

## Sensing Properties of Gas Sensor Based on Adsorption of NO<sub>2</sub> with Defect, Pristine, Fe and Si-MoS<sub>2</sub> Layer

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Two-dimensional (2D) layered materials are currently being considered as entrant for future electronic devices. Molybdenum disulphide (MoS<sub>2</sub>) belongs to a family of layered transitional metal dichalcogenides (TMDS), has a unique characteristics of showing intrinsic semiconducting nature is being considered a major advantageous over graphene (which has no intrinsic band gap) as a two-dimensional (2D) channel material in field effect transistors (FET). In the paper, the results of investigations are presented concerning the affects of adsorption of NO<sub>2</sub> gas on the surface of MoS<sub>2</sub>, defect-MoS<sub>2</sub>, Si-MoS<sub>2</sub> and Fe-MoS<sub>2</sub> layer. The changes density of states (DOS) and electrostatic difference potential of Si-MoS<sub>2</sub> by applying different gate voltage were studied. We proposed that, NO<sub>2</sub> might play an important role on MoS<sub>2</sub> layer that can be used as gas sensor. In the research, it has been shown that in the case of gas sensor, the adsorption of NO<sub>2</sub> with MoS<sub>2</sub>, Fe-MoS<sub>2</sub>, Si-MoS<sub>2</sub> and defect-MoS<sub>2</sub> play an important rule for sensing behavior.

**Keywords:** DOS, Electrostatic difference potential, 2D MoS<sub>2</sub>.

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### 1. INTRODUCTION

Two dimensional (2D) graphene synthesis and theoretical observation of Molybdenum disulphide - based devices have attracted broad attention of scientists in assorted disciplines of science and technology due to its unique structural, mechanical, and electronic properties [1]. The unique characteristics of MoS<sub>2</sub> suggest that to use as chemical vapor sensors, photosensor, high performance photo-detector and photovoltaic [2-5]. The performances of MoS<sub>2</sub>-based devices are generally determined by the electronic properties of MoS<sub>2</sub> as a result experimental and theoretical studies have been conducted to understand the interactions of the materials with different chemical species for improving its chemical and physical properties [6, 7]. The previous researches in this area have focused on the interactions of small gas molecules, such as adsorption of CO<sub>2</sub>, NO<sub>2</sub> and NH<sub>3</sub> with the pristine MoS<sub>2</sub> in theory [8] and CO<sub>2</sub> sensing using MoS<sub>2</sub> sheet in experiment [9]. After introducing dopants into 2D nanosheets of MoS<sub>2</sub>, the interactions between small molecules and MoS<sub>2</sub> can be highly enhanced [7, 10]. Recently, the functionalized MoS<sub>2</sub> have also been investigated extensively [11, 12]. Monolayer MoS<sub>2</sub> improved performances when working as chemical sensors [13]. It has been found that organic electron acceptors [14], donors [15], for instance, can induce significant changes in the electronic structure of MoS<sub>2</sub>. Metal dopant [16] and defect [17] can be used to tune MoS<sub>2</sub>'s magnetic property. These theoretical studies could give us clear insight into understanding the bio/chemical sensing behaviors of MoS<sub>2</sub> and thus direct us in designing novel microdevices with optimized performances. A level of 50 ppm NO<sub>2</sub> has been designated by the US National Institute for Occupational Safety and Health (NIOSH) as immediately dangerous to life and health [18], and several groups have worked on fabricating microdevices for detecting the toxic mole-

cule. Again, it was found that the surface modification of ZnO nanowires with Pd nanoparticles can highly enhance the performances of NO<sub>2</sub> sensors [19]. While the chemical sensors based on carbon nanotubes [20] and graphene [21, 22] were also investigated extensively. To the best of our knowledge, there is no report in literature concerned with the NO<sub>2</sub> adsorption effect on DOS and electrostatic difference potential on Si-MoS<sub>2</sub> layer by applying different gate voltage. Here in we report a systematic theoretical study of NO<sub>2</sub> sensing ability of MoS<sub>2</sub> doped with elements including Si and Fe. The interactions between NO<sub>2</sub> molecule and MoS<sub>2</sub> have been investigated carefully for understanding the effects of dopants and defects on the electronic properties of MoS<sub>2</sub>. It was found that the electronic properties of MoS<sub>2</sub> can be modified effectively by introducing dopants and defects into the 2D sheets.

