Supporting Information File

Reduced Graphene Oxide/ZnO Nanocomposites: One-Step Solid State Preparation for Room Temperature Photo-sensing and Photoelectrical Gas Sensing Capabilities

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Sensor's measurement setup and ppm calculation

The Keysight 3472A data acquisition unit (DAQ) was utilized to measure the sensor's conductivity during gas sensing experiments. All measurements were conducted at standard room temperature (25°C) and a relative humidity (RH) of 65%. To monitor and regulate the humidity levels within the sensing chamber, a high-precision HygroClip 2 advanced series HC2A-S hygrometer was employed, capable of detecting even minor changes in RH within the chamber.

To evaluate the sensing performance, the sensor device was positioned inside a 1.2 L sealed sensing chamber. A UV source with a wavelength of 365 nm and the intensity of 250 W/m^2 illuminated the device through a quartz window.

The intensity (I) was calculated using the formula (Equation 5):

$$I = P/A \tag{5}$$

Where P and A represent applied power and area of incident light. Putting the values of P and A in the formula, the intensity of the light is obtained as:

$I = 5/0.02\ m^2 = 250 W/m^2$

A schematic representation of the sensing system is provided in Figure 7a, while Figure S6 showcases optical photographs of the laboratory setup used to measure the sensor's performance.

For the preparation of VOC vapors, the respective VOC solvents were allowed to evaporate inside airtight bottles sealed with rubber corks to maintain a stable and saturated vapor concentration. These VOC vapors were then introduced into the sensing chamber using a gas-tight syringe. The ppm concentration of the VOCs was calculated using the Equation 2:

$$\text{ppm concentration} = \frac{Vapor\ pressure\ (VP)\ of\ VOC\ solvent\ (Pa)}{atmospheric\ pressure\ (pa)} \times 10^6 \tag{2}$$

Here the atmospheric pressure was 101,325 pa and the VP of all VOCs was evaluated using the following Antoine's formula (Equation 3).[1]

$$\log_{10}(\text{Pi}) = \text{A} - \frac{B}{C+T} \tag{3}$$

where A, B, and C are Antoine constants available in the NIST database,[2] and T is the temperature in Celsius (25°C).

For sensor measurements, a specified concentration of VOC vapors was introduced into the sensing chamber. Once the sensor achieved its full response, the VOCs were purged from the chamber using an external air pump to facilitate sensor recovery. This process was repeated for various VOC concentrations to evaluate the sensor's performance.

The concentration of VOC vapors introduced into the chamber, expressed in ppm, was calculated using the equation 4:[3]

$$\text{Ppm conc.} = \frac{Concentration\ of\ evaporated\ vapor\ in\ ppm \times Quantity\ of\ vapor\ in\ syringe}{Volume\ of\ sensor\ chamber\ (ml)} \tag{4}$$

The corresponding ppm conversion table is given here

Table S1. Ppm calculation for TEA.

VOC n-butylamine	**Vapor pressure (kPa)**	**Evaporated PPM of VOC conc.**	**Final gas conc.**	
			mL conc. in syringe	**PPM in chamber**
Triethylamine	7.199	71048	2.4	142
			4.8	284
			9.6	568
			19.2	1136

Similarly evaluation for ethanol, benzene, and acetone was carried out.

