904 \mu_B$, which

is higher than that observed in other configurations. The highest magnetic moment was recorded for the Mn-doped AlNNS, where the total magnetic moment reached $4.961 \mu\text{B}$, primarily resulting from the spin polarization of the Mn atoms ($4.99 \mu\text{B}$), with only slight contributions from the N (approximately $0.217 \mu\text{B}$) and Al (approximately $0.469 \mu\text{B}$) atoms.

Additionally, the local magnetic moments for other configurations were as follows: the Cr-doped AlNNS exhibited a magnetic moment of $4.319 \mu\text{B}$, V-doped nanosheets showed $\sim 3.151 \mu\text{B}$, while Co- and Fe-doped nanosheets had local magnetic moments of $\sim 3.287 \mu\text{B}$ and $\sim 4.361 \mu\text{B}$, respectively.

4. Data Availability Statement

Data sets generated during the current study are available from the corresponding author on reasonable request.

5. Conclusions

The study systematically explored the structural, electronic and magnetic properties of transition metal-doped AlN nanosheets using density functional theory. The results reveal that the pristine AlN nanosheet is a nonmagnetic, wide-bandgap semiconductor with a band gap of 4.21 eV . Upon doping with transition metals (Cr, Mn, Fe, Co, Cu), the magnetic behavior of the material changes significantly, with doping introducing magnetic moments and altering the structural integrity of the nanosheet.

Specifically, doping with Cr and Cu leads to the emergence of half-metallic ferromagnetism, with 100% spin polarization, making these materials highly suitable for spintronic applications. The computed magnetic moments show that Cr and Mn dopants contribute significantly to the overall magnetic properties, with Mn-doped AlN nanosheets exhibiting the highest magnetic moment ($\sim 4.99 \mu\text{B}$), primarily from the Mn dopant, along with slight contributions from neighboring N and Al atoms. Conversely, Cu-doped AlN nanosheets exhibit a lower magnetic moment, with the primary contribution from the neighboring nitrogen atoms rather than copper. In particular, Cr- and Cu-doped AlN nanosheets, which display half-metallicity and 100% spin polarization, are ideal candidates for spintronic devices, offering high efficiency for spin injection. Furthermore, while V- and Fe-doped AlN nanosheets show weak fer-

romagnetism, they retain semiconducting behavior, with smaller magnetic moments and less pronounced spin splitting.

The results of this study pave the way for further investigation into the precise tuning of doping concentrations and the exploration of other transition metals, with an eye toward developing high-performance nanodevices. These findings contribute to the broader understanding of transition metal-doped AlN nanosheets as promising candidates for spintronic applications and provide guidance for future experimental and theoretical investigations in the field.

