Energetic and Electronic Properties of NH₃, NO₂ and SO₂ Interacting with GaN Nanotube: A DFT Study

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Energetic and electronic properties of NH_3 , NO_2 and SO_2 interacting with GaN nanotube: A DFT study

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Abstract In this work, the interaction of GaN nanotube (GaNNT) with common air pollutants of industrialized cities, such as NH_3 , NO_2 and SO_2 in different configurations was studied. For this study, the single-walled (10,0) GaNNT was used. The analysis was done via the density functional theory implemented in the SIESTA simulation software. The analysis of the results shows that the air pollutants alter the properties of nanotubes when they interact with them. The stability analysis shows that the most stable configurations are those in which adsorption occurs through a chemical process. The systems remain semiconductors, but in the case of NO_2 and SO_2 molecules interacting with GaNNT, there was a significant reduction in the energy gap. Our results also indicate that GaNNT is a promising material to detect and remove NH_3 and NO_2 molecules from the environment, however it may be not applicable to detect or remove SO_2 , because the latter interacts strongly with the nanotube, which prevents the GaNNT from being reused.

Keywords GaN nanotubes · DFT · Electronic properties · Air pollutants

1 Introduction

In the last decades, there has been a major technological advance in the world, but the implementation of these technologies despite the benefits has also brought harmful effects such as air pollution. Pollutants such as ammonia (NH_3), nitrogen dioxide (NO_2) and sulfur dioxide (SO_2) are by-products of various chemical and biological processes and considered dangerous for our

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environment. NH_3 is a widely used chemical that can be found in a variety of common industrial environments, while NO_2 is the precursor to a series of harmful secondary air pollutants, such as nitric acid, aerosols and photooxidants [1]. SO_2 is a toxic gas that can cause health problems and is found mainly in automobiles and oil industries [2]. The most common method of controlling pollutants is through air filtration, where the porous substances in the air filter retain part of the gases generated by burning the fuel. To enhance the action of filters, catalysts (composed of noble metals) are used, which interact with combustion gases and produce gases less toxic to the environment. The adsorption of pollutants in the filtrations gradually decreases the performance of the filters, so it is necessary to use materials with greater durability than those already used. Nanostructured materials are an option, as recent studies show that the shape and size of these materials can affect their original properties. Nanostructures such as nanotubes, nanowires and nanorods have been studied due to their potential applications in nanoelectronic and optoelectronic devices, due to their unique electronic and optical properties. [3]. On the other hand, the adsorption of gases in nanotubes has potential applications in fuel cells, gas sensors and hydrogen storage [4]. There are different types of nanotubes investigated for adsorption of gas molecules, such as the carbon nanotube, [5], boron nitride nanotubes [6], silicon carbide nanotubes [7], among others [8-10].

Gallium nitride (GaN) nanomaterials have drawn great attention as a promising candidate for use in short-wavelength optoelectronic devices, such as light-emitting diodes (LEDs), laser diodes (LDs), as well as high-power operating devices and high temperature [11]. In particular, studies show that GaNNTs are stable and can be synthesized under some extreme conditions [12-15]. For example, Goldberger et al. [14] synthesized GaNNT using the epitaxial casting method and characterized through electron microscopy. They found that GaNNTs are robust, electrically and optically active, and therefore are interesting nanostructures for biochemical electronic sensing and optoelectronics applications. Due to their excellent properties, GaNNTs can be used as materials for gas detection, and for this reason, Khan et al. [16] used the density functional theory to investigate the interactions between the (4,4) GaNNT with the NH_3 and NO_2 molecules using the Gaussian 09 software [17]. They found that GaNNT may be a prominent sensor candidate for the NH_3 and NO_2 gas molecules. Due to the lack of research with GaNNT acting as a sensor for toxic gas molecules in the literature, in this work we report the study of zigzag (10,0) GaNNT interacting with NH_3 , NO_2 and SO_2 molecules of toxic gas.

