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ABSTRACT

Recent reports have raised exciting prospects for the use of C$_3$N monolayers exhibiting excellent adsorptive properties in nanodevice applications. In this study, we carried out first-principle calculations to investigate the adsorption of NO$_2$, NO, CO, HCN, NH$_3$, CO$_2$, H$_2$, N$_2$, CH$_4$, H$_2$O, O$_2$, and N$_2$O gas molecules on a C$_3$N monolayer as well as its potential applications in gas sensor devices. Our results reveal that the chemisorption of NO$_2$ can significantly influence the electronic properties of the C$_3$N monolayer (e.g., changing semiconducting behavior to conducting behavior). In contrast, physisorption of the other gas molecules had little effect on the electronic properties of the C$_3$N monolayer. These results suggest that the C$_3$N monolayer is much more sensitive and selective to NO$_2$ than to the other gases. The recovery time of NO$_2$ at $T = 300$ K is only 0.62 s. Moreover, the optical properties of the C$_3$N monolayer can be modified as a result of the adsorption of different molecules, especially the NO$_2$ molecule. Thus, the C$_3$N monolayer is a promising and desirable candidate for use as a suitable material in gas sensors for NO$_2$ detection.

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I. INTRODUCTION

Nitrogen dioxide (NO$_2$), which is produced mainly in vehicle exhaust gases, from industrial byproducts, and in fuel combustion, is a toxic compound with a pungent odor that is harmful to the environment, being a major cause of acid rain and photochemical smog.$^{1-3}$ Moreover, the reactions of NO$_2$ gas with moisture, ammonia, hydrocarbons, and other compounds generate minute particles, which can cause inflammation of the airways in human beings.$^4$ In response to this increasing risk to health and to minimize the effects of prolonged NO$_2$ inhalation, almost all countries have established regulatory and legislative standards to deal with this issue.$^5$ For example, the European Commission suggests an hourly exposure to NO$_2$ concentrations of no more than $\sim$106 ppb no more than 18 times per year. Exposure levels above this limit result in an increased incidence of acute respiratory illness. It would seem highly desirable, therefore, that the development and fabrication of highly sensitive and selective NO$_2$ gas sensors be given special attention, particularly for the detection of NO$_2$ gas at the parts per billion level for commercial applications in environmental monitoring and health care.

Since the discovery of graphene$^6$ and the various studies that have since been carried out on this remarkable material with regard to its potential for NO$_2$ gas sensing (even the detection of NO$_2$ gas at the parts per billion level),$^{7-14}$ carbon-based two-dimensional (2D) nanomaterials have become widely used in gas sensing applications and have attracted growing attention due to their excellent advantages, such as large surface-to-volume ratio, high carrier mobility, gas adsorption capabilities, and quantum confinement.$^{15-26}$ In particular, metal-free carbon nitride-based 2D nanomaterials are of great interest due to their novel structures and physicochemical properties as well as their potential applications in photocatalysis, gas sensing and capture, and lithium-ion batteries, among others.$^{27-32}$ Recently, 2D polyaniline (C$_3$N), which displays a hole-free honeycomb structure in which nitrogen and carbon atoms have homogeneous and ordered distributions, has been successfully synthesized by the polymerization of 2,3-diaminophenazine$^3$ or the direct pyrolysis of hexa-aminobenzene trihydrochloride...
single crystals. It's outstanding electronic, mechanical, thermal, and chemical properties promise that C\(_3\)N monolayers will be suitable as gas-sensing materials.

In this study, in order to explore the gas-sensing properties of C\(_3\)N monolayers, we systematically investigated the adsorption behaviors and electronic properties of various gas molecules, including NO\(_2\), NO, CO, HCN, NH\(_3\), CO\(_2\), H\(_2\), N\(_2\), CH\(_4\), H\(_2\)O, O\(_2\), and N\(_2\)O, on C\(_3\)N monolayers using the first-principles method based on density functional theory (DFT). Specifically, the optimum adsorption structures, adsorption strength, charge transfer between molecules and the C\(_3\)N monolayer, changes in electronic properties [such as density of states (DOS) and band structures] before and after molecule adsorption, and work functions were investigated. Our results have revealed that C\(_3\)N monolayers are promising candidates for use as gas sensors for NO\(_2\) detection and, more interestingly, that C\(_3\)N monolayers can be used as potential optical gas sensors.

