Chemiresistive Sensors for Environmental Monitoring

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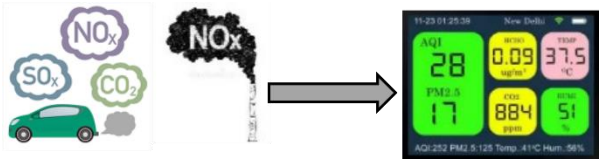
Abstract: Climate change is one of the major challenges in front of mankind. Air pollution is one of the reasons for climate change and hence, monitoring air quality followed by air pollution abatement is essential to preserve the environment. Air quality monitoring can be done efficiently by developing compact, low power, and low cost sensors for sensing the air pollutants. We have developed MoS_2 based sensors to detect NO_2 at room temperature. A compact and low cost electronic circuit was designed and assembled to replace the table top read out circuit and make the device portable. The assembled circuit board can also facilitate interfacing the existing sensors that are available in the market such as temperature, humidity, CO. This work provides a proof-of-concept of developing a portable resistive sensor for detecting some of the air pollutants.



Keywords: *Environmental Monitoring, Interfacing Electronics, NO_2 sensor, chemiresistive sensors, Air Quality Monitoring (AQM).*

1. Introduction

Climate change is affecting the lives of the global population in adverse manner [1]. This is caused primarily due to burning of fossil fuels and other anthropogenic activities because of which greenhouse gases and other pollutants get introduced to the environment. Central pollution control board (CPCB) India identified NO_2, NH_3, CO, Pb, O_3, SO_2, PM_{10}, and $PM_{2.5}$ as the important air pollutants that need continuous monitoring and constitute the air quality index

(AQI) of a particular area [2], [3], [4]. The safe limit of NO_2 and the effects on human health is as shown in Table. 1.

Table. 1. Effects of NO_2 on human health[5]

S. No	Concentration of NO_2 (ppm)	Time of Exposure	Effects
1	0.06-0.1	2-3 years	Increase in acute respiratory disease.
2	Up to 0.1	6 months	Increase in acute bronchitis in school children.
3	0-12	< 24 hrs.	Human olfactory threshold.
4	5	10 minutes	Increase airway resistant.
5	90	30 minutes	Pulmonary edema.

It can be observed from Table 1 that even a low concentration of the marked pollutants are unsafe to be exposed to. Also, it has been understood by governing bodies of multiple conutries that it is necessary to generate continuous and huge data of AQI of a particular area for a specified period to be able to take precautionary measures to combat air pollution. Hence, an effort towards engaging different societies and individual citizens in creating such databases have begun to be made. The success of these efforts heavily relies on availability of portable and low cost sensors that can accurately detect the air pollutants. Existing techniques like olfactory [6], spectroscopy [7], gas chromatography [8], and optical [9], suffer from poor accuracy, high power consumption, need for bulky and sophisticated laboratory instruments, high maintainance, and need of skilled expertise. Resistive sensors, being portable are emerging as suitable alternative to the continuous air quality monitoring [10].

Sensing material is the most important part of a resistive sensor. Several nanomaterials have already been explored for their resistive sensing capabilities but transition metal dichalcogenides (TMDs) owing to their tunable bandgaps, outstanding electronic properties and easy synthesis methods have fetched a lot of attention of the scientific community in the past few years. One of the TMDs is molybdenum di-sulphide (MoS_2). The molybdenumis a transition metal having the

atomic number 42 located in period 5 and group 6. Sulphur is a chalcogenide having the atomic number 16 located in period 3 and group 16.

2. Work Done (Hardware)

2.1. MoS_2 nanoflakes synthesis

The 2D MoS_2 nanoflakes were synthesized by the liquid-phase exfoliation method as has also been reported by our group [11]. Briefly, 45% EtOH was prepared by adding 45 mL of ethanol to 55 mL of DI water. Then 180 mg of MoS_2 bulk powder was added to the solution and ultrasonicated for 12 hours at room temperature. The ultrasonicated solution has been centrifuged at 5000 rpm for 10 min. Then the light green in colour supernatant was collected and taken for further characterizations and the device fabrication.