TGA-DSC

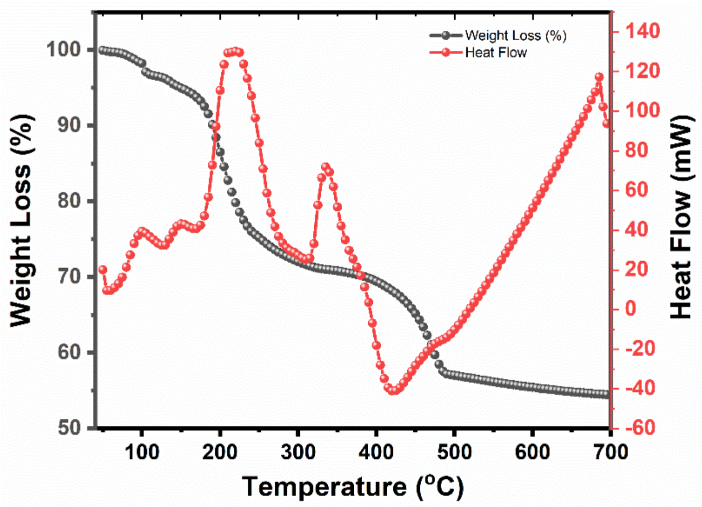

Figure S1. TGA-DSC graphs of raw 10%G@ZnO nanocomposite sample.

FTIR spectroscopy

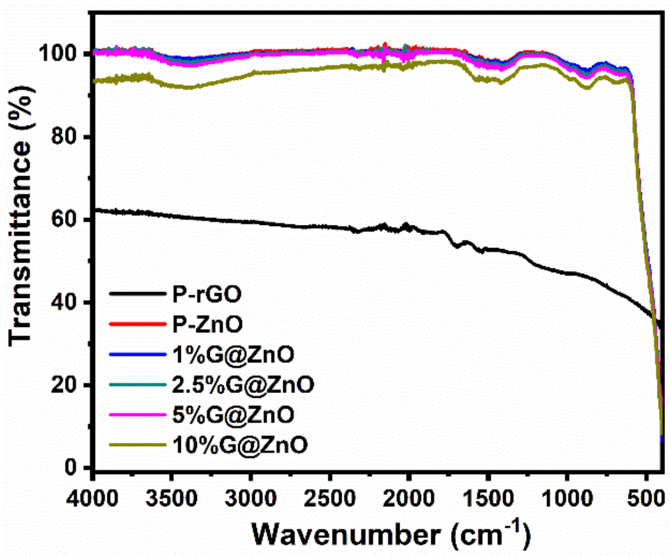

Figure S2. FTIR spectra of synthesized P-rGO, P-ZnO and G@ZnO samples.

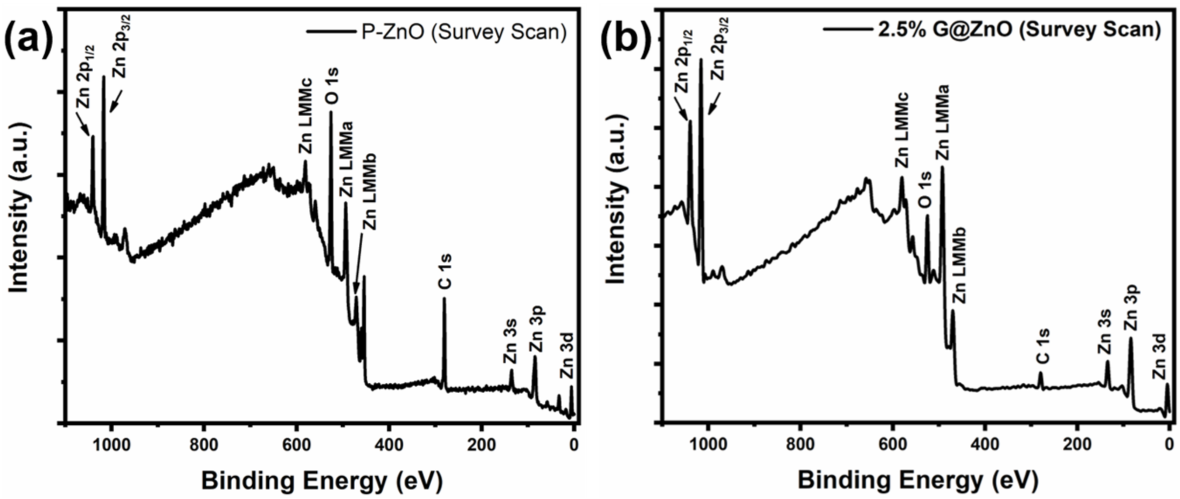

Figure S3: Survey spectra of (a) ZnO, (b) 5%G@ZnO.

