



# Highly selective ammonia gas sensor using Ga<sub>2</sub>O<sub>3</sub>/MoO<sub>3</sub> nanocomposite at ambient atmospheric conditions

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## ABSTRACT

The β-Ga<sub>2</sub>O<sub>3</sub> and MoO<sub>3</sub> nanocomposite with varying concentration of MoO<sub>3</sub> at 2.5 %, 5 % and 7.5 % were synthesized through hydrothermal method followed by physical mixing. Obtained nanocomposites were characterized to study its morphological, structural and optical properties through XRD, SEM, EDAX, TEM, XPS and UV–Visible spectroscopy. Surface area analysis was done using BET analysis method. Ammonia (NH<sub>3</sub>) sensing studies were conducted at room temperature for synthesized composites. Nanocomposite with increased MoO<sub>3</sub> concentration showed increase in the response towards ammonia detection and highest response of 420.12 % for 100 ppm NH<sub>3</sub> at relative humidity (RH) of 69 % with response and recovery time of 53.75 s and 27.44 s respectively. Studies on humidity dependent sensing have been conducted for the same synthesized nanocomposites. The enhanced sensing of NH<sub>3</sub> in room temperature is attributed to sensing mechanism mediated by the adsorbed humidity and oxygen on the surface of the sensing material in addition to the chemical and electronic sensitization effects.

## 1. Introduction

Ammonia (NH<sub>3</sub>) is a colorless gas with a pungent odor, widely recognized for its toxic and corrosive properties. The detection of ammonia (NH<sub>3</sub>) is critical in various fields, including environmental monitoring, agriculture, and industrial safety, due to its toxicity and potential health hazards [1,2]. Exposure to ammonia can lead to a range of acute and chronic health effects, primarily affecting the respiratory system. Short-term exposure to high concentrations of ammonia can cause severe irritation of the eyes, nose, and throat, resulting in symptoms such as coughing, wheezing and difficulty breathing [3,4]. In more severe cases, ammonia exposure can lead to chemical burns on the skin and eyes, as well as pulmonary edema, which is a potentially life-threatening condition characterized by fluid accumulation in the lungs [5–7]. Since 16–28 % of the ammonia gas concentration in the atmosphere is thought to be lethal, proper monitoring of the gas concentration is essential for a healthy environment [8,9]. Therefore, it is important for both academia and industry to create effective gas sensors that can detect NH<sub>3</sub> at room temperature at lower concentrations (100 ppm). Typically, a variety of techniques were used to detect hazardous gases, such as gas chromatography, optical spectroscopy,

electrochemical methods, and semiconductors [10–13]. Because of their sophisticated sensing response to different gases, transition metal oxide semiconductor gas sensors were shown to be more efficient and cost-effective than other methods [14–16].

Among the other transparent conducting materials, gallium oxide (Ga<sub>2</sub>O<sub>3</sub>) has gathered significant attention in the field of gas sensing due to its remarkable properties and versatility. It has wide bandgap (ranging from approximately 4.2 to 5.2 eV) and depending on its crystalline phase, Ga<sub>2</sub>O<sub>3</sub> exhibits excellent electrical and optical characteristics that make it suitable for various sensing applications [17,18]. The β-Ga<sub>2</sub>O<sub>3</sub> is the most stable phase, is particularly noteworthy for its potential in high-temperature gas sensing, as it maintains structural integrity and functionality even in harsh environments [19,20]. The sensitivity of Ga<sub>2</sub>O<sub>3</sub> to various gases, including oxygen, ammonia, and nitrogen dioxide, is a key factor that underpins its role as a gas sensor. This sensitivity can be enhanced through the engineering of defects and the introduction of dopants, which modify the electronic properties of the material. For instance, doping Ga<sub>2</sub>O<sub>3</sub> with tin has been shown to improve its conductivity and gas sensing performance, allowing for more accurate detection of target gases [21]. Furthermore, the nano structuring of Ga<sub>2</sub>O<sub>3</sub>, such as the formation of nanowires or

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nanoparticles, increases the surface area-to-volume ratio, thereby enhancing the interaction with gas molecules and improving sensor response times [22,23]. **Recent advancements in metal oxide-based gas sensors have demonstrated that surface modification, hetero-structure formation, and humidity-assisted adsorption processes can significantly enhance gas sensing performance [24–27].** The composite formation of  $\text{Ga}_2\text{O}_3$  with other materials can lead to synergistic effects that further enhance gas sensing capabilities. For example, composites of  $\text{Ga}_2\text{O}_3$  with MWCNTs or other metal oxides can result in improved selectivity and sensitivity, making them suitable for detecting low concentrations of gases [28–30].

$\text{MoO}_3$ , on the other hand, is recognized for its versatile crystalline phases and high reactivity, which contribute to its effectiveness in gas sensing [27]. A variety of gases, such as nitrogen dioxide, ammonia, and volatile organic compounds (VOCs), can be detected using  $\text{MoO}_3$  because to its exceptional electrical conductivity and stability [31–33]. The material is more applicable in real-world situations where energy efficiency is crucial because of its capacity to operate efficiently at comparatively low operating temperatures [34]. Abdullah et al., has fabricated the  $\text{SnO}_2$  coated  $\text{Ga}_2\text{O}_3$  nanobelt for  $\text{H}_2$  gas sensor. According to the obtained results, authors concludes that the  $\text{SnO}_2$ -coated  $\text{Ga}_2\text{O}_3$  gas sensor operates at room temperature up to  $200^\circ\text{C}$  and has a reversible response to a wide range of  $\text{H}_2$  concentrations (33–1000 ppm) with low power consumption [35].

The integration of  $\text{Ga}_2\text{O}_3$  and  $\text{MoO}_3$  into a single nanocomposite represents a promising advancement in the field of gas sensor technology, particularly for the detection of ammonia ( $\text{NH}_3$ ). Both materials exhibit unique properties that, when combined, can enhance the sensitivity and selectivity of gas sensors. The gas sensing mechanism of  $\text{Ga}_2\text{O}_3$  and  $\text{MoO}_3$  is primarily based on their interaction with gas molecules, leading to changes in their electrical resistance. When exposed to  $\text{NH}_3$ , these metal oxides undergo surface reactions that alter their charge carrier concentration, resulting in measurable changes in conductivity [36,37]. **The Table 1 presents the list of different chemiresistive  $\text{NH}_3$  gas sensors fabricated using different nanoparticles along with their sensing parameters.**

In the present work the hydrothermally synthesized  $\beta\text{-Ga}_2\text{O}_3$  along with the different percentages of  $\text{MoO}_3$  (2.5 %, 5 % and 7.5 %) was used to study the gas sensing property towards  $\text{NH}_3$  gas. The composite material was also tested under different relative humidity (RH) condition under room temperature (RT).

## 2. Experimental details

### 2.1. Synthesis of $\text{Ga}_2\text{O}_3/\text{MoO}_3$ nanocomposite

The hydrothermal process was used to synthesize the  $\text{Ga}_2\text{O}_3$  and  $\text{MoO}_3$  nanoparticles. First, 20 ml of deionized (DI) water is used to dissolve 0.51 g of Gallium (III) Nitrate Hydrate ( $\text{Ga}(\text{NO}_3)_3 \cdot n\text{H}_2\text{O}$ ) and 0.116 g of Sodium Dodecyl Sulphate (SDS), which are then agitated for 20 min. Using 1 N NaOH (0.4 g NaOH in 10 ml of nano-pure water), the

pH of the above-prepared solution was kept at 10 while stirring continuously for an hour. After that, the mixture was put into a Teflon-coated autoclave and heated to  $120^\circ\text{C}$  for 12 h, producing a white precipitate of gallium oxide hydroxide ( $\text{GaOOH}$ ). The sample was then cooled and repeatedly cleaned with alcohol and DI water before being dried for five hours at  $70^\circ\text{C}$  in an oven. The  $\beta\text{-Ga}_2\text{O}_3$  nanoparticles were subsequently created by calcining the resultant powder for three hours at  $1000^\circ\text{C}$ .

