Supplementary Information

Simultaneous microwave-assisted reduction and B/N co-doping of graphene oxide for selective recognition of VOCs

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Results:

Concentrations of methanol and ethanol vapours (C) were determined from the amount of acetone and ethanol, added to the analysis chamber through the equation:

$$C_{ppm} = \frac{2.46 V_a \rho}{V_c M w} 10^7 \text{ ……………………….. (S1)}$$

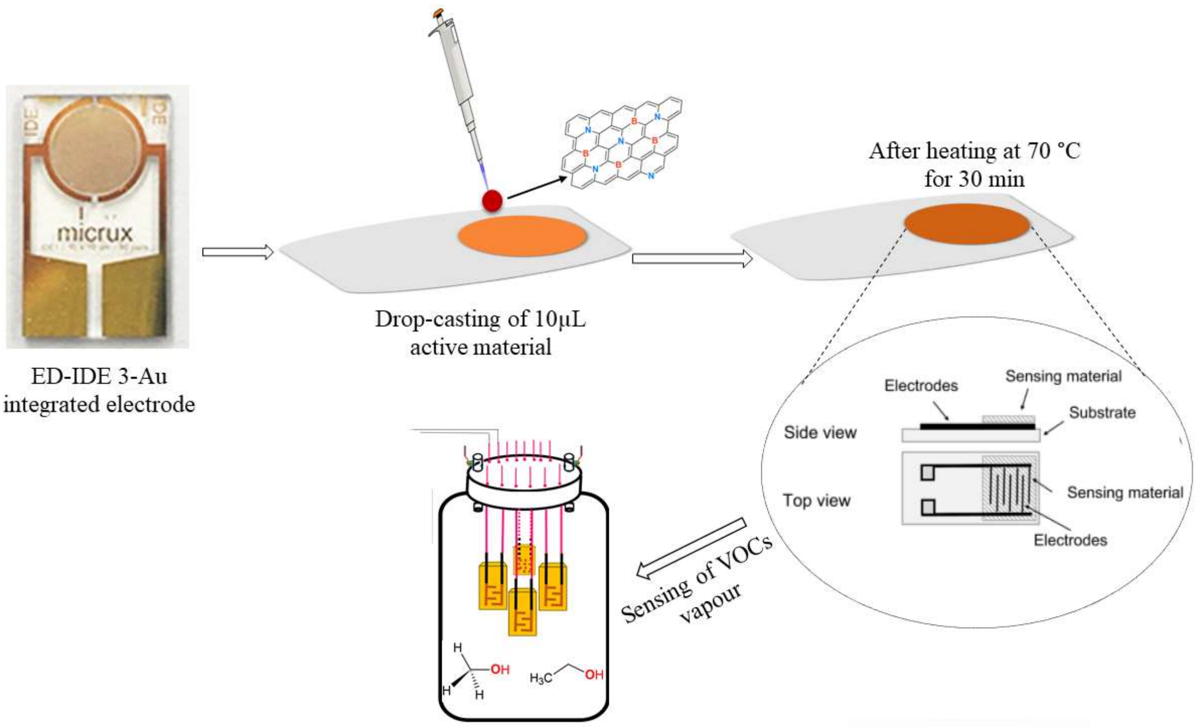
where V_a represents the volume (in µL) of the analyte added to the chamber, V_c is the volume (in mL) of the analysis chamber, ρ is the density of analyte (in gmL^{-1}) and *Mw* is the molecular weight of analyte in gM^{-1}. The response (*Resp*), limit of detection (*LoD*) and sensitivity (*S*) were given by

$$\Delta R/R_0 = (R_f - R_0)/R_0 \text{ ……………………… (S2)}$$

$$LoD = Rb + 3db \text{ ……………………………… (S3)}$$

$$S = dResp/dC \text{ ……………………………… (S4)}$$

where, R_f is the impedance of the sensor when exposed to analyte and R_0 the resistance of the sensor in ambient condition, *Rb* is the average impedance, *db* is the standard deviation of the device impedance without analyte, and *C* is an analyte concentration.



