First principle insights of NO$_2$ detection via III-V nitride nanoribbons with armchair edges

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Abstract
The development of low-dimensional and robust nano-sensors is an area of potential research and development. In this direction, here, we investigated the sensing of NO$_2$ gas molecules adsorbed on the edges of III-V nitride nanoribbons with armchair edges (AXNNR, X = B/Al/Ga). Five different adsorption sites are considered for the adsorption of NO$_2$ molecules and the adsorption assisted modulation of electronic and transport properties has been observed for detection purpose. Interestingly, a semiconducting to metallic transition has been noticed in considered AXNNR due to NO$_2$ interaction. The selectivity of NO$_2$ with respect to N$_2$ is found to be higher as compared to that of O$_2$. Further, some of the selected structures exhibit an interesting negative differential resistance (NDR) phenomenon which suggest that NO$_2$ adsorbed AXNNR could also be useful for designing of the fast switching devices and oscillators applications.

1. Introduction

Nowadays, high performance and highly sensitive gas sensors have gained enormous attention for air quality monitoring, chemical/gaseous detection, medical diagnosis etc. The magnitude of air pollutants in breathable air such as CO, SO$_2$, NO$_2$ etc increases day by day which causes various health issues for the mankind. NO$_2$ is the major pollutant available in our environment which is released during burning of fossil fuels, motor vehicles exhaust, combustion in factories and thermal power plants. The presence of NO$_2$ gas in atmosphere is responsible for photochemical smog, acid rain, ozone layer thinning and respiratory related diseases. Thus, maintaining the quality of environment is a major concern all over the world which demands for the development of next generation sensing devices. The successful synthesis of nitride based mono-layers and nanoribbons [1–4] has revolutionized the research community due to their promising physical, chemical and electronic properties. Nitride (BN, AlN, GaN etc) based nanoribbons posses hexagonal honeycomb structure identical to graphene nanoribbons [5, 6]. Depending upon the edge shape, nanoribbons are mainly divided into two category: zigzag edged nanoribbons and armchair edged nanoribbons [7]. It is reported that nitride based nanoribbons exhibit fascinating electronic, chemical, mechanical and thermal properties [8–10] which makes them a promising building blocks for various nano-device applications [11, 12]. In case of nanoribbons, owing to dangling bonds, edges are more reactive as compared to their central region [13]. Therefore, due to edge functionalization, the electronic properties of nanoribbons could be efficiently tailored for various technological applications. It is reported that armchair nitride nanoribbons (AXNNR, where X = B/Al/Ga) are wide band gap semiconductor and the variation in band gap has been noticed with increasing ribbon width [14–16]. The half-metallicity in edge hydrogenated armchair boron nitride nanoribbon is predicted by Rai et al [17]. The theoretical investigations reveal that edges of boron nitride nanoribbons decorated by different functional group exhibit variation in the electronic properties of the nanoribbons [18]. Similarly, the effect of the dangling bonds on the electronic and magnetic properties of AlN nanoribbons has also been investigated by Zhang et al [19]. Various studies also conclude that nitride based nanoribbons exhibits excellent candidature for sensing of gas molecules [12, 20–22]. However, a fair comparison among all nitride nanoribbons is highly warranted to select...
the most potential member for designing the efficient sensing devices. Thus, here we compared the sensing capability of armchair edged nitride (BN, AlN and GaN) nanoribbons towards detection of harmful pollutant NO2.

