First-principles predictions of tunable half metallicity in zigzag GaN nanoribbons with possible applications in CO detection and spintronics

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September 8, 2022

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Abstract

Based on systematic first-principles density-functional theory (DFT) simulations, we predict that the zigzag GaN nanoribbons (ZGaNNR) can be used both as highly efficient CO detectors as well as spin filters. Our calculations, performed both on infinitely long nanoribbons, and also on finite strands, suggest that: (a) CO binds strongly at the edges of ZGaNNRs, and (b) that several of the resultant configurations exhibit half-metallic behavior. We considered various edge-passivation sites and found that all the resultant structures are thermodynamically stable. The metallic, half-metallic, and semiconducting configurations are observed as a function of CO passivation coverage. We also compute the current-voltage (I-V) characteristics of various structures using the Landauer formalism, and find that the devices made up of half-metallic configurations act as highly-efficient spin filters. The effect of CO concentration is also investigated which suggests a viable way to not just tune the electronic band gap of ZGaNNRs, but also their half metallicity. Our simulations thus suggest a new direction of research for possible device applications of III-V heterostructures.

• Keywords: Nanoribbons, Gallium Nitride, Zigzag, Carbon monoxide, detection/capturing, spin filtering.

Introduction

2-D materials [1, 2, 3, 4] exhibit potential candidature as a building block in upcoming sensing devices due to their higher surface to volume ratio, unique electron confinement and mature synthesis techniques compared to their 1-D counterparts [5, 6, 7, 8, 9, 10]. Their outstanding electronic, magnetic and transport properties, higher carrier mobility also makes them center of attraction for various technological applications [11, 12, 13, 14, 15, 16, 17, 18, 19]. It is reported that nanoribbons can be realized either by cutting [20] mechanically exfoliated nanosheet [21] or by patterning epitaxially grown nanosheet [22, 23]. The obtained nanoribbons are in the form of zigzag, armchair and chiral [24, 25, 26]. Edge shape play a vital role in case of nanoribbons as all the electronic, magnetic and transport properties are significantly influenced by their edge geometries [27, 28, 29, 30, 31, 32, 26]. GaN nanoribbons are successfully synthesized using various technique [33, 34, 2, 35]. The electronic and magnetic properties of nanoribbons make them a good candidate for various applications [36].

Continuous advancement in industries and growth of traffic increases the pollution rate day by day. Therefor, the development of highly efficient sensors is one of the most active area of research nowadays. The exceptional electronics properties and edge reactivity of 2D material makes them a good candidate for detection of gas molecule at very low concentration [37, 38, 39, 40]. GaN nanoribbons exhibit wide band gap and a promising material for optoelectronic and high power applications. On the other hand, its investigations towards sensing devices are very limited [41, 10, 42]. The application of GaN in sensing devices could be superior compared to graphene which
is restricted via zero band gap behavior \cite{43, 44}. As CO is one of the most common environment pollutant gas, it is highly warranted to develop CO sensing/capturing devices in near future. On the other hand, the intrinsic wide band gap of GaNNR could obstruct its path for semiconducting device applications. The interaction of CO with GaNNR edges may affect their electronic properties. Therefore, the present study, CO passivation with GaN based zigzag nanoribbons (ZGaNNR) is investigated towards possible CO detection and its effect on the band gap modulation. In our study we focused on the electronic behavior of the material through which we have also analyzed the charge transfer due to the passivation of gas molecule on ZGaNNR. Typically, the charge transfer to the molecule or from the molecule, also induces change in electric resistivity of the material.

**Model and Methodology**

The present investigations were performed using first-principles self-consistent calculations based on density functional theory (DFT). We used QuantumATK DFT code \cite{45} for the present simulation results. The generalized gradient approximation (GGA) in the form of Predew-Burke-Ernzerhof (PBE) was used as exchange correlation potential \cite{46}. The considered configurations of ZGaNNR were modelled with periodic boundary conditions having repetition along Z-axis whereas X and Y directions were kept confined. The norm-conserving pseudo-potential with 70 Ry energy mesh cut-off value was adopted to define the fineness of the grid. Further, double $\zeta$ polarized basis set has been considered for all constituent atoms. The Monkhorst-Pack Grid \cite{47} for k-point sampling was selected as $1 \times 1 \times 50$ for defining the sampling of the Brillouin zone centered at $\Gamma$. To avoid inter-ribbon interactions, ribbons were separated using a cell padding vacuum of 10Å along the confined directions. During the geometry optimization, we used Pulay mixer algorithm with $1 \times 10^{-5}$Ry tolerance for self-consistent iteration loop and all the atoms were free to change their positions during optimization to attain the minimum energy configuration. The geometries were relaxed without any constraint till the force and stress on each atom reduces to a criterion of 0.05 eV/Å and 0.05 eV/Å$^3$ respectively. The ribbon width is defined in the conventional manner i.e. the number of Ga-N bonds across the transverse direction \cite{48, 49}. Five different passivation sites on ZGaNNR are considered for CO molecule as illustrated in Fig. 1.

