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Theoretical study of two dimensional Nano sheet for gas sensing application

Deepak Dubey[1], Dr.Ajazul Haque[2], Dr.J.C.Jain[3], Ramashankar Prajapati[4]
[1](Viva Institute of Technology, University of Mumbai,, India)
[2](Viva Institute of Technology, University of Mumbai,, India)
[3](Viva Institute of Technology, University of Mumbai,, India)
[4](Viva Institute of Technology, University of Mumbai,, India)

Abstract :*This study is focus on various two dimensional material for sensing various gases with theoretical view for new research in gas sensing application. In this paper we review various two dimensional sheet such as Graphene, Boron Nitride nanosheet, Mxene and their application in sensing various gases present in the atmosphere.*

Keywords *-Two dimension, Gas sensor, Graphene, Mxene. Boron Nitride*

I. INTRODUCTION

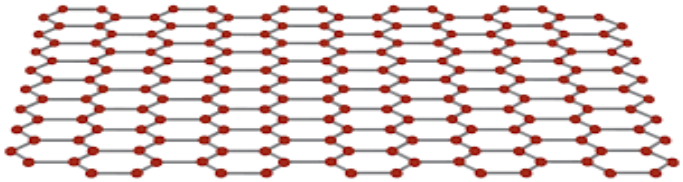
Due to industrialization gas usage has increased in various applications. Gas sensing material has an increasing application in the automobile industry, environmental studies and in the medical field In this century air pollution causing major damage to various countries in their progress. Also increasing pollution increases at a particular level that will cause huge impact on citizens' health living in that particular area. An accurate, effective and efficient gas sensor is needed in today's world which can precisely sense the various gases present in the atmosphere. Chemiresistive sensors detect gases by a chemical reaction when the gases are in direct contact with the sensor's surface which causes change of its electrical resistance depending upon sensing materials and gas concentration. Sensors need to be accurate, sensitive and selective. Two dimensional Nano sheet has successfully developed by various scientist around the globe. In this study we review in detail about various two dimensional Nano sheet structure and their application in sensing various gases in atmosphere.Nanosheet is an important segment of nanophysics it has attracted interest in the field of nanotechnology due to unique mechanical, thermal, chemical properties.

II.GRAPHENE SHEET

Graphene sheet has connected carbons in sp^2hybridization it is a crystalline allotrope of carbon and a zero band gap semiconductor, it's conduction band and valence band meet at Dirac point with the thinnest 2D material with largest surface area ,highest strength and stiffness. Graphene's fascinating properties make it very important material for various applications. Graphene properties could be improved by two different method by doping different atoms in pristine graphene or by decorating surface with atoms. Different group of scientist have reported Boron and nitrogen doped graphene, AL-doped graphene.

one of the research carried out by Zheng, et al for Graphene sheets doped by different elements acts as a sensor for sensing CO2 greenhouse gas present in the environment. In their work in graphene Nano sheets one carbon atom is doped by (B,N,P,Al). They studied the interaction of CO_2 gas molecules with this metal doped graphene~(MG).

From their studies they found Al-MG to be more sensitive to CO_2 gas molecules than other metal atoms. Wedong wang , et al studied the adsorption of CO molecules on doped graphene they investigated various suitable sites and orientation for CO adsorption on doped graphene. Pristine graphene can only physisoabsorb CO molecules, the interaction between CO and N-doped graphene has certain enhancement, but still belongs to physical adsorption.

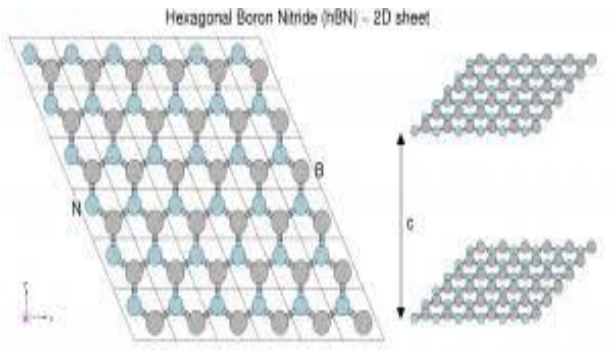


Al-doped graphene is strongly reactive to CO molecule, and Al-doped graphene will be a good candidate for sensing CO gas.