1. N.A. Ismaylova, S.H. Jabarov, J.A. Guliyev. Semi-metal ferromagnetism V-doped GaN nanosheet application in a spintronic device. *Ukr. J. Phys.* **69**, 754 (2024).
2. S.G. Asadullayeva, N.A. Ismaylova, E.H. Alizade, N.T. Mamedov, A.I. Bayramov, M.A. Musayev, I.I. Abbasov. Photoluminescence and spectroscopic ellipsometry of single crystal MnGa_2S_4 . *Bull. Mater. Sci.* **47**, 115 (2024).
3. N.A. Ismaylova, S.Q. Asadullayeva. First principle calculation of magnetic properties of doped Mn: ZnGa_2S_4 . *J. Supercond. Nov. Magn.* **35**, 1107 (2022).
4. C.M. Lieber. Nanowire superlattices. *Nano Lett.* **2**, 81 (2002).
5. Z. Wu, J.B. Neaton, J.C. Grossman. Charge separation via strain in silicon nanowires. *Nano Lett.* **9**, 2418 (2009).
6. V. Meunier, C. Roland, J. Bernholc, M. Buongiorno Nardelli. Electronic and field emission properties of boron nitride/carbon nanotube superlattices. *Appl. Phys. Lett.* **81**, 46 (2002).
7. C.Y. Hsieh, S.L. Chung. High thermal conductivity epoxy molding compound filled with a combustion synthesized AlN powder. *J. Appl. Polym. Sci.* **102**, 4734 (2006).
8. A. Madan, I.W. Kim, S.C. Cheng, P. Yashar, V.P. Dravid, S.A. Barnett. Stabilization of cubic AlN in epitaxial AlN/TiN superlattices. *Phys. Rev. Lett.* **78**, 1743 (1997).
9. L.J. Shi, L.F. Zhu, Y.H. Zhao, B.G. Liu. Nitrogen defects and ferromagnetism in Cr-doped dilute magnetic semiconductor AlN from first principles. *Phys. Rev. B* **78**, 195206 (2008).
10. S.H. Wei, X.G. Gong, G.M. Dalpian, S.-H. Wei. First-principles study of Mn-induced local magnetic moments in host semiconductors. *Phys. Rev. B* **71**, 144409 (2005).
11. Y. Yang, Q. Zhao, X.Z. Zhang, Z.G. Liu, C.X. Zou, B. Shen, D.P. Yu. Mn-doped AlN nanowires with room temperature ferromagnetic ordering. *Appl. Phys. Lett.* **90**, 092118 (2007).
12. Y.J. Zhang, H.-L. Shi, S.X. Wang, P. Zhang, R.W. Li. Electronic structure and magnetic coupling properties of Gd-doped AlN: first-principles calculations. *Eur. Phys. J. B* **77**, 345 (2010).
13. H. Li, H.Q. Bao, B. Song, W.J. Wang, X.L. Chen, L.J. He, W.X. Yuan. Ferromagnetic properties of Mn-doped AlN. *Physica B* **403**, 4096 (2008).

