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Adsorption of SO2 air pollutant gas molecule on the pure and Al-doped graphene nano sheet: A DFT study

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***Abstract*---**The interaction of pure graphene nano sheet and Al-doped graphene nano sheet with SO_2 pollutant gas molecules was examined by density functional theory (DFT). Adsorption energies and the transferred Mulliken charge were calculated. Doping Al on the graphene improved adsorption and electronic properties of graphene. Dos plots and HOMO-LUMO band gaps showed that pure graphene and Al-doped were semiconductor materials. The results revealed that sensitivity of graphene-based materials was enhanced by doping Al on the surface of pure graphene. Thus, Al-doped graphene was found to be a better detector of SO_2 gas molecules.

Keywords*---*DFT; Adsorption; Graphene; nanosheet; DOS.

Introduction

Two-dimensional materials (2D) consist of a single layer of atoms with honeycomb structure on nanometer scale [1-4]. A growing body of research is carried out on a wide variety of 2D materials [5-6] due to their fascinating electronic properties and their applications in nano-scale design [7-9]. Of these 2D materials, graphene has been studied more extensively [10-12]. Discovered in 2003 by Andre Geim,

Graphene was the first 2D material composed of carbon atoms [13, 14] whose stacked form is called graphite [15, 16]. Graphene is a magnificent new material which is million times thinner than paper and stronger than diamond [17-19], in which each atom is connected to another neighboring atoms with a strong σ-bond [20, 21]. Generally, graphene is a semimetal with unusual electronic properties, which can be described by condensed matter and band theory [22, 23]. Defects created on the graphene sheet contribute to improving electronic properties [24-26]. Doping different atoms is the most famous manipulation applied to the 2D materials and graphene surface [27-30]. Graphene sheet and Al-doped graphene sheet are significant adsorbents of pollutant gas molecules, namely SO2, CO2, O3 and etc. [31-33]. Of these pollutant gas molecules, Sulfur dioxide (SO2) is a colorless, reactive air pollutant with a strong odor [34-36], the main sources of which are fossil fuel combustion and natural volcanic activity [37-41] [42,43]. High concentrations of SO_2 can be hazardous for human health [44-48] [49-52]. These molecules are adsorbed by different kinds of graphene sheets or carbon nanotubes consisting of carbon atoms as well [53-56]. Density functional theory is the theoretical method for studying the adsorption process [57, 58]. Research demonstrates that graphene and doped graphene has high capability to adsorb different gas molecules [59-61] and can be considered as a sensor of gas molecules [62-64] due to these three properties: (1) being single layer; (2) having band gap on the surface; and having extremely low Johnson noise [65-67].

In this study, we examined adsorption properties of pure and Al-doped graphene to determine which one is a more suitable SO2 molecule adsorbent. Sensing properties have been calculated using DOS plots and adsorption energies. All calculations were theoretical and performed by DFT.

Methods:

All the calculations related to the interaction between graphene and Al-doped graphene with SO2 gas molecule were carried out using the density functional theory (DFT) by OPENMX3.9 code [68]. All structures were optimized by the General Gradient Approximation (GGA) functional [69], and exchange correlation interactions were taken into account by Perdew-Burke-Emzerhof (PBE) [70, 71]. Cut off energy, the electronic temperature, and the pressure were 100 Ry, 300 K, and 10^{-5} Gpa, respectively. The design of the supercell was 3*3*1 and 16 carbon atoms. Adsorption energies for the current study were calculated by [72]:

