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Electric field modulated half-metallicity of semichlorinated GaN nanosheets



^a College of Materials Science and Engineering, Xi'an Shiyou University, Xi'an 710065, People's Republic of China

^b Institute of Environmental Health and Pollution Control, School of Environmental Science and Engineering, Guangdong University of Technology,

Guangzhou 510006, People's Republic of China

^c College of Materials Science and Engineering, Xi'an University of Science and Technology, Xi'an 710054, People's Republic of China

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ABSTRACT

Through density-functional theory calculations, we investigated the half-metallic properties of semichlorinated gallium nitride (Cl–GaN) nanosheets (NSs) under an electric field *F*. The results show that the electric field can modulate Cl–GaN NSs efficiently from ferromagnetic metals to half-metals. More interestingly, under a broad range of electric field intensity ($-0.10 \sim -1.30$ V/Å), Cl–GaN NSs have the excellently half-metallic properties with the band gaps (3.71-0.96 eV) and maximal half-metallic gaps with 0.30 eV in spin-up states and metallic behaviors in spin-down states. Moreover, the total magnetic moment decreases (increases) depending on the negative (positive) *F*, mainly induced by the unpaired N atoms. Our studies demonstrate that the electronic and magnetic properties of GaN NSs can be delicately tuned by the combined surface modification and electric field, indicating the potential of GaN NSs for developing high-performance spintronic nanodevices.

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1. Introduction

Nowadays, realizing the spintronic devices has the potential advantages of nonvolatility, increasing data processing speed, decreasing electric power consumption, and increasing integration densities compared with conventional semiconductor devices [1,2]. In spintronics, half-metals are highly desirable for one metallic spin channel and the other one semiconducting channel [3]. Exploring half-metallic nanostructures is a crucial solution for developing high-performance spintronic devices [4]. Recently, the various nanosheets (NSs) have attracted a broad research interest due to their unique electronic and magnetic properties [5,6], such as silicone [7–9], AlN [10–12], and GaN [13–15] NSs.

External electric field and surface modification are promising methods for tuning the electronic and magnetic properties of semiconductor nanomaterials [16–22]. It has been reported that an external electric field can induce a direct-to-indirect band gap transition in ZnO nanowires [23,24] and a transition from semiconducting to metallic behavior in Si nanowires [25]. Applying a transverse electric field significantly reduces the band gap of MoS₂ armchair nanoribbon [26], and induces the tensile MoS₂ one with

a ferromagnetic (FM) metal [27]. Moreover, an electric field normal to NSs can act as a catalyst to facilitate semiconductor NSs with surface modification [28–30], such as hydrogenation of graphene [31] and silicene [32]. The applied electric field perpendicular to the hydrogenated bilayer graphene allows continuous tuning of the band gap and leads to a transition from semiconducting to metallic state [33]. Note that a transverse electric field induces the hydrogenated graphene nanoribbon with half-metallic behavior [34]. These researches demonstrated the resonant effects of electric field and surface modification on the electronic and magnetic properties of semiconductor nanomaterials.

Gallium nitride (GaN) with extraordinary physical properties has attracted increasing attention due to its excellent performance in optics, electronics, and photoelectronics [35]. For GaN NSs terminated with (0001) surfaces, barely and fully hydrogenated GaN NSs have a semiconductor-to-metal transition dependent on the thickness of GaN NSs because of the partially occupied surface states [36], and monolayer GaN NSs exhibit half-metallic character through particular Ga-defects [37]. The electronic and magnetic properties of GaN NSs can be controlled by decoration on one-side Ga atoms. For example, the semihydrogenated and semichlorinated GaN NSs exhibit FM behaviors except for semifluorinated monolayer with antiferromagnetic (AFM) state [13– 15]. Moreover, AlN NSs with chlorination on surface Al atoms have a transition from the half-metallic into metallic FM behaviors [38], while the semichlorinated GaN NSs maintain metallic properties



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^{*} Corresponding authors. *E-mail addresses:* mxxiao@xsyu.edu.cn (M.X. Xiao), zhimin.ao@gdut.edu.cn (Z.M. Ao).

regardless of thickness [15]. Thus, it is interesting to investigate whether GaN NSs maintain the metallicity in the context of combined effects of semichlorination and electric field.

In this work, we employ density-functional theory DFT-D calculations approach within the Grimme scheme [39] to explore the electronic and magnetic properties of semichlorinated two-bilayer GaN NSs under electric field. It is interesting to find the possibility of tuning half-metallic properties of the GaN NSs, which provide a unique way for the design and fabrication of novel spintronic devices.