II. MODELS AND METHODS

The spin-polarized DFT calculations were performed within the generalized gradient approximation (GGA) using the DMol\(^3\) module in Materials Studio.\(^{29,30}\) The Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional\(^{39}\) with the van der Waals (vdW) correction under the Grimme scheme\(^{40}\) was also used. All-electron core treatment and a double numerical basis set including the \(d\) polarization function (i.e., DNP) were used to describe the electron ion–core interactions, and the charge analysis used the Hirshfeld method.\(^{41}\) Guerra et al.\(^{37,38}\) have studied various types of charge analysis, including Mulliken, Bader, Hirshfeld, Weinhold, and the Voronoi deformation density (VDD), and recommended the Hirshfeld method because it yields chemically meaningful charges. The Brillouin zone was sampled using \(9 \times 9 \times 1\) special \(k\)-points using the Monkhorst–Pack scheme.\(^{26}\) A minimum distance of 20 \(\AA\) vacuum spaces was set in order to hinder interactions between the supercell and its periodic images. The convergence criteria for the energy and electron density were set as \(1 \times 10^{-6}\) hartrees and \(1 \times 10^{-6}\) e/bohr\(^2\), respectively, in the self-consistent field calculations. In addition, convergence criteria of \(1 \times 10^{-3}\) hartrees/bohr on the gradient and displacement and \(1 \times 10^{-5}\) hartrees on the total energy were set in the geometrical optimization. The PBE with the Grimme correction method has been successfully used in the investigation of the CN system.\(^{25,30,35,36}\)

We used a \(3 \times 3 \times 1\) supercell of a C\(_3\)N monolayer involving 18 N atoms and 54 C atoms as the substrate to investigate the adsorption of molecular gases. The adsorption energy (\(E_a\)) is defined as \(E_a = E_{\text{tot}} - E_{\text{CN}} - E_{\text{mol}}\), where \(E_{\text{tot}}\), \(E_{\text{CN}}\), and \(E_{\text{mol}}\) are, respectively, the total energy of each molecule adsorbed on the C\(_3\)N monolayer, the energy of the corresponding C\(_3\)N monolayer, and the energy of the pristine molecule. According to this definition, a negative value of \(E_a\) indicates the exothermic adsorption and the adsorption site with the largest \(E_a\) is the most energetically favorable one.

III. RESULTS AND DISCUSSION

We first optimized a \(3 \times 3 \times 1\) supercell of a C\(_3\)N monolayer, which is shown in Fig. 1. The optimized lattice parameters were \(a = b = 4.862\) \(\AA\), and the C\(_3\)N monolayer had an indirect bandgap of 0.437 eV in the electronic structures, both of which are in good agreement with previous predictions.\(^{29,32,35,36}\) We then investigated the interaction between the molecules and the C\(_3\)N monolayer. To obtain the most stable configurations of molecules adsorbed on the C\(_3\)N monolayer, we considered all possible adsorption sites [i.e., two top sites (C and N), one hole site (H), and five bridge sites (B\(_n\), \(n = 1–5\)], as shown in Fig. 1 and the orientation of the molecules (parallel or vertical) to each site. The most stable configurations of molecules adsorbed on the C\(_3\)N monolayer are shown in Figs. 2 and 3, and the corresponding results are summarized in Tables I and II.

