JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. **6** No 4, 04004(3pp) (2014)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том **6** № 4, 04004(3cc) (2014)

Sensing Properties of Gas Sensor Based on Adsorption of NO_2 with Defect, Pristine, Fe and Si-MoS_2 Layer

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(Received 04 July 2014; revised manuscript received 28 November 2014; published online 29 November 2014)

Two-dimensional (2D) layered materials are currently being considered as entrant for future electronic devices. Molybdenum disulphide (MoS_2) 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_2 gas on the surface of MoS_2, defect-MoS_2, Si-MoS_2 and Fe-MoS_2 layer. The changes density of states (DOS) and electrostatic difference potential of Si-MoS_2 by applying different gate voltage were studied. We proposed that, NO_2 might play an important role on MoS_2 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_2 with MoS_2, Fe-MoS_2, Si-MoS_2 and defect-MoS_2 play an important rule for sensing behavior.

Keywords: DOS, Electrostatic difference potential, 2D MoS_2.

PACS number: 07.07.Df

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_2 suggest that to use as chemical vapor sensors, photosensor, high performance photo-detector and photovoltaic [2-5].The performances of MoS_2-based devices are generally determined by the electronic properties of MoS_2 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_2, NO_2 and NH_3 with the pristine MoS_2 in theory [8] and CO_2 sensing using MoS_2 sheet in experiment [9]. After introducing dopants into 2D nanosheets of MoS_2, the interactions between small molecules and MoS_2 can be highly enhanced [7, 10]. Recently, the functionalized MoS_2 have also been investigated extensively [11, 12]. Monolyer MoS_2 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_2. Metal dopant [16] and defect [17] can be used to tune MoS_2's magnetic property. These theoretical studies could give us clear insight into understanding the bio/chemical sensing behaviors of MoS_2 and thus direct us in designing novel microdevices with optimized performances. A level of 50 ppm NO_2 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 molecule. Again, it was found that the surface modification of ZnO nanowires with Pd nanoparticles can highly enhance the performances of NO_2 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_2 adsobing effect on DOS and electrostatic difference potential on Si-MoS_2 layer by applying different gate voltage. Here in we report a systematic theoretical study of NO_2 sensing ability of MoS_2 doped with elements including Si and Fe. The interactions between NO_2 molecule and MoS_2 have been investigated carefully for understanding the effects of dopants and defects on the electronic properties of MoS_2. It was found that the electronic properties of MoS_2 can be modified effectively by introducing dopants and defects into the 2D sheets.

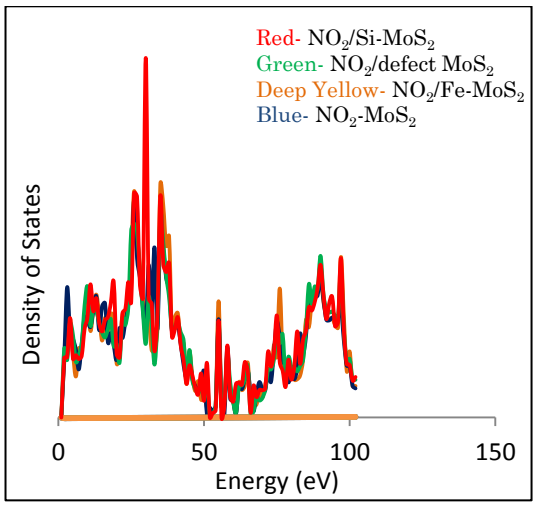

Fig. 1 – Density of States of NO_2 with pristine-, defect-, Fe- and Si-MoS_2

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2. MODELING AND ANALYSIS

To better understand the change in the electronic structure arouse by NO_2 gas adsorption, the electronic densities of states (DOSs) are calculated for the systems of NO_2 on pristine, defect and Fe-MoS_2, Si-MoS_2. Fig. 1 shows the DOS for the representative systems. The adsorption energies calculated reveal that the interaction between NO_2 and the pristine MoS_2 is weak. The DOS structure of NO_2/ MoS_2 system shows little change after the adsorption of NO_2 molecule, clearly verifies the weak interaction again. In contrast, the DOS of NO_2 on defect MoS_2 changed due to the strong molecule-MoS_2 interactions. Compared to that of pristine MoS_2, the DOS of defect-MoS_2 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_2 is expected in comparison with the pristine MoS_2. After the chemisorption of NO_2 molecule, the system becomes more like a semiconductor and exhibits a drop of the DOS near the Fermi level.