14. M. Ayoubi-Chianeh, M.Z. Kassaei. Detection of bendamustine anti-cancer drug via AlN and Si-doped C nanocone and nanosheet sensors by DFT. *Struct. Chem.* **31**, 2041 (2020).
15. W. López-Pérez, L. Ramírez-Montes, A. González-García, C. Pinilla, J. Rivera-Julio, R. González-Hernández. Charged vacancy defects in an AlN nanosheet: A first-principles DFT study. *Comput. Condens. Matter* **14**, 153 (2018).
16. M. Beyranvand, T. Movlaroo, F.B. Baghsiyahi. Magnetic phase stability of transition metals doped (4,4) AlN nanosheet. *J. Magn. Magn. Mater.* **497**, 166028 (2020).
17. Y. Peng, C. Xia, H. Zhang, T. Wang, S. Wei, Y. Jia. Tunable electronic structures of *p*-type Mg doping in AlN nanosheet. *J. Appl. Phys.* **116**, 044306 (2014).
18. G. Xiao, L.-L. Wang, Q.-Y. Rong, A.-M. Hu, W.-Z. Xiao. Magnetic properties in AlN nanosheet doped with alkali metals: A first-principles study. *Phys. Status Solidi B* **253**, 1816 (2016).
19. H. Cao, P. Lu, Z. Yu, J. Chen. Electronic and magnetic properties of vanadium doped AlN nanosheet under in-plane biaxial strains. *Superlattices Microstruct.* **73**, 113 (2014).
20. K. Zhang, M. Pan, Z. Liu, J. Wang, Y. Wang, H. Deng. Theoretically evaluating transition metal activated two-dimensional bilayer tetragonal AlN nanosheet for high-performance HER/OER/ORR electrocatalysts. *Comput. Mater. Sci.* **232**, 112634 (2024).
21. L. Yang, H. Zou, X. Wang, C. Wang, Q. Wang, C. Liu. Synthesis, magnetism and photoluminescence of Mn doped AlN nanowires. *J. Lumin.* **243**, 118657 (2022).
22. Y. Zhang, H. Shi, R. Li, P. Zhang. Magnetic coupling properties of Mn-doped AlN nanowires: First-principles calculations. *Phys. Lett. A* **375**, 1686 (2011).
23. J. Gao, C. Ma, A. Kumar. Au-decorated semiconducting AlN nanosheet as an electronic sensor for theophylline drug. *Mol. Simul.* **47**, 500 (2021).
24. Sh. Valedbagi, A. Fathalian, S. Mohammad Elahi. Electronic and optical properties of AlN nanosheet: An ab initio study. *Opt. Commun.* **309**, 153 (2013).
25. W.A. Abdul-Hussein, F.H. Hanoon, L.F. Al-Badry. Control the electronic and optical properties of AlN nanosheet by the electric field. *Results Opt.* **11**, 100423 (2023).
26. P. Hohenberg, W. Kohn. Inhomogeneous electron gas. *Phys. Rev.* **136**, B864 (1964).
27. Synopsys. QuantumATK. <https://www.synopsys.com/manufacturing/quantumatk.html>.
28. B. Ahmed, B.I. Sharma. Structural and electronic properties of AlN in rocksalt, zinc blende and wurtzite phase: A DFT study. *Dig. J. Nanomater. Bios.* **16**, 125 (2021).
29. J.H. Edgar ed. Properties of Group III Nitrides. EMIS Datareviews Series No. 11. INSPEC, The Institution of Electrical Engineers, London (1994).
30. M. Noei, H. Soleymanabadi, A.A. Peyghan. Aluminum nitride nanotubes. *Chem. Pap.* **71**, 881 (2017).
31. H. Wu, B. Xu, R. Zheng, Z. Yan. First-principle studies on ferromagnetism of Fe-doped AlN diluted magnetic semiconductors. *Mater. Sci.* **22**, 472 (2016).
32. T. El-Achari, F. Goumrhar, L.B. Drissi, M.D. El Bouzaïdi, R.A. Laamara. Electronic and magnetic properties of V- and Cr-doped zinc-blende AlN. *Commun. Theor. Phys.* **73**, 125702 (2021).
33. Y.Q. Fan, X. Yao. Half-metallic and optical properties of Cu and Cr codoped AlN. *Adv. Mater. Res.* **842**, 205 (2014).
34. W. Jia, P. Han, M. Chi, S. Dang, B. Xu, X. Liu. Electronic structure and ferromagnetic properties of Cu-doped AlN from first principles. *J. Appl. Phys.* **101**, 113918 (2007).
35. L. Li, T. Li, Y. Hu, C. Cai, Y. Li, X. Zhang, B. Liang, Y. Yang, J. Qiu. Mechanism of the trivalent lanthanides' persistent luminescence in wide bandgap materials. *Light Sci. Appl.* **11**, 51 (2022).
36. Q.Y. Wu, Z.G. Huang, R. Wu, L.J. Chen. Cu-doped AlN: A dilute magnetic semiconductor free of magnetic cations from first-principles study. *J. Phys.: Condens. Matter* **19**, 056209 (2007).
37. G. Yao, G. Fan, H. Xing, S. Zheng, J. Ma, Y. Zhang, L. He. Electronic structure and magnetism of V-doped AlN. *J. Magn. Magn. Mater.* **331**, 117 (2013).
38. X.D. Gao, E.Y. Jiang, H.H. Liu, W.B. Mi, Z.Q. Li, P. Wu, H.L. Bai. Structure and RT ferromagnetism of Fe-doped AlN films. *Appl. Surf. Sci.* **253**, 5431 (2007).
39. N.A. Ismayilova, D.P. Rai. Half-metallic ferromagnetism in TM-doped GaN nanosheet – a potential candidate for spintronics device application. *NANO* **19**, 2450045 (2024).
40. S.G. Asadullayeva, N.A. Ismayilova, N.T. Mamedov, A.H. Bayramov, M.A. Musayev, Q.Y. Eyyubov, E.K. Kasumova, I.G. Afandiyeva, Kh.O. Sadig. Photoluminescence and density functional theory analysis of BaTiO₃:Mn. *Solid State Commun.* **372**, 115307 (2023).
41. N.A. Ismayilova, S. Asadullayeva. Computationally predicted energies and properties of defects. *Indian J. Phys.* **98**, 1103 (2024).
42. S.G. Asadullayeva, N.A. Ismayilova. Effect of rare earth ions on the optical and electronic properties of defect chalcopyrite: Experimental and theoretical investigation. *Solid State Commun.* **394**, 115725 (2024).
43. A.O. Dashdemirov, S.G. Asadullayeva, A.S. Alekperov, N.A. Ismayilova. Electronic and optical properties of GeS and GeS:Gd. *Int. J. Mod. Phys. B* **35**, 2150305 (2021).
44. N.A. Ismayilova. Electronic and magnetic properties of Mn-doped CdSe nanoribbon: First-principles calculations. *Eur. Phys. J. Plus* **139**, 321 (2024).
45. N.A. Ismayilova. Room-temperature ferromagnetism in ZnTe nanosheet doped by transition metal atom. *J. Supercond. Nov. Magn.* **38**, 80 (2025).
46. N.A. Ismayilova, Z.A. Jahangirli, S.H. Jabarov. Mn impurity in InN nanoribbon: An ab initio investigation. *J. Supercond. Nov. Magn.* **36**, 1983 (2023).
47. N.A. Ismayilova, Z.A. Jahangirli. Electronic, optical and magnetic properties of TM-doped CdTe nanosheet: First-principles calculations. *J. Magn. Magn. Mater.* **626**, 173079 (2025).

