

Sensing Properties of Gas Sensor Based on Adsorption of NO₂ with Defect, Pristine, Fe and Si-MoS₂ Layer

S.R. Shakil*, S.A. Khan†

Robotics Research Lab, School of Engineering and Computer Science, BRAC University, Bangladesh

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Two-dimensional (2D) layered materials are currently being considered as entrant for future electronic devices. Molybdenum disulphide (MoS₂) 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 NO₂ gas on the surface of MoS₂, defect-MoS₂, Si-MoS₂ and Fe-MoS₂ layer. The changes density of states (DOS) and electrostatic difference potential of Si-MoS₂ by applying different gate voltage were studied. We proposed that, NO₂ might play an important role on MoS₂ 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 NO₂ with MoS₂, Fe-MoS₂, Si-MoS₂ and defect-MoS₂ play an important rule for sensing behavior.

Keywords: DOS, Electrostatic difference potential, 2D MoS₂.

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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 MoS₂ suggest that to use as chemical vapor sensors, photosensor, high performance photo-detector and photovoltaic [2-5]. The performances of MoS₂-based devices are generally determined by the electronic properties of MoS₂ 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 CO₂, NO₂ and NH₃ with the pristine MoS₂ in theory [8] and CO₂ sensing using MoS₂ sheet in experiment [9]. After introducing dopants into 2D nanosheets of MoS₂, the interactions between small molecules and MoS₂ can be highly enhanced [7, 10]. Recently, the functionalized MoS₂ have also been investigated extensively [11, 12]. Monolayer MoS₂ 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 MoS₂. Metal dopant [16] and defect [17] can be used to tune MoS₂'s magnetic property. These theoretical studies could give us clear insight into understanding the bio/chemical sensing behaviors of MoS₂ and thus direct us in designing novel microdevices with optimized performances. A level of 50 ppm NO₂ 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 NO₂ 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 NO₂ adsorbing effect on DOS and electrostatic difference potential on Si-MoS₂ layer by applying different gate voltage. Here in we report a systematic theoretical study of NO₂ sensing ability of MoS₂ doped with elements including Si and Fe. The interactions between NO₂ molecule and MoS₂ have been investigated carefully for understanding the effects of dopants and defects on the electronic properties of MoS₂. It was found that the electronic properties of MoS₂ can be modified effectively by introducing dopants and defects into the 2D sheets.

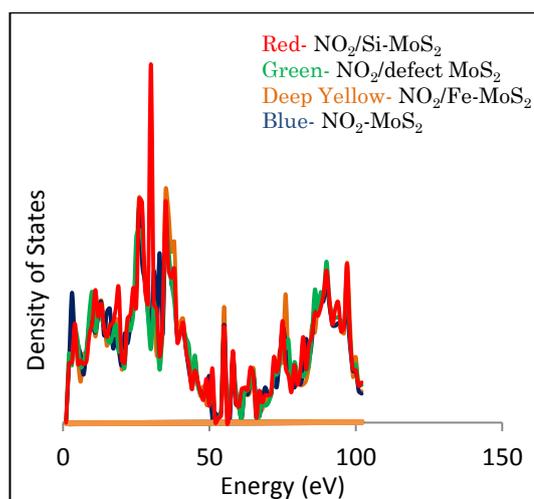


Fig. 1 – Density of States of NO₂ with pristine-, defect-, Fe- and Si-MoS₂

* shifur.shakil@gmail.com

† khan.sabbir@bracu.ac.bd

2. MODELING AND ANALYSIS

To better understand the change in the electronic structure arise by NO_2 gas adsorption, the electronic densities of states (DOSs) are calculated for the systems of NO_2 on pristine, defect and Fe-MoS₂, Si-MoS₂. Fig. 1 shows the DOS for the representative systems. The adsorption energies calculated reveal that the interaction between NO_2 and the pristine MoS₂ 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 MoS₂ changed due to the strong molecule-MoS₂ interactions. Compared to that of pristine MoS₂, the DOS of defect-MoS₂ 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-MoS₂ is expected in comparison with the pristine MoS₂. 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.