2. Computational methods

Our calculations are implemented using the DMol³ code [40,41] with employing spin-polarized DFT-D, where generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) is chosen as the exchange-correlation functional [42]. For the geometric, electronic, and magnetic calculations, the 2×2 unit cells of GaN NSs are used with a vacuum space of 15 Å to avoid interlayer interactions between neighboring cells. All the atoms are allowed to relax without any constraints. The DFT semicore pseudopots is implemented for relativistic effects [43,44]. In addition, the double numerical plus polarization (DNP) basis sets are adopted in all calculations [40]. The Brillouin zone integration is performed with $17 \times 17 \times 1$ k-points [45]. Smearing technique is also used to achieve the self-consistent field convergence with a smearing value of 0.001 Ha (1 Ha=27.2114 eV). The convergence tolerances of energy of 1.0×10^{-5} Ha, the maximum force of 0.002 Ha/Å, and the maximum displacement of 0.005 Å are taken in the geometry optimization.

3. Results and discussion

The bare two-bilayer GaN NS with polar (0001) surfaces forms a planar graphitic structure, which is constructed from bulk wurtzite structure. Note that the graphitic GaN NS exhibits a nonmagnetic (NM) semiconductor at the ground state in well consistent with the previous results [36,46]. Similar to BN and ZnO NSs [47,48], since Ga and N sites in GaN NSs are chemically nonequivalent [14], the two-bilayer GaN NS transforms to be FM metal through chlorination on one-side Ga atoms (denoted as Cl-GaN NSs) in the insert of Fig. 1(a), but remains NM behavior through chlorination on one-side N atoms [15]. In order to investigate the probability of electric field F tuning ferromagnetic half-metallicity of the Cl-GaN NSs, we calculate three magnetic configurations in NM, FM and AFM states (the insets of Fig. 1) under different strength of vertical electric field. Herein, we describe that a vertical electric field *F* along the upward direction is defined as positive "+", i.e., from the surface Cl atoms to the surface N atoms while F along the downward direction is defined as negative "-". The energy differences $\Delta E_{\rm FM-NM}$ between FM and NM states and $\Delta E_{\text{FM-AFM}}$ between FM and AFM states are dependent on electric field strength F in Fig. 1, respectively. It can be seen that the energies of Cl-GaN NSs in FM states between N atoms are energetically lowest than those in NM and AFM configurations under the electric field strength F from -1.50 to +0.50 V/Å. Our results confirm that the structures of Cl–GaN NSs in FM states remarkably are energetically most stable under electric field. Thus, we mainly investigate the structural, electronic and magnetic properties of Cl-GaN NSs in FM states under different electric field.

To further assess the structural stability of Cl–GaN NSs in FM states under electric field, the binding energies E_b of these systems are calculated as follows: $E_b = (E_{Cl-GaN} - E_{GaN} - n_{Cl}E_{Cl})/n_{Cl}$. E_{Cl-GaN}



Fig. 1. (Color online) The atomic structures and the energy difference ΔE between FM and NM or AFM states of two-bilayer GaN NSs with chlorinated Ga atoms (a) in side view, (b) NM, (c) FM and (d) AFM states in top views. The large (light pink) and middle (dark blue) spheres represent Ga and N atoms, respectively, while the smallest light blue spheres represent Cl atoms. The subscript number indicates the bilayer number.



Fig. 2. (Color online) Calculated binding energies E_b (in eV) of two-bilayer Cl–GaN NSs in FM states as a function of electric field strength *F*, where the insets show the bond lengths of atomic structures at *F*.

and E_{GaN} are the total energies of the semichlorinated and bare GaN NSs. E_{CI} and n_{CI} is the energy and number of single Cl atoms. Fig. 2 presents the binding energies E_b of the Cl–GaN NSs in FM states as a function of electric field *F*. We find that chlorination on Ga atoms of GaN NSs is still energetically favorable, suggesting the feasible study of chlorination on Ga atoms of GaN NSs in FM states.

