



Adsorption of CO and CO₂ molecules on nitrogen-doped armchair silicene/graphene nanoribbons as a gas sensor

Majeed Ali Habeeb, Hamad Rahman Jappor, and Sameer Hassan Hadi Al-Nesrawy

Department of Physics, College of Education for Pure Sciences, University of Babylon, Hilla, Iraq

Abstract: The adsorption of CO and CO₂ molecules on pristine and nitrogen-doped silicene/graphene nanoribbons (N-doped SiGNR) has been studied using density functional theory (DFT). The electronic structure, energy gap, density of states and adsorption energies are obtained. The adsorption energies of CO molecules on pristine and N-doped SiGNR is a strong chemisorption with adsorption energies being larger than 1.0 eV, therefore, SiGNR could catalyse or activate this adsorbate due to the strong interaction, suggesting the possibility of Ndoped SiGNR as a metal-free catalyst. Also, our results show that the adsorption energy of CO₂ on N-doped SiGNR is between -2.17 and -3.23 eV, indicating that SiGNR could be a good CO₂ sensor and more sensitive to the adsorption of CO₂ than pristine and N-doped SiGNR. Thus, the sensitivity of gases on SiGNR can be significantly improved by introducing nitrogen as dopants. Moreover, the energy gap of pristine and N-doped SiGNR is opened upon adsorption of CO and CO₂ in various ways. In general, the energy gap for CO molecule on SiGNR are larger than those of CO₂ molecules on SiGNR.

Keywords: Adsorption, silicene/graphene, nanoribbons, gas sensor.

Introduction

Graphene is one of the most important two dimensional honeycomb structure that has been extensively studied in the last few years because of its potential applications mechanical and exceptional electronic and properties¹⁻⁵. Graphene was discovered at the focus for nanotechnology and mesoscopic directed by Novoselov and Geim⁶. After the successful synthesis of graphene followed by a surge of studies novel two dimensional materials, a daunting quest was to obtain silicene.

Silicene is similar to graphene, which is a two-dimensional crystal of Si atoms on a honeycomb lattice, has recently attracted intensive interest because of its electronic properties⁷⁻⁹. Unlike graphene, atomic structure of silicene is buckled. However, silicene/graphene nanoribbons (SiGNRs), a hexagonal structure consisting of silicon and carbon, have a large band gap and high exciting binding up to energy 2.0 eV¹⁰⁻¹¹. Theoretical calculations have been shown that SiGNR is similar to graphene which is a planar, has a stable two-dimensional honeycomb structure, in addition to tis a good semiconductor¹².

Carbon based materials is used for gas sorption, storage, and separation, due to its high abundance, robust pore structure, light-weight, high thermal and chemical stability¹³⁻¹⁵. Lately, the reports¹⁶⁻¹⁸, show that graphene is an exciting candidate for usage as a gas sensor due to its extraordinary sensitivity, which is attributed to its high electron mobility. Experimentally¹⁹, it was shown that the NO₂, CO, NH₃ adsorbates are only physisorbed on graphene, therefore, graphene cannot detect these gas molecules. On the other hand, it has been reported that

silicene shows a high reactivity towards O₂, SO₂ and NO₂. Moreover, NH₃ and NO can be adsorbed on silicene, demonstrating that silicene could be a good NH₃ or NO sensor²⁰. Substituting the carbon atoms by other elements is one way to dope the layer. However, nitrogen belongs to the most studied dopants for graphene²¹⁻²³. It is assumed that N incorporation modifies the graphene structure and destroys its quality²⁴⁻²⁵. Taking into consideration the potential applications of graphene and the high reactivity of silicene and development of gas sensor, we have investigated the effects of N doping on the electronic, and structural properties of SiGNR and the adsorption of CO and CO₂ gas molecules on N-doped SiGNR using DFT calculations to improve the sensitivity for gases in SiGNR. Density DFT is an efficient method to fine-tune the structural stability and electronic properties of some nanostructures²⁶⁻²⁹.

2. Computational Details

DFT calculations were performed using Gaussian 09 package³⁰ with Perdew–Burke–Ernzerhof (PBE) functional³¹ at 6-31G basis set, to investigate N doping on the adsorption effect of gas molecules CO₂ and CO on the electronic structure SiGNR. We used armchair silicene/graphene nanoribbon (SiGNR) consist of 42 atoms (21carbon+21 silicon) with a doped atom substituting a Si atom or C atom and a single CO₂ and CO molecule adsorbed onto it. The corresponding dopant concentration is about 2.3%. The optimized bond lengths for C-Si are 1.83Å. These values are in agreement with other calculations for and SiC nanoribbons³² and silicene/graphene (SiG) hybrid³³.