The optimized structures of NO\(_2\) adsorbed on the C\(_3\)N monolayer are shown in Fig. 2. We found that O atoms in the NO\(_2\) molecule point down the C–N surface, and the NO\(_2\) molecule is vertical to a C–N bond in the most stable configuration (the so-called NO\(_2\)-1 structure), the adsorption energy of which was \(-0.702\) eV. The shortest distance between the NO\(_2\) molecule and the C\(_3\)N monolayer was 2.56 \(\AA\). More importantly, there was an apparent charge transfer of 0.406 e from the C\(_3\)N monolayer to the NO\(_2\) molecule. The angle between the two bonds of the O–N–O
molecule was reduced from $133.5^\circ$ for the isolated NO$_2$ state to $122.7^\circ$ as a result of the interaction between NO$_2$ and the C$_3$N monolayer. These results indicate that NO$_2$ adsorption is, in fact, weak chemisorption and is not strong enough to prevent desorption at room temperature, which is similar to the results reported in a previous study.$^{35}$ We also obtained other adsorption configurations, as shown in Figs. 2(b) and 2(c), where we found that the energy difference between different adsorption configurations was very small (<0.1 eV) and the distances between the molecule and the C$_3$N monolayer and the extent of charge transfer were all consistent with the most stable configuration (NO$_2$-1 structure). Furthermore, we also investigated their band structures and densities of states (DOSs). The band structure and DOS of only the NO$_2$-1 structure are shown in Fig. 4 because of the similarity of the electronic features of the NO$_2$-1, NO$_2$-2, and NO$_2$-3 structures. For these NO$_2$-adsorbed C$_3$N structures, compared with the band structure and DOS of the pure C$_3$N monolayer shown in Fig. 4(a), holes of the valence band maximum (VBM) are the majority charge carriers due to $p$-type doping in a way that electrons could transport easily in the valence bands and conduct electricity as well. In such cases, it can be seen in Fig. 4(b) that the Fermi level is shifted below the neutral one [Fig. 4(a)], which make the unfolded energy bands intersect the Fermi level, indicating semiconductor-metal transition for such cases. The adsorption of the NO$_2$ molecule induced impurity states in the valence bands very near the Fermi level, which results in the generation of the majority carriers, and more importantly, these impurity states crossed the Fermi level, which makes the semiconducting behavior of the pure C$_3$N monolayer change to a conducting behavior. This indicates that adsorption of NO$_2$ molecules can significantly enhance the conductance of the C$_3$N monolayer, where the system will exhibit metallic behavior following adsorption, which is a useful property for application in gas sensors. These features are also found in NO and NO$_2$ molecule adsorption on other 2D nanomaterials.$^{34-40}$

Furthermore, we constructed several C$_3$N structures with different supercell sizes, namely, $2 \times 2 \times 1$, $3 \times 2 \times 1$, and $4 \times 4 \times 1$

![FIG. 3. Top and side views of the most stable configurations of C$_3$N monolayer adsorption with (a) CO, (b) NO, (c) NH$_3$, (d) HCN, (e) CH$_4$, (f) CO$_2$, (g) H$_2$, (h) H$_2$O, (i) N$_2$, (j) O$_2$, and (k) N$_2$O. The white balls are H atoms.](image-url)

### TABLE I. Adsorption energy ($E_a$), adsorption distance ($D$), charge transfer ($Q$), band energy gap ($E_g$), recovery time ($\tau$), and work function ($\Phi$) for NO$_2$ adsorbed on the C$_3$N monolayer.

| System | $E_a$ (eV) | $D$ (Å) | $Q$ (e) | $E_g$ (eV) | $\tau$ (s) | $\Phi$ (eV) |
|--------|-----------|--------|--------|-----------|------------|------------|
| NO$_2$-1 | $-0.702$ | $2.56$ | $-0.406$ | $0$ | $0.62$ | $3.76$ |
| NO$_2$-2 | $-0.671$ | $2.65$ | $-0.403$ | $0$ | $0.19$ | $3.78$ |
| NO$_2$-3 | $-0.613$ | $2.42$ | $-0.445$ | $0$ | $0.02$ | $3.84$ |

### TABLE II. Adsorption energy ($E_a$), adsorption distance ($D$), charge transfer ($Q$), band energy gap ($E_g$), recovery time ($\tau$), and work function ($\Phi$) for the most stable structures of NO$_2$ adsorbed on the C$_3$N monolayer with different concentrations.

| Super cell | $E_a$ (eV) | $D$ (Å) | $Q$ (e) | $E_g$ (eV) | $\tau$ (s) | $\Phi$ (eV) |
|-----------|-----------|--------|--------|-----------|------------|------------|
| $2 \times 2 \times 1$ | $-0.634$ | $2.57$ | $-0.344$ | $0$ | $0.05$ | $4.14$ |
| $3 \times 2 \times 1$ | $-0.668$ | $2.58$ | $-0.377$ | $0$ | $0.17$ | $3.95$ |
| $3 \times 3 \times 1^a$ | $-0.702$ | $2.56$ | $-0.406$ | $0$ | $0.62$ | $3.76$ |
| $4 \times 4 \times 1$ | $-0.710$ | $2.54$ | $-0.415$ | $0$ | $0.85$ | $3.62$ |