![Figure 1: The schematics of zigzag GaN nanoribbon with passivation of CO on (a) CO-ZGaN-CO, (b) CO-ZGaN-H, (c) H-ZGaN-CO, (d) CO-ZGaN and (e) ZGaN-CO at width-8.](image-url)
Table 1: Calculated bond lengths and bond angles of CO passivated zigzag GaN nanoribbons

|                | Bond length (Å) | Bond angle (°) |
|----------------|----------------|----------------|
| C-O (Ga edge)  | 1.81           | 116.39         |
| C-O (N-edge)   | 1.19           | 116.87         |
| C-Ga (Ga edge) | 1.90           | 118.08         |
| Ga-N (Ga edge) | 1.86           | 131.20-126.58  |
| Ga-H (N-edge)  | 1.53           | 115.73         |

Results and discussion

Structural Stability

To find out the most suitable passivation sites, various possible configurations have been modeled. It is noticed that bonding of CO molecule with the GaN nanoribbons takes place via C side as shown in Fig. [1]. The variation in bond length and bond angle has been illustrated in Table 1. To avoid an ambiguity, the structural stability of CO passivated GaN nanoribbons is further discussed in separate subsections for ZGaNNR.

The reported lattice constant of zigzag GaN nanoribbon is 3.18Å which shows good agreement with our results (3.32Å) [50]. All the properties of nanoribbons are highly dependent on their edge shape and ribbon width. First we investigate the structural stability of bare and H-passivated nanoribbons.

Table 2: Variation of adsorption energy ($E_{ad}$), binding energy (BE), band gap ($E_g$) and Fermi energy ($E_F$) of H-passivated and bare zigzag GaN nanoribbons as a function of ribbon width.

| Width ($N_Z$) | ZGaNNR (eV) | H-Passivated | Bare |
|---------------|-------------|--------------|------|
|               | $E_{ad}$    | $E_g$        | $E_F$| BE  | $E_g$ | $E_F$ |
| 4             | -5.65       | 3.40         | -3.17| -5.83| M     | -4.96 |
| 6             | -5.69       | 3.04         | -3.55| -6.02| M     | -4.99 |
| 8             | -5.70       | 2.86         | -3.68| -6.12| M     | -4.98 |

To insure the structural stability we have calculated the binding energy (BE) for bare ribbons and adsorption energy for H-passivated ribbons respectively and the calculated values are depicted in Table 2. To calculate the BE following relation has been used [51, 52]:

$$BE = \frac{1}{m+n}[E_{total} - m(E_{Ga}) - n(E_N)]$$

(1)

where $E_{total}$, $E_{Ga}$ and $E_N$ are, the total energies of bare ribbon, isolated Ga, and N atom. Similarly, m and n represented the number of Ga and N atoms in the nanoribbon respectively. As per the definition adopted here, negative binding or adsorption energy exhibits exothermic nature while the magnitude signifies thermodynamic stability. It is noticed that structural stability increases with the ribbon width. To find the most stable CO passivated nanoribbon, we calculate adsorption energy ($E_{ad}$) of considered configurations including H passivation. The following relation has been utilized for $E_{ad}$ calculation: [53, 54]

$$E_{ad} = \frac{1}{n}[E_T - E_{bare} - nE_{H/CO}]$$

(2)

where $E_T$, $E_{bare}$, $E_{H/CO}$ are the total energies of considered configuration after attachment of CO/H, bare nanoribbon, isolated CO molecule/H atoms, respectively and n is number of passivated molecules/atoms.
Table 3: Variation of adsorption energy ($E_{ad}$), Fermi energy ($E_F$) and band gap ($E_g$) of zigzag GaN nanoribbons with CO passivation as a function of ribbon width.