2. Methodology

For present results, First-principle investigations were performed under the flagship of density functional theory (DFT) coupled with non-equilibrium Green's function as employed in Quantum-ATK code [23]. The generalized gradient approximation (GGA) in the form of Perdew, Burke and Ernzerhof was used for accounting the exchange correlations [24]. All the considered configurations of nitride based armchair nanoribbons (AXNNR, X = B/Al/Ga) with NO2 adsorption are modelled with periodic boundary conditions. To analyze the structural stability, electronic properties and transport properties of AXNNR, five different configurations for NO2 adsorption are considered as illustrated in figure 1. The considered structures are: figure 1 (a) NO2 molecule adsorbed on both edges of nanoribbon (NO2-AXNNR-NO2), in configurations (b) and (c) one of the edge atom is adsorbed by NO2 while other is H passivated [NO2(H)-AXNNR-H(NO2)], similarly, in configurations (d) and (e) NO2 is adsorbed only at one of the edge atom [NO2-AXNNR or AXNNR-NO2]. A vacuum space of 10 Å was introduced along non-periodic directions to eliminate the spurious interactions between periodic replicas of the structures. Nanoribbons of width Na = 5, 7 and 9 are considered to comment on the width effects. The Monkhorst-Pack Grid [25] was used for k-point sampling and set to 1 x 1 x 50 in the first Brillouin zone and centred at Γ. For the geometry optimization, 70 Ry energy cut-off was used whereas the force and stress between participating atoms were reduced to be less than 0.05 eV Å−1 and 0.05 eV Å−3 respectively. During the process of optimization, no constraint was imposed on the supercell or its constituent atoms. Furthermore, to calculate the current-voltage (I-V) characteristics of NO2 adsorbed AXNNR, we have used two-probe model. The I-V characteristics is calculated using following relation [26]:

\[ I(V) = G_0 \int_{\mu_L}^{\mu_R} T(E, V) \left( f(E - \mu_L) - f(E - \mu_R) \right) d\varepsilon \]  

(1)

where, G0 is the quantum of conductance while \( \mu_L \) and \( \mu_R \) are the chemical potentials of left and right electrodes respectively. T represents the transmission spectra which is a function of energy and bias voltage and governs the electron transitions from left to right electrodes through central scattering region.

3. Structural stability

To identify the structural stability of NO2 adsorbed AXNNR, first we have investigated the structural stability of bare AXNNR as depicted in table 1. After optimization, the observed bond lengths between B-N, Al-N, Ga-N, B-H, Al-H, Ga-H and N-H are found to be (1.39 Å to 1.44 Å), (1.79 Å to 1.81 Å), (1.83 Å to 1.85 Å), 1.21 Å, 1.58 Å, 1.52 Å and 1.02 Å respectively which show good agreement with previous available data [16, 20, 27, 28]. To
investigate the structural stability of bare AXNNR we have calculated the binding energy using following relation [29]:

$$BE = \frac{1}{p + q}[E_{\text{Total}} - p(E_X) - q(E_N)]$$

(2)

where $E_{\text{Total}}, E_X, E_N, p$ and $q$ are the total energies of bare ribbon, isolated X atom, isolated N atom, total numbers of X and N atoms in the nanoribbon respectively. To explore the most energetically favourable configuration, we have compared the adsorption energies ($E_{\text{ad}}$) of NO$_2$ adsorbed AXNNR calculated as [20]:

$$E_{\text{ad}} = \frac{1}{n}[E_{\text{Tot}} - E_{\text{bare}} - nE_{\text{Guest}}]$$

(3)

where $E_{\text{Tot}}, E_{\text{bare}}, E_{\text{Guest}}$ are the total energies of considered configuration after adsorption of (NO$_2$ and H), bare nanoribbon, isolated NO$_2$ molecule and isolated H atoms respectively and $n$ is number of adsorbed guest atoms/molecules.