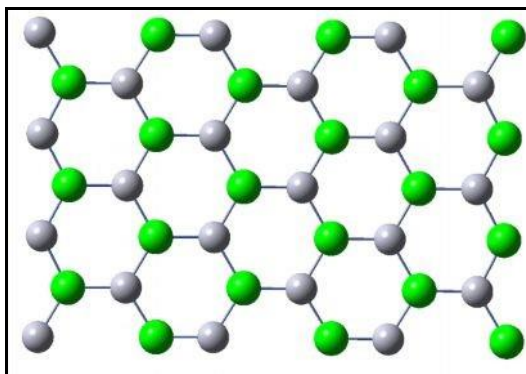


Figure 1: Geometric structures of armchair silicene/graphene nanoribbon SiGNR. The gray and green spheres are denoted as C, Si atoms, respectively.

In order to calculate the adsorption energy (E_a), the adsorption energy is difference between the total energy of the system (gas+SiGNR) and the sum energy of pristine SiGNR (E_{SiGNR}) and the molecule (E_{gas})³⁴.

$$E_a = E_{\text{total}} - (E_{\text{SiGNR}} + E_{\text{gas}}) \quad (1)$$

And it is a physical quantity reflecting the adsorption strength, the adsorption energy is generally negative, and adsorption is unstable when we get the positive values. The greater the absolute value of adsorption energy is, the more stable the system will be. Generally, the smaller ones can testify the instability of the adsorption

3. Results and Discussion

In order to find the favourable adsorption configuration, the adsorption of gas molecules (CO and CO₂) on pristine SiGNRs is placed at the possible adsorption sites: The top (T₁) site directly above the carbon atom, top (T₂) site directly above the silicon atom as shown in Figure 2. Its known that CO is a non-irritating and colourless gas, when it enters the body of human, CO combines with blood haemoglobin that prevents the union of oxygen and haemoglobin, leading to body tissue hypoxia and suffocation³⁵. As a usual kinds of toxic gases, CO plays a central role in environmental monitoring, space missions, control of chemical processes, agricultural and medical applications³⁶⁻³⁷.

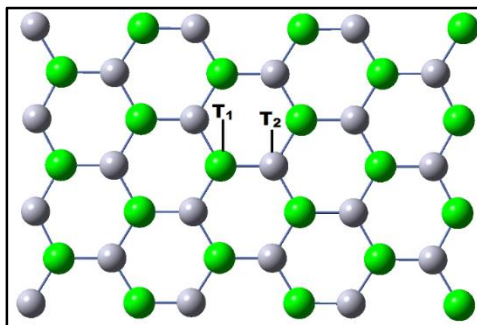


Figure 2: The position of the CO and CO₂ molecules on the pristine SiGNRs.

The most stable configurations after the relaxation of CO and CO₂ adsorption on pristine SiGNR is shown in Figure 3. The gray, green and red spheres are denoted as C, Si, and O atoms, respectively. Figures 3(a) and 3(b) give the structure of CO adsorption on pristine SiGNR. We find that C atom binds with the T₁ site of SiGNR with the C-C distance of 1.35Å, while the C-C-O angle is 165.5°, agreement with the other result [38, 39], meanwhile, the bond length with T₂ site Si-C is 1.87Å and the Si-C-O angle is 176.5°, which is consistent with other similar studies¹⁹. Figures 3(c) and 3(d) show the CO₂ adsorption is on SiGNR, the perpendicular distance between SiGNR and CO₂ is found to be about 1.37Å in the T₁ site, and a C-C-O of angle 165.5°, while C atom binds with the T₂ site of SiGNR with the Si-C distance of 1.87Å and a Si-C-O of angle 176.5°, which are analogous to the adsorption of CO on SiGNR. As far as we know that, at $E_a < 0$, the reaction is exothermic because the energy of the absorption system is less than the total energy of pristine SiGNR and gas molecules. Greater adsorption energy releases more energy during the reaction process. On the other hand, owing to the energy required when $E_b > 0$, it is relatively difficult for the reaction to continue. Table 2 clarify the effect of CO and CO₂ adsorption on the electronic properties of pristine SiGNR, the adsorption energy CO molecule on pristine SiGNR are larger than 1eV, corresponding to strong chemisorption⁴⁰. The adsorption energy for pristine SiGNR at site T₁ is 4.2 eV, in agreement with the previous results⁴¹.