2 Method of calculation

The investigation of the adsorption of NH_3 , NO_2 and SO_2 molecules in different sites of the (10,0) GaNNT was made through density functional theory (DFT) calculations [18]. The SIESTA code [19] was used to perform the full self-

consistent calculations to solve the Kohn Sham equations [20]. The interaction of valence electrons with ionic cores was described through norm conserving pseudopotentials [21] in Kleinman-Bylander form [22]. A double zeta basis set with polarization function was used in all the calculations [23]. The electronic relaxation was converged to 1.0×10^{-4} . Eighteen special k-points along the Γ -X directions using Monkhorst-Pack method [24] sampled the Brillouin zone. The generalized gradient approximation (GGA) with the parametrization of Perdew et al. [25] was used for the exchange-correlation term. The charge density was represented by a cutoff of 250 Ry for the grid integration. In all calculations were used supercell approximation and the periodic boundary conditions.

A zig-zag (10,0) GaNNT with 80 atoms ($\text{Ga}_{40}\text{N}_{40}$) and total length of 11.60 Å was chosen as the initial model. In order to assure that the tubes in neighboring cells do not interact, the supercell dimensions in directions perpendicular to the tube axis are taken as 15.0 Å. A conjugated gradient procedure was used to perform the structural optimizations. Furthermore, the atomic positions of the structure were relaxed until all the force components were smaller than 0.05 eV/Å.

The binding energies (E_b) calculated for all systems were obtained through the following formula:

$$E_b = E_T[X + \text{GaNNT}] - E_T[\text{GaNNT}] - E_T[X] \quad (1)$$

where $E_T[X + \text{GaNNT}]$ is the total energy of the GaNNT with the adsorbed molecules, $E_T[\text{GaNNT}]$ is the total energy of the pristine GaNNT and $E_T[X]$ is the total energy of the isolated molecules (NH_3 , NO_2 or SO_2).

3 Results and discussion

NH_3 interacting with GaNNT

First of all, the geometry of the pristine GaNNT was optimized to compare some of its structural and electronic properties with the literature. Therefore, after the geometry optimization, the Ga-N bond length was approximately 1.87 Å along the tube axis and 1.81 Å otherwise, which is in agreement with the works of Sodre et al. [26] and Ribeiro et al. [27]. The interaction of the NH_3 molecule with the GaNNT surface was performed according the following configurations: (i) the N atom of the molecule over the Ga atom of the nanotube, (ii) the N atom of the molecule over the N atom of the nanotube, (iii) the N atom of the molecule in the center of one of the nanotube hexagons and (iv) the NH_3 molecule inside the nanotube. The optimized geometries for each studied configuration above are shown in Figure 1. According to the binding energies, the most stable configuration was the first configuration (i), in which a bond is formed between the N atom of the molecule and the Ga atom of the nanotube [see Figure 1 (a)], with a binding energy of approximately 1.20 eV, calculated through the Equation 1, and a bond length of around 1.99 Å.

Fig. 1 Optimized structures representation for GaNNT interacting with NH_3 molecule. The pink, grey and blue spheres indicate Ga, N, H atoms, respectively.

Table 1 shows the binding energy (E_b) calculated through the Equation 1, the distance from the molecule center to the tube surface (D), the energy gap (E_g) and the charge transfer (CT) for each configuration shown in Figure 1. From the Table 1, we can see that all binding energies have negative values, which indicates that these structures are stable. Moreover, the interaction between NH_3 molecule with the GaNNT, in the configuration of the Figure 1 (a), occurs through a chemical process, whereas in the configurations of the Figures 1 (b) and (c), the interactions occur through a physical process. This is due to the analysis carried out by Machado et al. [28], which shows that binding energy values less than or equal to 0.83 eV are considered low values and correspond to a physical adsorption, whereas binding energies above this value correspond to a chemical adsorption process.

