

Supporting Information

Graphene loading with polypyrrole nanoparticles for trace-level detection of ammonia at room temperature

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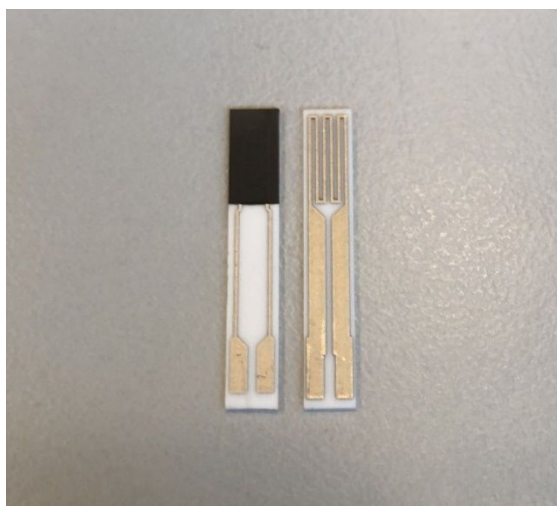


Figure S1. Layer of graphene nanoflakes loaded with PPy NPs onto alumina substrate.

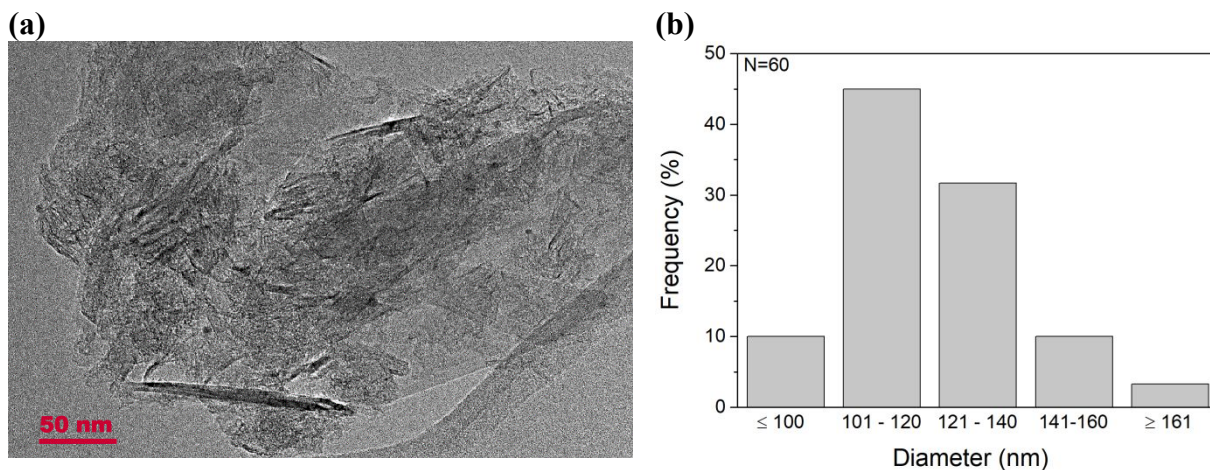


Figure S2. (a) HRTEM image at a lower magnification of the bare graphene. (b) PPy nanoparticle size distribution histogram. Above 75% of PPy NPs have diameter in the range of 101 to 140 nm.

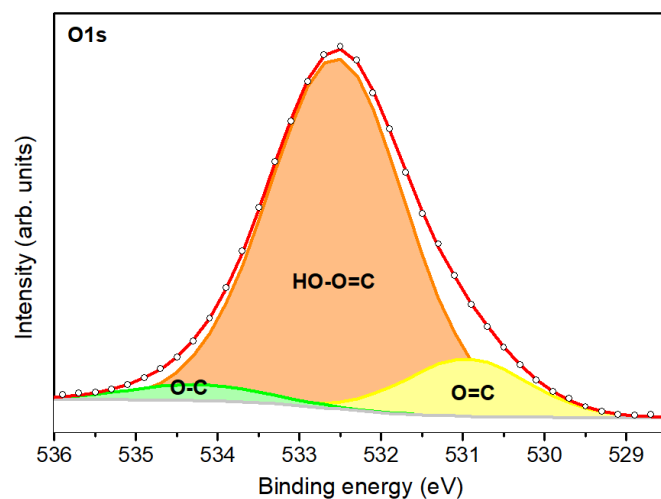


Figure S3. XPS O1s core level obtained for the bare PPy NPs.