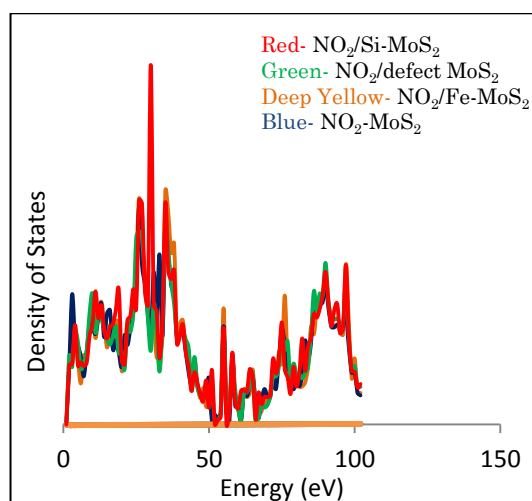


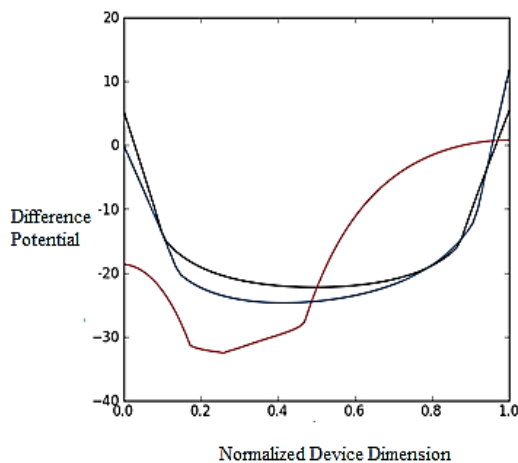
Fig. 1 – Density of States of NO<sub>2</sub> with pristine-, defect-, Fe- and Si-MoS<sub>2</sub>

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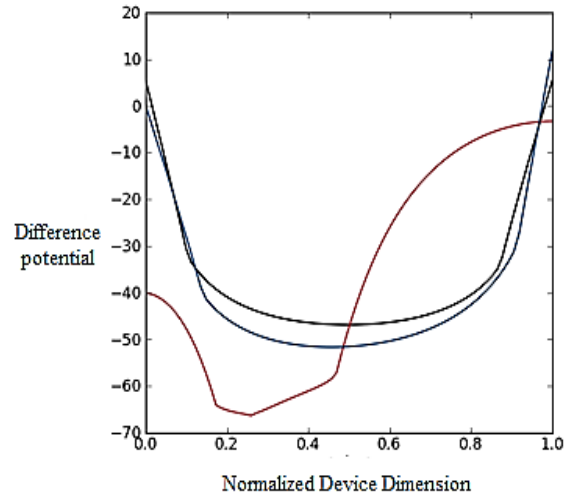
## 2. MODELING AND ANALYSIS

To better understand the change in the electronic structure arise by  $\text{NO}_2$  gas adsorption, the electronic densities of states (DOSs) are calculated for the systems of  $\text{NO}_2$  on pristine, defect and Fe-MoS<sub>2</sub>, Si-MoS<sub>2</sub>. Fig. 1 shows the DOS for the representative systems. The adsorption energies calculated reveal that the interaction between  $\text{NO}_2$  and the pristine MoS<sub>2</sub> is weak. The DOS structure of  $\text{NO}_2/\text{MoS}_2$  system shows little change after the adsorption of  $\text{NO}_2$  molecule, clearly verifies the weak interaction again. In contrast, the DOS of  $\text{NO}_2$  on defect MoS<sub>2</sub> changed due to the strong molecule-MoS<sub>2</sub> interactions. Compared to that of pristine MoS<sub>2</sub>, the DOS of defect-MoS<sub>2</sub> exhibits a large peak appearing just above the Fermi level. This peak indicates that the system is strongly metallic and a significant increase in the conductivity of defect-MoS<sub>2</sub> is expected in comparison with the pristine MoS<sub>2</sub>. After the chemisorption of  $\text{NO}_2$  molecule, the system becomes more like a semiconductor and exhibits a drop of the DOS near the Fermi level.

