Electronic Supplementary Information (ESI)

Ammonia vapour sensing properties of *in-situ* polymerized conducting PANI-nanofiber/WS_2 nanosheet composites

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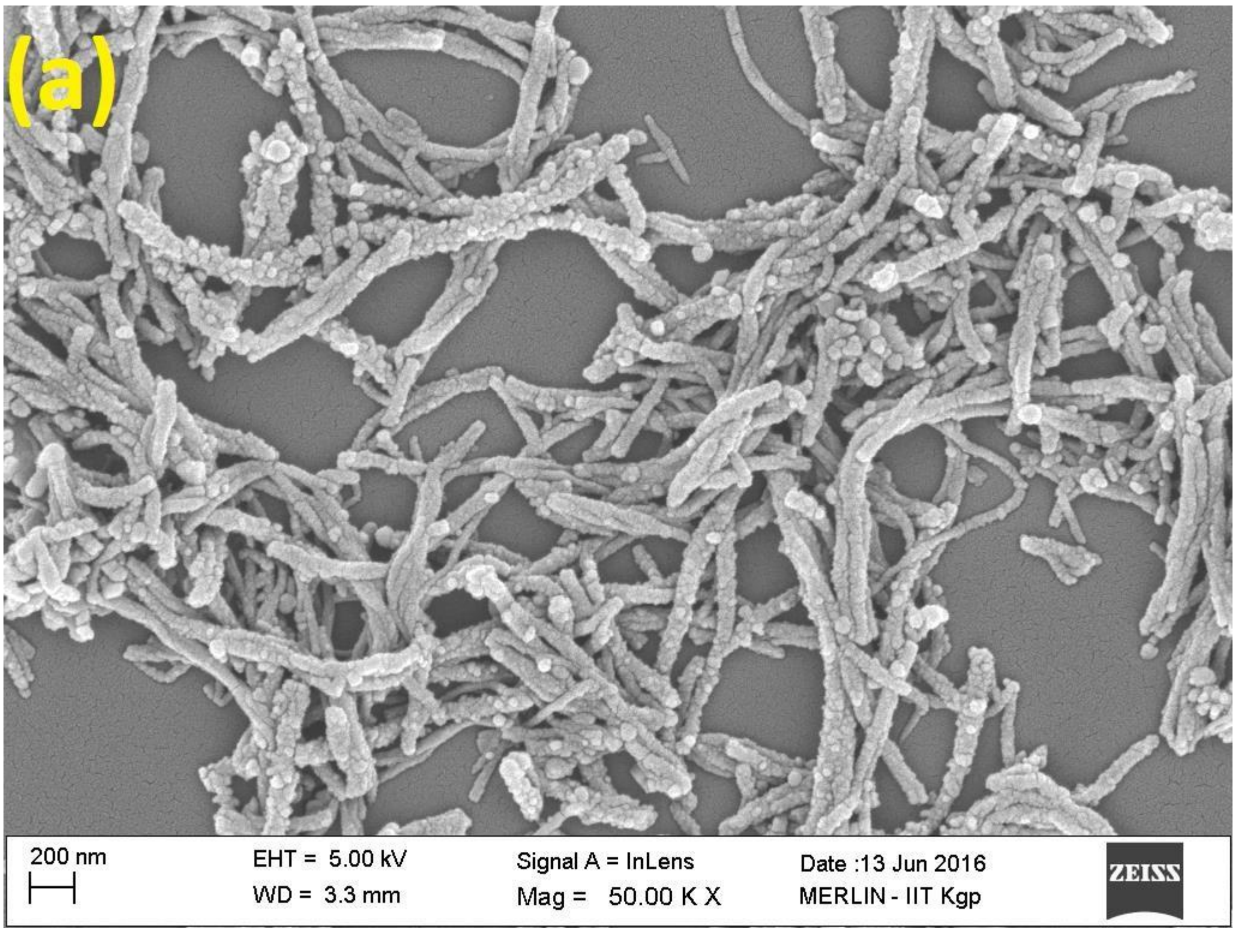