Scheme S1: Sensing device preparation and sensing set-up.

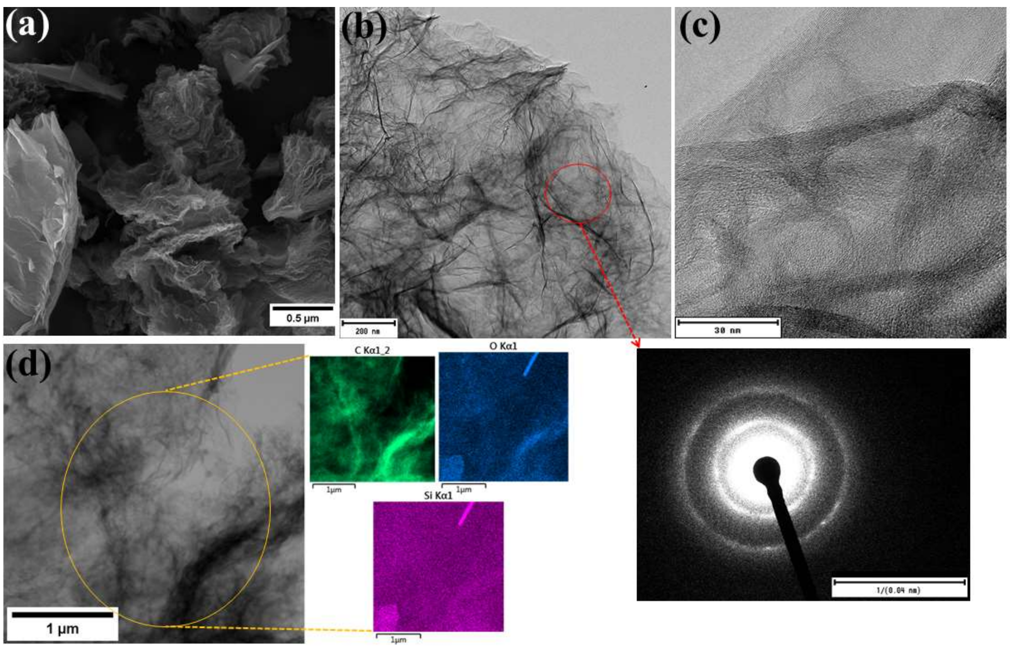


Figure S1: Morphology of the rGO sample based on (a) SEM, (b) low magnification TEM, (c) high magnification TEM with SAED, and (d) TEM elemental mapping.