In order to synthesize  $\text{MoO}_3$  nanoparticles, 0.392 g of Ammonium Molybdate ( $(\text{NH}_4)_2\text{MoO}_4$ ) was dissolved in 10 ml of DI water. The solution was vigorously stirred for 15 min, and then 5 ml of concentrated  $\text{HNO}_3$  was added and stirred for 1 h. The solution is transferred to autoclave at  $180^\circ\text{C}$  for 24 h. Collected and washed product was calcinated at  $500^\circ\text{C}$  for 2 h to obtain  $\text{MoO}_3$  nanoparticles.

The obtained pristine materials were mixed in different weight ratio of 2.5 %, 5 % and 7.5 % by grinding them in mortar pestle to get the desired composite material.

### 2.2. Gas sensing measurements

Detailed fabrication process of gas sensor is described in our previous work [34]. The obtained nanocomposites along with the  $50\ \mu\text{l}$  NMP is mixed well and coated on IDEs as shown in Fig. 1. The gas sensing measurements were taken with the help of Keysight B2912A instrument in indigenously built set up for measuring sensing results. Synthetic air is used as a reference and diluting gas throughout the experiment.

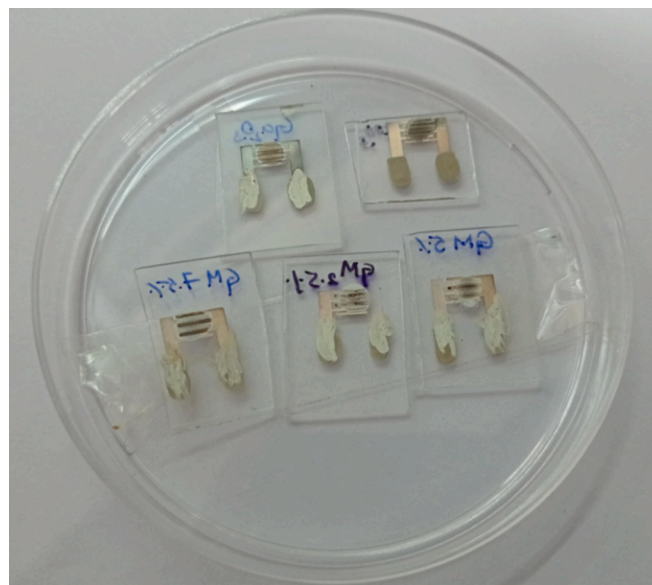


Fig. 1.  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  nanocomposite coated on Au IDEs.

**Table 1**  
Chemiresistive  $\text{NH}_3$  gas sensor for different materials.

Sensor Material	Working temperature ( $^\circ\text{C}$ )	Sensing response	Response time ( $T_{\text{res}}$ ) sec	Recovery time ( $T_{\text{rec}}$ ) sec	$\text{NH}_3$ concentration (ppm)	References
$\text{Ga}_2\text{O}_3/\text{MoO}_3$	RT	420.12 %	53.75	27.44	100	Present work
ZnO	RT	52 %	49	59	50	[38]
h- $\text{MoO}_3$	200	36 %	230	267	5	[39]
$\text{Ga}_2\text{O}_3$	RT	160 %	42	30	100	[40]
PtNps@ $\text{TiO}_2\text{-WO}_3$	RT	92.28	23	8	50	[41]
Polypyrrole/zinc-porphyrin	RT	104.3 %	42	223	1000	[42]
Sn doped $\text{Ga}_2\text{O}_3$	RT	274.98 %	–	–	200	[43]
$\text{MoS}_2/\text{WO}_3$	200	207 %	80	70	200	[44]
$\text{In}_2\text{O}_3/\text{Ga}_2\text{O}_3$	400	238 %	18	90	200	[45]
ZnO/rGO	RT	10.96	153	79	50	[46]

### 3. Results and discussion

#### 3.1. XRD analysis

The Fig. 2 shows the XRD result of synthesized nanocomposites which are recorded using Rigaku-miniflex with copper source of 1.5406 Å wavelength. The crystallinity and homogeneity of the synthesized nanoparticles are confirmed by the strong and evident peaks in the pristine  $\text{Ga}_2\text{O}_3$  and  $\text{MoO}_3$  nanoparticles XRD patterns. The XRD data is analyzed using the HighScore Plus tool for all the pristine and nanocomposite samples. It was confirmed that the produced  $\text{Ga}_2\text{O}_3$  nanoparticles matched ICDD No. 00-041-1103 and exhibited a stable monoclinic crystal structure [40]. The pristine  $\text{MoO}_3$  has hexagonal crystal structure that matches the ICDD No. 00-021-0569 with lattice constants  $a = 10.5310 \text{ Å}$ ,  $b = 10.5310 \text{ Å}$ ,  $c = 14.8760 \text{ Å}$ ,  $\alpha = \beta = 90^\circ$  and  $\gamma = 120^\circ$  [47]. The nanocomposite with different concentration of  $\text{MoO}_3$  showed the prominent peak of  $\text{MoO}_3$  peak around  $25.8^\circ$  (marked as \* in composite XRD graph) confirming the presence of  $\text{MoO}_3$  and the intensity of this peak increases with the increase in the concentration of  $\text{MoO}_3$ . The crystallite size of the pristine and nanocomposite samples was calculated using Scherrer formula. It was found to be 22.86 nm, 38.87 nm for pristine  $\text{Ga}_2\text{O}_3$  and  $\text{MoO}_3$  material respectively. The composite crystallite size for 2.5 %, 5 % and 7.5 %  $\text{MoO}_3/\text{Ga}_2\text{O}_3$  composite was 39.56, 39.24 and 35.6 nm respectively.

#### 3.2. Raman analysis

Raman spectroscopy was used to explore the structural characteristics of pristine  $\text{Ga}_2\text{O}_3$ ,  $\text{MoO}_3$  and their combined  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  nanocomposite. The Fig. 3 displays the Raman spectrum of pristine and nanocomposite material. Raman spectrum of pristine  $\text{Ga}_2\text{O}_3$  showed several peaks mainly in the  $140\text{--}750 \text{ cm}^{-1}$  range, consistent with its monoclinic  $\beta$ -phase structure [48]. For  $\text{MoO}_3$ , the distinct Raman peaks at  $123, 179, 222, 252, 399, 512, 689, 901$ , and  $990 \text{ cm}^{-1}$  were observed. These peaks reflect the well-known vibrational features of the  $\alpha$ - $\text{MoO}_3$  phase [49]. The lower wavenumber peaks ( $123\text{--}252 \text{ cm}^{-1}$ ) are typically associated with lattice vibrations and bending of O–Mo–O bonds, while the strong peak at  $990 \text{ cm}^{-1}$  corresponds to the stretching of terminal Mo=O bonds. Peaks at  $689$  and  $901 \text{ cm}^{-1}$  are linked to the vibrations of bridging oxygen atoms between Mo centres [50]. The peaks corresponding to  $\text{MoO}_3$  are marked \* in the  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  composite Raman spectra. When both oxides were combined in the  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  nanocomposite, a slight shift in the peak position can be noticed. These changes suggest that there are interactions between  $\text{Ga}_2\text{O}_3$  and  $\text{MoO}_3$  at the structural level, possibly due to lattice strain or chemical bonding at the interface [51,52].

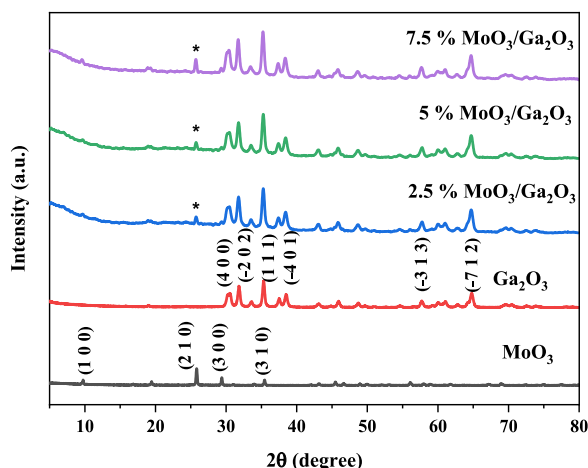


Fig. 2. XRD pattern of pristine  $\text{Ga}_2\text{O}_3$ ,  $\text{MoO}_3$  and  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  nanocomposite.