For the studied configurations, we consider the charge transfer (see Table 1) through the analysis of the Mülliken population, and although this analysis does not correspond to the correct values of partial charges, it indicates the correct tendency and order of the charge transfer process [29]. Therefore, in Table 1 we can infer that in the configuration of the Figure 1 (a), which corresponds to the most stable structure, the NH_3 molecule donates $0.38 e^-$, while in configurations of the Figures (b) and (c) the NH_3 donates only $0.05 e^-$ and receives $0.01 e^-$, respectively. These low amount of charge donated

Table 1 Binding energies (E_b), distance from the molecule center to the tube surface (D), energy gap (E_g) and charge transfer (CT) for each studied configuration of the (10,0) GaNNT interacting with the NH_3 molecule. The plus (minus) sign in the charge transfer values indicates that the NH_3 molecule donates (receives) electronic charge.

Configuration	E_b (eV)	D (Å)	E_g (eV)	CT (e^-)
(a)	-1.20	1.99	2.24	+0.38
(b)	-0.32	3.28	2.30	+0.05
(c)	-0.10	3.48	2.30	-0.01

and received in these last two systems is already expected due to their low interaction with the nanotube. Thus, we can infer that in all systems the NH_3 molecule behaves as an electron donor, except in the system of the Figure 1 (c).

Fig. 2 Electronic band structure for (a) pristine GaNNT and for [(b), (c) and (d)] different configurations of NH_3 interacting with the GaNNT, which correspond to the configurations shown in Figures 1 (a), (b) and (c), respectively. The red dotted line represents the Fermi level.

To investigate the modification on the electronic properties of the NH_3 molecule interacting with GaNNT, the band structure was plotted as shown in Figure 2. For comparison purposes, we plotted in Figure 2 (a) the band structure for the pristine (10,0) GaNNT, which shows that this nanomaterial

is a direct band gap semiconductor with an energy gap around 2.34 eV. This value is in good agreement with literature for GaNNTs with diameters between 8.50 Å to 9.80 Å [26, ?]. In all systems, the band gap is defined as the energy difference between the states of the bottom of the conduction band and the top of the valence band. The Figures 2 (b), (c) and (d) show the band structure of the configurations represented in Figures 1 (a), (b) and (c), respectively. By direct comparison with the pristine (10,0) GaNNT, we can observe that the NH_3 adsorption introduces new levels in valence and conduction bands that hybridize weakly with the GaNNT bands. These new levels are present mainly at the top of the valence band, where a degenerate level appears.

Fig. 3 Plots of the local density of states (LDOS) for the NH_3 molecule interacting with (10,0) GaNNT in all studied configurations. The plots are for the electronic structure, in the region around the Fermi level, of the Figures 2 (b)-(d), using an isovalue of 0.005 states/Ry.

In order to elucidate in more detail the localization of the states around the Fermi level, the local density of states (LDOS) was plotted. Thus, the LDOS for the band structure shown in Figure 2 (b) is represented in Figure 3 (a), where we can see in general that for the isosurface value of 0.005 states/Ry, the contributions around the Fermi level are mainly due to the N and Ga atoms of GaNNT, specially the Ga and N atoms near the NH_3 molecule. The Figures 3 (b) and (c) show the LDOS for the band structures of the Figures 2 (c) and (d), respectively, where we can see that the contribution is due to the N atoms of the nanotube and the molecule.

NO_2 interacting with GaNNT

The Figure 4 show the optimized geometries for all studied configurations of the NO_2 molecule interacting with the GaNNT. The most stable configuration is shown in Figure 4 (a), in which the N atom of the molecule was initially positioned over the N atom of the nanotube, and after the geometry optimization, the NO_2 molecule was adsorbed to the nanotube in such a way that its two O atoms each one formed a Ga-O bond (approximately 1.80 Å) with the Ga atoms of GaNNT, while its N atom formed a N-N bond of approximately