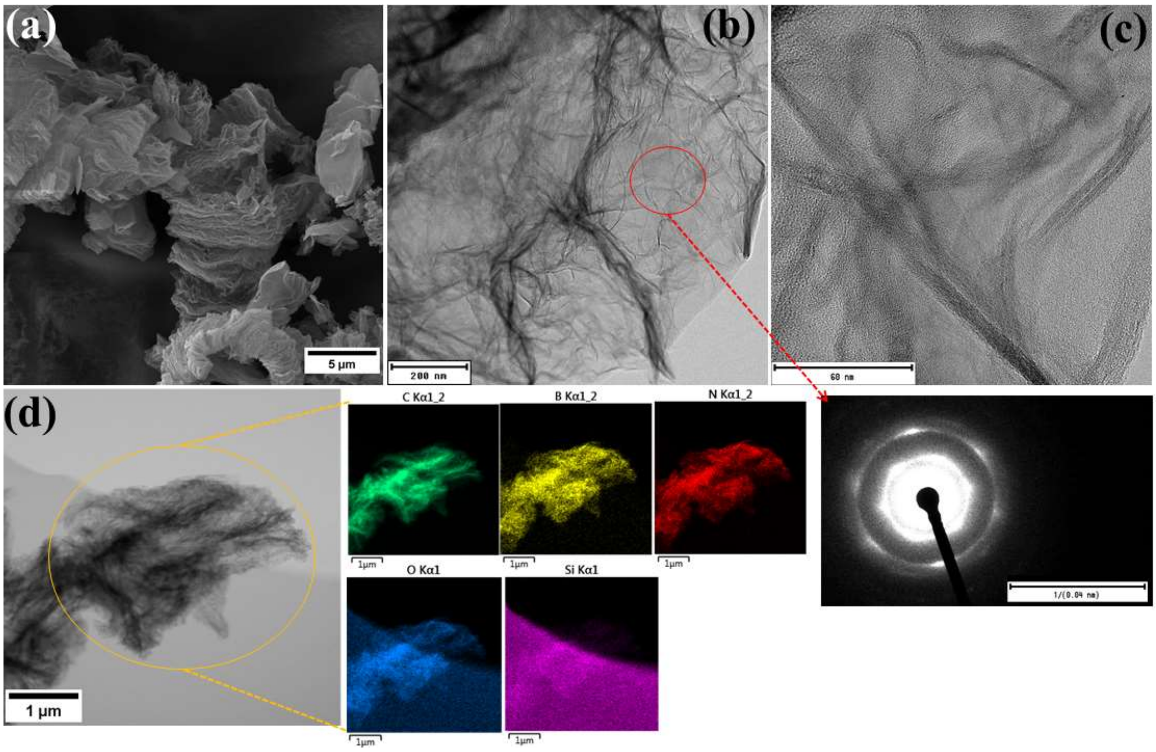


Figure S2: Morphology of the BN-GO$_{TMABH}$ sample based on (a) SEM, (b) low magnification TEM, (c) high magnification TEM with SAED, and (d) TEM elemental mapping.

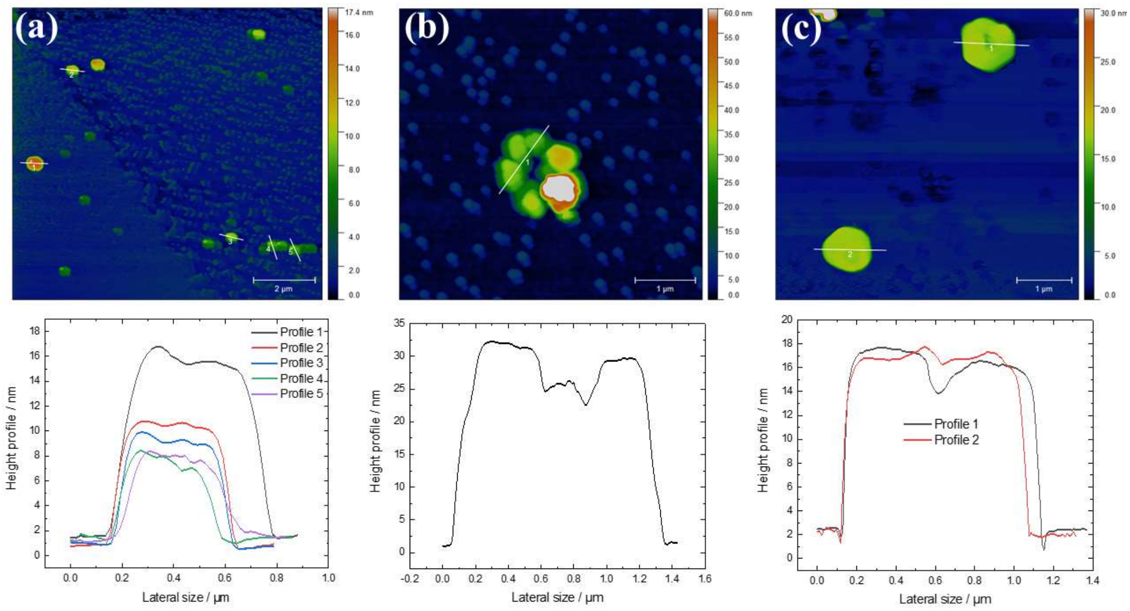


Figure S3: AFM micrographs of (a) pristine rGO, (b) BN-rGO$_{AB}$, and (c) BN-GO$_{TMABH}$ samples; corresponding height profiles.