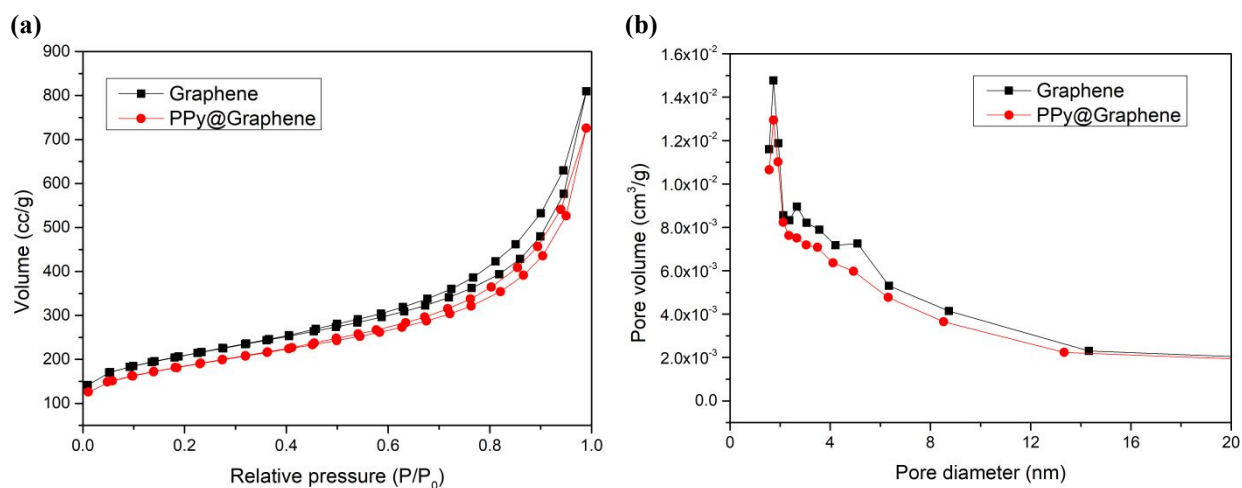


Figure S4. Adsorption-desorption isotherms for both samples (a). Pore diameter distribution for bare and PPy decorated graphene (b).

Table S1. Comparison of characterization results.

Sample	BET area (m ² /g)	Average pore diameter (nm)	Pore volume (cm ³ /g)
Graphene	730	1.730	1.037
PPy@Graphene	644	1.735	0.993

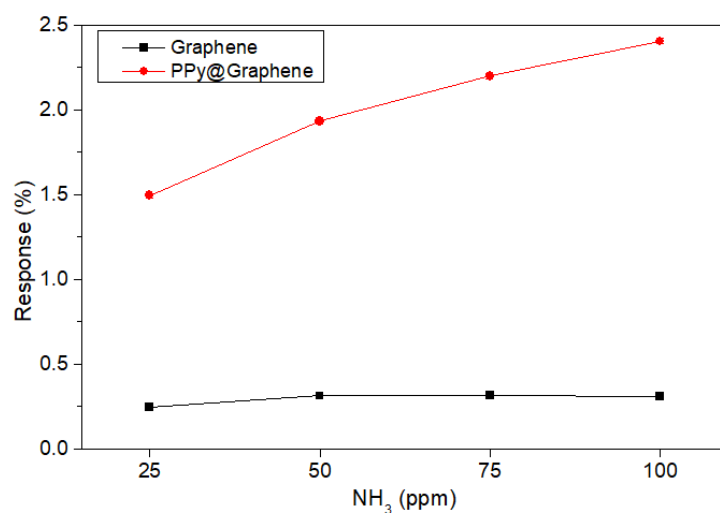


Figure S5. Calibration curves obtained for the detection of NH₃ (concentration range: 25-100 ppm).