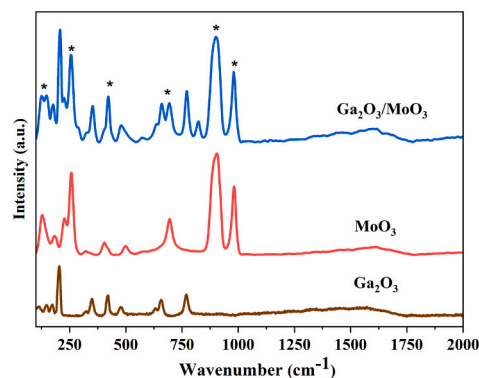


Fig. 3. Raman spectra of pristine  $\text{Ga}_2\text{O}_3$ ,  $\text{MoO}_3$  and  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  nanocomposite.

#### 3.3. Morphological and elemental analysis

The Fig. 4 shows the surface morphology of the synthesized  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  nanocomposite examined using SEM at various magnifications. The micrographs shed light on surface texture, particle dispersion, and nanostructure of the material. The SEM analysis confirms that the  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  nanocomposite consists of well-defined, densely packed nanorod like structures with uniform morphology. The porous texture and high surface area observed at lower magnifications are likely beneficial for gas-sensing applications [53]. The hierarchical structuring observed at different magnifications suggests that the synthesis approach effectively promoted the growth of nanostructured features with strong interfacial interactions between  $\text{Ga}_2\text{O}_3$  and  $\text{MoO}_3$ .

The compositional analysis of  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  sample was performed using the EDS technique as shown in Fig. 5. The figure shows that the sample shows the peak corresponding to Ga, Mo and O with no other additional peaks indicating the purity and it is compatible with the XRD results. Further Fig. 6 presents the EDS mapping for the sample with 7.5 %  $\text{MoO}_3$ , showing the distribution of Ga, O and Mo.

The Fig. 7(a–f) exhibit the TEM images of  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  nanocomposite. The images in Fig. 7(a–c) shows the arrangement of rod like  $\text{Ga}_2\text{O}_3$  and  $\text{MoO}_3$  particles in the nanocomposite. A distinguished lattice fringes measuring  $0.628$  and  $0.372 \text{ nm}$  were observed in the Fig. 7(d–e) corresponding to  $\text{Ga}_2\text{O}_3$  and  $\text{MoO}_3$  respectively. The selective area electron diffraction (SAED) pattern of the synthesized sample is shown in Fig. 7f and it is in good agreement with the corresponding XRD pattern. The effective synthesis of a well-crystallized  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  nanocomposite with clear grain boundaries and high structural integrity is confirmed by TEM images.

#### 3.4. Optical analysis

The UV–Vis absorption spectra of  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  nanocomposites with varying  $\text{MoO}_3$  weight percentages 2.5 %, 5 %, and 7.5 % are displayed in Fig. 8(a). The UV–Vis absorption spectra of  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  nanocomposites demonstrate notable variations in their optical absorption behaviour. Wide bandgap semiconductors are characterized by a prominent absorption edge in the ultraviolet spectrum, which is present in all samples. However, a significant redshift in the absorption edge is seen as the  $\text{MoO}_3$  content increases. The 7.5 %  $\text{MoO}_3$  sample has the most noticeable red-shift, while the 2.5 % sample displays the absorption edge at a shorter wavelength. This shift indicates that the presence of more  $\text{MoO}_3$  introduces changes in the electronic structure, possibly due to stronger interaction between the  $\text{Ga}_2\text{O}_3$  and  $\text{MoO}_3$  phases or the formation of defect states [54]. Additionally, the increase in overall absorbance with higher  $\text{MoO}_3$  content suggests better light absorption capabilities, which could enhance the material's performance in applications like photocatalysis or sensing [55].



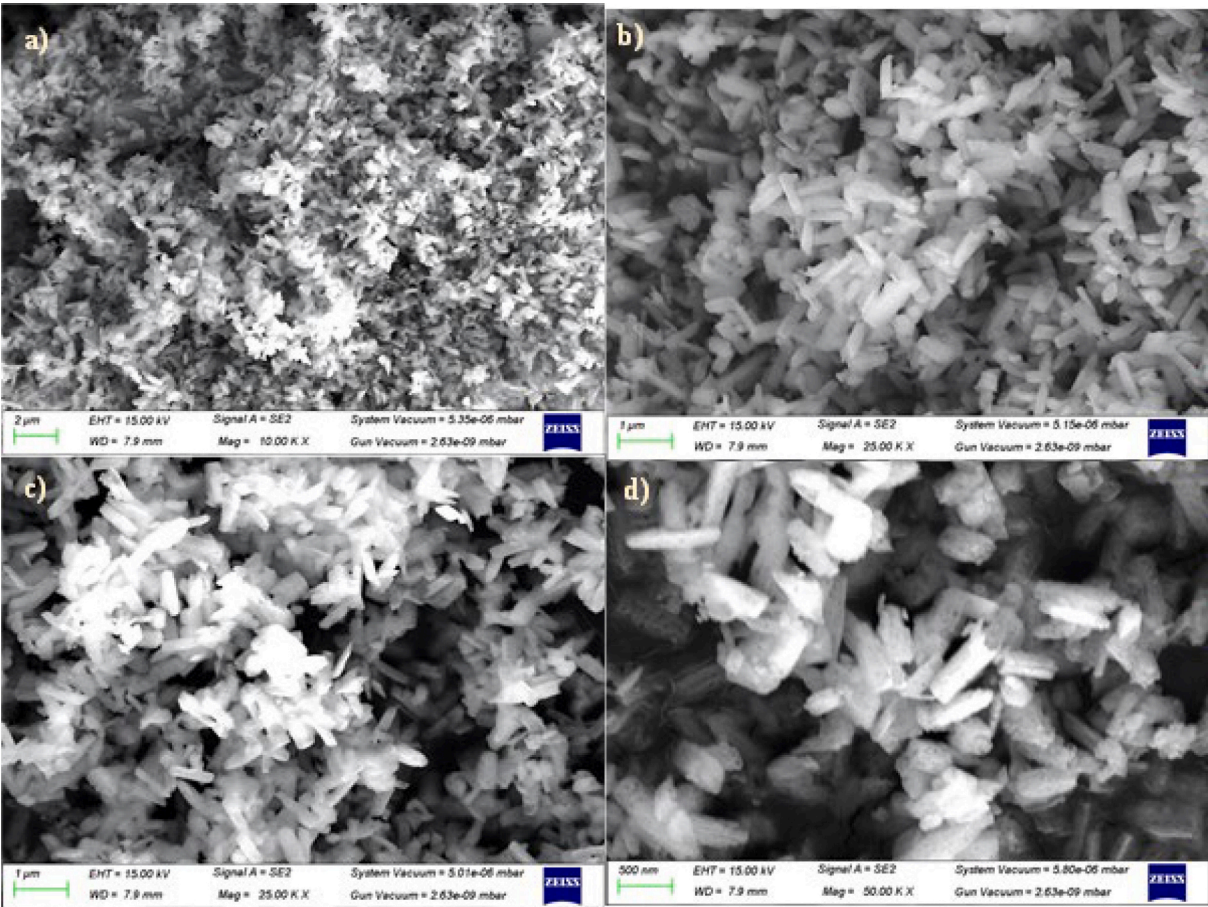


Fig. 4. SEM images of  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  nanocomposite.