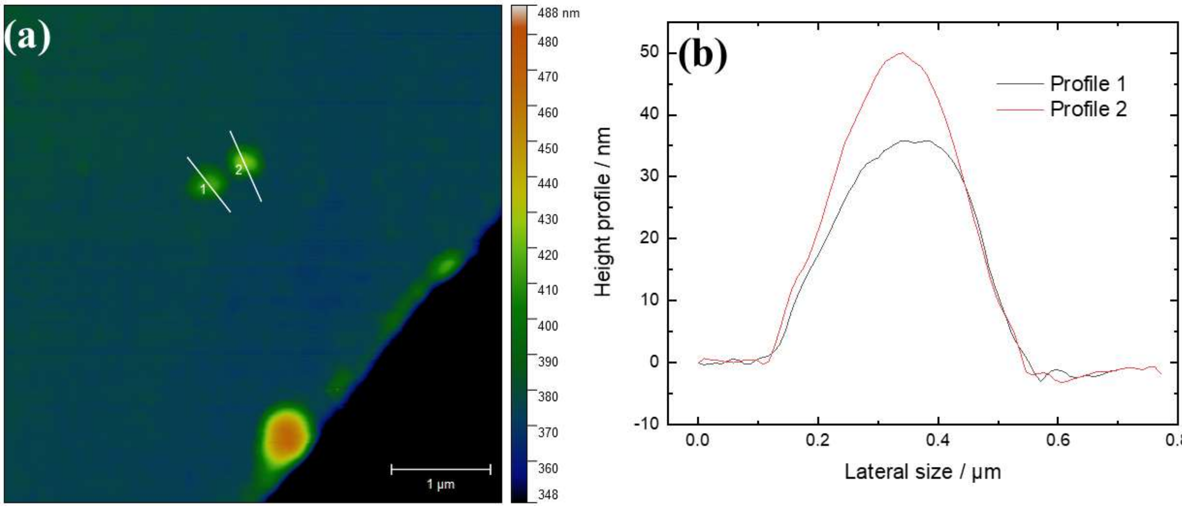


Figure S4: (a) AFM micrographs and (b) corresponding height profiles of the nanosheets on the integrated electrode.