$^a$To have a perceptual and systematic comparison, we also show the related results of a $3 \times 3 \times 1$ supercell (see Table I).
expected for the above-mentioned supercell size \((3 \times 3 \times 1)\), to examine the effects of different concentrations of NO\(_2\) adsorbates on the adsorption behaviors. After optimization, we found that the most stable configurations of NO\(_2\) on different C\(_3\)N supercells are the same as the most stable one of NO\(_2\) on the C\(_3\)N within the \(3 \times 3 \times 1\) supercell as shown in Fig. 2(a). The \(E_g\) gradually decreases with the increase in the C\(_3\)N supercell size (shown in Table II), which means that the interaction strength between NO\(_2\) molecules and C\(_3\)N is inversely proportional to the concentration. In addition, the increasing \(E_g\) is always accompanied with enhanced charge transfer between the C\(_3\)N monolayer and the NO\(_2\) molecule, indicating that the enhanced charge transfer would lead to stronger NO\(_2\)-C\(_3\)N interaction. From the analysis of electronic properties, there is always a transition from semiconducting behaviors to conducting behaviors due to the adsorption of NO\(_2\) molecules, no matter what the concentration of NO\(_2\) adsorbates is. Furthermore, the concentration of NO\(_2\) adsorption increases the majority carrier concentration, which leads to the Fermi energy level lower away from the conduction and pushed deeper into valence bands, facilitating the participation of the hole band in the carrier transport.

We then considered other molecules (NO, CO, HCN, NH\(_3\), CO\(_2\), H\(_2\), N\(_2\), CH\(_4\), H\(_2\)O, O\(_2\), and N\(_2\)O) adsorbed on the C\(_3\)N monolayer, of which the most stable configurations are shown in Fig. 3. We found that all of these molecules were only weakly adsorbed on the C\(_3\)N monolayer, with adsorption energies of less than \(-0.33\) eV. Based on the results of previous studies, an adsorption energy \(<-0.5\) eV can differentiate chemisorption from physisorption, which means that the adsorption of molecules on surfaces should be that of chemisorption when the adsorption energy is \(<-0.5\) eV. Therefore, based on only the adsorption energy, we can confirm that all of these molecules were physically adsorbed on the C\(_3\)N monolayer. Little charge transfer (\(<0.1\) e) and large distances between the molecules (except for NO and O\(_2\)) and the C\(_3\)N monolayer were found, further demonstrating physical adsorption. However, the unambiguous charge transfer of 0.147 e (or 0.182 e) between the NO (or O\(_2\)) molecule and the C\(_3\)N monolayer suggests that the interaction between the NO (or O\(_2\)) molecule and the C\(_3\)N monolayer will be stronger than for CO, HCN, NH\(_3\), CO\(_2\), H\(_2\), N\(_2\), CH\(_4\), H\(_2\)O, or N\(_2\)O adsorption, resulting in a slightly larger adsorption energy of \(-0.327\) eV (or \(-0.319\) eV). Furthermore, we studied the band structures and DOSs of these molecules adsorbed on the C\(_3\)N monolayer, which are shown in Figs. 5 and 6.

Since adsorption of H\(_2\), NH\(_3\), and CH\(_4\) gave similar band structures and DOSs, while adsorption of CO, H\(_2\)O, HCN, CO\(_2\), N\(_2\), and N\(_2\)O also gave similar band structures and DOSs, only the band structures and DOSs of CH\(_4\) and CO\(_2\) adsorption are shown as examples. We found that the adsorption of H\(_2\), NH\(_3\), CH\(_4\), CO, H\(_2\)O, HCN, CO\(_2\), and N\(_2\) molecules did not introduce any impurity states into the bandgaps and thus had little effect on the bandgap widths of the C\(_3\)N monolayer (see Table III). Specifically, H\(_2\), NH\(_3\), and CH\(_4\) molecules introduce fully occupied states into the valence bands, which are generally far away from the Fermi level, while CO, H\(_2\)O, HCN, CO\(_2\), N\(_2\), and N\(_2\)O molecules not only induce fully occupied states (located at \(<-3\) eV under the Fermi level) in the valence bands but also give rise to some impurity states (located at \(>2\) eV above the Fermi level) within the conduction bands. In contrast, NO and O\(_2\) molecules can give rise to some impurity states within the bandgaps of the pure C\(_3\)N monolayer, thereby modifying the electronic properties of the C\(_3\)N monolayer to some extent.

**FIG. 4.** The band structures and densities of states (DOSs) of (a) the C\(_3\)N monolayer and (b) NO\(_2\) adsorption on the C\(_3\)N monolayer. The LDOS of molecules is also given as cyan filled area under the DOS curve. The Fermi level is set to zero.