FESEM images

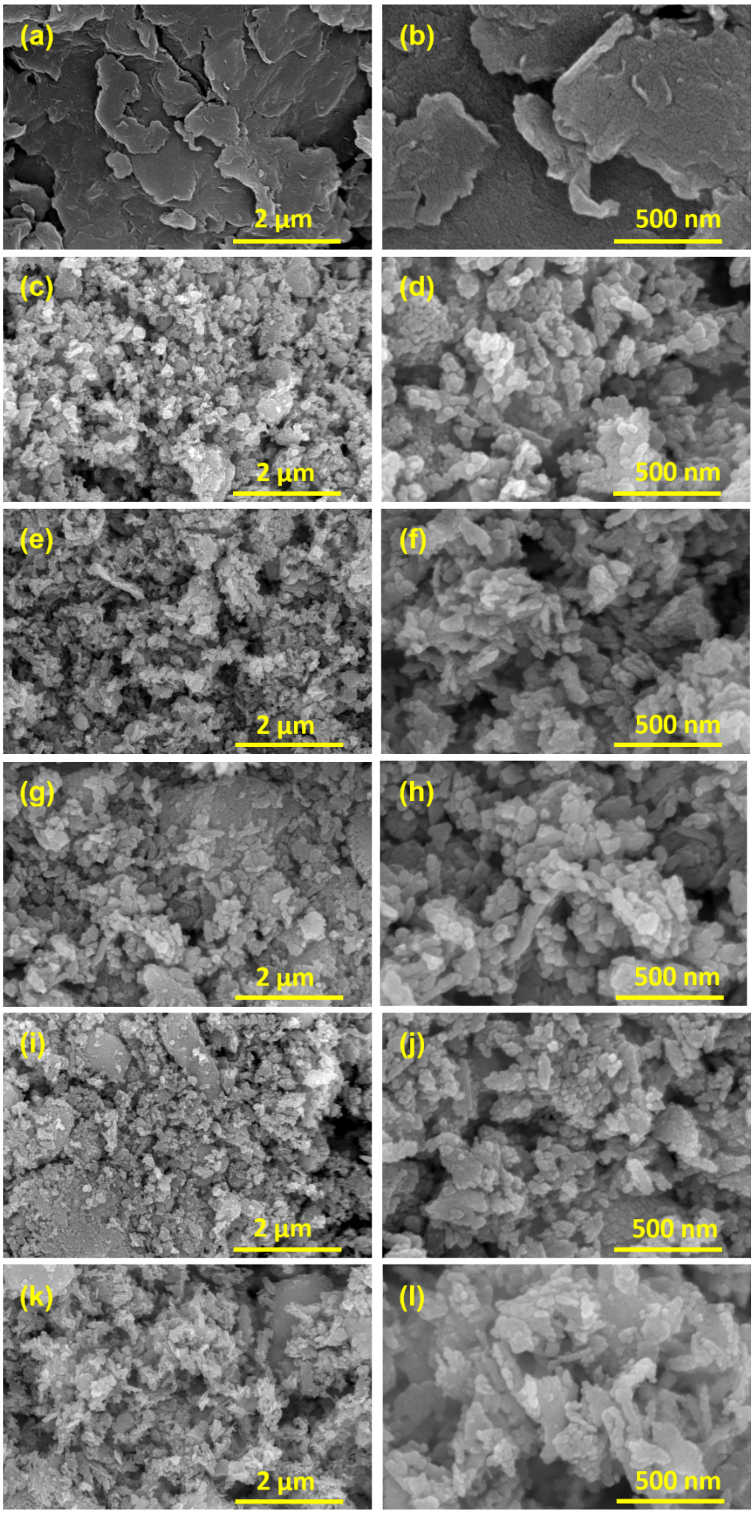

Figure S4. FESEM images of (a, b) P-rGO, (c, d) P-ZnO, (e, f) 1%G@ZnO, (g, h) 2.5%G@ZnO, (i, j) 5%G@ZnO, and (k, l) 10%G@ZnO samples each at low and high magnification respectively.