| Configurations  | Width ($N_Z$) | $E_{ad}$(eV) | $E_F$(eV) | Spin up | Spin down | $E_g$ (eV) |
|----------------|----------------|---------------|-----------|---------|-----------|------------|
| CO-ZGaN-CO    | 4              | -1.64         | -3.44     | M       | 0.5       |            |
|                | 8              | -1.66         | -3.41     | M       | 0.5       |            |
|                | 4              | -3.67         | -3.06     | M       | 3.0       |            |
| CO-ZGaN-H     | 6              | -3.71         | -3.05     | M       | 2.6       |            |
|                | 8              | -3.71         | -3.04     | M       | 2.5       |            |
|                | 4              | -3.64         | -3.43     | 2.5     | 1.0       |            |
| H-ZGaN-CO     | 6              | -3.68         | -3.53     | 2.1     | 0.9       |            |
|                | 8              | -3.69         | -3.64     | 2.0     | 0.9       |            |
|                | 4              | -1.19         | -4.49     | M       | M         |            |
| CO-ZGaN       | 6              | -1.20         | -4.44     | M       | M         |            |
|                | 8              | -1.75         | -4.81     | M       | M         |            |
|                | 4              | -2.65         | -3.51     | 1.0     | 0.2       |            |
| ZGaN-CO       | 6              | -2.69         | -3.55     | 0.9     | 0.2       |            |
|                | 8              | -2.68         | -3.63     | 0.8     | 0.2       |            |

For sensing of CO molecules, five different passivation sites are considered as illustrated in Fig. 1. The structural stability of all considered geometries of ZGaNNR are tabulated in Table 3. The magnitude of adsorption energy is much higher than thermal excitation energy ($\approx 25$ meV) which suggests that all the configurations are thermally stable. Interestingly, it is also noticed that the most energetically favorable configuration is CO-ZGaNN-H followed by H-ZGaNN-CO from which we conclude that the presence of passivating H atoms effectively increases the stability of ZGaN nanoribbon. Similarly, the order of least favorable configurations are CO-ZGaN, CO-ZGaNN-CO and ZGaNN-CO. The Fermi energy also varies as the ribbon width increases. In all the configurations the Fermi level shifts in downward direction with respect to its bare counterpart. The downward shifting of Fermi level is analogous to p-type doping candidature. It is also concluded that after passivation of CO, ZGaN nanoribbons are stable in antiferromagnetic (AFM) ground state. We tried to incorporate the effect of vdW corrections however, there was no change in the ground state energy of the structures. This is due to the reason that all the adsorbed CO molecules form stable chemical bonds with the host nanoribbons. Therefore, the weak physical interactions are not affecting the ground state of the system [55, 56].

Electronic properties

The electronic band structures of ZGaNNR with passivation of CO on the edges of nanoribbon are illustrated in Fig. 2. It is reported that zigzag bare GaNNR is metallic in nature whereas H-passivation exhibits a band gap [42, 57]. Also, zigzag bare and H-passivated GaNNR, both are stable in non-magnetic ground states, respectively. It is revealed that presence of CO on the edges of ZGaNNR profoundly affects the electronic properties of ZGaNNR. After passivation of CO, ZGaNNR is stable in AFM ground state. The observed AFM ground state could be further explained on the basis of electronegativity difference between C and the host edge atoms (Ga and N). The electronegativity of C is greater (smaller) than the Ga (N) atoms. Owing to this, an unequal charge transfer takes place between the adsorbed CO molecule and the edge Ga/N atoms. It creates a difference between the electric potentials of the opposite edges which in turn favors the AFM ground state. Similar magnetic behavior has been previously reported for graphene nanoribbons functionalized with different atoms/groups [58]. Interestingly, when both edges of nanoribbon are containing CO molecule [Fig. 1] and when CO is passivated on the Ga edge and N edge posses H atom [Fig. 1(b)] then half metallic nature is noticed as depicted in Fig. 2(b). Another important thing we have observed is the pure metallic character when CO is located at the Ga edge of the ribbon [Fig. 2(d)]. However, when Ga edge is passivated by H atom or left bare, finite band gap is observed [Fig. 2(c) and (e)]. The calculated band gap is 2.0 eV for spin-up carrier whereas 0.9 eV for spin-down charge carrier of H-ZGaNN-CO configuration at ribbon width-8. Similarly, ZGaNN-CO configuration posses band gap [0.8 eV (spin-up) and 0.2 eV (spin-down)]. It is reported that H-passivated ZGaNNRs exhibit indirect band gap [57] and after passivation of CO the behavior remains same [Fig. 2(c) and (e)].
Figure 2: The spin polarized band structure of zigzag GaNNR with CO passivation for (a) CO-ZGaNNR-CO, (b) CO-ZGaNNR-H, (c) H-ZGaNNR-CO, (d) CO-ZGaNNR and (e) ZGaNNR-CO at width-8. The solid (black) and dashed (red) lines correspond to electronic states of spin up (majority spin) and spin down (minority spin) electrons respectively. The horizontal dotted line at 0 eV represents the Fermi level.