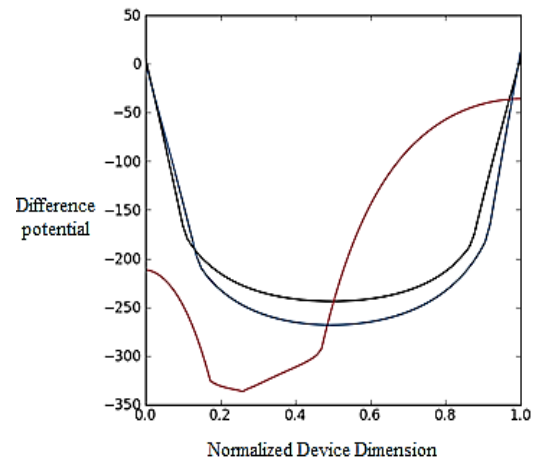


**Fig. 2** – Electrostatic difference Potential (applied gate voltage of 0.2 V)

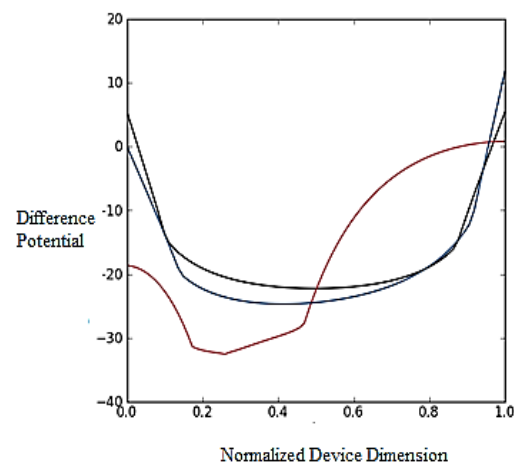
The DOS analysis also indicates that the interaction between  $\text{NO}_2$  and the defect-MoS<sub>2</sub> is stronger than that of pristine MoS<sub>2</sub>. The adsorption of  $\text{NO}_2$  onto the surface of defect-MoS<sub>2</sub> can move the major band features to a higher energy; in other words, the Fermi level of the system shifts towards lower energy. It is consistent with the results based on the analysis of adsorption energy values of the two systems. Such an enhancement in the interaction between  $\text{NO}_2$  molecule and defect-MoS<sub>2</sub> can be directly associated with the rearrangement of the sheet structure of MoS<sub>2</sub> in the presence of  $\text{NO}_2$  molecule [23]. In case of  $\text{NO}_2/\text{Si-MoS}_2$ , there is a peak before Fermi level which indicates the adsorption of  $\text{NO}_2$  on that place. The falling of peak just before the Fermi level also represents the semi-conductive behavior. As the result, of electron density shows that Fe-MoS<sub>2</sub> is more suitable than Si-, defect-, pristine MoS<sub>2</sub> which we discuss before but in case of DOS Si-MoS<sub>2</sub> behaves more for sensing property than others. The electrostatic difference potential of  $\text{NO}_2$  adsorbed Si-MoS<sub>2</sub> has a gate voltage of 0.2 V are shown in Fig. 2.



**Fig. 3** – Electrostatic Difference Potential (Applied gate voltage of 0.4 V)



**Fig. 4** – Electrostatic Difference Potential (Applied gate voltage of 1 V)



**Fig. 5** – Electrostatic Difference Potential (Applied gate voltage of 2 V)

We have considered bias voltage from 0 to 1 V to show where the adsorption process mainly take place. The red color line shows the direction of X-axis, the blue color line shows the direction of Y-axis, and the

black color line shows the direction of Z-axis. Fig. 2 illustrates that the adsorption of NO<sub>2</sub> has occurred in near 0.2 to 0.4 bias voltage. If we increase the gate voltage up to 0.4 V which is shown in Fig. 3 illustrates that the electrostatic difference potential changes dramatically. The effect of increasing gate voltage around 1 and 2 voltage are shown in Fig. 4 and Fig. 2d. In last, we make a conclusion that with the increase of gate voltage, it is possible to increase electrostatic difference potential of NO<sub>2</sub> doped Si-MoS<sub>2</sub>.

### 3. CONCLUSION

In summary, DFT calculations divulge that MoS<sub>2</sub> with Fe and defect exhibit highly enhanced NO<sub>2</sub> sens-

ing behaviors, compared to that of pristine MoS<sub>2</sub> when exposed to gaseous NO<sub>2</sub> molecule. Doping adsorption with N or B is not a promising route for improving NO<sub>2</sub> molecule adsorption. In contrast, NO<sub>2</sub> can be adsorbed on MoS<sub>2</sub> surface strongly when lattice defect, or doping Si, Fe are introduced into the MoS<sub>2</sub> layer. It is found from electron density that metal doped on MoS<sub>2</sub> layer especially Fe shows high sensitivity with NO<sub>2</sub>. Again from DOS, it is found that NO<sub>2</sub>-Si / MoS<sub>2</sub> has shown high sensitivity rather than NO<sub>2</sub> on Fe-, defect-MoS<sub>2</sub>. The changes of DOS by varying gate voltage shows a negotiable effect on NO<sub>2</sub> / Fe-MoS<sub>2</sub>, NO<sub>2</sub> / Si-MoS<sub>2</sub> and NO<sub>2</sub> / defect-MoS<sub>2</sub> and have a little bit effect on NO<sub>2</sub>-MoS<sub>2</sub>.

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