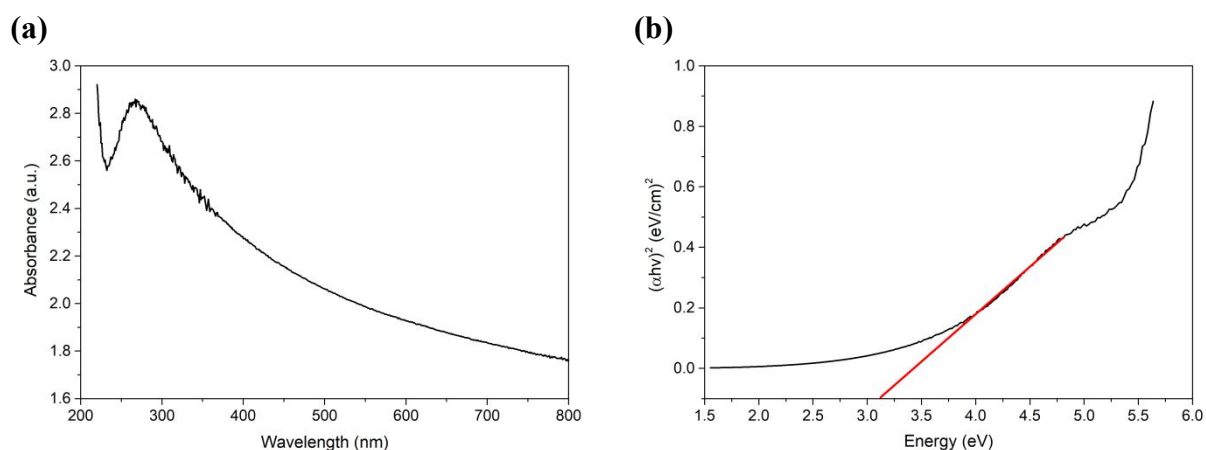


Figure S6. UV-Vis absorption spectrum for graphene nanoflakes **(a)** and Tauc plot for calculating their direct bandgap **(b)**. Sample preparation comprised 5 mg of graphene added to 2 ml of ethanol in a 10 x 10 mm fluorescence quartz cuvette. Afterwards, the cuvette was sealed and subsequently deaerated by purging with an Ar gas stream for 10 minutes.

(a)

(b)

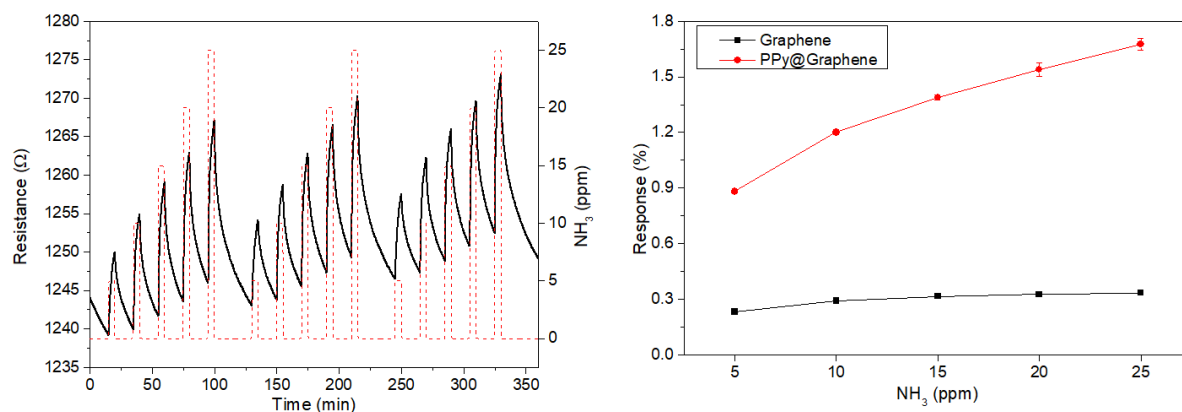


Figure S7. Example of electrical responses when detecting NH₃ at the concentration range of 5-25 ppm for the PPy@Graphene sensor (a). Comparison of the calibration curves obtained for bare and PPy loaded graphene (b). Higher responses and sensitivity can be observed for the PPy@Graphene sample.