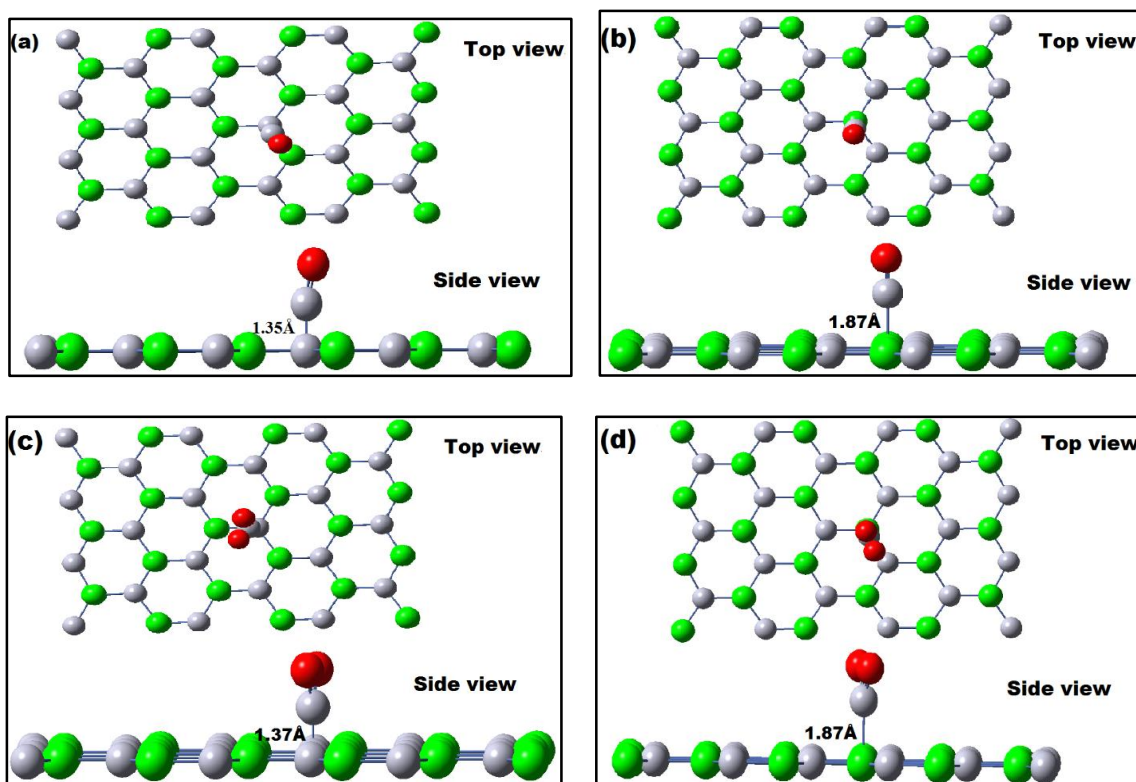


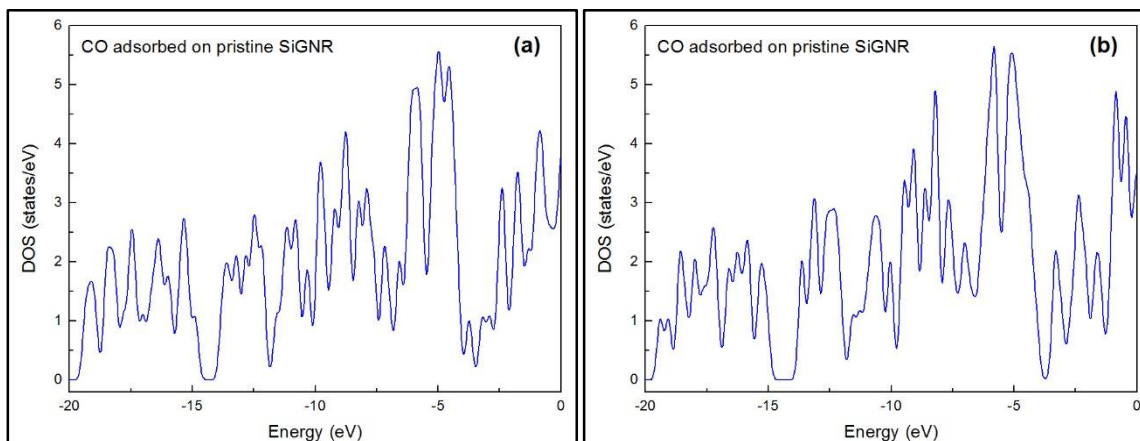
Figure 3: Structural model of CO and CO₂-SiGNRs adsorptive systems, (a) CO molecule adsorbed on the site T₁, (b) CO molecule adsorbed on the site T₂, (c) CO₂ molecule adsorbed on the site T₁ and (d) CO₂ molecule adsorbed on the site T₂.