For two-bilayer Cl–GaN NSs in FM states, the Ga and N atoms become sp³ hybridized with the bonded Cl atoms, which distorts the planar geometries of GaN NSs and forms zigzag configurations. The optimized atomic structures (the insets of Fig. 2) indicate the semichlorinated Cl–GaN NSs with wurtzite configurations rather than the graphitic ones under electric field. The optimized Ga₂–Cl bond lengths (2.208 Å) involve the formation of the chemical bonds between Cl and surface Ga atoms. With increasing negative (positive) *F*, the bond lengths of Ga₂–Cl and Ga₁–N₁ bonds elongate (shrink) slowly, and those of Ga₂–N₂ and Ga₂–N₁ bonds remain unchanged, indicating the deteriorative and strengthening interactions between Cl and Ga₂ atoms or between Ga₁ and N₁ atoms. Note that the change of bond lengths between undecorated N and neighboring Ga atoms results in a transition from semiconductor



Fig. 3. (Color online) Band gaps in spin-up states (solid squares) and spin-down states (hollow squares), and half-metallic gaps in spin-up states (hollow circles) dependent on electric field strength *F* for two-bilayer Cl–GaN NSs in FM states, where the insets give band structures at F = -0.10 V/Å, at F = -0.25 V/Å, at F = -0.30 V/Å, at F = -0.30 V/Å, at F = -1.30 V/Å, at F = -1.30 V/Å, and at F = -1.35 V/Å, at F = -0.30 V/Å, at F = -1.35 V/Å, at F = -0.30 V/Å.

or half-metallic into metallic behavior for the semidecorated GaN NSs [15]. Therefore, the chlorination-derived effects are significantly modulated by the bonding variation under electric field, which is an important factor for the electronic and magnetic properties of the GaN NSs.

To verify whether the two-bilayer Cl-GaN NSs can exhibit halfmetallicity in the presence of the vertical electric field, we calculate the band structures, partial density of states (PDOS) and magnetic moment of the two-bilayer Cl-GaN NSs in FM states. In pristine GaN NSs, the charge transfer from Ga to N atoms and the orbital hybridization make electrons paired, thus the system is NM [36]. However, the two-bilayer Cl-GaN NSs without electric field are FM metals in Fig. 3, where both the spin-up and spin-down states become metallic and spin polarization is obvious in the band structure and PDOS in Fig. 4(a) and (b). By applying a positive electric field with the strength from 0 to +0.5 V/Å, the fully-metallic behavior maintains in both spin-up and spin-down states. We select the band structure and PDOS of two-bilayer Cl-GaN NSs at F = +0.50 V/Å (Fig. 4(c) and (d)) to illustrate the fully-metallic fact. More careful examination of PDOS in Fig. 4(b) and (d) reveals that Ga atoms are covalently bonded with Cl atoms forming sp³ hybridization, leading to 2p orbitals of N₁ atoms unpaired. Thus, the induced magnetism is attributed primarily by the unsaturated N atoms (2p orbitals) and Cl atoms (3p orbitals), which is similar to the results in BN NSs [47].

Now, we turn to study the effects of negative electric field on the properties of Cl-GaN NSs in the FM state. Fig. 3 shows the band gaps and half-metallic gaps in spin-up and spin-down states under an electric field, where half-metallic gap is defined as the difference between the Fermi level and the valence maximum band (VBM). It is clearly seen that once a negative electric field is applied, the valence band maximum in the spin-up state rapidly shifts downwards, but the spin-down state remains metallic behavior. When the electric field strength increases to -0.10 V/Å, Cl– GaN NS becomes a FM half-metal, where spin-up state transforms into a semiconductor with band gap of 3.44 eV and half-metallic gap of 0.10 eV, while spin-down state maintains metallic behavior. Detailed analysis of PDOS reveals that the half-metallic behavior is determined by the occupied energy band of Cl 3p orbital in spinup state lower than the Fermi level in Fig. 5(a). With increasing strength of the negative electric field, a metallic behavior in spindown state remains unchanged and the direct band gap and halfmetallic gap are enlarged in spin-up state. The resonant effects of the movement upwards or downwards of the conduction band minimum (CBM) and VBM on the band gaps and half-metallic gaps are induced by the electric field. The direct band gap in the spinup state is 3.70 eV at F = -0.20 V/Å where the CBM reaches to the highest energy level of 3.49 eV, while the half-metallic gap increases to 0.21 eV. At F = -0.25 V/Å, the movement downward of the energy levels of CBM and VBM leads to Cl-GaN NS with the maximum band gap of 3.71 eV and half-metallic gap of 0.29 eV in the spin-up state. However, at F = -0.30 V/Å, the VBM arrives at the lowest energy level of -0.30 eV, indicating that the maximum of half-metallic gap is 0.30 eV, and the direct band gap in the spinup state becomes 3.62 eV. With higher strength of negative electric field, the energy levels of CBM and VBM continuously shift near the Fermi level, leading to the band gaps and half-metallic gaps in spin-up states monotonously decrease. At F = -1.30 V/Å, the Cl-GaN NSs has a direct band gap of 0.96 eV and 0.01 eV in the spin-up state, respectively. From the PDOS in Fig. 5(b), the CBM and VBM are contributed by Ga₂ 4p and N₁ 2p orbital. However, our calculation shows that a too strong electric field would destroy the half-metallicity of semiconductor NSs. Applying a stronger negative electric field, Cl-GaN NSs could transform into metallic character. To more evidently demonstrate this case, the band structure and PDOS of Cl–GaN NS under F = -1.50 V/Å are shown in Fig. 6. It can be obviously seen that N₁ 2p orbitals across Fermi level in both spin-up and spin-down states, indicating the fullmetallicity for Cl-GaN NSs in FM states. More interestingly, the electric field and chlorination on Ga atoms present the resonant effects on the half-metallic behaviors of GaN NSs at a broad range from F = -0.10 V/Å to F = -1.30 V/Å. For other materials, the zigzag AlN [3] and graphene [49] nanoribbons can exhibit half-metallicity under a relatively narrower range of $-0.20 \sim -0.05 \text{ V/Å}$ and $+0.30 \sim +0.80$ V/Å, respectively. Our results of effectively tuning half-metallic properties of GaN NSs by electric field and surface modification may open their novel potential applications in spintronic devices.