For the further understanding of electronic properties of ZGaNNR with CO passivation, we have also calculated the density of states (DOS) of all the considered geometries [Fig. 3]. It is revealed that the DOS profile exhibits good compatibility with band structure results. The similar half metallic character is also noticed in DOS of CO-ZGaN-CO and CO-ZGaN-H configurations. Similarly, the absence of energy states near the Fermi level is witnessed in H-ZGaN-CO and ZGaN-CO configuration, whereas the DOS of CO-ZGaN clearly exhibits metallic behavior.

Figure 3: The spin polarized DOS of zigzag GaNNR with CO passivation for (a) CO-ZGaNNR-CO, (b) CO-ZGaNNR-H, (c) H-ZGaNNR-CO, (d) CO-ZGaNNR and (e) ZGaNNR-CO at width-8. The solid (black) and dashed (red) lines correspond to electronic states of spin up (majority spin) and spin down (minority spin) electrons respectively.

In realistic devices, there will be finite fragments of nanoribbons between the electrodes, unlike the infinitely
long structures considered for computing the band structure. Therefore, we have also investigated the electronic properties of finite fragments of CO-ZGaNRR-CO consisting of five unit cells (repetitions) as illustrated in Fig. 4. Our calculations reveal that even this finite fragment exhibits half-metallic character with a finite band gap for spin down electrons \( (E_g = 0.55 \text{ eV}) \), and a negligible one \( (E_g = 0.06 \text{ eV}) \) for spin up electrons. Hence, only the spin-up electrons will participate in conduction, leading to a spin-polarized current.

Figure 4: Energy levels of up- (b) and down-spin (c) electrons for the CO-ZGaNRR-CO fragment consisting of five repeat units (a). The solid (black) and dashed (red) lines correspond to electronic states of spin up (majority spin) and spin down (minority spin) electrons respectively. The blue dotted line at 0 eV represents the Fermi level.

For further verification of the observed half-metallic character and understanding the splitting of electronic states around the Fermi level, Bloch states have been analysed. We elected the highest valence band and the lowest conduction band for this (Bloch) analysis as these are mainly responsible for governing the electronic transport in the material. The spin polarized Bloch states for CO-ZGaNRR-CO are depicted in Fig. 5. Perusal of this figure reveals that different spins are populated at opposite edges of the ribbon. The localized behavior of electrons is also be noticed in Fig. 5 (a)-(d). Additionally, there exists a phase change of \( \pi \) between spatially separated charges on the two edges, further confirming the AFM ordering in the system.
Transport Properties

The two-probe model is used for transport studies as shown in Fig 6. The calculated I-V characteristic of ZGaNNR containing CO are illustrated in Fig 7.

It is revealed that CO-ZGaN configuration exhibits maximum current followed by CO-ZGaN-CO. In these two structures, current increases linearly up to ~0.6 V beyond which it starts to saturate. In contrast, an interesting behavior is noticed for rest of the other I-V characteristics. For H-ZGaN-CO, the current remains zero for entire bias window as the corresponding band gap is significantly larger (2.5 eV) than applied biasing. For remaining three structures, the current initially increases and attains a maximum value (~14 µA for bare/CO-ZGaN-H and ~ 11.6 µA for ZGaN-CO) around 0.5 V. As the biasing is further increased, the current starts to decline and approaches 0 near 1 V. Thus, a clear signature of negative differential resistance (NDR) phenomena is obtained in these three structures.
Figure 7: The calculated I-V characteristic of bare and CO passivated ZGaN nanoribbons with higher peak to valley ratio (PVR).

The observed I-V characteristics could be further understood on the basis of transmission spectra as shown in Fig 8. For CO-ZGaN and CO-ZGaN-CO, the transmission coefficient is found to be maximum (i.e. 4) which supports highest current in these structures. For the structures showing NDR behavior, a relatively small but finite transmission coefficient is noticed around the Fermi level. Upon increasing the biasing, reduction in the transmission takes place which is responsible for the observed NDR phenomenon.