As per the definition adopted here, negative binding or adsorption energy exhibits exothermic nature while the magnitude signifies thermodynamic stability. It is observed that, in bare AXNNR the binding energy improves with increasing the ribbon width. In addition, the order of energetic feasibility is found to be BN $>$ AlN $>$ GaN i.e. moving downward in the periodic table, the stability of AXNNR decreases. This is due to the fact that difference between atomic radii of X = B/Al/Ga and N atom increases. Owing to this, the X − N bond length increases from B to Ga and their binding energy decreases. After analyzing the structural stability of bare AXNNR, we further explore the structural stability of NO$_2$ adsorbed AXNNR as depicted in table 2. To identify the most energetically favourable adsorption configuration for NO$_2$ gas molecules, five different adsorption sites are considered here. Investigations revealed that all the configurations are expected to be thermodynamically stable in non-magnetic ground state. Out of five configurations, NO$_2$-AXNNR-H was found to be most energetically favorable followed by the H-AXNNR-NO$_2$. It is noticed that the bonding of NO$_2$ takes place via formation of stable chemical bonds with the edge atoms of ribbons. The optimized angle for isolated NO$_2$ molecule was $\angle$ONO $= 132.77^\circ$, whereas after adsorption on AXNNR it varies with the adsorption site. After adsorption on AXNNR, the calculated angle $\angle$ONO $= 122.71^\circ, 117.59^\circ, 110.36^\circ$ is

### Table 1. Variation of binding energy (BE), Fermi energy ($E_F$) and the band gap ($E_g$) as a function of ribbon width ($N_a$) for bare AXNNR.

| Width ($N_a$) | ABNNR (eV) | AAlNNR (eV) | AGaNNR (eV) |
|--------------|------------|-------------|-------------|
|              | $E_B$      | $E_F$       | $E_g$       | $E_B$      | $E_F$       | $E_g$       | $E_B$      | $E_F$       | $E_g$       |
| 5            | $-8.61$    | $-3.44$     | $3.66$      | $-6.69$    | $-4.69$     | $1.84$      | $-5.81$    | $-4.66$     | $1.81$      |
| 7            | $-8.82$    | $-2.99$     | $4.02$      | $-6.91$    | $-4.54$     | $1.99$      | $-5.99$    | $-4.50$     | $1.94$      |
| 9            | $-8.94$    | $-2.88$     | $4.12$      | $-7.03$    | $-4.48$     | $2.05$      | $-6.10$    | $-4.42$     | $2.00$      |

### Table 2. Variation of adsorption energy ($E_{\text{ad}}$) and band gap ($E_g$) for NO$_2$ adsorbed AXNNR as a function of ribbon width ($N_a$). Here, all numerical values (except the ribbon widths) are presented in eV while M represents the metallic character of the structure.

| Configurations | Width ($N_a$) | ABNNR | AAlNNR | AGaNNR |
|----------------|--------------|-------|--------|--------|
| NO$_2$-AXNNR-NO$_2$ | 5 | $-0.39$ | $0.8$ | $-2.81$ | $2.4$ | $-2.42$ | $2.2$ |
|                 | 7 | $-0.39$ | $0.8$ | $-2.81$ | $2.4$ | $-2.16$ | $2.2$ |
| NO$_2$-AXNNR-H   | 9 | $-0.39$ | $0.8$ | $-2.80$ | $2.3$ | $-2.42$ | $2.2$ |
|                 | 5 | $-3.97$ | $3.3$ | $-4.53$ | $2.5$ | $-4.13$ | $2.7$ |
|                 | 7 | $-3.99$ | $3.2$ | $-4.36$ | $2.5$ | $-4.22$ | $2.7$ |
| H-AXNNR-NO$_2$   | 5 | $-3.23$ | $3.3$ | $-3.93$ | $2.9$ | $-3.77$ | $2.7$ |
|                 | 7 | $-3.08$ | $3.3$ | $-3.24$ | $3.1$ | $-3.76$ | $2.6$ |
|                 | 9 | $-3.09$ | $3.3$ | $-3.24$ | $2.9$ | $-3.26$ | $2.5$ |
| NO$_2$-AXNNR     | 5 | $-1.82$ | $M$   | $-2.41$ | $M$   | $-1.70$ | $M$   |
|                 | 7 | $-1.54$ | $M$   | $-2.34$ | $M$   | $-1.66$ | $M$   |
|                 | 9 | $-1.52$ | $M$   | $-2.32$ | $M$   | $-1.64$ | $M$   |
| AXNNR-NO$_2$     | 5 | $-1.62$ | $M$   | $-3.19$ | $M$   | $-2.74$ | $M$   |
|                 | 7 | $-1.54$ | $M$   | $-2.87$ | $M$   | $-2.53$ | $M$   |
|                 | 9 | $-1.54$ | $M$   | $-2.88$ | $M$   | $-2.53$ | $M$   |
obtained for B edge, Al edge and Ga edge respectively. Thus, an overall reduction in the bond angle of NO$_2$ is witnessed for B to Ga. It is also noticed that after optimization, the NO$_2$ adsorbed from O-side in case of AGaNNR whereas in BN and AlN nanoribbons it is attached from N-side.