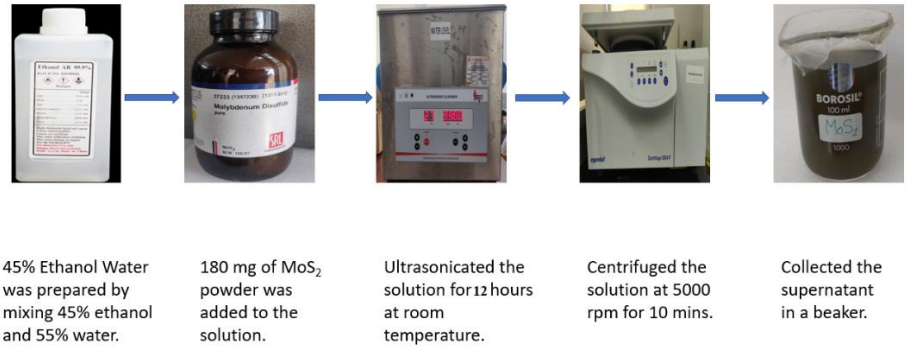


Fig. 1. Synthesis procedure of MoS_2 nanoflakes.

2.2. MoS_2 Nanoflakes characterization

The thickness of the synthesized nanomaterials was studied using a Park Systems NX 10 atomic force microscope (AFM). The average thicknesses of MoS_2 nanoflakes were found to be 8 nm (Fig. 2 (a)). The morphology of the MoS_2 sample was examined using Carl Zeiss Gemini 300 field emission scanning electron microscopy (FESEM) and found to be nanoflakes of size 3.61 µm (Fig. 2(b)). The bandgap of the synthesized MoS_2 sample was ascertained through the Tauc plots derived from the UV-Vis spectra of the samples (Fig. 2 (c, d)). The bandgap was found to be 1.71 eV, which confirms the semiconducting nature of the sample.

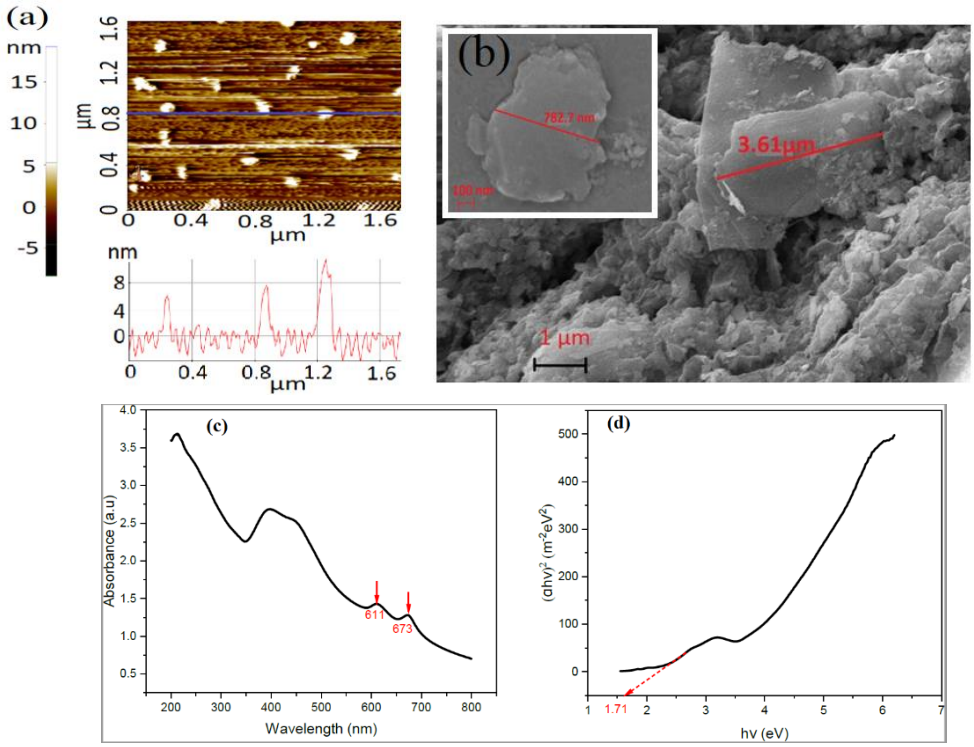


Fig. 2. (a) AFM image (b) SEM image (c) Absorption spectra (d) Tauc plot of Mo_2C MoS_2 sample.