Figure 8: The calculated transmission spectra of CO passivated ZGaN nanoribbons for (a) bare, (b) CO-ZGaN-CO (c) CO-ZGaN-H, (d) H-ZGaN-CO, (e) CO-ZGaN and (f) ZGaN-CO.

To further confirm the half metallic behavior in selected structures as observed in the band structures [Fig. 2 (a), (b)], we computed spin polarized I-V characteristics. Fig 9 depicts the spin dependent currents for CO-ZGaN-CO and CO-ZGaN-H structures. It is clearly visible in both of these images that the entire current conduction takes place only due to spin up (majority spin) electrons. As the current due to spin down (minority spin) electrons remains essentially zero, it confirms the observed HM property of these structures.
Spin filtering efficiency

The spin I-V characteristics of considered structures exhibit interesting features. We find that for a given voltage, the magnitude of the current due to one spin orientation is much more than that due to the other. This imbalance between the current contributed by the two different spin orientations is an important parameter for spin filtering device applications. The ability of a material or a device to select a particular spin direction can be quantified in terms of spin filtering efficiency ($S_{FE}$) defined as \[ S_{FE} = \frac{I_{\text{spin}^\uparrow} - I_{\text{spin}^\downarrow}}{I_{\text{spin}^\uparrow} + I_{\text{spin}^\downarrow}} \times 100\% \] (3)

where, $I_{\text{spin}^\uparrow}$ and $I_{\text{spin}^\downarrow}$ are the magnitudes of the currents for spin-up and spin-down electrons, respectively. Fig 10 shows the behavior of spin filtering efficiency as a function of applied voltage for CO-ZGaNNR-CO and CO-ZGaNNR-H structures. With respect to the applied bias voltage, we note the following trends: (a) for CO-ZGaNNR-CO, $S_{FE}$ varies in the range 86%-100%, while (b) for CO-ZGaNNR-H, $S_{FE}$ stays constant at 100%. This behavior is fully consistent with the variation of the currents of the two spin orientations, with the applied bias voltage, for the two types of nanoribbons (see Fig 9). These results suggest that if one is looking for a perfect spin filter, CO-ZGaNNR-H is a strong candidate for the purpose.
Different CO concentration

In the present work we have also study the different CO concentration effect on the of most energetically favorable configuration (CO-ZGaN-H). Different edge coverage (0% to 100% with interval of 25%, where 0% means absence of CO and 100% means all edges are passivated by CO molecule.) of CO is obtained for the analysis of the electronic properties of CO-ZGaN-H (Fig 11).

It is noticed that the different edge coverage of CO profoundly alter the electronic properties of considered structures. The band structures of CO-ZGaN-H with different CO concentrations is illustrated in Fig 12. Interestingly, it is noticed that as the edge coverage of CO increases, the band gap decreases. The magnitude of obtained band gap is 1.5 eV (spin-up) & 1.9 eV (spin-down), 1.5 eV (spin-up) & 1.1 eV (spin-down), 0.9 eV (spin-up) & 2.1 eV (spin-down), metallic (spin-up) & 1.1 eV (spin-down), and metallic eV (spin-up) & 2.6 eV (spin-down) for 0%, 25% and 50% CO coverage. In contrast, for 75% and 100% CO coverage, the half metallic behavior is obtained as already discussed in the previous section. Thus, variation in the CO coverage could be a potential way to tailor the electronic band gap of ZGaNNR.

![Figure 10: The calculated spin filtering efficiencies of CO-ZGaN-CO and CO- ZGaNNR-H.](image)

![Figure 11: The Schematic diagrams of different concentration of CO on most energetically favorable configuration CO-ZGaN-H for (a) 0%, (b) 25%, (c) 50%, (d) 75% and (e) 100% at width-8 and 4 repetition.](image)
In summary, our DFT based first-principles calculations demonstrate that after passivation of CO molecule on one or both the edges of ZGaNNR, the nanoribbons exhibit metallic to half metallic character. Of the two possible CO-passivated configurations, we find that the nanoribbons passivated with CO on one edge (CO-ZGaNNR-H) are not only more stable as compared to the ones passivated with it on both the sides (CO-ZGaNNR-CO), but also they exhibit better spin-filtering efficiency. Furthermore, we also observe variations in Fermi energy as a function of passivation, suggesting that the edge passivation can also be used to achieve doping in these systems. The negative differential resistance observed in these structures also suggests their possible applications in fabricating oscillators and amplifiers. Therefore, we believe that structures can be used to fabricate a variety of devices such as CO sensors, spin filters, oscillators, and amplifiers.

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