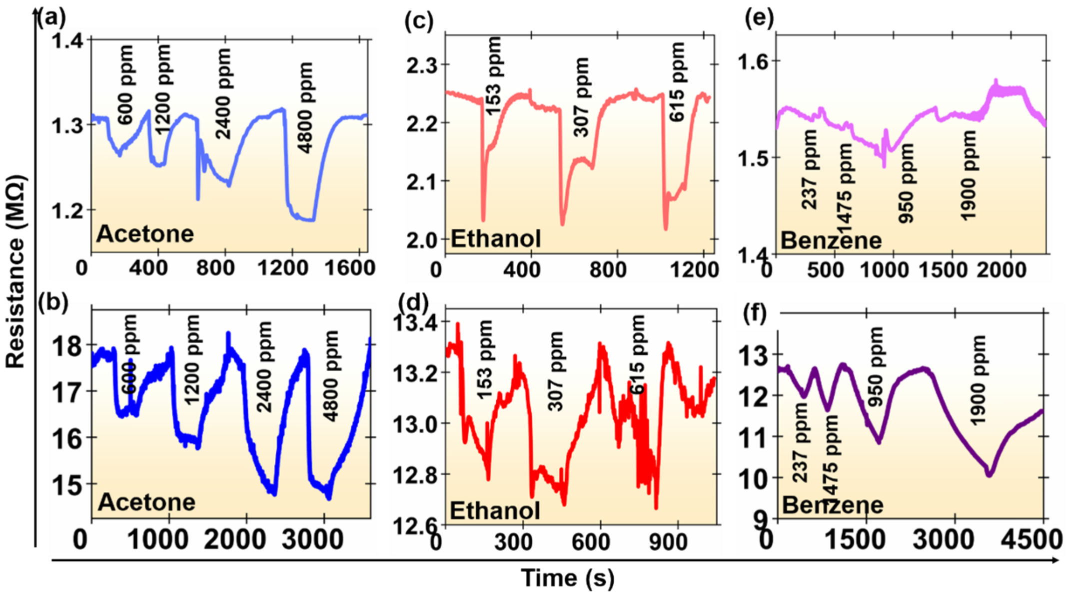

Figure S5. Photoelectrical gas sensing performance of P-ZnO and 2.5%G@ZnO nanocomposite sensors against acetone (a and b), ethanol (c and d) and benzene (e and f) respectively.

LOD Calculation

From the Figure S5, baseline was utilized for D value calculation which further provided the LOD value.

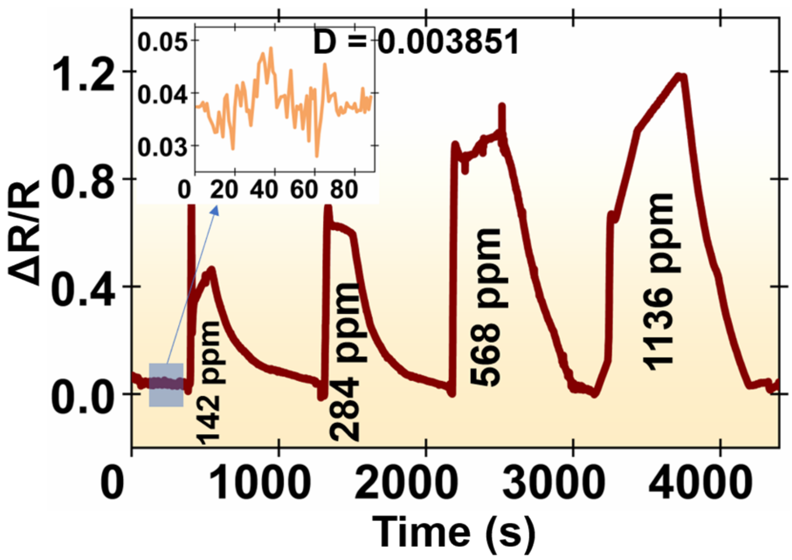

Figure S6. Response curve of 2.5G@ZnO sensor against TEA which was used for the calculation of LOD.

