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An Efficient Polyimide Ammonia Sensor

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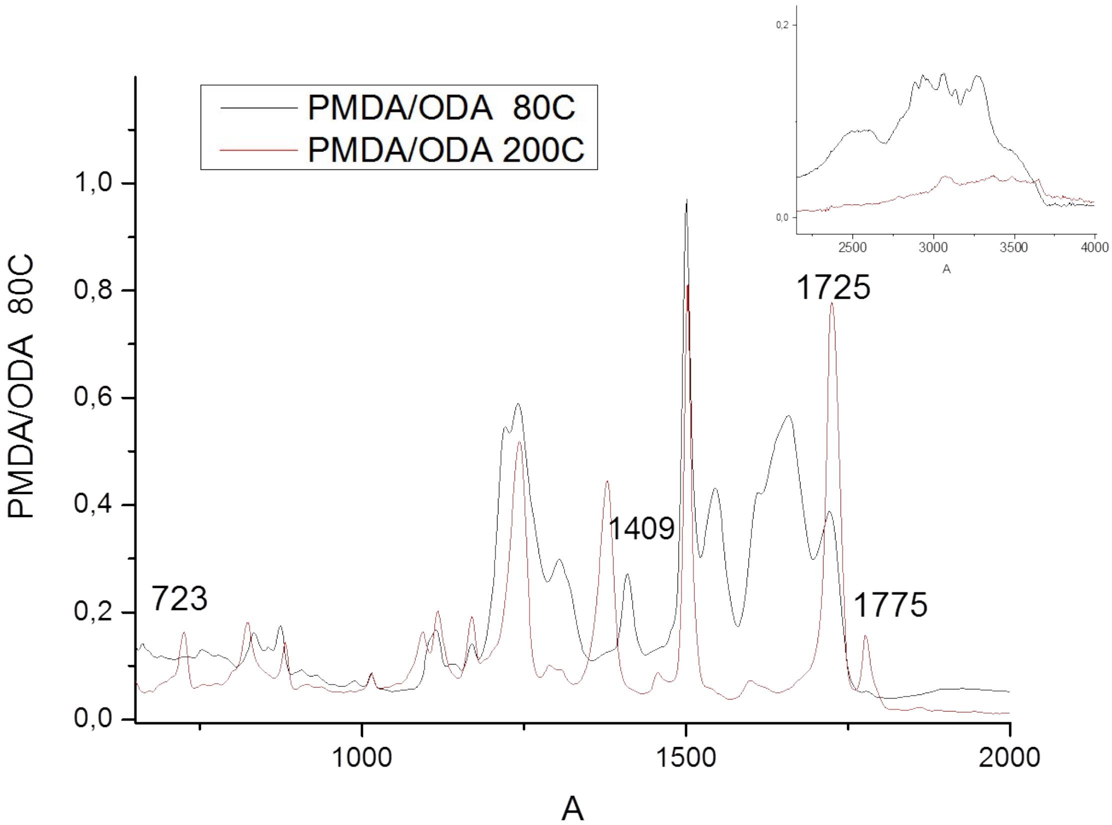
Supporting Information

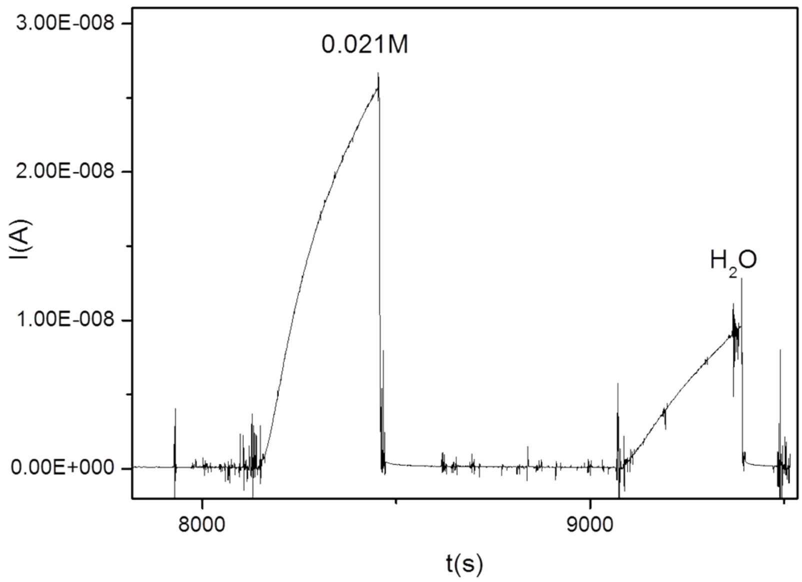
S1: PMDA-ODA curing



S1: FTIR spectra of the uncured (blue) and cured (red) PMDA-ODA films.