2.3. Sensor fabrication and testing

The synthesized MoS_2 nanoflakes were drop casted onto an interdigitated electrode (IDE) to get the sensor device. The details and respective dimensions of the IDE are shown in Fig. 3 (a).

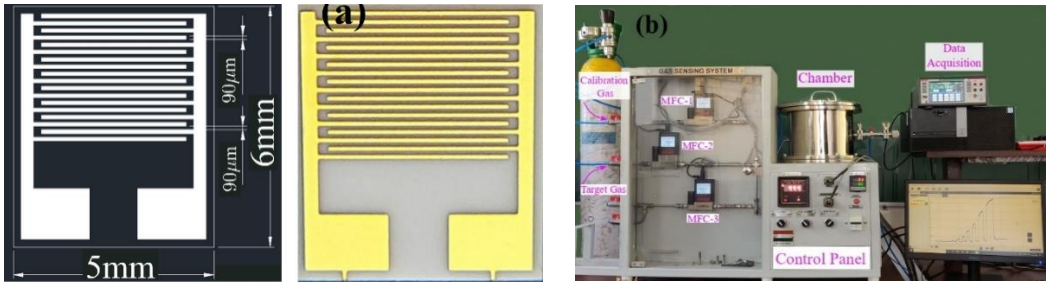


Fig. 3. Schematic of the (a) IDE and (b) Gas sensing set-up

These MoS_2-coated IDE was probed inside an airtight stainless-steel chamber of the gas sensing test setup (Fig. 3 (b)). The gas sensing setup comprises mass flow controllers (MFCs) to maintain the concentrations of the analytes inside the chamber, a data acquisition system (Keithley 6510) through which the resistance of the sensing layer was continuously acquired and stored at an interval of 1 s on a computer. The gas tests started by purging the 100 standard cubic centimetres

per minute (sccm) of calibration gas (dry air) for around an hour till the baseline resistance of the sensor was stable. Next, different concentrations of the target gases viz. NO_2, NH_3, and 2-NT were introduced into the chamber individually through the second MFC. This was done by changing the proportion of the flow rates of the two MFCs (one passing the dry air and other passing the target gas).

2.4. Sensing Results

The response of the sensor was calculated using the relation shown in equation (1)

$$Response(\%) = \frac{|R_{tar} - R_{cal}|}{R_{cal}} \times 100 \quad \text{----------} \quad (1)$$

Where R_{tar} is the resistance of the sensors in the presence of the targeted vapors and R_{cal} is the baseline resistance which was observed when the vapors were not the proximity of the devices. The comparative response of the MoS_2 sensing layer for different analytes was as shown in Fig. 4. The response was found to be highest for NO_2 and was around 41% at 150 ppm.

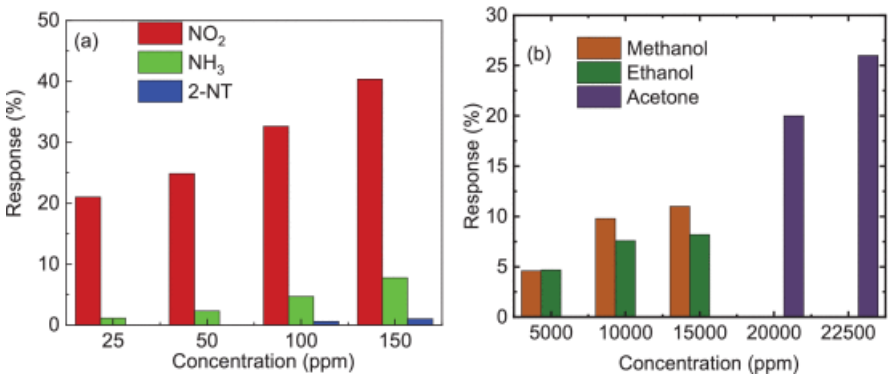


Fig. 4. Comparative response of MoS_2 sensors for (a) 25-150 ppm of NO_2, NH_3, 2-NT (b) higher concentrations of CH3OH, C2H5OH, and (CH3)2CO at 25 °C.