4. Electronic properties

The AXNNR can be used for sensing applications if the changes in the electronic properties due to NO$_2$ adsorption are easily measurable. To investigate the electronic properties of NO$_2$ adsorbed AXNNR, first we have studied the electronic properties of bare AXNNR. The electronic band structures of bare AXNNR are illustrated in figure 2.

It is observed that obtained band gaps of bare ribbons are lower than those of H-passivated counterparts of respective AXNNR $[12, 16]$. Further, the magnitude of obtained $E_g$ as presented in table 1 follows the trend of BN $>$ AlN $>$ GaN similar to previous available reports $[28, 30, 31]$. The electronic band structures of NO$_2$ adsorbed AXNNR are depicted in figure 3. The variation in electronic properties of AXNNR are highly sensitive to adsorption sites of NO$_2$ molecules. Similar findings were recently reported for SO$_2$ molecules $[32]$. It is noticed that NO$_2$-AXNNR-NO$_2$ configuration reveals lower band gap as compared to NO$_2$- AXNNR-H and H-AXNNR-NO$_2$ whereas NO$_2$-AXNNR and AXNNR-NO$_2$ configurations exhibit metallic character irrespective of the type of nanoribbons i.e. BN/AlN/GaN (figure 3).

To verify the obtained electronic band structures, we have also studied the electronic density of states (DOS) as depicted in figure 4. The DOS profile of all the considered configurations exhibits excellent agreement with their corresponding band structures i.e. availability of electron peaks across the Fermi level for NO$_2$-AXNNR and AXNNR-NO$_2$ while the absence of electronic states near Fermi level for remaining all configurations. Thus, the noticed NO$_2$ assisted changes in the electronic properties of AXNNRs are significant. A remarkable change in the band gap as well as semiconductor to metallic transition has been confirmed which could to be utilized for sensing device application.

5. Transport properties

In order to investigate the measurement of changes in electronic properties of AXNNR due to NO$_2$ adsorption, we next investigated the transport properties by computing current-voltage (I-V) characteristics using standard two-probe models $[33]$ as depicted in figure 5. The two-probe model consists of scattering region in the centre which is seamlessly coupled with right and left electrodes. As the proposed sensing devices are expected to be operating under low bias condition, we calculated I-V characteristics within 0–1 V and selectively for NO$_2$-AXNNR and AXNNR-NO$_2$ as shown in figure 6.

As the remaining structures exhibit $E_g = 0.8$ eV or larger, the magnitude of current remains almost zero within the selected bias range (0–1 V). It is revealed that AXNNR-NO$_2$ structures exhibit overall larger current that NO$_2$- AXNNR. In later, the maximum current is observed for BN nanoribbon which also displays a negative differential resistance (NDR) phenomenon whereas linear behavior is noticed for AlN nanoribbon. On the other
hand, for AXNNR-NO$_2$ configuration, the order of current is noticed as GaN > AlN > BN with a perfect NDR behavior noticed for GaN and AlN nanoribbons. The observed NDR behavior could be explained on the basis of corresponding electronic band structures (figures 3(d$_1$)–(d$_3$) and (e$_1$)–(e$_3$)). It is revealed that configurations exhibiting NDR phenomenon have discrete and quantized electronic states near the Fermi level. As the biasing is applied across the electrodes, current continue to increase through two-probe device as long as the channel states lie between the chemical potential of left and right electrodes. Further increment of applied biasing shifts the electrode chemical potentials such that no channel states are available for electronic conduction between them which in turn results in the reduction of the current and causes NDR behavior.