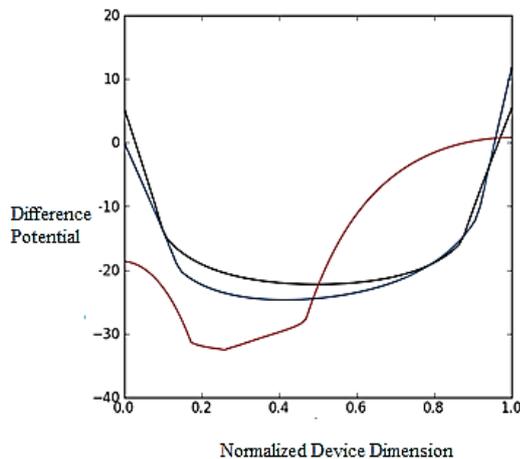


Fig. 2 – Electrostatic difference Ppotential (applied gate voltage of 0.2 V)

The DOS analysis also indicates that the interaction between NO_2 and the defect-MoS₂ is stronger than that of pristine MoS₂. The adsorption of NO_2 onto the surface of defect-MoS₂ 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-MoS₂ can be directly associated with the rearrangement of the sheet structure of MoS₂ in the presence of 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 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-MoS₂ is more suitable than Si-, defect-, pristine MoS₂ which we discuss before but in case of DOS Si-MoS₂ behaves more for sensing property than others. The electrostatic difference potential of NO_2 adsorbed Si-MoS₂ has a gate voltage of 0.2 V are shown in Fig. 2.

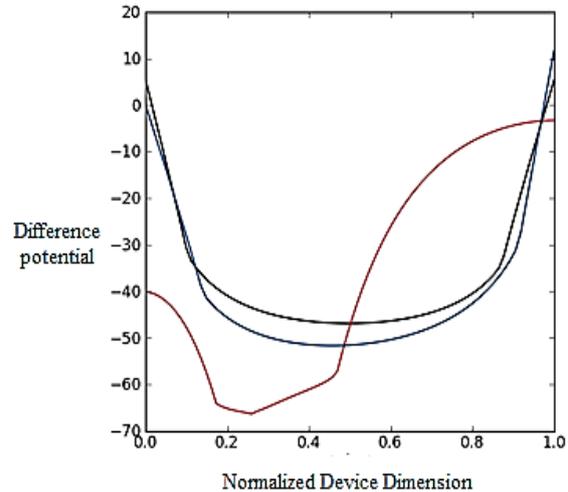


Fig. 3 – Electrostatic Difference Potential (Applied gate voltage of 0.4 V)

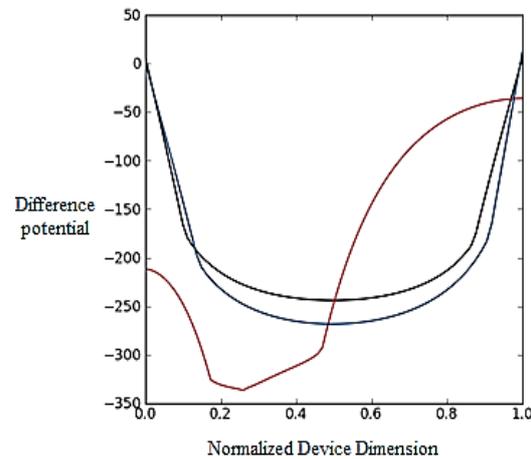


Fig. 4 – Electrostatic Difference Potential (Applied gate voltage of 1 V)

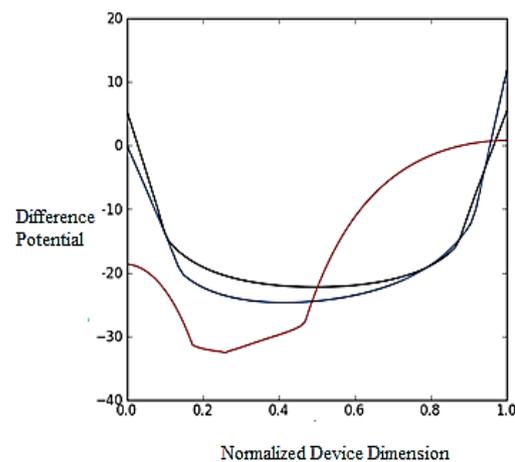


Fig. 5 – Electrostatic Difference Potential (Applied gate voltage of 2 V)

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 NO₂ 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 NO₂ doped Si-MoS₂.