2.5. Interfacing Electronics

Next, in an attempt to develop a portable prototype of the resistive sensor, efforts to replace the table top DAQ and personal computer was made to make the system compact and low power consuming. We have designed a PCB level circuit to interface with the IDE based sensor and display the concentration levels of the pollutants of interest, the ambient temperature and humidity levels (Fig. 5 and 6). The gas sensor interface board uses ATmega 328P microcontroller

to read and display the parameters of the sensor modules. The microcontroller was connected with 0.96 inch I2C OLED to display the parameters. The circuit board uses a 3.7 V 1050 mAH Lithium polymer rechargeable battery to power all the peripherals and microcontroller. As 3.7V may not be sufficient and cause fluctuation in the voltage if we take voltage directly from the battery, a DC-DC boost converter was used to regulate and boost the voltage to 5 V supply.

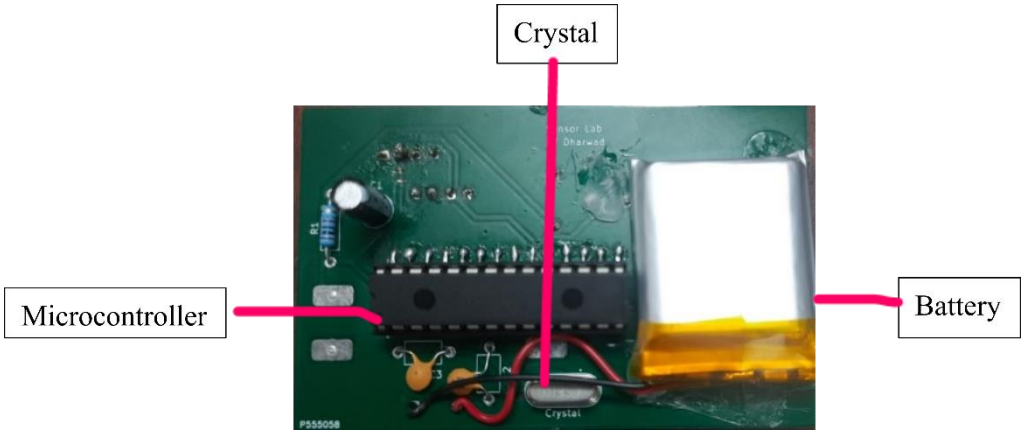


Fig. 5. Gas sensor Interfacing board (Top View)

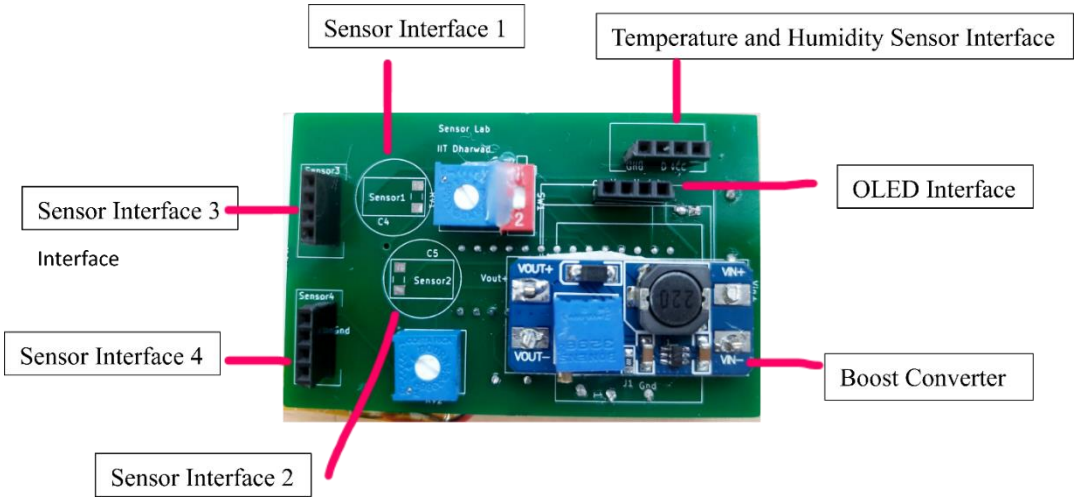


Fig. 6. Gas sensor Interfacing board (Bottom View)