1.46 Å with the N atom of the GaNNT [see Figure 4 (a)], which deformed three nanotube rings. This structure was already expected, since the N atom in the Lewis structure of NO_2 has a positive charge, and as the N atom of the GaNNT has an unpaired electron pair and also a negative partial charge, so the formation of a N-N bond in this system with a high binding energy (-1.28 eV) is not surprising. The Ga-N bond lengths near the region where the

Fig. 4 Optimized structures representation for GaNNT interacting with NO_2 molecule. The pink, grey, blue and red spheres indicate Ga, N, H and O atoms, respectively.

molecule was adsorbed are approximately 2.00 Å, while all others Ga-N bonds are around 1.81 and 1.87 Å, as in the (10,0) pristine GaNNT.

In configuration 4 (b), the molecule was initially positioned in the center of one of the GaNNT hexagons, and after the geometry optimization, the molecule moved over the Ga atom of the nanotube, where a Ga-O bond was formed with approximately 1.86 Å. Another stable configuration occurred when the N atom of NO_2 was initially positioned on the Ga atom of the nanotube, and after the geometry optimization, the N atom formed a bond with the Ga atom of approximately 1.94 Å. Even though the N in the Lewis structure of NO_2 having a positive charge, however, it also has an unpaired electron that gives rise to the geometry of this molecule, therefore, a bond between the N of NO_2 and the Ga was also expected, but as the results shows us, this is not the most favorable configuration, which can be explained by the positive charge on the N of the NO_2 Lewis structure.

The Table 2 lists the binding energies calculated through Equation 1, the bond lengths between the NO₂ and the GaNNT, the energy gap and the charge transfer (between the NO₂ and the GaNNT) for each system represented in the Figure 4. The binding energies values indicate that in the configurations 4 (a), (b) and (c), the interaction occurs through a chemical adsorption process, while in the configuration 4 (d) the interaction occur through a physical adsorption process. The charge transfer, calculated through the Mlliken population, indicated that the nanotube donates 0.21 e⁻, 0.12 e⁻ and 0.07 e⁻ to the NO₂, in the systems of the Figures 4 (a), (b) and (d), respectively. While the system of Figure 4 (c) was the only one in which the NO₂ molecule donates charge (0.04 e⁻) to the nanotube.

Table 2 Binding energies (E_b), the bond lengths and the distances between the NO₂ and the nanotube surface (D), energy gap (E_g) and the charge transfer (CT) for each system represented in Figure 4. The minus sign in charge transfer values indicates that the nanotube receives charge, while the plus sign indicates that the nanotube donates electronic charge.

Configuration	E_b (eV)	D (Å)	E_g (eV)	CT (e ⁻)
(a)	-1.28	$D_{N-N} = 1.46$; $D_{Ga-O} = 1.86$	1.16	-0.21
(b)	-1.07	$D_{Ga-O} = 1.86$	0.11	-0.12
(c)	-0.96	$D_{Ga-N} = 1.94$	0.39	+0.04
(d)	-0.32	4.05	0.34	-0.07

The electronic band structure around the Fermi level was plotted in Figure 5 for all systems with the NO₂ interacting with the (10,0) GaNNT, where the Fermi level is represented by the red dotted line, located at zero. The Figure 5 (b) shows the band structure for the structure of Figure 4 (a), which corresponds to the most stable configuration, where we can see significant changes in the electronic structure when the NO₂ molecule is adsorbed on the GaNNT surface. Two deep flat levels emerge in the gap region and are strongly localized. One of these levels is occupied and located at approximately 0.66 eV above the top of the valence band, and the other level is empty and located at around 2.03 eV below the bottom of the conduction band. These impurity states are located very far from the edges of the bands, which, in principle, the charge carriers could not participate in the transport of the current. We can also observe the appearance of degenerate levels at the top of the valence band and in the bottom of the conduction band, due to the interaction of NO₂ molecule with nanotube. On the other hand, the introduction of impurities levels in the gap region, reduces the energy gap from 2.34 eV to 1.16 eV, approximately. To better elucidate the localization of these states, we have plotted the local density of states (LDOS) around the Fermi level in the Figure 6, for the isosurface value of 0.005 states/Ry. Thus, we can see that, for this system, the energy levels around the Fermi level belong exclusively to the N atom of molecule, as shown in the Figure 6 (a).