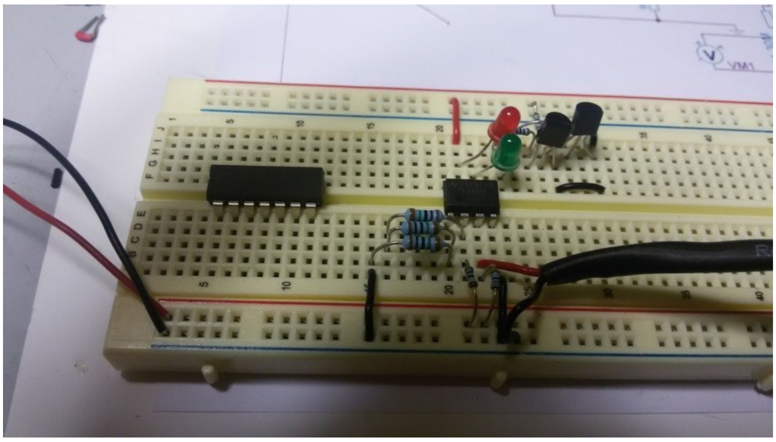
The PMDA-ODA curing involves the condensation of the amide group and hydroxyl group (carried out at 200°C) following the mechanism proposed by Jwo-Huei Jou et al.[1]. As expected, the cured sample shows the typical peak due to $(CO)_2NC$ imide symmetrical stretching centred at 1775 cm^{-1}, meaningful of an efficient curing procedure. This was further confirmed by the band at 3000 cm^{-1}, due to H-bond typical of NH_2 and OH, that disappears after curing. In addition, the absorption peaks at 1550 cm^{-1} (amide I, CNH vibration) and 1409 cm^{-1} disappear, whereas two new peaks appear at 1380 cm^{-1} (imide II, C-N stretching vibration) and 725 cm^{-1} (imide IV, vibration of cyclic C=O)[2].

S2: Water response vs analyte

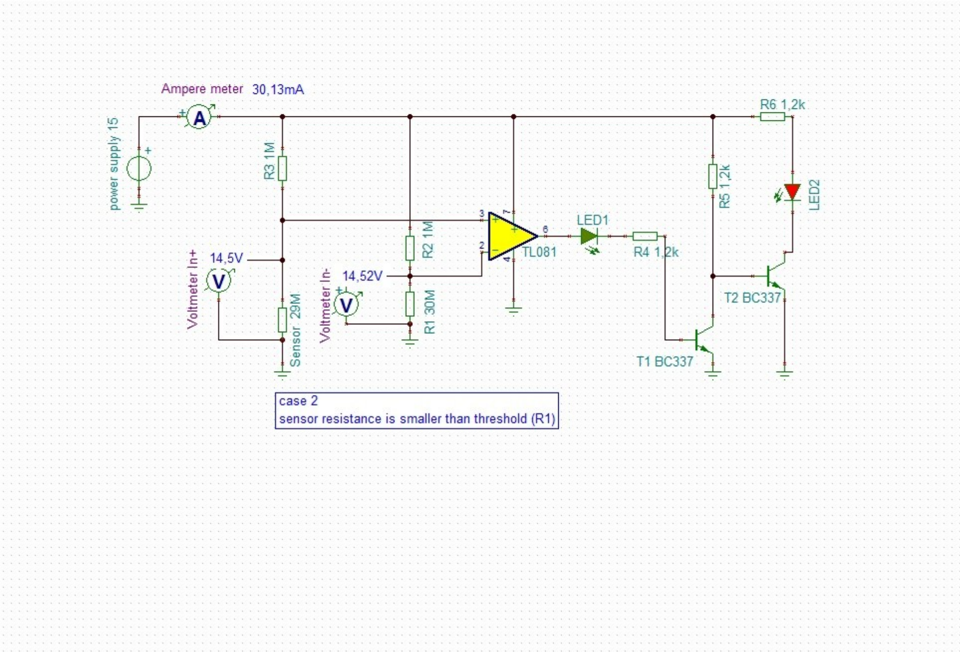


The sensor response for 0.021 M ammonia solution and water. The increase of the electrical current in the presence of water, is much smaller than in the present of ammonia.

S3: Device



S3a: The electrical circuit.