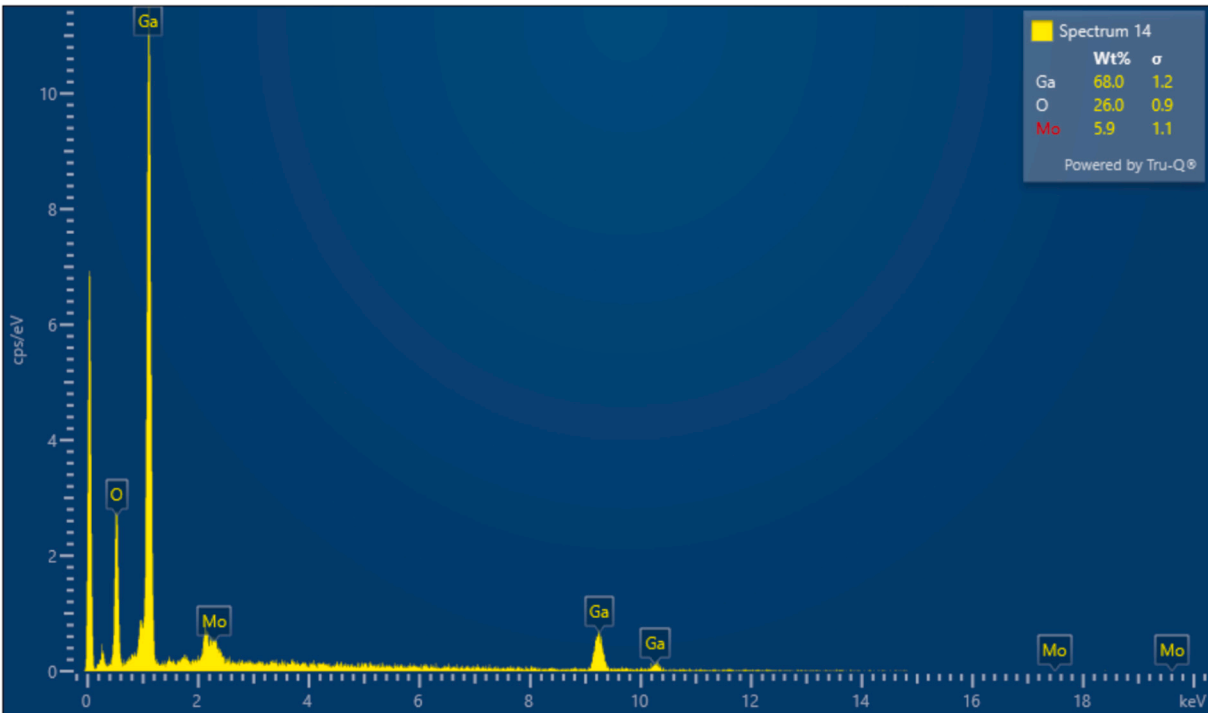


Fig. 5. EDS spectrum of 7.5 %  $\text{MoO}_3/\text{Ga}_2\text{O}_3$  nanocomposite.



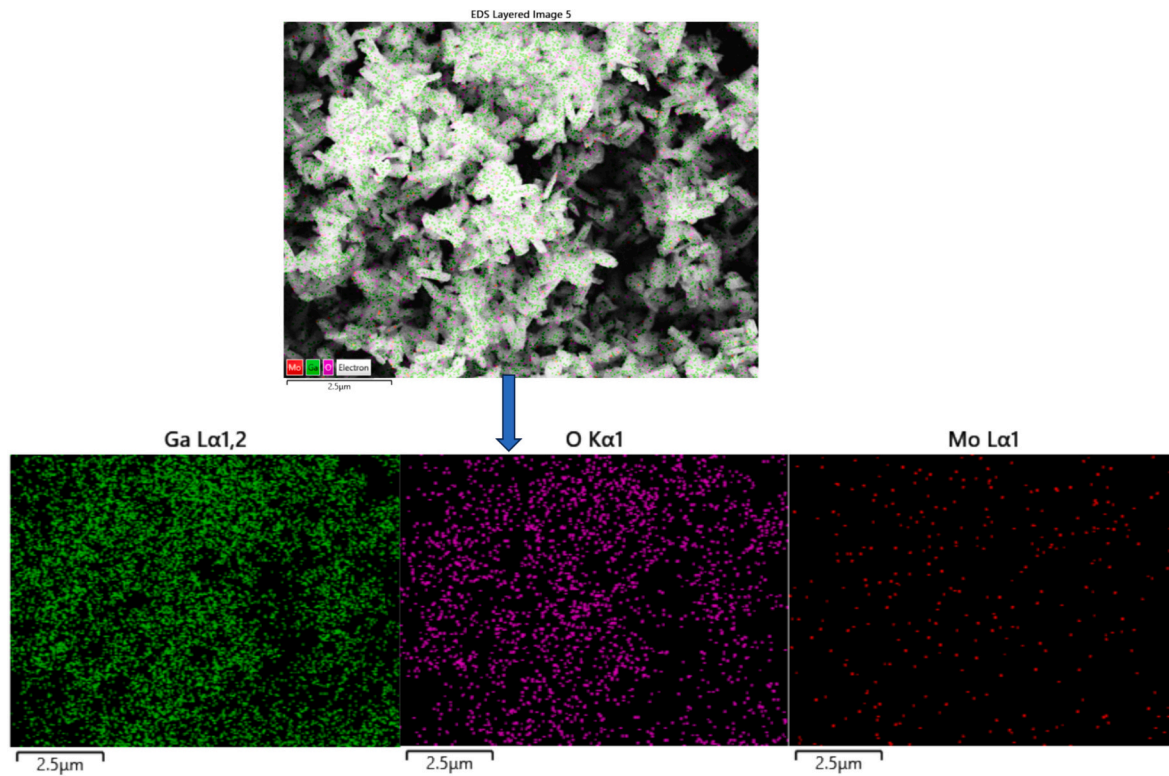


Fig. 6. EDS Elemental mapping of 7.5 %  $\text{MoO}_3/\text{Ga}_2\text{O}_3$  nanocomposite.

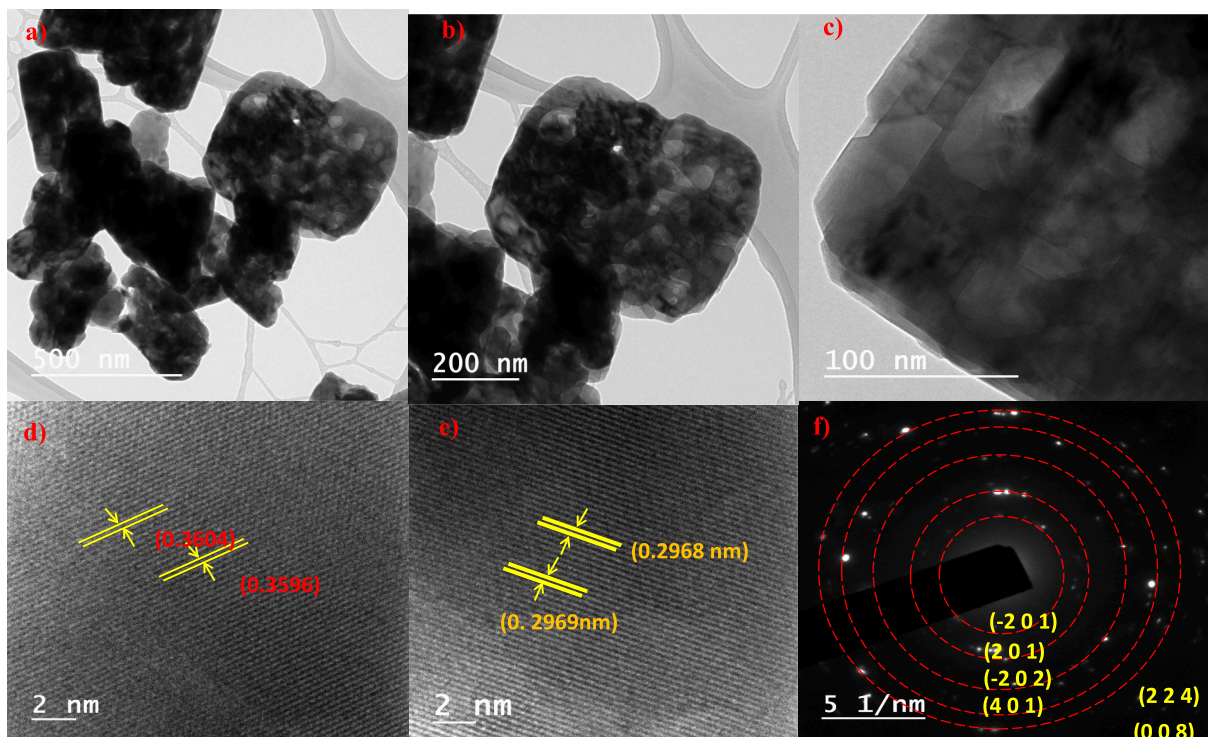


Fig. 7. TEM images of  $\text{Ga}_2\text{O}_3/\text{MoO}_3$  nanocomposite.