Fig. 5 Electronic band structures for (a) the pristine GaNNT, and for [(b)-(e)] different configurations of NO_2 interacting with the GaNNT, which correspond to the configurations shown in Figures 4 (a)-(d), respectively. The red dotted line represents the Fermi level.

Fig. 6 Plots of the local density of states (LDOS) for the NO_2 molecule interacting with (10,0) GaNNT in all studied configurations. The plots are for the electronic structures, in the region around the Fermi level, of the Figures 5 (b)-(e), using an isovalue of 0.005 states/Ry.

The band structures of the Figures (c) and (d) have similar behavior, since in all systems the localized levels appear in the energy gap region and degenerate levels appear at the top of the valence band. In addition, the energy gap has been significantly reduced, due to the presence of defect levels that emerge in the energy gap region. In the band structures of the Figures (c) and (d), the energy gap was reduced from 2.34 eV to 0.11 eV and 0.39 eV, respectively, compared to the (10,0) pristine GaNNT. The LDOS of these two systems, around the Fermi level, show that these defect levels in the gap region are contribution mainly from the NO_2 orbitals [see Figure 6 (b) and (d)].

The band structure for the configuration in which the NO₂ molecule is inside the nanotube is shown in Figure 5 (e), and as we can see, new levels appear in the energy gap region when compared directly to the (10,0) pristine GaNNT. These levels are characteristic levels from the molecule, and they contribute to the reduction of the energy gap from 2.34 eV to 0.34 eV, when compared to the pristine system. The LDOS plot, around the Fermi level, shows that the energy levels in this region are contributions from the orbitals of N atoms of both GaNNT and NO₂ [see Figure 6 (d)].

SO₂ interacting with GaNNT

The configuration shown in the Figure 7 (a) corresponds to the most stable system with the SO₂ molecule. In this configuration, the SO₂ molecule was adsorbed to the nanotube wall, forming a Ga-O bond of approximately 1.85 Å and a N-S bond of approximately 1.77 Å. The SO₂ molecule inside the nanotube was predicted as the second most stable configuration [Figure 7 (b)], with a binding energy of -1.53 eV. In the configuration of the Figure 7 (c), the S atom of the molecule was initially positioned in the center of the hexagon, and after the geometry optimization, the molecule SO₂ remained positioned in the center of the hexagon, and the distance between the molecule center and the hexagon center is approximately 1.92 Å.

Table 3 lists the binding energies (E_b) calculated according to the equation 1, the bond lengths (D), the energy gap (E_g) and the charge transfer between the molecule and the GaNNT for each system shown in the Figure 7. According to the analysis of the binding energies, the interactions between the SO₂ molecule and the (10,0) GaNNT occur both by chemical and physical adsorption processes, depending on the position of the molecule in relation to the nanotube. Thus, in the configurations of Figure 7 (a) and (b) a chemical adsorption process occurs, while in the configuration of Figure 7 (c) a physical adsorption process occurs.

According to the charge transfer shown in Table 3, calculated through the Mülliken population, we note that the SO₂ molecule behaves as an electron acceptor in all systems, in which in the configurations of the Figures 7 (a), (b) and (c), the GaNNT donates 0.17, 0.14 and 0.05 e⁻ to the SO₂ molecule, respectively.

The Figure 8 shows the electronic band structure for all systems with the SO₂ interacting with the GaNNT, however, the band structure for the (10,0) pristine GaNNT was also plotted for comparison purposes [see Figure 8 (a)]. Therefore, we can see that significant changes around the Fermi level occurred in the band structures of all systems, when compared to the pristine system (see Figure 8).