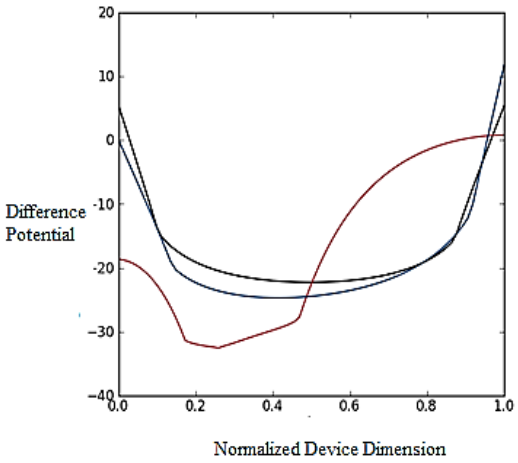

Fig. 2 – Electrostatic difference Ppotential (applied gate voltage of 0.2 V)

The DOS analysis also indicates that the interaction between NO_2 and the defect-MoS_2 is stronger than that of pristine MoS_2. The adsorption of NO_2 onto the surface of defect-MoS_2 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 NO_2 molecule and defect-MoS_2 can be directly associated with the rearrangement of the sheet structure of MoS_2 in the presence of NO_2 molecule [23]. In case of NO_2/ Si-MoS_2, there is a peak before Fermi level which indicates the adsorption of NO_2 on that place. The falling of peak just before the Fermi level also represents the semiconductive behavior. As the result, of electron density shows that Fe-MoS_2 is more suitable than Si-, defect-, pristine MoS_2 which we discuss before but in case of DOS Si-MoS_2 behaves more for sensing property than others. The electrostatic difference potential of NO_2 adsorbed Si-MoS_2 has a gate voltage of 0.2 V are shown in Fig. 2.

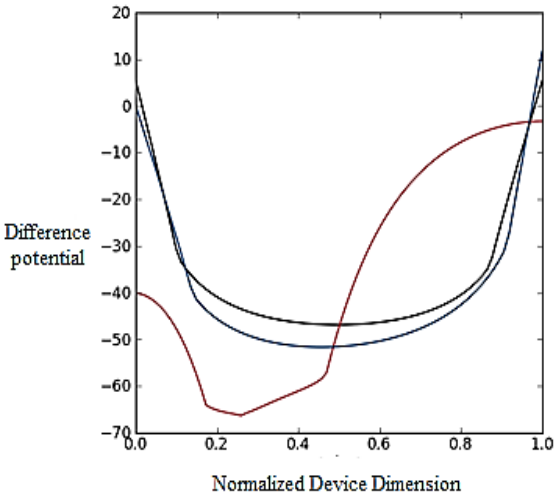

Fig. 3 – Electrostatic Difference Potential (Applied gate voltage of 0.4 V)

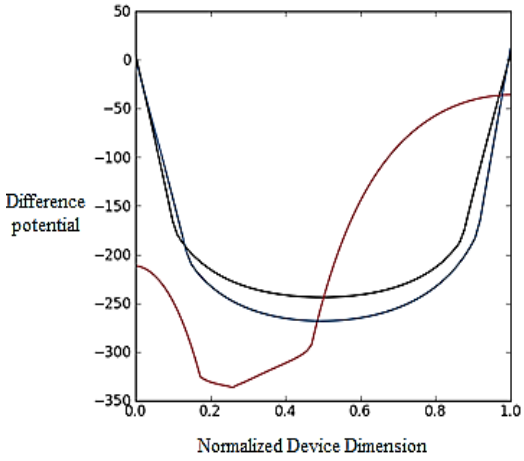

Fig. 4 – Electrostatic Difference Potential (Applied gate voltage of 1 V)

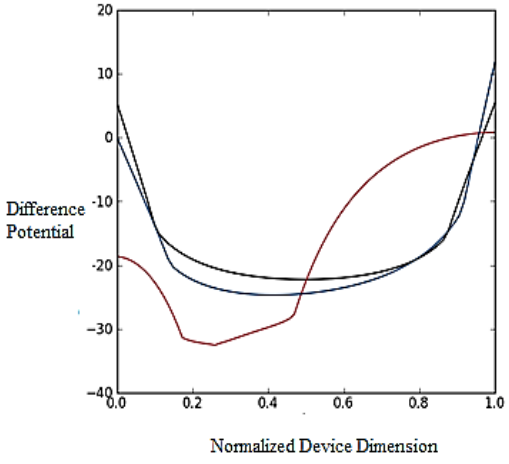

Fig. 5 – Electrostatic Difference Potential (Applied gate voltage of 2 V)

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_2 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_2 doped Si-MoS_2.

3. CONCLUSION

In summary, DFT calculations divulge that MoS_2 with Fe and defect exhibit highly enhanced NO_2 sensing behaviors, compared to that of pristine MoS_2 when exposed to gaseous NO_2 molecule. Doping adsorption with N or B is not a promising route for improving NO_2 molecule adsorption .In contrast,NO_2 can be adsorbed on MoS_2 surface strongly when lattice defect, or doping Si, Fe are introduced into the MoS_2 layer. It is found from electron density that metal doped on MoS_2 layer especially Fe shows high sensitivity with NO_2.Again from DOS, it is found that NO_2-Si / MoS_2 has shown high sensitivity rather that NO_2 on Fe-, defect-MoS_2.The changes of DOS by varying gate voltage shows a negotiable effect on NO_2 / Fe-MoS_2, NO_2 / Si-MoS_2 and NO_2 / defect-MoS_2 and have a little bit effect on NO_2-MoS_2.

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