III. Boron Nitride Nano sheet

Boron nitride Nano sheet is a two-dimensional crystalline form of the hexagonal boron nitride (h-BN), which has a thickness of one to few atomic layer. BN Nano sheets consist of sp^2-conjugated boron and nitrogen atoms that form a honeycomb structure. They contain two different edges: armchair and zig-zag. The armchair edge consists of either boron or nitrogen atoms, while the zig-zag edge consists of alternating boron and nitrogen atoms. These 2D structures can stack on top of each other and are held by Van der Waals forces to form few-layer boron nitride Nano sheets. In these structures, the boron atoms of one sheet are positioned on top or below the nitrogen atoms due to electron-deficient nature of boron and electron-rich nature of nitrogen's. It is similar in geometry to its all-carbon analog graphene, but has very different chemical and electronic properties – contrary to the black and highly conducting graphene, BN Nano sheets are electrical insulators with a band gap of ~5.9 eV, and therefore appear white in color.

In particular, we propose to study the functionalization of Nano sheet by various effective functionalization methods and study its interaction with various molecules such as CO, CO_2, O_2, CH_4, etc.



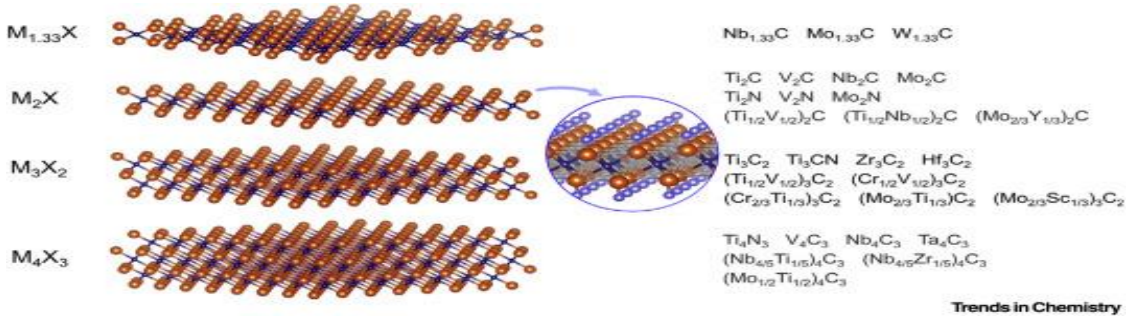
Hexagonal BN sheets possess polar B–N bonds and a wide band gap Zhang et al. have investigated adsorption mechanisms of carbon monoxide on BN sheets with various modifications, including Al doping, monovacancies, and Stone–Wales defects via density functional theory (DFT). It was found that the modified sheet is more sensitive than the pristine sheet for detecting CO molecules. In this work, by means of DFT calculations, we investigate the adsorption of N2O molecules on pristine and Al-doped BN sheets to verify whether or not the sheets can be used as gas sensors in environmental monitoring. Besides the interest in N2O as a greenhouse gas, there is also a need to monitor N2O gas. The adsorption of phosgene (COCl2) on pristine, Al- and Si-doped boron nitride Nano flakes (BNNFs) is studied using density functional theory calculations. The adsorption energies of the most stable complexes, formed from interaction between $COCl_2$ and the pristine, Al- and Si-doped BNNFs are −28.97, −78.71 and −171.60 kJ/mol at the M06-2X/6-31 + G* level of theory, respectively. It is found that COCl2 experiences a chemisorption interaction over the doped BNNFs, significantly altering its structure with respect to the gas-phase molecule. The $COCl_2$ adsorption can also induce a change in the HOMO–LUMO or SOMO–LUMO energy gap of the surface. In particular, the adsorption of $COCl_2$ is found to decrease the HOMO–LUMO energy gap of Al-doped BNNF by about 30%. It is suggested that the Al- or Si-doped BNNFs can be considered as a potential material for detecting toxic $COCl_2$.