In general, the adsorption energy in the results indicate that SiGNR is strongly reactive to CO in all sites except the adsorption energies in the range of (1.28–4.169) eV, corresponding to a strong chemisorption. therefore, due to gases slow desorption from pristine SiGNR, the SiGNR is not suitable as the sensor of CO. However, SiGNR could activate or catalyse this adsorbate due to the strong interaction, suggesting the possibility of SiGNR as a metal-free catalyst. The CO₂ adsorption on pristine SiGNR demonstrated that the adsorption energy for at site T₂ is larger than 1eV (6.33eV); adsorption of CO₂ is a strong chemisorption. On the other hand, the binding strength of CO₂ with pristine SiGNR at site T₁ is intermediate with the adsorption energy is 0.36 eV. Thus, SiGNR can be used to detect CO₂ since the adsorption–desorption equilibrium of CO₂ on SiGNR at T₁ site is easily built. We can recognize in Table 3, ionization energy (IP), electron affinity (EA) and fermi energy (E_F) for CO molecule on pristine SiGNR at site T₂ is larger than that at site T₁. Also, the energy gap for CO molecule on pristine SiGNR at site T₂ is smaller than that at site T₁. Conversely, the IP, EA and E_F for CO molecule on pristine SiGNR at site T₁ is smaller than that at site T₂. It is known that the small value of IP and EA may refer to that, this system needs to a small energy to remove an electron to become cation, it has ability to donating an electron in comparison with other adsorbed SiGNR and pristine. Electron affinity plays an important role on both plasma physics and chemical sensors⁴².

Table 1: Structural and electronic properties of adsorption of CO molecule on SiGNR.

Property (eV)	CO ₂ adsorbed on pristine SiGNR		CO adsorbed on pristine SiGNR	
	at site T ₂	at site T ₁	at site T ₂	at site T ₁
E _a	6.33	0.36	1.28	4.17
E _g	0.016	0.011	0.14	0.18
IP (= -E _{HOMO})	4.99	5.01	5.161	5.001
EA (= -E _{LUMO})	4.98	4.99	5.019	4.985
E _F	-4.99	-5.00	-5.02	-4.99

We found that high value of E_{HOMO} is -5.161 eV, this value indicates a propensity of the molecule to donate electrons, while the lower the value of E_{LUMO} is -4.98 eV, this value indicate a tendency of the molecule to accept electrons. Figures 4(a) and 4(b) illustrated the density of states (DOS) of CO adsorption on pristine SiGNR, according to the results of the system of CO molecules adsorbed on pristine SiGNR is a semiconductor with energy gap ranging from (0.14 to 0.18) eV. The highest number of degenerate states in the conduction and valence bands are approximately 6. However, the adsorption CO₂ on SiGNR at sites T₁ and T₂ leads to an increase in the DOS in the conduction and valence bands with comparison the system of CO molecules adsorbed on pristine SiGNR as depicted in Figures 4(c) and 4(d). Since that in all DOS there are many main peaks, there are states available for occupation at high DOS for a specific energy level and no states can be occupied at a zero- density of states for energy level.