The Figures 8 (b) and (c) show the band structure for the two most stable configurations, which correspond to the configurations shown in Figures 7 (a) and (b), respectively. We can see that in the band structures of the Figures 8 (b) and (c), new degenerates states appear in the valence and conduction

Fig. 7 Optimized structures representation for GaNNT interacting with SO_2 molecule. The pink, grey, yellow and red spheres indicate Ga, N, S and O atoms, respectively.

Table 3 Binding energies (E_b), the bond lengths and the distances between the NO_2 and the nanotube surface (D), energy gap (E_g) and the charge transfer (CT) for each system represented in the Figure 7. The minus sign in the charge transfer values indicates that SO_2 molecule receives electronic charge.

Configuration	E_b (eV)	D (Å)	E_g (eV)	CT (e^-)
(a)	-2.55	$D_{S-N} = 1.77$; $D_{Ga-O} = 1.86$	2.29	-0.17
(b)	-1.53	$D_{S-N} = 1.84$; $D_{Ga-O} = 1.86$	2.22	-0.14
(c)	-0.30	$D_{Ga-O} = 1.92$	0.91	-0.05

bands when compared to the pristine system [Figure 8 (a)]. We also observed new delocalized levels mainly in the valence band, and as these new levels are not characteristic of a molecular system, so it can be inferred that they belong to new chemical bonds formed between the SO_2 molecule and nanotube atoms. These new bonds are possible due to the high binding energies found for these two systems (-2.55 and -1.53 eV, respectively), as show in Table 3. In addition, these systems remained semiconductors, with no significant reduction in energy gaps [see Figures 8 (a) and (b)]. Through the LDOS analysis, with an isovalue of 0.005 states/Ry, for the most stable configuration, we verified that the localization of the states, in the region around the Fermi level, are

contributions from both the N atoms of GaNNT and the S and O atoms of the molecule [see Figure 9 (a)].

Fig. 8 Electronic band structure for (a) the pristine (10,0) GaNNT, and for [(b), (c), and (d)] different configurations of SO_2 interacting with GaNNT, which correspond to the configurations shown in Figures 7 (a)-(c), respectively. The red dotted line represents the Fermi level.

The band structure of the Figure 7 (c) has some levels localized in the region of the energy gap, as can be seen in Figure 8 (d). These levels correspond to defect levels introduced by the molecule, which contribute to the energy gap reduction from 2.34 eV to 0.90 eV. Moreover, these states are flat, which indicate a localized character. Therefore, the optical properties of the GaNNT must be affected, since these impurity states will give rise to new bound states in the band gap, which will change the optical response of this material. The LDOS plot, around the Fermi level, shows that these energy levels are mainly a contribution from the atoms of the molecule, but there is also a contribution from the N atoms of the nanotube [see Figure 9 (c)].

The use of GaNNT to filter and detect pollutants is promising, since the interaction between the nanotube and the NO_2 , NH_3 and SO_2 molecules is suf-

Fig. 9 Plots of the local density of states (LDOS) for the SO_2 molecule interacting with (10,0) GaNNT in all studied configurations. The plots are for the electronic structures, in the region around the Fermi level, of the Figures 8 (b)-(d), using an isovalue of 0.005 states/Ry.

ficient to capture these molecules. If this interaction occur through a physical process, the nanotube can still be reused, however, in case of a chemical process, this interaction alters the nanotube properties, so it cannot be reused. In addition, the energy gap will change according to each interaction, when compared to the isolated nanotube, so the wavelength of light will also accompany this change.

So far, GaNNT are still little explored, as we can see in the literature, so there is a vast field of research and technological applications still open involving these systems. It is known that through functionalization there are ways to increase the applicability of nanotubes. Thus, studies considering other pollutants and also considering a greater number of pollutants interacting with the surface of the nanotube are necessary to better understand these systems.