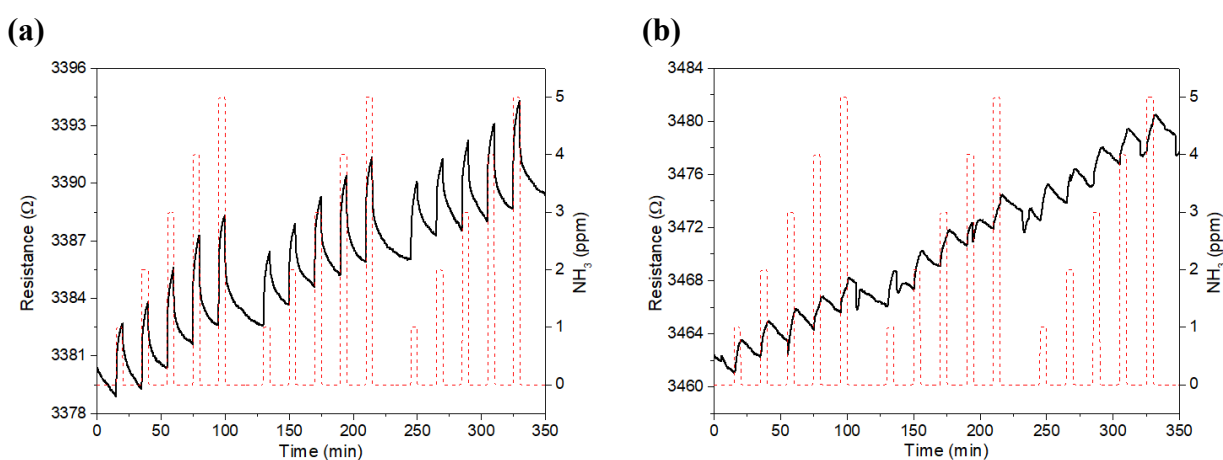


Figure S8. Examples of electrical responses when detecting low concentrations of NH₃ for the bare graphene sensor in dry (a) and humid (b) conditions.

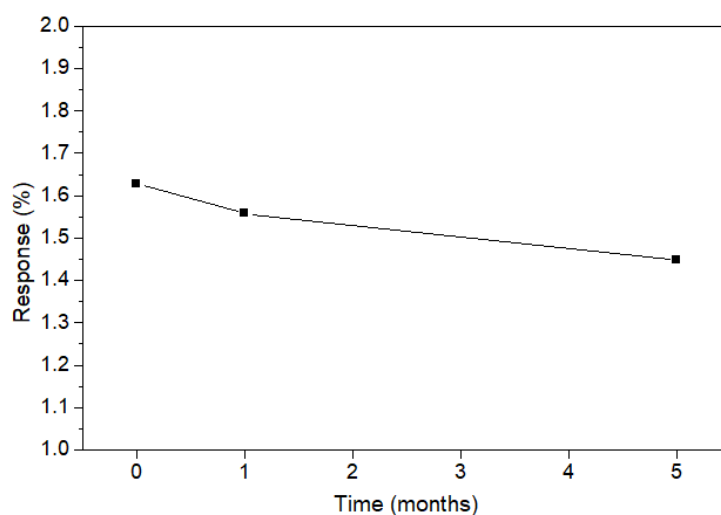


Figure S9. Stability study of the PPy@Graphene sensor, 50 ppm of NH₃ were measured over a 5-month period. A slightly higher slope during the first month can be observed. Nonetheless, during the following months, the slope was lowered, revealing a high sensor stability in the long term.

Table S2. Relative area (%A) of the different components obtained from the C 1s core level peak. The comparison was done with the freshly synthesized sample before the gas sensing measurements and after 5-months of use for detecting NH₃.