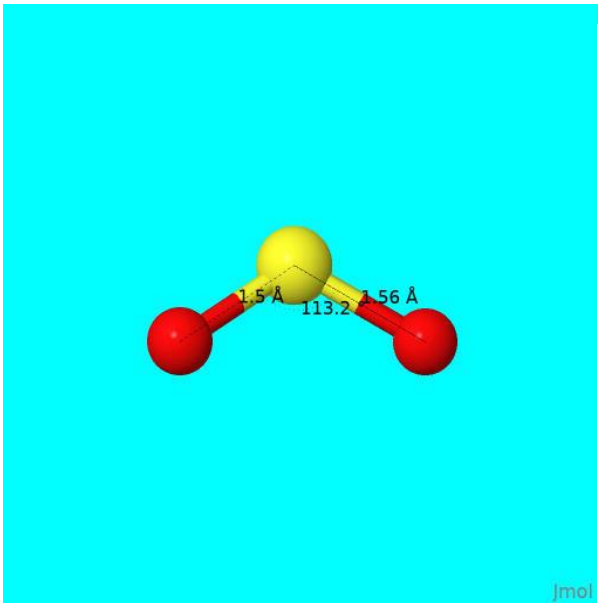
$$E_{ad} = E_{(gas+graphene\text{-}doped} - E_{(gas)} - E_{(graphene)}$$

where E_{ad} , $E_{(gas+graphene\text{-}doped}$, $E_{(gas)}$ and $E_{(graphene)}$ denote adsorption energy, adsorbed of combined system, gas molecule energy and, isolated doped-graphene energy, respectively.

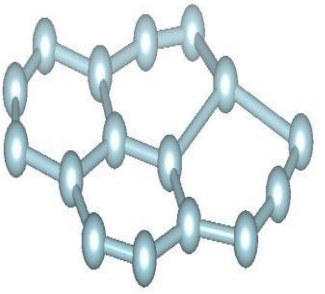
Mulliken charge model was applied to calculate the transferred charge between graphene and SO2 and also between graphene-doped and SO2 gas molecules. VESTA, and Jmol codes were employed to visualize numerical results.

Results

The steadiest adsorption configurations of SO_2 on the pure and Al-doped graphene sheet were acquired (Figure 1). After relaxation, oxygen atoms of SO_2 molecule were correlated with the pure and Al-doped graphene sheet (Figure 2). Oxygen atoms were coordinated on the pure and Al-doped graphene sheet, which occurred on one side of SO2 molecule in pure graphene sheet. According to the optimized geometry configuration values for SO_2 molecule adsorption (i.e., the bond lengths and angles) (Table 1), C-O and Al-O bond lengths decreased, thus shortening adsorption process for the two types of carbon material the pure and Al-doped graphene sheet. This results in transferring electronic density from the newly formed C-O and Al-O bonds to S-O bonds between pure and Al-doped graphene sheet and SO2 molecule. Furthermore, adsorption process decreased O-S-O angle after adsorption in two carbon materials (Table 1), leading to a relatively strong band formation on both graphene sheet surfaces.



a)



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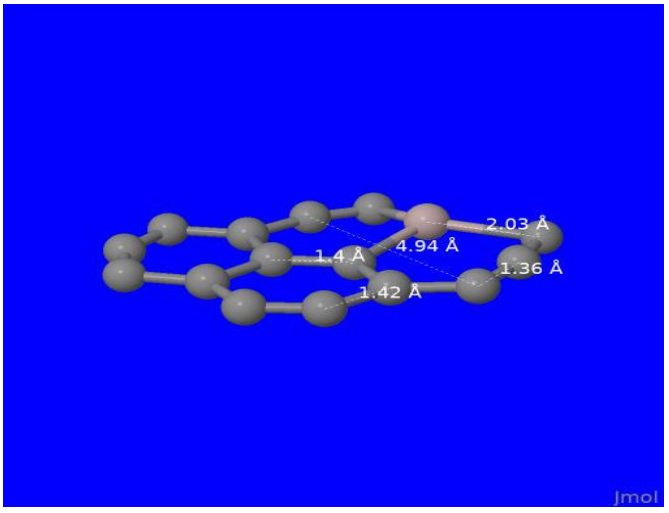
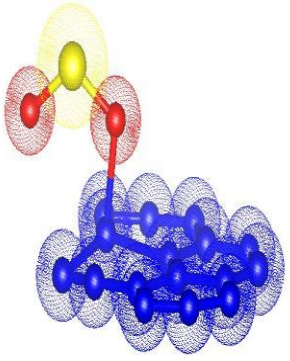
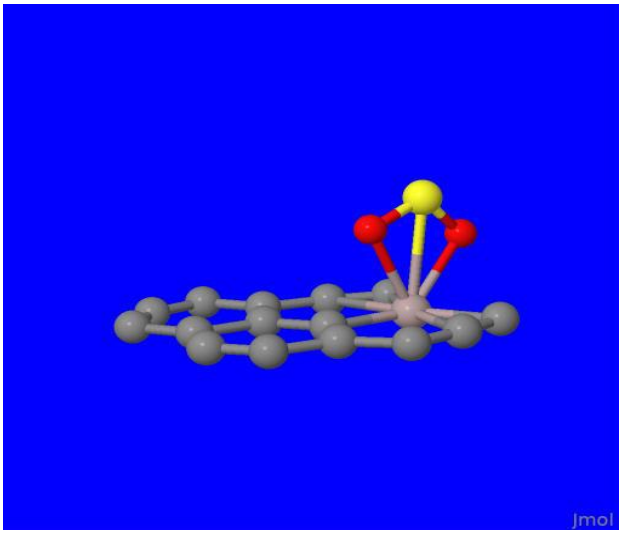