For further understanding of the origin of NDR behavior, the computed transmission spectra for AXNNR-NO$_2$ has been depicted in figure 7. It is revealed that highest transmission coefficient is noticed for AGaNNR (with a magnitude of 4) in the vicinity of Fermi level. This highest transmission is consistent with the observed largest current through this structure. In addition to this, a transmission gap is also witnessed near 0.5 eV which continues upto ~1 eV. This transmission gap is responsible for the peculiar NDR behavior in AGaNNR. As soon as the biasing shifts the chemical potential of the electrodes within this gap, current decreases rapidly and eventually results in NDR behavior. Similar transmission gap is noticed in the transmission spectra of AlN and BN nanoribbons. However, the decay of transmission peak around the Fermi level is slower in BN compared to AlN. It causes delay in the decrement of the current through BN nanoribbon which looks like saturated I-V characteristics. Remarkably, it is observed that only integer transmission peaks exist for AXNNR which points towards the quantized transport through the ribbons.

The maximum current value obtained for AlNNR-NO$_2$ is 5.67 μA whereas for AGaNNR-NO$_2$ it reaches upto 12.81 μA (at 0.5 V). Although, after achieving the maximum value it decreases upto 0.22 μA and 0.51 μA respectively for AlN and GaN nanoribbons. Thus, the peak to valley ratio (PVR) is obtained upto 25.77 and 25.12 respectively for AlN and GaN nanoribbons in AXNNR-NO$_2$. The obtained PVR magnitude indicates that NO$_2$ could be further explored for the chemical edge functionalization of AXNNR towards potential application in upcoming nano-electronic devices.

Figure 3. The electronic band structures of NO$_2$ adsorbed AXNNRs for (a$_1$)–(a$_3$) NO$_2$–AXNNR–NO$_2$, (b$_1$)–(b$_3$) NO$_2$–AXNNR–H, (c$_1$)–(c$_3$) H–AXNNR–NO$_2$, (d$_1$)–(d$_3$) NO$_2$–AXNNR and (e$_1$)–(e$_3$) AXNNR–NO$_2$ for ribbon of width $N_a = 9$. The dotted line at 0 eV represents the Fermi level.
6. Selectivity

To identify the selectivity of AXNNRs towards targeted NO$_2$ molecules, we further analyzed the selectivity as a function of temperature with respect to two most abundant environmental gases (i.e. N$_2$ and O$_2$) as shown in figure 8. The selectivity of NO$_2$ on the edges of AXNNR, is calculated using following equation [34]

$$S_{NO_2/O_2/N_2} = \frac{A_{NO_2}}{A_{O_2/N_2}} e^{(-E_{O_2/N_2}+E_{NO_2})/k_BT}$$

(4)

where A is the interaction pre-factor taken for NO$_2$ as well as O$_2$/N$_2$ equal to the reported value of A = 10$^{11}$ [35]. The $E_{O_2/N_2}$, $E_{NO_2}$ represents the adsorption energies of O$_2$/N$_2$ and NO$_2$, $k_B$ is Boltzmann constant and T is the temperature in Kelvin.

It is noticed that temperature has a profound effect on the selectivity of NO$_2$ (figure 7). Moreover, the selectivity of NO$_2$ with respect to O$_2$ is low as compared to that of N$_2$ which is consistent with previous results for zigzag ribbons of similar materials [36]. The graphical representation of selectivity of NO$_2$ with respect to N$_2$ suggests that NO$_2$-AXNNR-NO$_2$ configuration is the most preferred one amongst all considered structures.
followed by NO$_2$-AXNNR-H and H-AXNNR-NO$_2$ respectively. On the other hand, AXNNR-NO$_2$ configuration is found to be least preferred from selectivity point of view. Overall, the most preferred material for better selectivity of NO$_2$ with respect to N$_2$/O$_2$ is predicted to be ABNNR followed by AAlNNR and AGaNNR respectively.