The bandgap energy was calculated by means of the Kubelka-Munk (K-M) algorithm and plot is given in Fig. 8(b). The bandgap energy of the composites was 2.86 eV, 2.63 eV and 2.41 eV for 2.5 %, 5 % and 7.5 %  $\text{MoO}_3$  respectively. The 2.5 wt%  $\text{MoO}_3$  sample shows the highest bandgap energy, while the 7.5 wt% sample exhibits the lowest. This red

shift in the absorption edge suggests enhanced electronic interaction between  $\text{Ga}_2\text{O}_3$  and  $\text{MoO}_3$ , possibly due to the introduction of defect states or modified electronic structure at the interface [56]. Based on these results, it is possible to effectively customize the optical characteristics of the composite for certain functional applications by adjusting

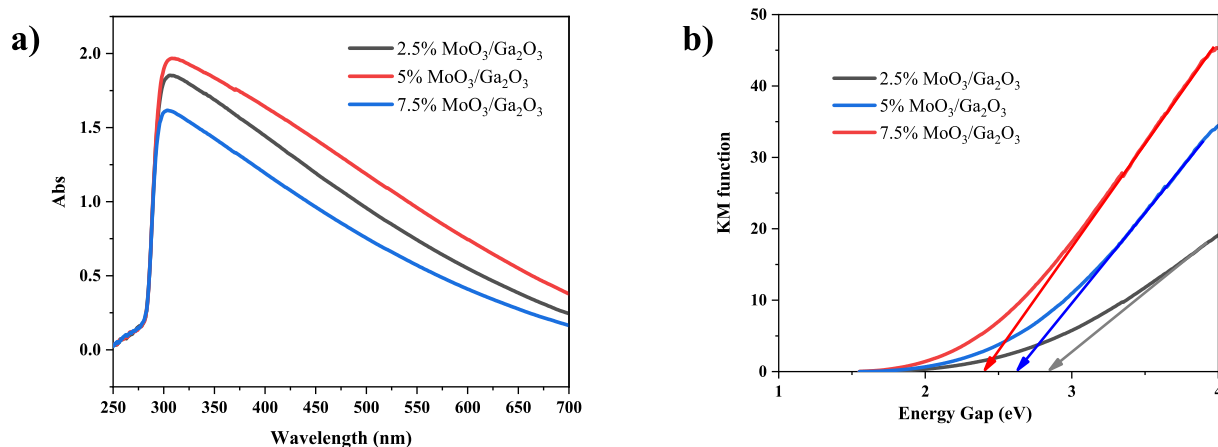


Fig. 8. a) Absorption spectra b) KM plot of Ga<sub>2</sub>O<sub>3</sub>/MoO<sub>3</sub> nanocomposite with 2.5 %, 5 % and 7.5 % MoO<sub>3</sub>.

the concentration of MoO<sub>3</sub> in the composite.

### 3.5. XPS studies

The Fig. 9 shows the results of XPS characterisation, which was utilized to determine the composition and chemical bonding states of the composite under investigation. The composition with 7.5 % MoO<sub>3</sub>/

Ga<sub>2</sub>O<sub>3</sub> XPS survey spectra is presented in Fig. 9(a), where photoelectron spectra with Ga (3d, 3p, 3s, 2p and LMM), Mo (3d), O (2s, 1s), and C (1s) peaks have been identified [57,58].

The C—C bond at 284.3 eV from unexpected surface contamination serves as the calibration for all binding energies [47]. The Fig. 9(b) display the O—Ga bond for lattice O<sup>2-</sup> ions is represented by the core level of O 1s, which is located at 532.4 eV [59,60]. The peak at 21.5 eV

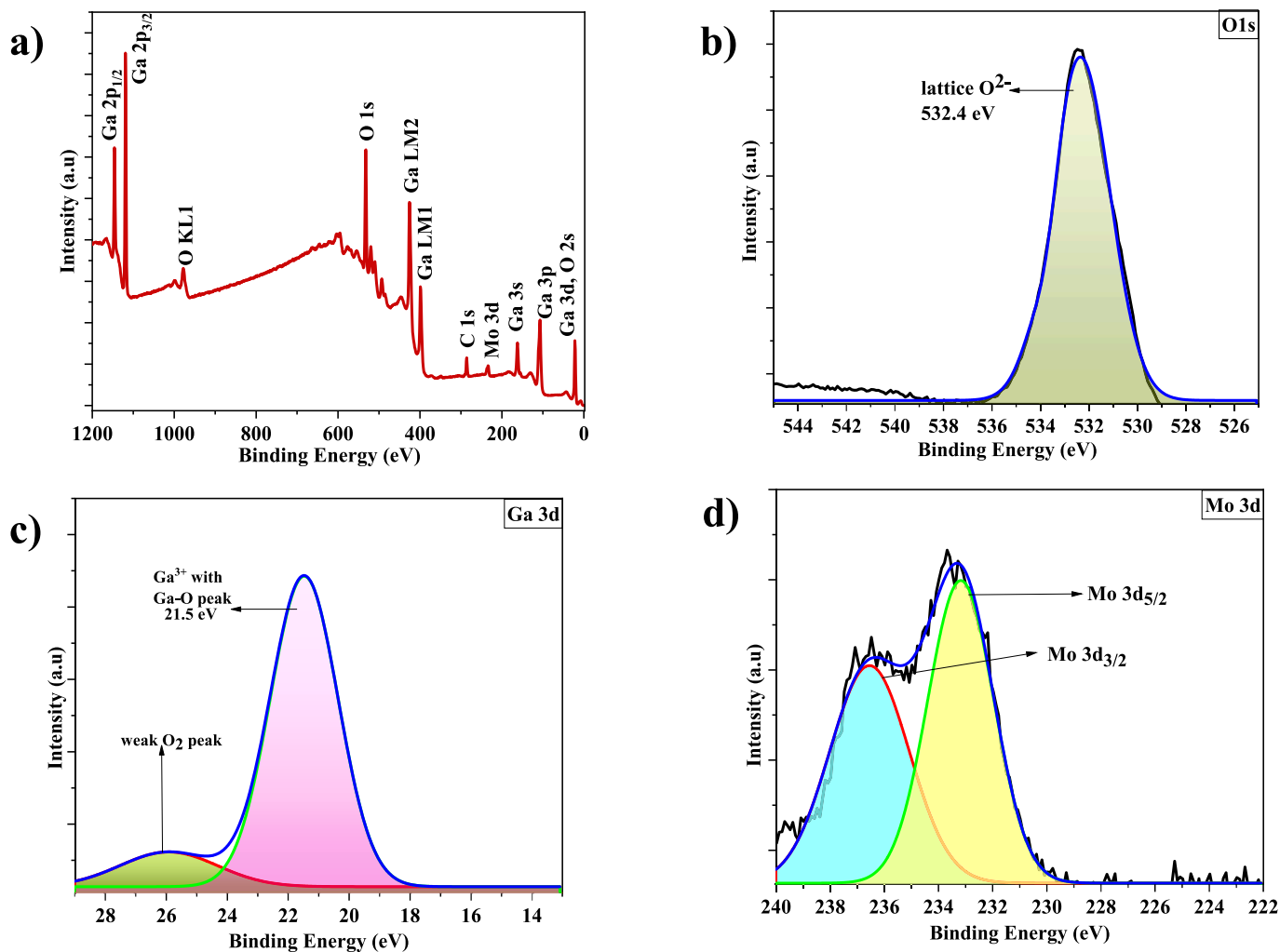


Fig. 9. XPS spectra of a) Ga<sub>2</sub>O<sub>3</sub>/ MoO<sub>3</sub> nanocomposite b) O 1s c) Ga 3d d) Mo 3d.

is attributable to the Ga 3d with Ga—O bond, is depicted in Fig. 9(c). In addition to the peak, a weak O 2s peak can be observed at 26.05 eV [60–62]. The high resolution XPS spectra in Fig. 9(d) show doublet peaks that match to the molybdenum 3d state of the material at 233.2 eV and 236.5 eV, respectively, representing the 3d<sub>5/2</sub> and 3d<sub>3/2</sub> states [63,64].