(c)

Fig.1 . (a) SO_2 gas molecule, (b) pure graphene nano sheet, (c) Al-doped graphene nano sheet; Yellow: Sulfur (S) atom ; red: Oxygen (O) atoms , gray and blue: Tin (Sn) atoms, and pink: Aluminum (Al) atom. Angstrom (Å)





(a) (b)

Fig. 2 . Optimized geometry configurations, after adsorption of SO2 on the pure graphene sheet (a), Al-doped graphene sheet (b), Yellow: Sulfur (S) atom ; red: Oxygen (O) atoms; blue and gray : Tin atoms, pink: Aluminum (Al) atom .

Carbon Materials	Newly formed C-O	Newly formed Al-O	C-O	Al-O	SO2 angles (before-after) of adsorption
SO2 adsorption					
graphene	1.95	-	2.00	-	118.6-113.2
Al-graphene	-	1.98	-	3.05	118.6-115.3

Table1. Bond lengths (Å), angles (degrees) for adsorption of SO2 on the pure and Al-doped graphene nanosheet.

Adsorption energies of SO_2 molecule on the pure and Al-doped graphene sheet (Table2) indicate that adsorption of SO_2 molecule on both pure and Al-doped graphene sheet was relatively strong while the strength of adsorption on Al-doped graphene sheet was more substantial. The dipole moment of SO2 on the pure and Al-doped graphene sheet (Table 2) showed that dipole moment was so small in pure graphene sheet and had a slight increase after SO2 adsorption. But in Al-doped graphene sheet, doping Al atom increased dipole moment which increased dramatically after SO2 adsorption, thereby increasing adsorption energy.

Carbon Materials	E_{ad}	Q_T	Debye before adsorption	Debye after adsorption	HOMO-LUMO band gap (before adsorption)	HOMO-LUMO band gap (after adsorption)
graphene	-0.26	0.002	0.003	0.1	~ Zero	0.003
Al-graphene	-0.55	0.025	0.24	2.39	0.03	0.05

Table 2. Adsorption energies (E_{ad}/eV), and charge transfers (Q_T/e) , dipole moment (Debye), HOMO-LUMO energies (eV) for SO2 adsorption of SO2 on the pure graphene sheet and Al-doped graphene sheet.

For graphene case, HOMO-LUMO band gap energy increased from zero to 0.003 eV after SO2 adsorption (Table 2), thereby creating semiconductor properties on the pure graphene sheet. As a semiconductor with HOMO-LUMO band gap energy of 0.03 eV before adsorption (Table 2), Al-doped graphene sheet showed an increase in its band gap energy to 0.05 eV after adsorption, improving semiconductor characteristics on the Al-doped graphene sheet.

Density of states (DOS) plots (Figure 3) illustrate that DOS plots changed in graphene sheet after SO2 adsorption and that DOS value around Fermi level increased slightly. Graphene sheet was thus identified as a detector for sensing SO2 gas molecule in this study. Changes in DOS of Al-doped graphene sheet (Fig 3) before and after adsorption were considerable, especially around Fermi level. As a result, some wrinkles were created between 10 eV and 20 eV. This suggests that Al-doped graphene sheet had a stronger detection of SO2 compared with the pure graphene sheet.