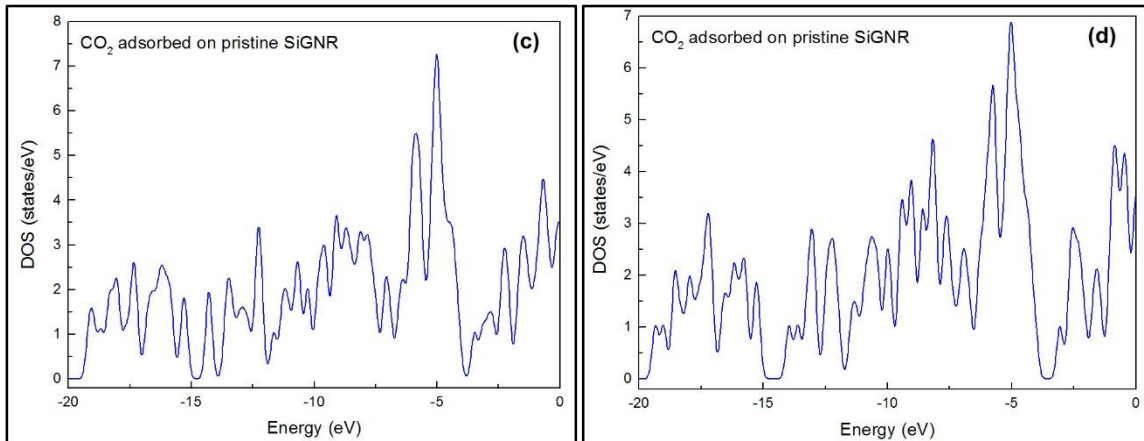


Figure 4: DOS of different systems, SiGNR for: (a) CO adsorbed on pristine at site T₁, (b) CO adsorbed on pristine at site T₂ (c) CO₂ adsorbed on pristine at site T₁ and (d) CO₂ adsorbed on pristine at site T₂.

In order to calculate the electronic structure of adsorption of CO and CO₂ molecules on nitrogen-doped silicene/graphene nanoribbons (N-doped SiGNR), we examine two states, the first state (model A) is substituting one of carbon atoms by a nitrogen atom, and the other state (model B) is substituting one of silicon atoms with a nitrogen atom, and then we bind CO or CO₂ molecules on the top site of N atom with O upwards, as we say that, the simulated system consists of 21 carbon+21 silicon, therefore, the corresponding dopant concentration is about 2.3%. The N-doped SiGNR retain a planar form after the relaxation, and the corresponding models are shown in Fig. 5, The gray, green, red and blue spheres are denoted as C, Si, O, and N atoms, respectively. Compared with the bond length for C-Si which is 1.83 Å, the carbon-nitrogen and silicon-carbon atom distances in the CO adsorption are found to be 1.76 Å and 1.85 Å, respectively, while the carbon-nitrogen and silicon-carbon atom distance are 1.79 Å and 1.89 Å, respectively, for the CO₂ adsorption.