The circuit board facilitates interfacing of temperature and humidity sensor and four more slots for sensor modules. Two of the four slots are meant for the inter digitated electrode (IDE) based sensors and the other for 4 pin based MQ sensors that are commercially available. The components and their uses are as listed in the Table. 2.

Table. 2. Hardware components that were used and their uses

Component/Device	Usage
AT mega 328P (IC1)	Microcontroller to read and display the parameters such as Temperature, Humidity, and NO_2 gas concentration.
Crystal (Y1)	To generate clock
Capacitors, Resistors (R1, C1, C2, C3)	Add On components to make AT mega works fine.
Potentiometers (RV1,RV2)	To calibrate Sensor 1 and Sensor 2 respectively
Battery Cell (BT1)	3.7V 1050mAH Lithium Polymer Rechargeable Battery
Dip Switch (sw1)	To power On the Gas Sensor Interface Board
MT 3608 (Power Block (J1))	Boost Converter dc-dc (2v-24v)/ 2A
DHT 22 (IC2)	Temperature and Humidity Sensor Module
SSD 1306 (Brd1)	2.44 cm (0.96 Inch) I2C/IIC 4pin OLED Display (Module BLUE)
Sensor 1 (C4)	Slot 1 meant for laboratory made IDE based sensor
Sensor 2 (C5)	Slot 2 meant for laboratory made IDE based sensor
Sensor 3 (IC 3)	4 pin based slot 1 meant for MQ based sensors
Sensor 4 (IC 4)	4 pin based slot 2 meant for MQ based sensors

3. Software Architecture

The gas sensor interfacing board was designed using KiCAD EDA tool [12]. The schematics and the gas sensing board is as shown in Fig. 7. The PCB layout and the Gerber files were generated and the PCB was printed through PCB Power Market India, Gujarat. Arduino IDE 1.8.19 was used to program and import the code into the AT mega 328P microcontroller. The software and their uses are listed in the Table. 3.

Table. 3. Software that were used for the project

Component/Device	Usage
Arduino IDE 1.8.19	Integrated Development Environment to give commands to AT mega 328P microcontroller.
KiCAD EDA	To design the Gas Sensor Interface Board PCB