Fig. 7 displays the magnetic moments of different elements in Cl–GaN NSs under electric field, where the emergent spin polarization is primarily contributed by the unpaired N atoms on the surface, and other atoms contribute very slightly. As the electric strength *F* of positive (negative) electric field increases, the magnetic moments of all N and Ga atoms monotonically increase (decrease), while those of Cl atoms change in the opposite trend. The resulting total magnetic moments per unit cell increase (decrease) with increasing positive (negative) *F*. Note that the linear electric field effects on the magnetic properties are similar to the situation of zigzag MoS₂ nanoribbon [50].

Fig. 8 illustrates the Hirshfeld charges difference Δq of all the atoms defined as $\Delta q = q(F) - q(0)$, where q(F) and q(0) denote the Hirshfeld charges under electric field and F=0. The N₁ and Ga₁ atoms and Cl atoms have a large Hirshfeld charge change under an electric field. However, the charge transfer of Ga₂ and N₂ atoms keeps almost unchanged. Clearly, Δq of N₁ and Ga₁ atoms increase monotonously with the positive or negative F, but contrary to that of Cl atoms. Note that Cl atoms receive less electrons, indicating the weakened effects of semichlorination on the Ga atoms. Thus, the degree of hybridization on GaN NSs is a main reason for the band gap variation with F, which results in the transition from metallic into half-metallic behavior. Moreover, with increasing negative (positive) electric field, the surface N_1 atoms in Cl–GaN NSs gain more (less) electrons from other atoms, suggesting the unpaired character deteriorated (strengthened), which interprets the reason that the rule of total magnetic moment as a function of the electric field F. As it is well known, the electronic and magnetic properties of thinner semiconductor NSs with larger surface/



Fig. 4. (Color online) Band structures and PDOS of Cl–GaN NSs in FM states (a)–(b) without electric field and (c)–(d) at F=+0.50 V/Å, respectively.

volume ratio should be more sensitive to the combined electric field and surface modification.

4. Conclusions

We have systematically investigated the electronic and magnetic properties of semichlorinated GaN NSs under an electric field. Depending on the strength and direction of the electric field, the Cl–GaN NSs have a transition from fully-metallic into halfmetallic behaviors, and persist the half-metallic properties from electric field strength F = -0.10 V/Å to F = -1.30 V/Å where the band gaps (3.71–0.96 eV) and half-metallic gaps in spin-up states vary with F and the metallic behavior regardless of F. The total magnetic moment decreases (increases) with increasing negative (positive) F, which are mainly contributed by the unpaired N



Fig. 5. (Color online) PDOS of CI–GaN NSs in FM states (a) at F = -0.10 V/Å and (b) at F = -1.30 V/Å respectively.



Fig. 6. (Color online) Band structure and PDOS of Cl–GaN NSs in FM state at F = -1.50 V/Å.



Fig. 7. (Color online) The magnetic moment of Cl-GaN NS per unit cell as a function of electric field strength F.



Fig. 8. (Color online) The Hirshfeld charge difference Δq of every atom of Cl–GaN NS as a function of the electric strength *F*, the charge difference Δq is defined as $\Delta q = q(F) - q(0)$, where q(0) and q(F) denotes the Hirshfeld charge at F = 0 and different electric field strength.

atoms and slightly donated by other atoms. Therefore, the combined effects of electric field and surface modification by chlorination play a key role in tuning the electronic and magnetic properties of GaN NSs, which facilitate the design and optimization of semiconductor NSs in spintronic nanodevices.

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