Component	%A Before	%A After
sp ²	45.1	42.4
sp ³	34.9	36.9
C-O/C-N	11.4	11.7
C=O/C=N	5.8	6.5
O-C=O/N-C=O	2.8	2.5

Table S3. Relative area (%A) of the different components obtained from the N 1s core level peak. The comparison was done with the freshly synthesized sample before the gas sensing measurements and after 5-months of use for detecting NH₃.

Component	%A Before	%A After
NH	54	40
C=N	9	27
C-N ⁺	32.1	12.3
C=N ⁺	4.9	12.1
Amines	-	7.7

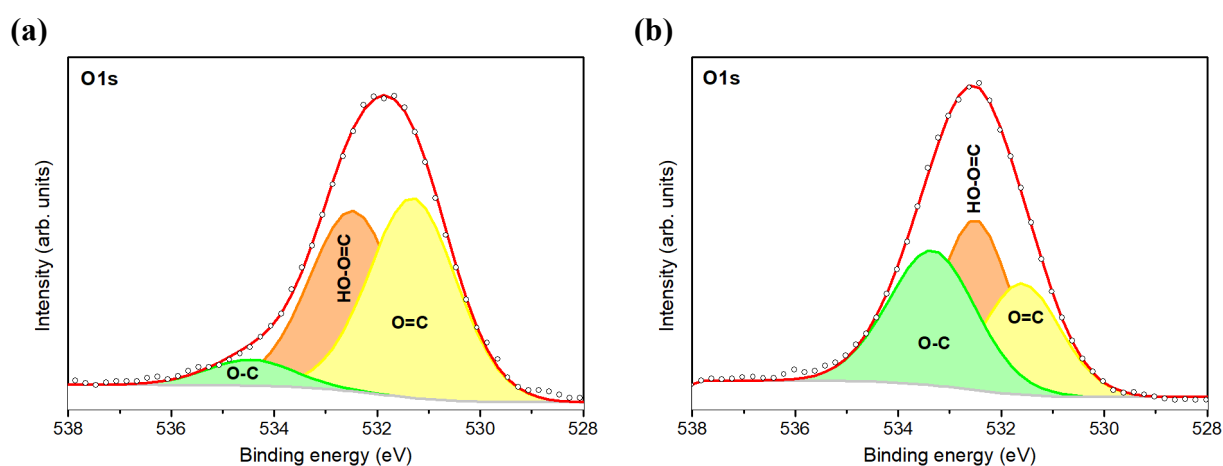


Figure S10. XPS O 1s core level obtained for the sample PPy@Graphene before (a) and after (b) NH₃ gas sensing.

Table S4. Comparison of the NH₃ sensing performance for polypyrrole (PPy)/graphene hybrids operated at room temperature. Sensitivity coefficients calculated as the response (%) / concentration applied. LOD: limit of detection. NA: not available data. *Color code:* Green and Red are for positive and negative features, respectively. Orange is not positive nor negative.

Nanomaterial	Polymerization procedure	Ease of synthesis	Solvent-free	Sensitivity Coefficient	Flow rate (sccm)	Carrier gas	LOD (ppb)	Stability test	Moisture cross-sensitivity test	Repeatability test	Reference
PPy NPs – Graphene	Chemical	Yes	Yes	0.88	100	Air	419	Yes	Yes	Yes	This work
PPy - GO	Chemical	Yes	No	0.029	NA	Air	NA	No	No	No	[1]
Thin PPy layer - Graphene	Electrochemical	No	No	1.7	1000	Air	NA	Yes	Yes	Yes	[2]
PPy – Single Layer Graphene	Electrochemical	No	No	7.5	NA	Air	0.04	No	No	Yes	[3]
PPy - rGO	Chemical	Yes	Yes	0.37	NA	Air/N ₂	NA	No	No	No	[4]
TiO ₂ NPs – Ppy - rGO	Chemical	Yes	No	2.04	NA	N ₂	1000	Yes	Yes	Yes	[5]
PPy film - GO	Electrochemical	Yes	No	0.1	1000	N ₂	NA	No	No	No	[6]

References

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