The limit of detection (LOD) of the sensor was calculated by the following equation

$$\text{LOD} = \frac{3D}{m} \qquad (4)$$

Where 3 denoted signal-to-noise ratio, D represented the standard deviation in the baseline of the TEA sensing curve before adding TEA and m was the slope of the fitted curve (sensitivity of TEA). The D was derived using 90 data points at the baseline in light-activated mode (D= 0.003851) in Figure S5.

$$\text{LOD} = \frac{3 * 0.003851}{0.000737}$$

LOD = 15 ppm.

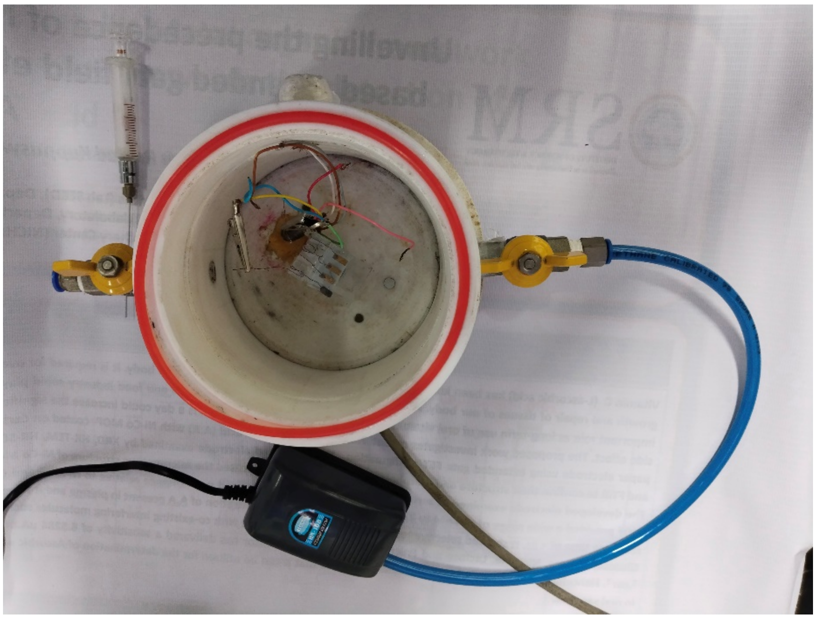

Figure S7. Static gas sensing setup.

References:

(1) Ghuge, R. S.; Shinde, M. D.; Kumar, V. H.; Arbuj, S. S.; Jayaraman, S. V.; Rane, S. B.; Di Natale, C.; Sivalingam, Y. The Emergence of MnFe2O4 Nanospheres-Based Humidity Sensor: A Methodical Investigation by Scanning Kelvin Probe and Its Deployment in Multitudinous Applications. *Mater. Adv.* **2023**.

(2) Marappan, G.; Manoharan, E.; Chidambaram, D.; Kandasamy, A.; Sivalingam, Y.; Di Natale, C.; Surya, V. J. Tunable Visible Light Enhanced Triethylamine Adsorption on PH Dependent ZnO Nanostructures: An Investigation by Scanning Kelvin Probe. *Surfaces and Interfaces* **2021**, *27*, 101507.

(3) Kalidoss, R.; Umapathy, S.; Anandan, R.; Ganesh, V.; Sivalingam, Y. Comparative Study on the Preparation and Gas Sensing Properties of Reduced Graphene Oxide/SnO 2 Binary Nanocomposite for Detection of Acetone in Exhaled Breath. *Anal. Chem.* **2019**, *91* (8), 5116–5124. https://doi.org/10.1021/acs.analchem.8b05670.