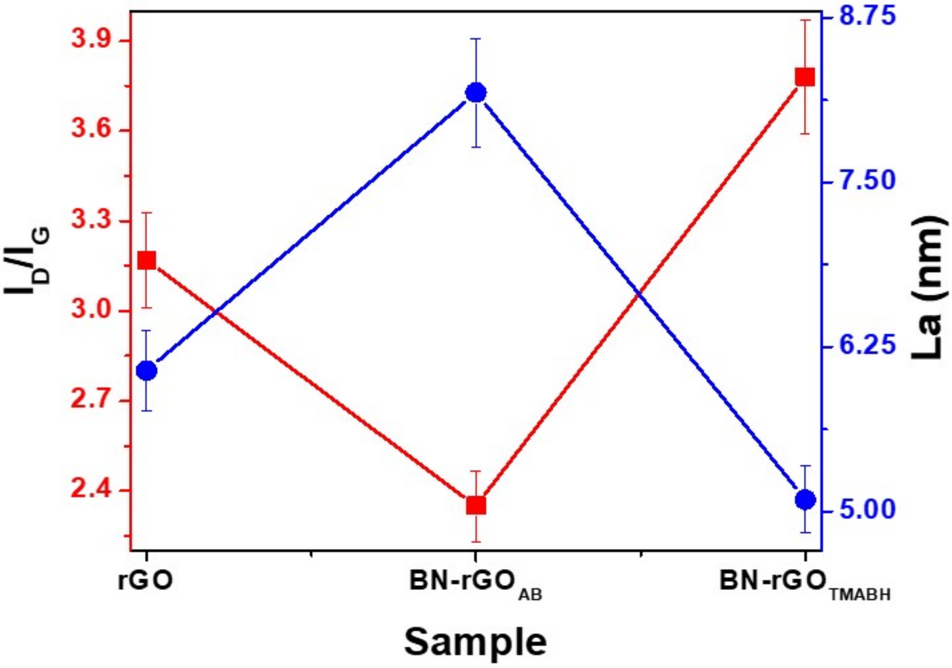


Figure S5: Defect density ratios and crystallite sizes for the pristine and variously co-doped rGO samples.

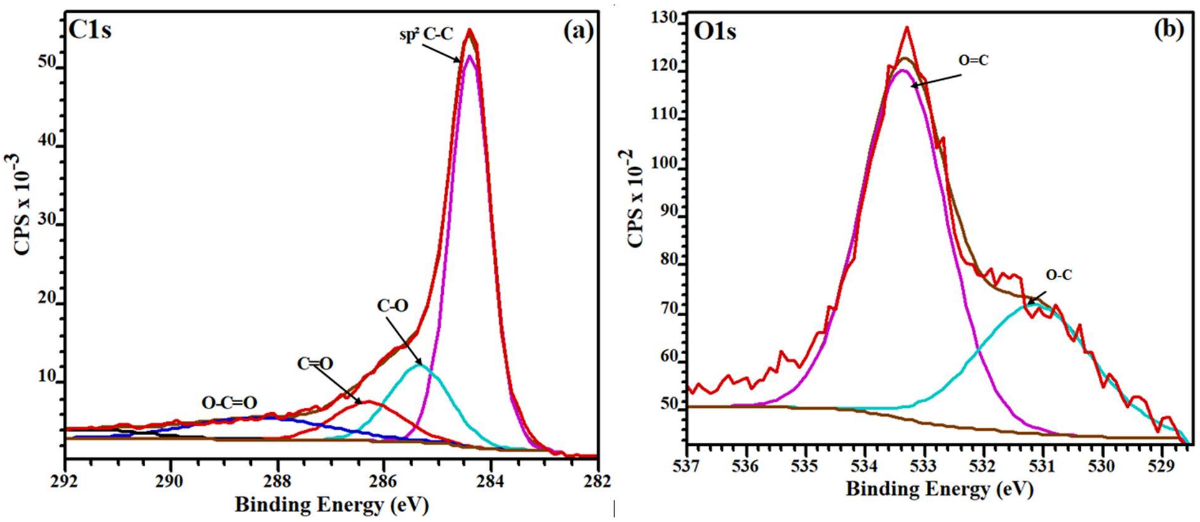


Figure S6: Deconvoluted (a) C1s and (b) O1s spectra of rGO sample.