IV. MXenes

A family of 2D transition metal carbides and nitrides, named as MXenes, is among the most recent 2D materials. The term MAX phases, a large group of ternary carbides and nitrides with hexagonal layered structure, reflect the chemical composition: $M_{n+1}X_nT_x$, where n = 1, 2, or 3 where "M" is an early transition metal, (Sc, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo,) "X" is carbon, nitrogen, or both and T_x stands for surface termination (for example OH, O, or F). About 70 different MXenes have been experimentally synthesized so far. The structures and properties of about dozens have been theoretically predicted. Such versatile chemistry of MXenes further allows their properties to be tailored for particular applications such as energy storage, electromagnetic interference shielding, water purification, gas and biosensors, lubrication, and catalysis. Some examples (Ti_2CTx_{16} , Ti_3CTx_{15} $Nb_4C_3Tx_{19}$).

Yu et al. using monolayer Ti_2CO_2 for NH_3 detection. Since only Ti_2CO_2 has semiconducting properties the Ti_2CO_2 was explored by the first-principles simulation. Based on O-functionalized monolayer Ti_2CO_2presenting the most stable structure, possible absorption sites of gas molecules were investigated to compute adsorption energy and charge transfer. As to NH_3, the strongest binding site was found where the N atom is located directly above the Ti atom in Ti_2CO_2 with −0.37eV adsorption energy and 0.174e charge transfer from NH3 to Ti_2CO_2 (In the density of state (DOS), the electronic charges are strongly overlapped, which causes orbital mixing and large charge transfer between NH_3 and Ti2CO2, suggesting chemisorption. Other gas molecules (H_2, CH_4, CO, CO_2, N_2, NO_2, and O_2) showed much lower gas adsorption energy and charge transfer than NH_3.

Junkaew et al. examined the adsorption behavior of gas molecules on four MXenes (M2C, M =Ti, V, Nb, Mo) and their O-terminated surfaces with the electronic charge properties. The O-terminated MXenes showed better selectivity toward particular gas species. For example, Ti_2CO_2 and Nb_2CO_2 absorb NH3 stronger than others, whereas Mo_2CO_2andV_2CO_2 preferto absorb NO.



V. METHODOLOGY

Theoretical simulation such as density functional theory (DFT)-based first-principles can be a very effective approach to analyze and predict gas sensing properties of materials. DFT-based first-principles simulation is a quantum mechanical method to investigate the electronic structure of materials using Schrödinger equation, from which physical properties are further to be predicted. In this theory, five basic physical constants were used; electron mass, electron charge, Planck constant, speed of light, and Boltzmann constant without any empirical constants. Recently, DFT has been upgraded to the density functional theory plus (DFT + U) method by adding the Hubbard U terms to the Hamiltonian, in which strong magnetic correlations between 5 f electrons were corrected for a more accurate description of structures and properties with a strong correlation system. Along with the DFT theory, the first-principles dynamics method combining the first-principles and the classical molecular dynamics methods has also been widely used. It became a popular tool for modeling collective interaction of atoms within classical mechanics with strong relevance to atomic coordination and their energy.

VI CONCLUSION

After reviewing various papers, we concluded that a two dimensional Nano sheet has tremendous scope and application in various fields of science. Two dimensional Nano sheets can be a potential candidate in gas sensing applications because of small size, large surface area Nano sheets can be very effective in selective absorption of various gas present in the atmosphere. There is a large scope for two dimensional Nano sheets in gas sensing applications which needs to explore in the coming future.

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