S3b: Schematic diagram of the circuit presented in S2a.

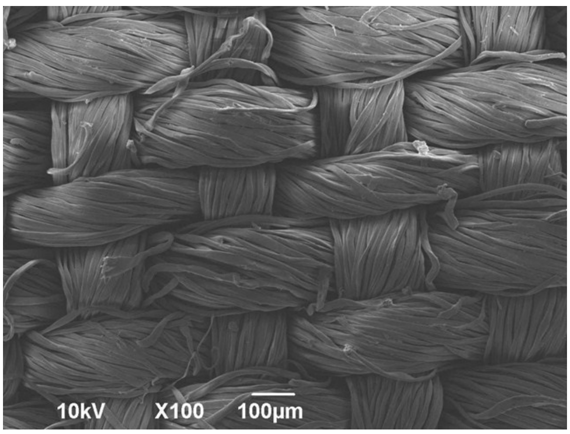
The electronic device to detect ammonia gas has as its core an operational amplifier in comparator configuration and a second stage with a transistor to drive any connected alarm device.

The operational amplifier compares two voltages in input port, V^+ and V^-, and computes their difference. The sensor voltage drop is V^+, a value that changes with the variation of resistivity when ammonia gas is present. V^- is the voltage drop of the threshold resistor (66MΩ), fixed as a limit for the activation of the alarm. The sensor is biased with +12 V. When V^+-V^->0, a voltage close to the one of the positive supply pole (+12V) will be the output. When V^+-V^-<0, a voltage close to the negative supply pole (0V) will be the output.

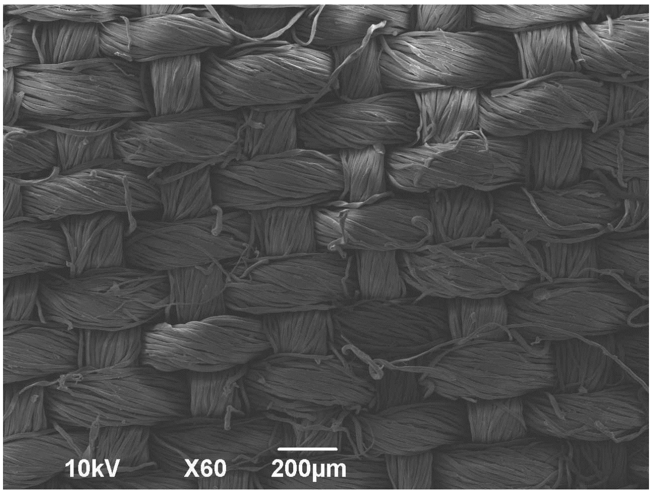
The output is connected to a green LED that indicates when ammonia vapor is not present. Finally, the output goes to a logic port, not with bjt technology, that can drive, when V^+-V^-<0 , a red LED or any other alarm device.

S4: PMDA-ODA on cotton textile

PMDA-ODA was dropped-casted on cotton textile and cured as described in Section 2.1. The polymer convoluted the fibers of the textile, rendering them a little darker than the untreated ones.



S4a: SEM image of the untreated textile, after the curing procedure.



S4b: SEM image of the cotton covered with PMDA-ODA, after curing.

S5: LOD calculation

The LOD was calculated using Henry's law constant as described in Ref. 3.

It is theoretically known that:

$$k_H^{cc} = \frac{c_a}{c_g} \quad (1)$$

where the Henry's solubility, k_H^{cc} , describing the solubility of a gas in an aqueous solution, is expressed as the dimensionless ratio between the aqueous-phase concentration, c_a, of a species and its gas-phase concentration c_g.

Furthermore,

$$k_H^{cc} = k_H \times RT \qquad (2)$$

Where , k_H, is Henry's constant and equals 60 mol/m^{3}Pa, R is the ideal gas constant (0.082 L atm/K mol) and T is the absolute temperature.

From (1) and (2) one can calculate c_g, when c_a is known (in the present case c_a=59.5 ppm).

1. Jou, J. H.; Huang, P. T., Effect of thermal curing on the structures and properties of aromatic polyimide films. *Macromolecules* **1991,** *24* (13), 3796-3803.
2. Nishino, T.; Kotera, M.; Inayoshi, N.; Miki, N.; Nakamae, K., Residual stress and microstructures of aromatic polyimide with different imidization processes. *Polymer* **2000,** *41* (18), 6913-6918.

3. R. Sander, Compilation of Henry's law constants (version 4.0) for water as solvent. Atmos. Chem. Phys., 15, 4399-4981, 2015.