**FIG. 5.** The band structures of the C\(_3\)N monolayer with molecule adsorption: (a) CH\(_4\), (b) CO\(_2\), (c) NO, and (d) O\(_2\). Black and red lines represent spin-up and spin-down states, respectively. The Fermi level is set to zero.
Next, we discuss the gas-sensing properties of the C$_3$N monolayer. We mainly investigated its sensitivity, selectivity, recovery time, and stability, which constitute the basic properties of effective gas sensing. The sensitivity can be evaluated by the change in electric conductivity ($\sigma$) before and after molecular adsorption, which is defined as $\sigma \propto \exp(-E_a/2kT)$, where $k$ is Boltzmann’s constant, $T$ is the temperature, and $E_a$ is the energy of the bandgap. As discussed above, the bandgap width of the C$_3$N monolayer changed from 0.439 to 0 eV due to the adsorption of NO$_2$, that is, the system changed from exhibiting semiconducting behavior to conducting behavior following NO$_2$ adsorption, resulting in the change in electric conductivity that is highly significant. The adsorption of other molecules (CO, HCN, NH$_3$, CO$_2$, H$_2$, N$_2$, CH$_4$, H$_2$O, and N$_2$O), however, had little effect on the electronic properties of the C$_3$N monolayer, while the adsorption of NO and O$_2$ had a small effect on its electronic properties, indicating that they scarcely enhanced the conductance of the monolayer. In particular, as discussed above, the physical adsorption of the N$_2$O molecule, which is a target of typical deNO$_x$ processes in industry and labs, hardly influences the structural and electronic properties of the C$_3$N monolayer, indicating that the C$_3$N monolayer is nonsensitive to N$_2$O gas and can differentiate NO$_2$ from N$_2$O. These results indicate that the C$_3$N monolayer shows ultrahigh sensitivity for NO$_2$ detection. From Tables I and II, it can be seen that the adsorption energy of NO$_2$ is much larger (approximately twice) than that of other molecules, indicating the high selectivity of the C$_3$N monolayer for NO$_2$ adsorption. The recovery time, which is defined as $\tau = 1/v_0\exp(-E_a/kT)$, where $v_0$ is the attempt frequency, $E_a$ is the adsorption energy, $k$ is Boltzmann’s constant, and $T$ is the temperature, can be used to evaluate the reusable performance of gas sensors. We assumed that the attempt frequency of all molecules is the same order of magnitude as that of the NO$_2$ molecule ($10^{12}$ s$^{-1}$) and then calculated the recovery times of all molecules at $T = 300$ K, which are summarized in Tables I and II. The recovery time of NO$_2$ is 0.62 s, which is very short for desorption of the NO$_2$ molecule from the C$_3$N monolayer. Although the other molecules have shorter recovery times, physisorption of these molecules makes the adsorption much weaker than chemisorption of NO$_2$ and, more importantly, physisorption hardly changes the electronic properties of the C$_3$N monolayer. Previous studies have demonstrated that the C$_3$N monolayer is thermodynamically stable enough to act as a promising candidate for CO$_2$ capture, lithium-ion batteries, and so on. Our results have revealed that NO$_2$ adsorption results in hardly any structural deformation of the C$_3$N monolayer, further suggesting its considerable stability. These results suggest that the C$_3$N monolayer exhibits high gas-sensing performance (high sensitivity and selectivity and rapid recovery time) for NO$_2$ detection.

With a view to introducing C$_3$N monolayers into applications for optical gas sensors because of the promising optical gas-sensing properties that these 2D nanomaterials have demonstrated, we calculated the work function (Φ) of the C$_3$N monolayer with and without molecular adsorption. The results are given in Tables I and II and are also shown in Fig. 7. Here, Φ is calculated from the equation $\Phi = E_{\text{vacuum}} - E_{\text{Fermi}}$, where $E_{\text{vacuum}}$ and $E_{\text{Fermi}}$ represent the potential energy of the vacuum level and the Fermi level, respectively. The Φ of the C$_3$N monolayer is 3.40 eV, smaller than that of other monolayer nanomaterials such as graphene (4.49 eV), silicene (4.77 eV), and MoS$_2$ (-4.05 eV). The work function was hardly changed as a result of adsorption of CH$_4$, CO, CO$_2$, H$_2$, N$_2$, NH$_3$, or N$_2$O. In contrast, the work functions increased from 3.40 to