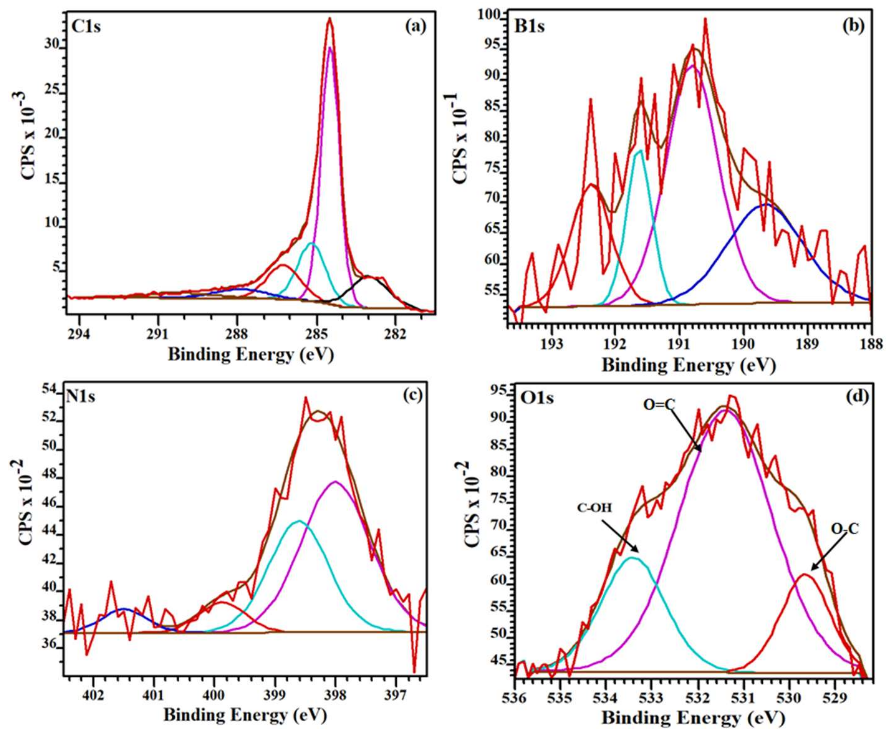


Figure S7: Deconvoluted (a) C1s, (b) B1s, (c) N1s, and (d) O1s spectra of BN-rGO$_{TMABH}$ sample.

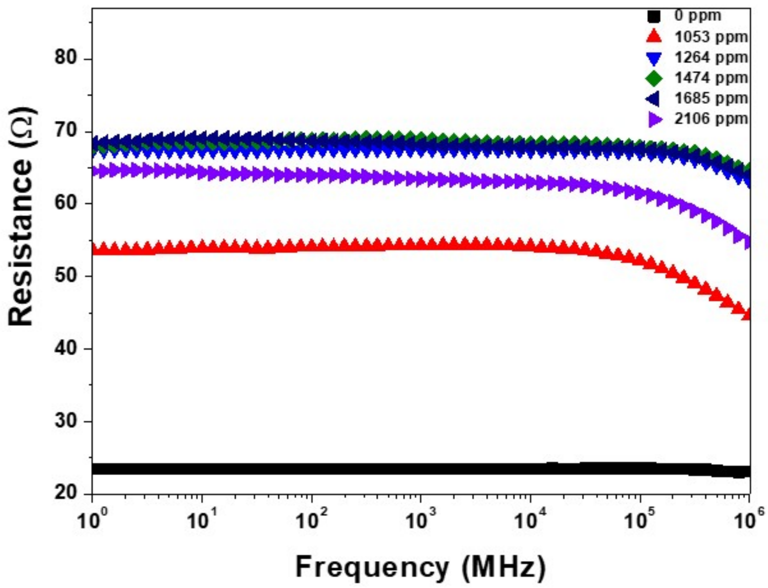


Figure S8: (a) Resistance as a function of frequency at increasing EtOH vapour concentration and (b) Nyquist plot for BN-rGO_{AB} sensor at 1100 ppm EtOH vapour concentration.