### 3.6. Surface area analysis

The Ga<sub>2</sub>O<sub>3</sub>/MoO<sub>3</sub> nanocomposites is subjected to Brunauer-Emmett-Teller (BET) surface area analysis to study the surface features and the result is given in Fig. 10. The nitrogen adsorption-desorption isotherm of the Ga<sub>2</sub>O<sub>3</sub>/MoO<sub>3</sub> nanocomposite displays a type IV curve accompanied by an H3-type hysteresis loop, which is characteristic of mesoporous materials, typically formed by aggregates of plate-like particles [65–67]. A larger BET surface area of 253 m<sup>2</sup> g<sup>−1</sup> and the pore volume V<sub>p</sub> = 0.55 cm<sup>3</sup> g<sup>−1</sup> implies that more active sites are available on the material's surface for gas molecule interaction, which is critical for enhancing sensor response and sensitivity [40,68,69].

The distribution of pore sizes is shown in the inset of Fig. 10, and it is clear that the Ga<sub>2</sub>O<sub>3</sub>/MoO<sub>3</sub> sample has a broad range of pore radii, peaking at RP = 19.65 nm. Additionally, the mesoporous framework enables efficient gas transport within the sensing layer, contributing to quicker response and recovery times. The integration of Ga<sub>2</sub>O<sub>3</sub> and MoO<sub>3</sub> not only modifies the surface and electronic properties but also contributes to a porous architecture that supports better gas adsorption dynamics and charge transfer which are key parameters in high-performance gas sensors.

### 3.7. Gas sensing studies

Sensing experiments on Ga<sub>2</sub>O<sub>3</sub>/MoO<sub>3</sub> nanocomposites with varying concentrations of analyte gas were conducted at RT by subjecting the sensor coated films, made using the drop casting technique. The sensing chamber, which is coupled to a high resistance electrometer, was used to expose sensor films to NH<sub>3</sub> vapours at different concentrations. The resistance the sensor film was noted in the ambient environment prior to injecting analyte vapours. Specific concentration of NH<sub>3</sub> vapours injected into the chamber and the variation of the sensor resistance was measured. The eq. (1) was used to compute the film's sensing responses to various NH<sub>3</sub> concentrations, in increments of 20 ppm from 10 ppm to 100 ppm.

$$S\% = \frac{I_a - I_g}{I_g} \quad (1)$$

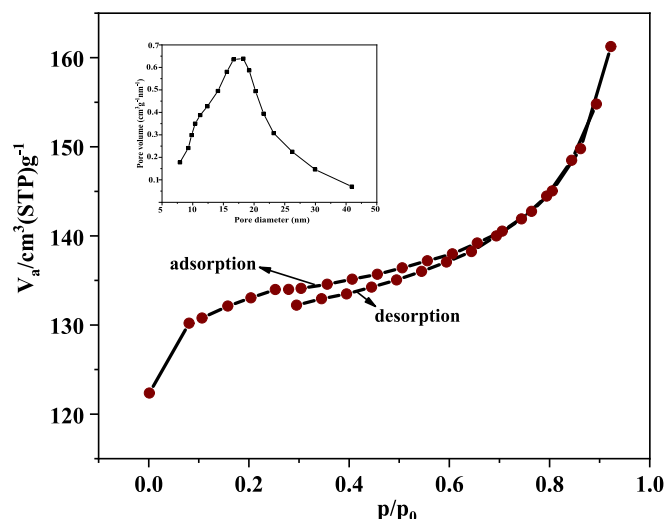


Fig. 10. BET analysis of Ga<sub>2</sub>O<sub>3</sub>/ MoO<sub>3</sub> nanocomposite.

where “S” denotes the sensing response, “I<sub>a</sub>” is the current flowing through the film in atmospheric air, and “I<sub>g</sub>” denotes the current when NH<sub>3</sub> is present. The sensor response was calculated for 2.5 %, 5 % and 7.5 % weight percentage concentration of MoO<sub>3</sub> in the composite. The results indicate that the pristine Ga<sub>2</sub>O<sub>3</sub> provides better response to NH<sub>3</sub> gas when compared to pristine MoO<sub>3</sub>, with the addition of low wt% (2.5 %, 5 %) MoO<sub>3</sub> to Ga<sub>2</sub>O<sub>3</sub> a slight increase in the response was observed. The composite with 7.5 % MoO<sub>3</sub>/Ga<sub>2</sub>O<sub>3</sub> showed the highest response of 420.12 % indicating that combined effect of Ga<sub>2</sub>O<sub>3</sub> and MoO<sub>3</sub> contribution in detecting the NH<sub>3</sub> vapours and the optimal mixing parameters for a porous mixture to achieve a successful Ga<sub>2</sub>O<sub>3</sub>/MoO<sub>3</sub> interaction [70]. Therefore, in comparison to pristine Ga<sub>2</sub>O<sub>3</sub> and MoO<sub>3</sub> based sensors, the Ga<sub>2</sub>O<sub>3</sub>/MoO<sub>3</sub> nanocomposite sensor has a higher gas detection response and it is shown in Fig. 11. The study was repeated at room temperature with different RH values and results were plotted.

The response and recovery time for the 7.5 % MoO<sub>3</sub>/Ga<sub>2</sub>O<sub>3</sub> composite is shown in Fig. 12 for 100 ppm of NH<sub>3</sub> gas. The response time is defined as the time for the sensor to reach 90 % of its maximum response after gas exposure, while the recovery time is defined as the time taken for the sensor to return to 90 % of its initial resistance after the gas is removed. The sensor demonstrated rapid performance, achieving a response time of 57.35 s when exposed to the target gas and recovering in 27.44 s after the gas was removed. These swift response and recovery characteristics indicate that the sensor is highly suitable for real-time applications.

### 3.8. The sensor's selectivity and sensitivity

The Fig. 13a displays the 7.5 % MoO<sub>3</sub>/Ga<sub>2</sub>O<sub>3</sub> sensor on/off cycles for 100 ppm of NH<sub>3</sub> gas at room temperature with 69 % relative humidity. The sensor's reaction is steady and reversible, as illustrated in the figure. The response of the sensor to varying concentrations in increments of 20 ppm is shown in Fig. 13b. A response of 33.3 % was noted towards 20 ppm of NH<sub>3</sub>, indicating the good sensitivity of the synthesized nanocomposite-based sensor. The Fig. 13c illustrates the linear relationship between the sensor response for varying NH<sub>3</sub> concentrations. According to the slope of the linear line, the sensor's sensitivity is 5.03 %/ppm, which is defined as the change in current response per 1 ppm of analyte gas [71]. In contrast to the other gases employed in the studies, the synthesized sensor shows strong selectivity to NH<sub>3</sub>, as determined by the selectivity study shown in Fig. 13d. The 7.5 wt% MoO<sub>3</sub> sensor was subjected to a selectivity test at RH with 69 % RH using 500 ppm concentrations of propanol, ethanol, toluene, formaldehyde, and acetone.