**Table III. Adsorption energy ($E_a$), adsorption distance (D), charge transfer (Q), band energy gap ($E_g$), recovery time ($\tau$), and work function (Φ) for molecules adsorbed on the C$_3$N monolayer.**

| System | $E_a$ (eV) | D (Å) | Q (e) | $E_g$ (eV) | $\tau$ (s) | Φ (eV) |
|--------|-----------|-------|------|-----------|-----------|--------|
| CO     | -0.173    | 2.84  | 0.033| 0.440     | $8.1 \times 10^{-10}$ | 3.43   |
| NO     | -0.327    | 2.67  | -0.147| 0.249     | $3.1 \times 10^{-7}$ | 3.51   |
| NH$_3$ | -0.288    | 2.45  | 0.050| 0.443     | $6.9 \times 10^{-8}$ | 3.37   |
| HCN    | -0.262    | 2.36  | -0.077| 0.439     | $2.5 \times 10^{-8}$ | 3.54   |
| CH$_4$ | -0.205    | 2.48  | -0.059| 0.440     | $2.8 \times 10^{-9}$ | 3.40   |
| CO$_2$ | -0.219    | 2.90  | 0.013| 0.441     | $4.8 \times 10^{-9}$ | 3.40   |
| H$_2$  | -0.130    | 2.80  | -0.028| 0.440     | $1.5 \times 10^{-10}$ | 3.40   |
| H$_2$O | -0.303    | 2.34  | -0.098| 0.436     | $1.2 \times 10^{-7}$ | 3.59   |
| N$_2$  | -0.191    | 2.86  | 0.013| 0.437     | $1.6 \times 10^{-9}$ | 3.40   |
| O$_2$  | -0.319    | 2.68  | -0.182| 0.334     | $2.3 \times 10^{-7}$ | 3.59   |
| N$_2$O | -0.244    | 3.04  | -0.005| 0.441     | $1.3 \times 10^{-8}$ | 3.40   |

**Fig. 6.** The densities of states (DOSs) of the C$_3$N monolayer with molecule adsorption: (a) CH$_4$, (b) CO$_2$, (c) NO, and (d) O$_2$. The LDOSs of molecules are also given as cyan filled areas under the DOS curves. The Fermi level is set to zero.
The calculated work function of the C$_3$N monolayer without and with adsorption of different molecules.

>3.7, 3.59, 3.54, 3.51, and 3.59 eV following NO$_2$, H$_2$O, HCN, NO, and O$_2$ adsorption, respectively, indicating that adsorption hinders the transfer of electrons to the vacuum level. For the adsorption of NO$_2$ with different concentrations, the work function of the NO$_2$-C$_3$N system increases with the increase in the concentration of NO$_2$ molecules, indicating that the concentration of NO$_2$ can be realized by measuring the work functions. Furthermore, there is a close relationship between the work function and the field emission ability. From the Fowler–Nordheim equation, where the field emission current density ($J$) is defined as $J = A(\beta E)^2 \exp(-\frac{4\sqrt{2m\Phi}}{\beta E})$, $A$ is a constant, $\beta$ is the field enhancement factor, $E$ is the intensity of electric field, and $m$ is electron mass, it can be seen that there is a close relationship between $\Phi$ and $J$. The adsorption of different molecules results in different work functions, which then induce different field emission abilities. On the basis of this analysis, the different values of $J$ of the C$_3$N monolayer with and without adsorption of different molecules under a constant voltage can be used to separate those molecules experimentally. Thus, the selective adsorption of molecules can modify the work function of the C$_3$N monolayer and can be characterized experimentally, making the C$_3$N monolayer a promising material for use in optical gas sensors.

IV. CONCLUSIONS

In summary, we have carried out first-principles calculations to investigate the adsorption geometries and electronic properties of the C$_3$N monolayer with adsorption of small gas molecules (NO$_2$, NO, CO, HCN, NH$_3$, CO$_2$, H$_2$, N$_2$, CH$_4$, H$_2$O, O$_2$, and N$_2$O). We found that only NO$_2$ can be chemisorbed on the C$_3$N monolayer with apparent adsorption energy and charge transfer and that the adsorption of NO$_2$ can significantly influence the electronic properties of the C$_3$N monolayer (e.g., semiconducting behavior changed to conducting behavior). In contrast, physisorption of the other gas molecules had little effect on the electronic properties of the C$_3$N monolayer, suggesting that the C$_3$N monolayer is much more sensitive and selective to NO$_2$ than to the other gases. The recovery time of NO$_2$ is only 0.62 s at $T = 300$ K. Moreover, the optical properties of the C$_3$N monolayer can be modified by the adsorption of different molecules. Our analysis of sensitivity, selectivity, recovery time, and change in optical properties suggests that the C$_3$N monolayer is a promising and desirable candidate for use as a suitable material in gas sensors for NO$_2$ detection.

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