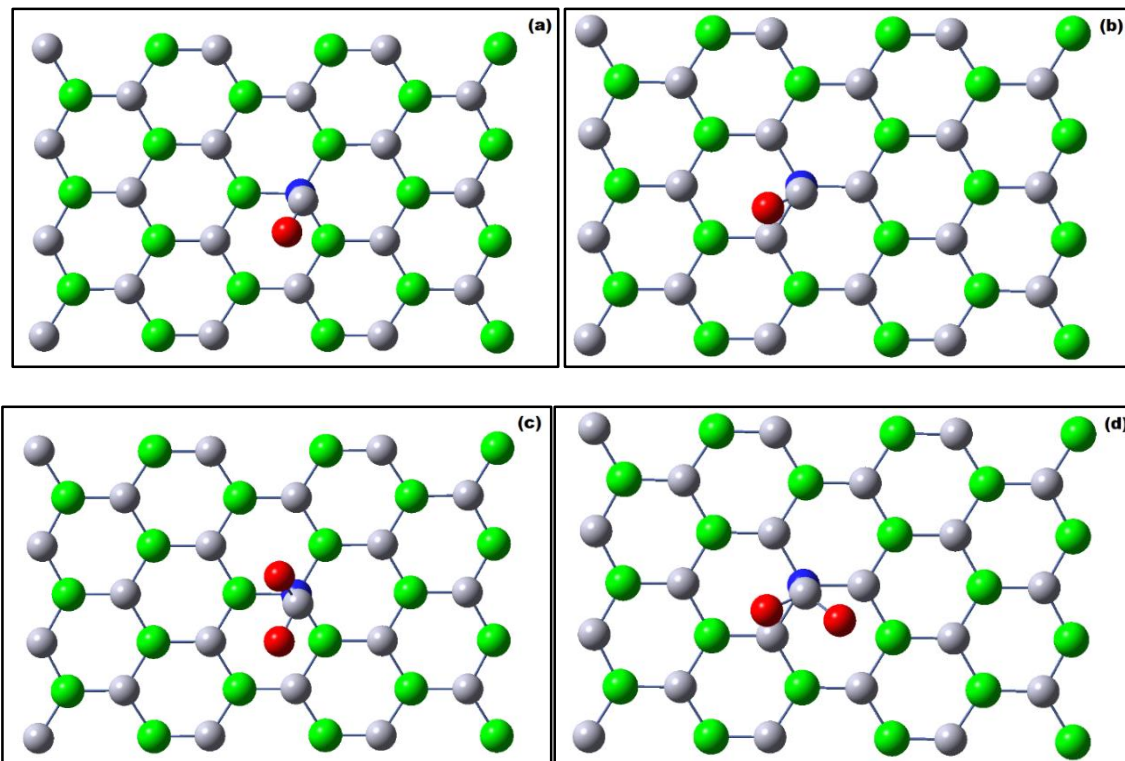


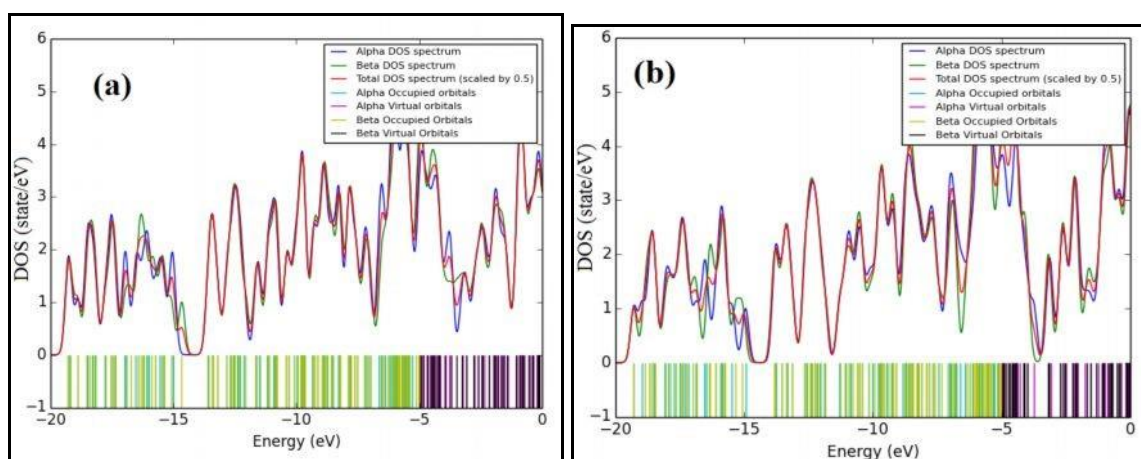
Figure 5: Top view of the configurations of the adsorption of CO and CO₂ on N-doped SiGNR after adsorption of: (a) molecule CO (model A), (b) molecule CO (model B), (c) molecules CO₂ (model A), (d) molecule CO₂ (model B).

Additional calculation results of the adsorbed systems were given in Table 2, where the model A) denotes substituting carbon atoms by nitrogen atom, model B denotes substituting silicon atoms with nitrogen atom. N-doped SiGNR can adsorb the CO₂ molecule with large adsorption energy of -3.24 and -2.18 eV for models A and B, respectively, which can show that N-doped SiGNR is sensitive to CO₂ molecule to a certain extent. The adsorption energies of CO molecules on N-doped SiGNR is a strong chemisorption with adsorption energies larger than 1.0 eV, therefore, SiGNR could activate this adsorbate due to the strong interaction, thus we can be using N-doped SiGNR as a metal-free catalyst. In Table 2, the energy gap is close to zero, after CO and CO₂ adsorption, the electronic properties structure is nearly the same to that of SiGNR at the neighborhood of the Fermi level. From the calculation, the N-doped SiGNR has a band gap larger than pristine in the CO₂ adsorption and smaller than pristine SiGNR in the CO adsorption. And Table 2 gives that the Fermi energy elevated to the conduction band on account of the alternative doping of nitrogen atom, which is due to the fact that a N atom has one more electron than a carbon atom³². Thus, the nitrogen atom acts as an n-type dopant. By doping nitrogen atom, impurity levels are introduced in the SiGNR band, which enhance the interaction between SiGNR and CO and CO₂.