48. S.G. Asadullayeva, Z.A. Jahangirli, T.G. Naghiyev, A.S. Abiyev. Systematic analysis of the optical properties of ZnGa_2Se_4 single crystal. *Curr. Appl. Phys.* **76**, 39 (2025).
49. Z.A. Jahangirli, S.G. Asadullayeva, I.R. Amiraslanov, Q.Y. Eyyubov, A.B. Rahimli, A.S. Abiyev. Ab initio and experimental investigations of the electronic and optical properties of pure and *p*-Aminopyridine-intercalated $\text{In}_{1.2}\text{Ga}_{0.8}\text{S}_3$. *Indian J. Phys.* **99**, 2087 (2025).
50. S.G. Asadullayeva, Z.A. Jahangirli, M.A. Musayev, Q.Y. Eyyubov, A.S. Abiyev. Near-infrared photoluminescence from ZnIn_2S_4 layered single crystals. *Phys. Solid State* **67**, 429 (2025).

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МАГНІТНІ ТА ЕЛЕКТРОННІ ВЛАСТИВОСТІ НАНОЛИСТІВ AlN , ЛЕГОВАНИХ ПЕРЕХІДНИМИ МЕТАЛАМИ: ДОСЛІДЖЕННЯ З ПЕРШИХ ПРИНЦИПІВ ДЛЯ ЗАСТОСУВАНЬ У СПІНТРОНІЦІ

У роботі *ab initio* на основі теорії функціонала густини досліджено структурні, електронні, магнітні й оптичні вла-

стивості наноліста AlN , легованого перехідними металами. На основі різниці повних енергій визначено стабільні конфігурації (феромагнітну й антиферомагнітну фази). Встановлено, що чистий наноліст AlN є немагнітним напівпровідником із широкою забороненою зоною (3,28 eV), тоді як атоми перехідних металів індукують магнітні моменти, що зумовлюють структурні зміни в ділянці навколо допанта й сусідніх атомів. Розраховані парціальні густини станів (DOS) свідчать про сильну гібридизацію *d*-орбіталей атомів перехідних металів із *p*-орбіталями азоту поблизу рівня Фермі, внаслідок чого напівпровідникові властивості змінюються на напівметалеві. Леговані атомами Cr і Cu нанолісти AlN , що виявляють 100% спінову поляризацію, є перспективними матеріалами для спінтронних пристроїв завдяки вираженим напівметалевим феромагнітним властивостям. Отримані результати вказують на перспективність застосування нанолістів AlN , легованих перехідними металами, у нанопристроях і спінтронних пристроях на основі низьковимірних наноструктур.

Ключові слова: атоми перехідних металів, спінова поляризація, нанолісти, магнітні моменти.