4 Conclusion

Through first principles calculations based on the density functional theory (DFT), we investigated the interactions of the GaN nanotube with the NH_3 , NO_2 and SO_2 molecules. The same configurations were used for all molecules. Among the studied molecules, NO_2 was the molecule that most originated different configurations after the geometry optimization, which can be concluded that NO_2 can be adsorbed on the nanotube through each of its atoms, and in different sites of the GaNNT. The binding energies obtained between NO_2 and the nanotube indicate that it will not be so difficult to remove this molecule after it is adsorbed, which makes GaNNT reusable to detect or remove more NO_2 molecules from the environment. In contrast, SO_2 interacts very strongly with GaNNT, which makes it non-reusable after adsorption. And the NH_3 molecule, in most of the studied configurations, has low adsorption energies with the nanotube. Therefore, our results indicate that GaNNT is applicable to detect and remove NH_3 and NO_2 molecules from the environment, since

they do not prevent GaNNT from being reused and do not need much energy to desorb them.

In addition, there was a significant reduction in the energy gap, when the molecules NO₂ and SO₂ were adsorbed on GaNNT, but the molecule of NO₂ was the one that most modified the electronic properties of GaNNT. However, it was also observed that, for all molecules, both the electronic properties and the energetic properties depend on the position of the molecules in relation to GaNNT. Thus, new applications in optoelectronic nanodevices can be achieved with GaNNT functionalized with these pollutants molecules.

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6 Declarations

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Availability of data and material: The data that support the findings of this study are available from the corresponding author upon reasonable request.

Code availability: N/A

Authors' contributions: A. J. Anchieta da Silva performed all the calculations presented in this study. All analyzes were performed by Silvette Guerini and A. J. Anchieta da Silva. The first draft of the manuscript was written by Silvette Guerini and Caio Vinícius Caetano. All authors contributed to the study conception and interpretation of results. The writing and revision of the final version of the manuscript were performed by Caio Vinícius Caetano.

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Figures

Figure 1

Optimized structures representation for GaNNT interacting with NH_3 molecule. The pink, grey and blue spheres indicate Ga, N, H atoms, respectively.

Figure 2

Electronic band structure for (a) pristine GaNNT and for [(b), (c) and (d)] different configurations of NH₃ interacting with the GaNNT, which correspond to the configurations shown in Figures 1 (a), (b) and (c), respectively. The red dotted line represents the Fermi level.

Figure 3

Plots of the local density of states (LDOS) for the NH₃ molecule interacting with (10,0) GaNNT in all studied congurations. The plots are for the electronic structure, in the region around the Fermi level, of the Figures 2 (b)-(d), using an isovalue of 0.005 states/Ry.

Figure 4

Optimized structures representation for GaNNT interacting with NO₂ molecule. The pink, grey, blue and red spheres indicate Ga, N, H and O atoms, respectively.

Figure 5

Electronic band structures for (a) the pristine GaNNT, and for [(b)-(e)] different configurations of NO₂ interacting with the GaNNT, which correspond to the configurations shown in Figures 4 (a)-(d), respectively. The red dotted line represents the Fermi level.

Figure 6

Plots of the local density of states (LDOS) for the NO₂ molecule interacting with (10,0) GaNNT in all studied configurations. The plots are for the electronic structures, in the region around the Fermi level, of the Figures 5 (b)-(e), using an isovalue of 0.005 states/Ry.

Figure 7

Optimized structures representation for GaNNT interacting with SO_2 molecule. The pink, grey, yellow and red spheres indicate Ga, N, S and O atoms, respectively.

Figure 8

Electronic band structure for (a) the pristine (10,0) GaNNT, and for [(b), (c), and (d)] different configurations of SO₂ interacting with GaNNT, which correspond to the configurations shown in Figures 7 (a)-(c), respectively. The red dotted line represents the Fermi level.

Figure 9

Plots of the local density of states (LDOS) for the SO₂ molecule interacting with (10,0) GaNNT in all studied configurations. The plots are for the electronic structures, in the region around the Fermi level, of the Figures 8 (b)-(d), using an isovalue of 0.005 states/Ry.