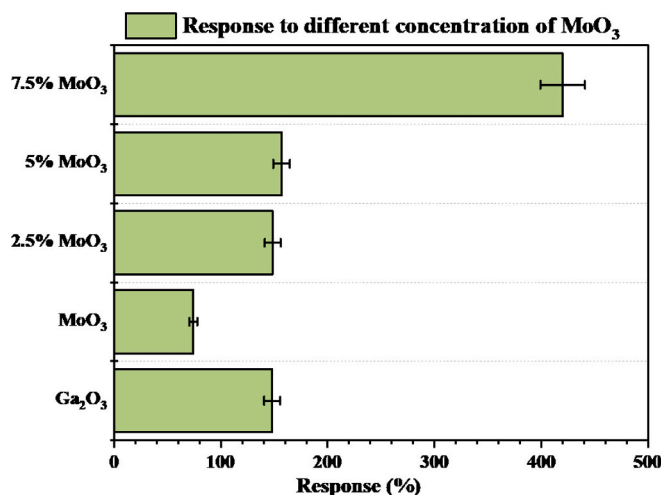


Fig. 11. Current Response of the pristine Ga<sub>2</sub>O<sub>3</sub>, MoO<sub>3</sub> and Ga<sub>2</sub>O<sub>3</sub>/ MoO<sub>3</sub> with different concentration.



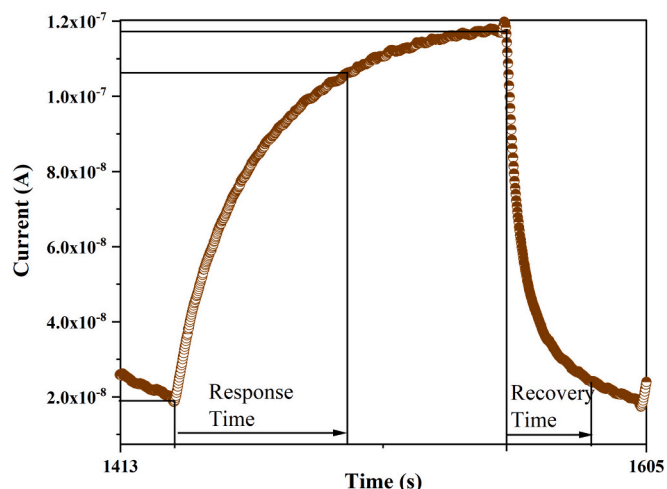


Fig. 12. Response and recovery time of 7.5 % MoO<sub>3</sub>/Ga<sub>2</sub>O<sub>3</sub> composite sensor for 100 ppm NH<sub>3</sub>.

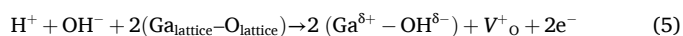
### 3.9. Sensing mechanism

Humidity is the main obstacle for the majority of semiconducting metal oxide gas sensors at room temperature because it interacts with the sensing material surface and restrict the sensing capability leading to the degradation of its performance [72]. Whereas according to reports,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is a potential option for room temperature humidity sensing applications [28,73]. Additionally, at room temperature, NH<sub>3</sub> and H<sub>2</sub>O react and enhance the sensing property. These two facts suggest two

potential modules of mechanisms based on adsorbed oxygen and humidity-assisted NH<sub>3</sub> sensing pathways.

#### 3.9.1. Humidity assisted sensing

At room temperature, humidity assisted detection of NH<sub>3</sub> vapours starts with the dissociative adsorption of H<sub>2</sub>O as H<sup>+</sup> and OH<sup>-</sup> on the surface of metal oxides, as shown in eq. (4). The ambient environment during sensing experiment refers to the wet environment with minimal humidity levels, where in one can assume that adsorption of one H<sub>2</sub>O molecule led to two adsorption active sites [74]. According to eq. (5), this dissociative adsorption causes the lattice to create an oxygen vacancy and a Ga<sup>δ+</sup> – OH<sup>δ-</sup> dipole. As seen in eq. (6), further interaction between H<sub>2</sub>O and these dipoles creates a liquid electrolyte medium, where NH<sub>3</sub> undergoes electrolytic dissociation to yield NH<sub>4</sub><sup>+</sup> and OH<sup>-</sup>. This electrolytic dissociation of NH<sub>3</sub> causes variations in ionic and electronic conduction on sensing material surface, which in turn causes variations in the electronic output.



#### 3.9.2. Sensing by adsorbed oxygen

Both Ga<sub>2</sub>O<sub>3</sub> and MoO<sub>3</sub> are n-type semiconductors, on exposure to air, ionized oxygen species (O<sub>2</sub><sup>-</sup>) can adsorb onto their surfaces and capture free electrons as shown in eq. (7), leading to the formation of a depletion layer near the surface. This process increases the resistance of the material. Upon exposure to NH<sub>3</sub>, the gas molecules interact with the adsorbed oxygen species. NH<sub>3</sub> acts as a reducing agent, donating

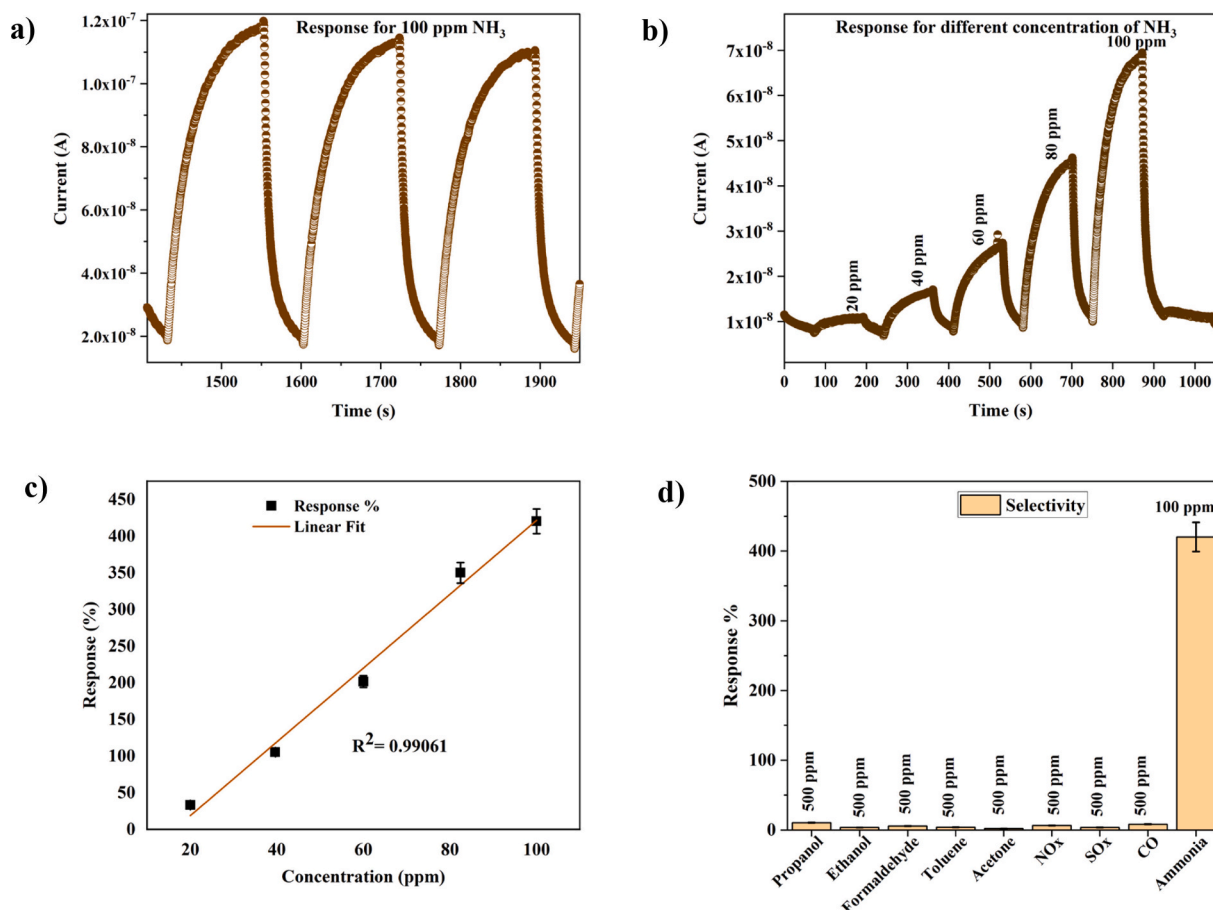
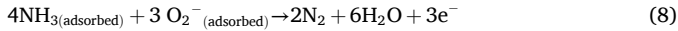
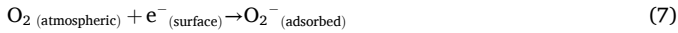


Fig. 13. a) Sensor response b) Sensitivity c) Linearity d) Selectivity of Ga<sub>2</sub>O<sub>3</sub>/ MoO<sub>3</sub> composite.

electrons to the semiconductor surface (eq. (8)). This interaction reduces the depletion layer's width, effectively lowering the resistance of the material and allowing for gas detection [75–77].