7. Sensitivity

As sensitivity is an important parameter for any sensing device, we next calculated the sensitivity of NO$_2$-AXNNR and AXNNR-NO$_2$ configurations (being metallic configurations as illustrated in figure 3). The following relation has been utilized for the calculation of sensitivity [37]:

$$S(\%) = \frac{|G - G_{\text{ref}}|}{G}$$

where $G$ and $G_{\text{ref}}$ are the zero bias conductance with NO$_2$ adsorbed AXNNR and bare AXNNR respectively. It is evident that all nanoribbons exhibit 100% sensitivity which shows good agreement with previously reported work on different inorganic materials [37, 38]. This is due to the fact that adsorption of NO$_2$ induces metallic character in intrinsically wide band gap AXNNR.
8. Recovery time

As recovery time plays a crucial role to decide the widespread acceptability of any sensing device, we next examined the recovery time of NO2-AXNNR and AXNNR-NO2 configurations. For every gas sensor, recovery time is a crucial parameter which predicts the reusability of the sensors. The following relation has been used for recovery time calculation [39–41]:

$$\tau = \frac{1}{v} e^{(-E_{ad}/k_B T)}$$

(6)

where \(v\), \(E_{ad}\), \(k_B\), and \(T\) are attempt frequency of bond breaking (assume to be \(10^{12}\) Hz similar to previous literatures [42, 43]), adsorption energy of NO2, Boltzmann constant and temperature.

The variation of recovery time as a function of temperature is shown in figure 9. The schematic of recovery time suggests that the recovery time and temperature both are inversely proportional to each other. It is evident that with increasing the temperature, recovery time is improved. The temperature dependent recovery time of ABNNR with NO2 adsorption is illustrated in figure 9(a), It is noticed that at 700 K, ABNNR took about 1 s time to recover whereas at higher temperature further reduction in recovery time has been witnessed. On the other hand, AAlNNR exhibit higher recovery time which suggest against their reusability; however, their disposable sensors could be further explored. AGaNNR shows interesting behaviour of recovery time. It is noticed that NO2-AGaNNR configuration is recovered within 5 s at 700 K, whereas at higher temperatures the recovery time further reduces. On the other hand, AGaNNR-NO2 configuration is predicted to take about \(1.79 \times 10^6\) s (at 700 K) to recover which is therefore not suggested for fast sensing devices. However, in a recent study, 2D tetragonal GaN is found to exhibit potential towards detection of NO and NO2 molecules with promising recovery time at room temperature [44]. The synthesis of BN nanosheets and their sensing application has also been reported by Lin et al [45] which involved the adsorption of gaseous molecules and subsequent changes in the resistivity measurements.

Figure 8. The calculated selectivity of NO2 with respect to O2 (upper panel) and with respect to N2 (lower panel) for (a) and (d) ABNNR, (b) and (e) AAlNNR and (c) and (f) AGaNNR.
9. Conclusion

In summary, our first-principle calculations predict that NO₂ adsorption significantly affects the electronic and transport properties of AXNNR presenting them as a building block for designing next generation sensing devices. It is noticed that NO₂ molecules form most stable chemical bonding with AAlNNR making it worst reusable sensing material. Further, NO₂-AXNNR-H is found to be energetically most preferred configuration for all AXNNR. The reduction in the band gap as well as semiconductor to metallic transition is also obtained in AXNNR due to NO₂ adsorption. Further, NDR phenomenon is witnessed in selective structures which suggest that NO₂ adsorbed AXNNR could also be explored for fast switching devices and oscillator applications.

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Data availability

All data that support the findings of this study are included within the article. Other data will be made available on request.

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Figure 9. The calculated recovery time as a function of temperature for (a) ABNNR, (b) AAlNNR and (c) AGaNNR.
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