Table 2: The electronic properties of adsorption of CO and CO₂ molecule on N-doped SiGNR.

Property (eV)	CO ₂ adsorbed on N-doped SiGNR		CO adsorbed on N-doped SiGNR	
	Model B	Model A	Model B	Model A
E _a	-2.18	-3.24	1	2.9
E _g	0.043	0.017	0.06	0.05
IP (= -E _{HOMO})	4.97	5.08	5.09	5.18
EA (= -E _{LUMO})	5.02	5.14	5.12	5.22
E _F	-4.99	-5.11	-5.1	-5.21

Figures 6 illustrated that the DOS of N-doped SiGNR with the adsorption of gas molecules are different from the corresponding pristine SiGNR. In the adsorption of gas molecules CO on SiGNR, the highest of peaks becomes less, in comparison with pristine SiGNR, i.e., the conduction and valence bands are less with the highest number of density of states.



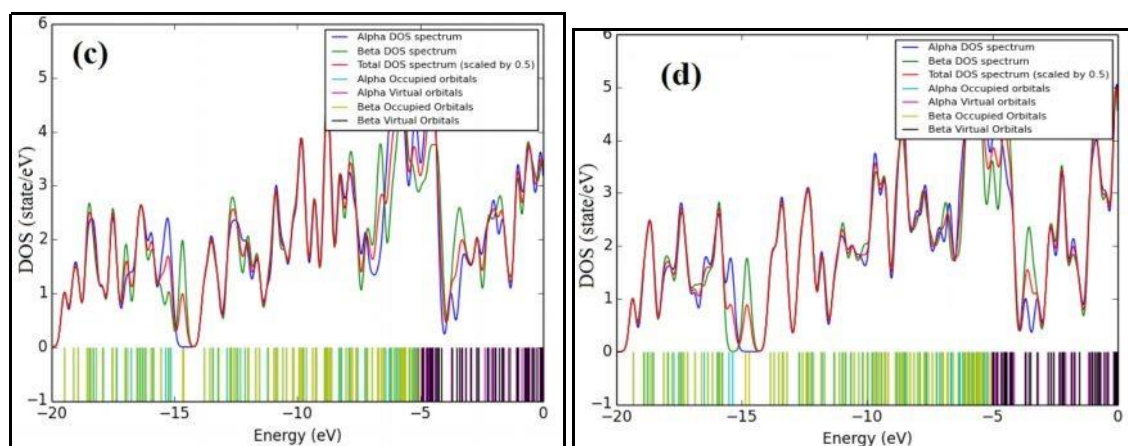


Figure 6: DOS of CO and CO₂ on N-doped SiGNR: (a) CO adsorbed on N-doped SiGNR (model A), (b) CO adsorbed on N-doped SiGNR (model B) (c) CO₂ adsorbed on N-doped SiGNR (model A), and (d) CO₂ adsorbed on N-doped SiGNR (model B).

4. Conclusions

We explore the adsorption of CO, and CO₂ on the surface of pristine SiGNR and N-doped SiGNR including two sites by DFT calculation at PBE/6-31 level of theory. In general, the adsorption energy in the results indicate that pristine SiGNR is strongly reactive to CO, and SiGNR is not suitable as a sensor of CO. Instead of this, SiGNR could catalyse or activate this adsorbate due to the strong interaction, suggesting the possibility of SiGNR as a metal-free catalyst. pristine SiGNR at site T₁ can be used to detect CO₂ at this site because it is weak physisorption. The adsorption energy for all adsorption of CO₂ on SiGNR is a strong chemisorption. The calculations show that all pristine SiGNR are positive adsorption energy corresponds to the endothermic reaction, and N-doped SiGNR can adsorb the CO₂ molecule with large adsorption energy. On the other hand, the adsorption energies of CO molecules on N-doped SiGNR is a strong chemisorption with adsorption energies larger than 1.0 eV. One can see that SiGNR could activate this adsorbate due to the strong interaction, thus we can be using N-doped SiGNR as a metal-free catalyst. Also, DOS shows that the adsorption of N-doped system is significantly different from pristine, the interaction between CO and N-doped SiGNR has certain enhancement, and may be a good candidate for sensing CO₂ gas to a certain extent.

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