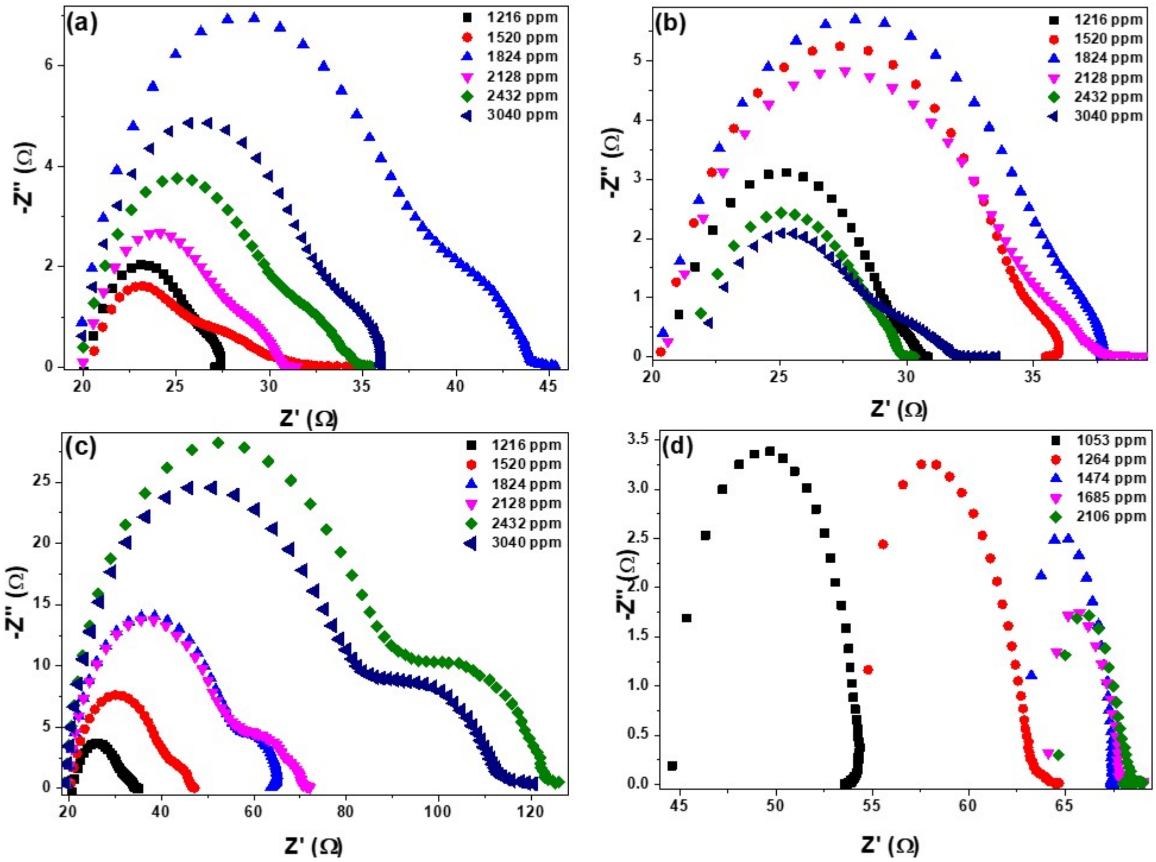


Figure S9: Nyquist plots for sensitivity of (a) rGO, (b) BN-rGO$_{AB}$, and (c) BN-rGO$_{TMABH}$ sensor devices with increasing MeOH vapour concentrations, and (d) for BN-rGO$_{AB}$ to EtOH vapour.

Table S1: Raman parameters for the pristine rGO and doped rGO samples.

Sample	**Peak position (cm^{-1})**		**Defect density ratio (I_D/I_G)**	**L_a (nm)**	**N_D/ $\times10^{11}$ cm^{-2} [a]**
	D-band	**G-band**			
rGO	1349.8	1584.3	3.17	6.07	9.50
BN-rGO$_{AB}$	1349.9	1584.3	2.35	8.18	7.04
BN-rGO$_{TMABH}$	1344.8	1577.9	3.78	5.09	11.3

$Defects\ density, n_D(nm) = \frac{2.4\times10^{22}}{\lambda_{laser}^4} \times I_D/I_G$ ....(S1^a)

Table S2: Textual properties of pristine and doped rGO samples.

Sample	BET surface area (m^2/g)	Monolayer Pore volume (cm^3/g)	Pore vol (cm^3/g)
rGO	185.8	42.7	0.77
BN-rGO$_{AB}$	432.6	99.8	1.94
BN-rGO$_{TMABH}$	325.4	74.8	1.50

Table S3: Atomic compositions of pristine and BN-rGO samples.

Samples	**Elements (at. %)**			
	C	**B**	**N**	**O**
rGO	93.02	-	-	6.98
BN-rGO$_{AB}$	75.69	7.33	2.61	14.48
BN-rGO$_{TMABH}$	84.87	2.94	2.09	10.09