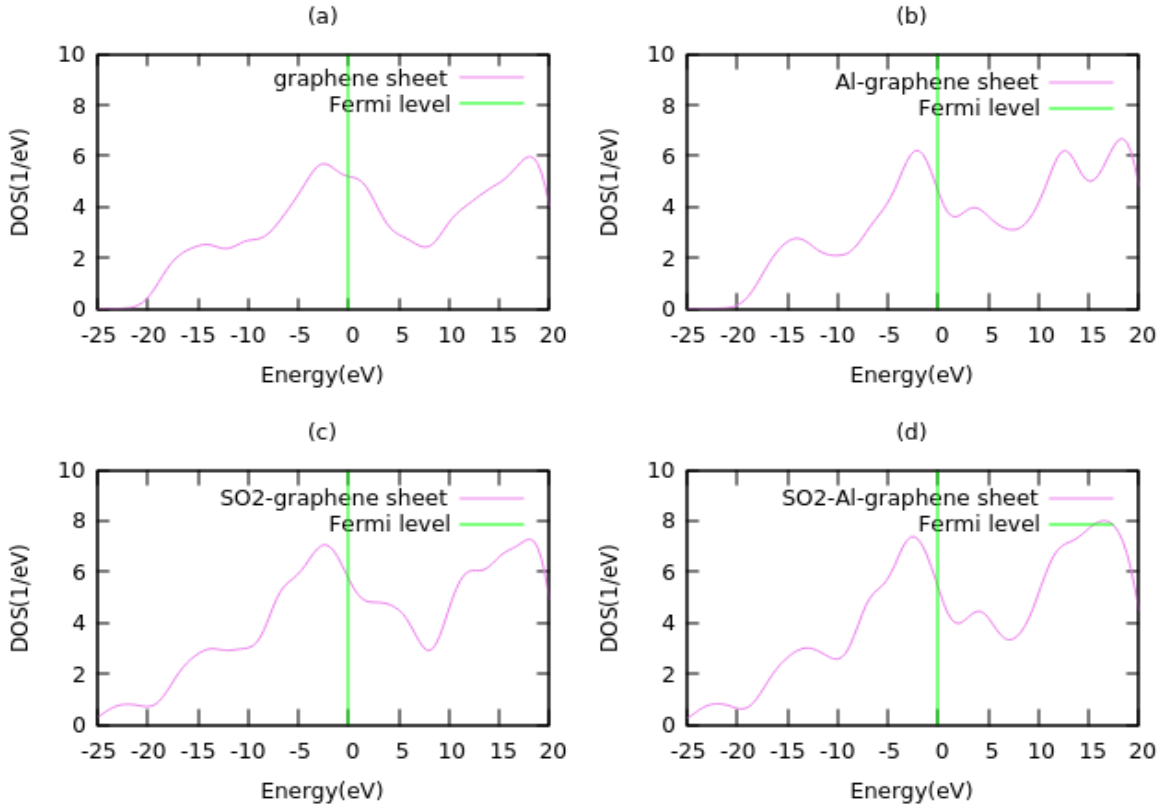


Fig3. Electronic density of state (DOS) of pure graphene sheet (a), Al doped graphene

(b), SO2–graphene sheet (c) and SO2–Al doped graphene sheet (d).

Conclusion

In this study, the calculations of adsorption energies of SO2 gas molecules on the pure and Al-doped graphene sheet indicated that Al-doped was a relatively stronger SO2 adsorbent due to its polarity. Dipole moments also showed that Al-doped had a larger polarity than pure graphene. Adsorption process increased semiconductor characteristics in two kinds of carbon materials. SO2 acted as an acceptor gas molecules, accumulating density charge around pure and Al-doped graphene sheet. DOS plots changes illustrated that the pure and Al-doped graphene sheet was a detector of SO2 and that Al-doped was a relatively stronger detector than pure graphene sheet.

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