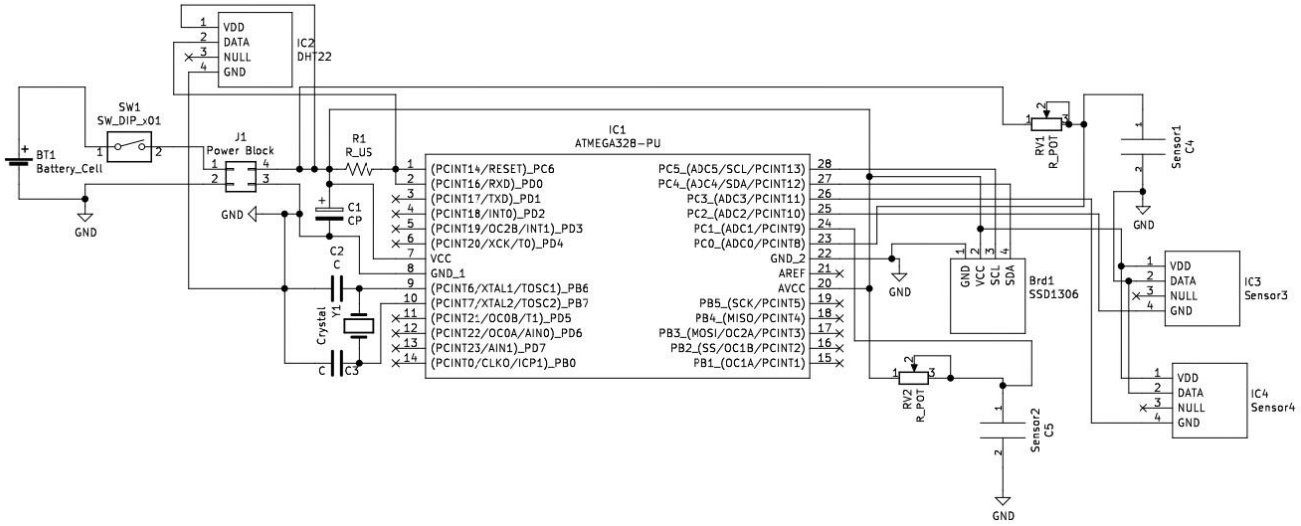


Fig. 7. Schematic of the gas sensing interfacing board

4. Challenges encountered and the approach to address the challenges.

- The response of the MoS2 sensor was reduced with time. The response was maintained above 90% of the original response for 21 days. Hence lifetime of the sensor has to be improved. Currently, we are working on composites to increase the lifetime of the sensor.
- While designing the PCB, we made the components of the through-hole. It would be better to have SMD components to look PCB thinner and more compact. We are developing the next PCB with advanced SMD components and additional microheaters.

5. Testing and Evaluation Results.

The MoS_2 nanoflakes coated IDE was connected to the sensor interface 1 of the circuit board and DHT 22 (Temperature and the humidity sensor) was mounted on the temperature and the humidity interface slot. A 0.96 inch 128×64 OLED display was mounted on the OLED slot of the board. The programmed ATmega328P IC was mounted on the IC slot and the peripherals were powered. The gas sensor interface board was kept in a air tight chamber which was defined and fabricated using 3 D printing, to carry out the gas test experiments. 100 ppm of NO_2 was introduced into the chamber through the mass flow controllers (MFCs) and the display was

device was observed to show a fluctuating value between 80 to 95 ppm. In addition to the NO_2, temperature (26º C) and humidity (54 % RH) were also displayed on OLED as shown in Fig. 8.

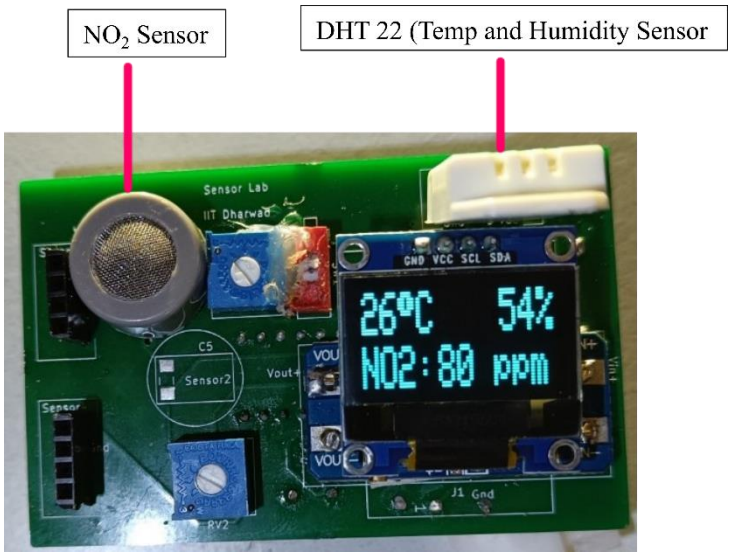


Fig. 8. Image of working of the gas sensing interfacing board

6. Pointer to the software repository and code

https://github.com/Sensorguru/Environmental-Sensors-Competition

7. Avenues for future work to improve the solution

So far, we have developed (a) MoS_2 based chemiresistive sensor for the detection of NO_2 and (b) gas sensor interfacing board as a portable alternative to the table top readout instruments. Though the MoS_2 sensor showing good accuracy, the base line stability was poor and need to go for metal oxides to maintain the stability. Generally, the metal oxides work at high temperatures (100ºC - 300ºC). So, a provision in the gas sensor interfacing board to add micro heater and closed loop system to maintain the constant temperature is to be created.

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