3. CONCLUSION

In summary, DFT calculations divulge that MoS₂ with Fe and defect exhibit highly enhanced NO₂ sens-

ing behaviors, compared to that of pristine MoS₂ when exposed to gaseous NO₂ molecule. Doping adsorption with N or B is not a promising route for improving NO₂ molecule adsorption. In contrast, NO₂ can be adsorbed on MoS₂ surface strongly when lattice defect, or doping Si, Fe are introduced into the MoS₂ layer. It is found from electron density that metal doped on MoS₂ layer especially Fe shows high sensitivity with NO₂. Again from DOS, it is found that NO₂-Si / MoS₂ has shown high sensitivity rather than NO₂ on Fe-, defect-MoS₂. The changes of DOS by varying gate voltage shows a negotiable effect on NO₂ / Fe-MoS₂, NO₂ / Si-MoS₂ and NO₂ / defect-MoS₂ and have a little bit effect on NO₂-MoS₂.

REFERENCES

1. H. Wang, L. Yu, Y.H. Lee, Y. Shi, A. Hsu, M.L. Chin, L.J. Li, M. Dubey, J. Kong, T. Palacios, *Nano Lett.* **12**, 4674 (2012).
2. F.K. Perkins, A.L. Friedman, E. Cobas, P.M. Campbell, G.G. Jernigan, B.T. Jonke, *Nano Lett.* **13**, 668 (2013).
3. N.P. López, Zhong Lin, et al, *2D Mater.* **1**, 011004 (2014).
4. M.R. Esmaeili-Rad, S. Sayeef, *Sci. Rep.* **3**, 2345 (2013).
5. M. Shanmugam, T. Bansal, D.A. Chiris, B.Yu, *Appl. Phys. Lett.* **100**, 153901 (2012).
6. M.T. Abuelma'atti, *Electronics, Communications and Photonics Conference (SIEPCP)*, 1 (Saudi International: 2013).
7. Z.M. Wang (Ed.), *MoS₂, Materials, Physics, and Devices XI*, 291 (2014).
8. Q. Yue, Z. Shao, S. Chang, J. Li, *Nanoscale. Res. Lett.* **8**, 425 (2013).
9. S. Zhao, J. Xue, W. Kang, *Chem. Phys. Lett.* **595-596**, 35 (2014).
10. Y.C. Lin, D.O. Dumcenco, H.P. Komsa, Y. Niimi, A.V. Krasheninnikov, Y.S. Huang, K. Suenaga, *Adv. Mater.* **26**, 2857 (2014).
11. H. Li, X. Qi, J. Wu, Z. Zeng, J. Wei, H. Zhang, *ACS Nano.* **7**, 2842 (2013).
12. C. Ataca, H. Sahin, E. Akturk, S. Ciraci, *J. Phys. Chem. C.* **115**, 10 (2011).
13. B. Liu, L. Chen, G. Liu, A.N. Abbas, M. Fathi, C. Zhou, *ACS Nano* **8**, 5304 (2014).
14. H. Ishii, K. Sugiyama, E. Ito, K. Seki, *Adv. Mater.* **11**, 605 (1999).
15. R. Gómez-Balderas, J.M. Martínez-Magadán, R. Santamaria, C. Amador, *Int. J. Quantum Chem.* **80**, 406 (2000).
16. N. Feng, W. Mi, Y. Cheng, Z. Guo, U. Schwingenschlögl, H. Bai, *Sci. Rep.* **4**, 3987 (2014).
17. M.R. Islam, N. Kang, U. Bhanu, H.P. Paudel, M. Erementchouk, L. Tetard, M.N. Leuenberger, S.I. Khondaker, *ArXiv:1404.5089* (2014).
18. *Documentation for Immediately Dangerous To Life or Health Concentrations (IDLHs)*, NIOSH Publications and Products, Centers for Disease Control and Prevention, 1600 Clifton Rd. Atlanta, GA 30333, USA.
19. Y. Xiao, L. Lu, A. Zhang, Y. Zhang, L. Sun, L. Huo, F. Li, *ACS Appl. Mater. Interface.* **4**, 3797 (2012).
20. D.R. Kauffman, D.C. Sorescu, D.P. Schofield, B.L. Allen, K.D. Jordan, A. Star, *Nano Lett.* **10**, 958 (2010).
21. Z. Jiang, J. Wang, L. Meng, Y. Huang, L. Liu, *Chem. Commun.* **47**, 6350 (2011).
22. Y. Dan, Y. Lu, N.J. Kybert, Z. Luo, A.T.C. Johnson, *Nano Lett.* **9**, 1472 (2009).
23. A.N. Enyashin, M.B. Sadan, L. Houben, G. Seifert, *J. Phys. Chem. C* **117**, 20 (2013).