The spilling effect of adding MoO<sub>3</sub> over the surface increases the chances that reactive oxygen or hydroxyl species will be adsorbed on the composite surface, providing more active sites for adsorption that could accelerate the kinetics of surface chemical processes [78,79]. The various methods that improve the NH<sub>3</sub> sensing capabilities of Ga<sub>2</sub>O<sub>3</sub>/MoO<sub>3</sub> composite in comparison to pristine Ga<sub>2</sub>O<sub>3</sub> at RT as shown in Fig. 14(a, b).

### 3.10. Humidity variation study

The response of 7.5 % MoO<sub>3</sub>/Ga<sub>2</sub>O<sub>3</sub> nanocomposite sensor with varying RH from 56 % to 80 % for 100 ppm of NH<sub>3</sub> was studied and the results are given in Fig. 15. It can be seen from that with increased RH the response of the sensor increases displaying maximum response at 69 % RH. Further increase in the RH decreases the response considerably. Research indicates that there exists an optimal humidity level where gas sensitivity is maximized without excessive interference. While low humidity may provide weak adsorption of NH<sub>3</sub>, excessively high humidity can lead to saturation and poor response due to the predominant adsorbate being water rather than the target gas itself. Therefore, increase in the humidity beyond optimal 69 % will considerably decreases the response of the sensor [28,73,76].

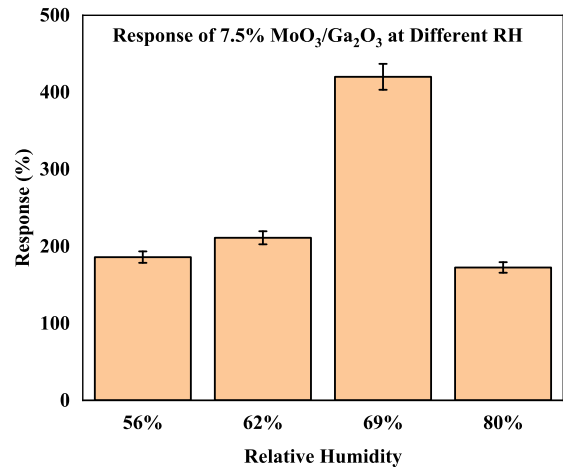


Fig. 15. Humidity study of Ga<sub>2</sub>O<sub>3</sub>/ MoO<sub>3</sub> composite.

### 3.11. Conclusion

NH<sub>3</sub> gas detection using a room temperature sensor based on Ga<sub>2</sub>O<sub>3</sub>/MoO<sub>3</sub> nanocomposites has been extensively researched. To synthesize Ga<sub>2</sub>O<sub>3</sub> and MoO<sub>3</sub> nanoparticles, a hydrothermal method was used. Through physical mixing of pristine samples at different weight ratios in NMP, the Ga<sub>2</sub>O<sub>3</sub>/MoO<sub>3</sub> nanocomposites were produced. The addition of MoO<sub>3</sub> alters the sensor's response to NH<sub>3</sub> gas. The addition of MoO<sub>3</sub> content is between 2.5 and 5 wt% shows a slight increase in the response of the sensor whereas to 7.5 wt% the response increase rapidly indicating that combined effect of Ga<sub>2</sub>O<sub>3</sub> and MoO<sub>3</sub> contribution in detecting the NH<sub>3</sub> vapours implying the ideal mixing conditions for a porous

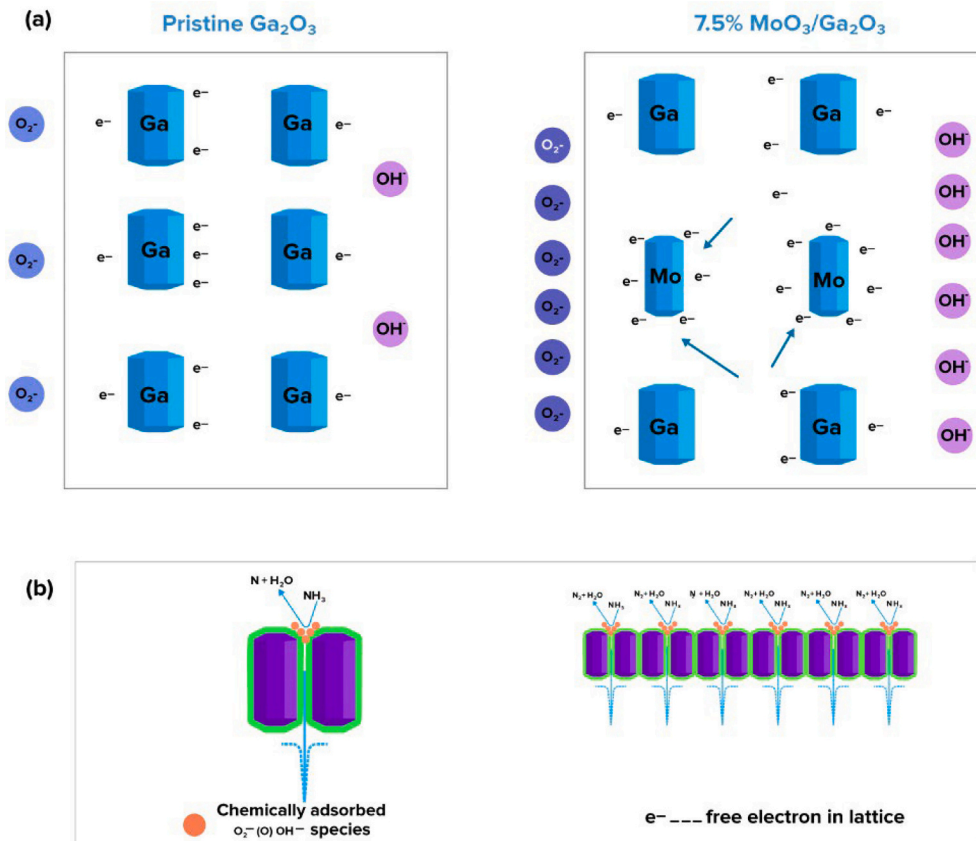


Fig. 14. Sensing mechanism of Ga<sub>2</sub>O<sub>3</sub>/MoO<sub>3</sub> for NH<sub>3</sub> detection a) adsorption oxygen and hydroxyl species b) electron and ionic conduction.

combination for effective Ga<sub>2</sub>O<sub>3</sub>/MoO<sub>3</sub> interaction. The sample with Ga<sub>2</sub>O<sub>3</sub> and 7.5 wt% MoO<sub>3</sub> exhibits maximum response (420.12 % for 100 ppm NH<sub>3</sub>) in RT at RH 69 %. The superior sensing performance can be attributed to the reduced crystallite size, enlarged surface area and higher surface-to-volume ratio, along with the development of a rod like morphology, all of which provide more active sites for gas adsorption and facilitate efficient charge transport. In addition, the sensor displays excellent selectivity for NH<sub>3</sub> when compared to other volatile organic compounds.

### CRedit authorship contribution statement

**Madhura N. Talwar:** Writing – review & editing, Writing – original draft, Visualization, Resources, Methodology, Investigation, Formal analysis, Data curation. **Asha P. Shirni:** Formal analysis, Data curation. **Rajendra Kumar R. T.:** Validation, Resources, Data curation. **Gnana Prakash A. P.:** Supervision.

### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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### Data availability

Data will be made available on request.

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