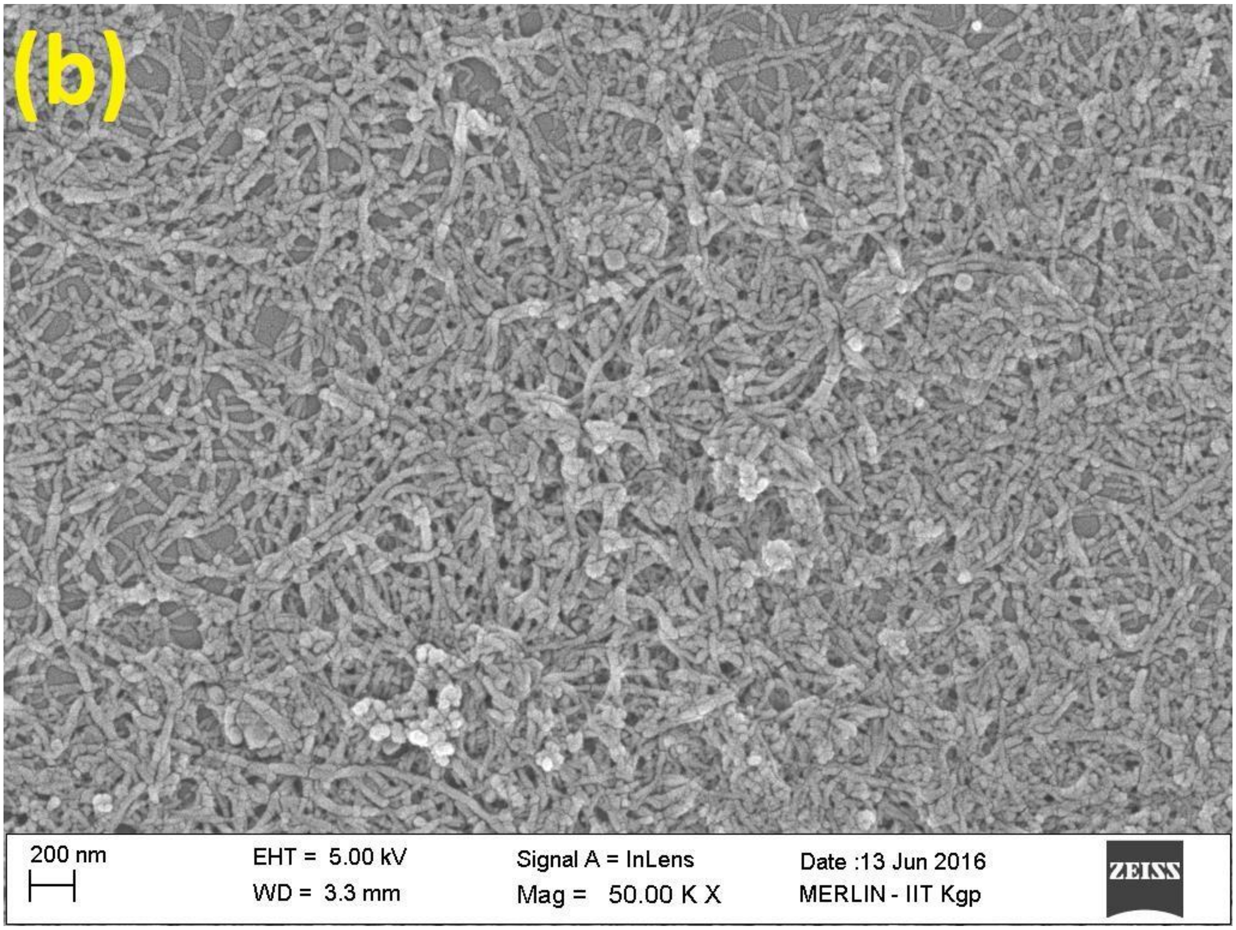
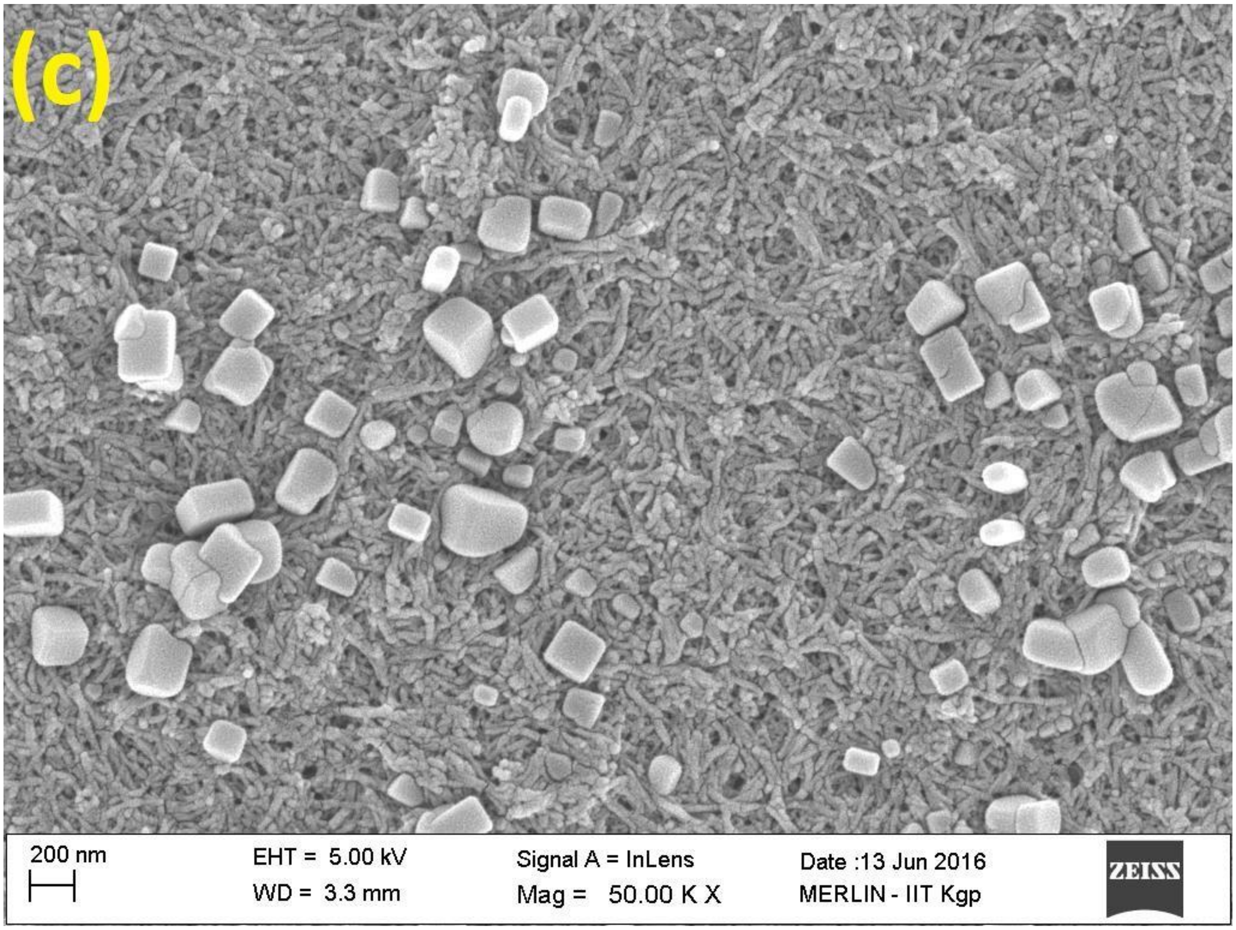
1. FESEM images




(b)
200 nm
EHT = 5.00 kV
WD = 3.3 mm
Signal A = InLens
Mag = 50.00 K X
Date :13 Jun 2016
MERLIN - IIT Kgp
ZEISS


(c)
200 nm
EHT = 5.00 kV
WD = 3.3 mm
Signal A = InLens
Mag = 50.00 K X
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MERLIN - IIT Kgp
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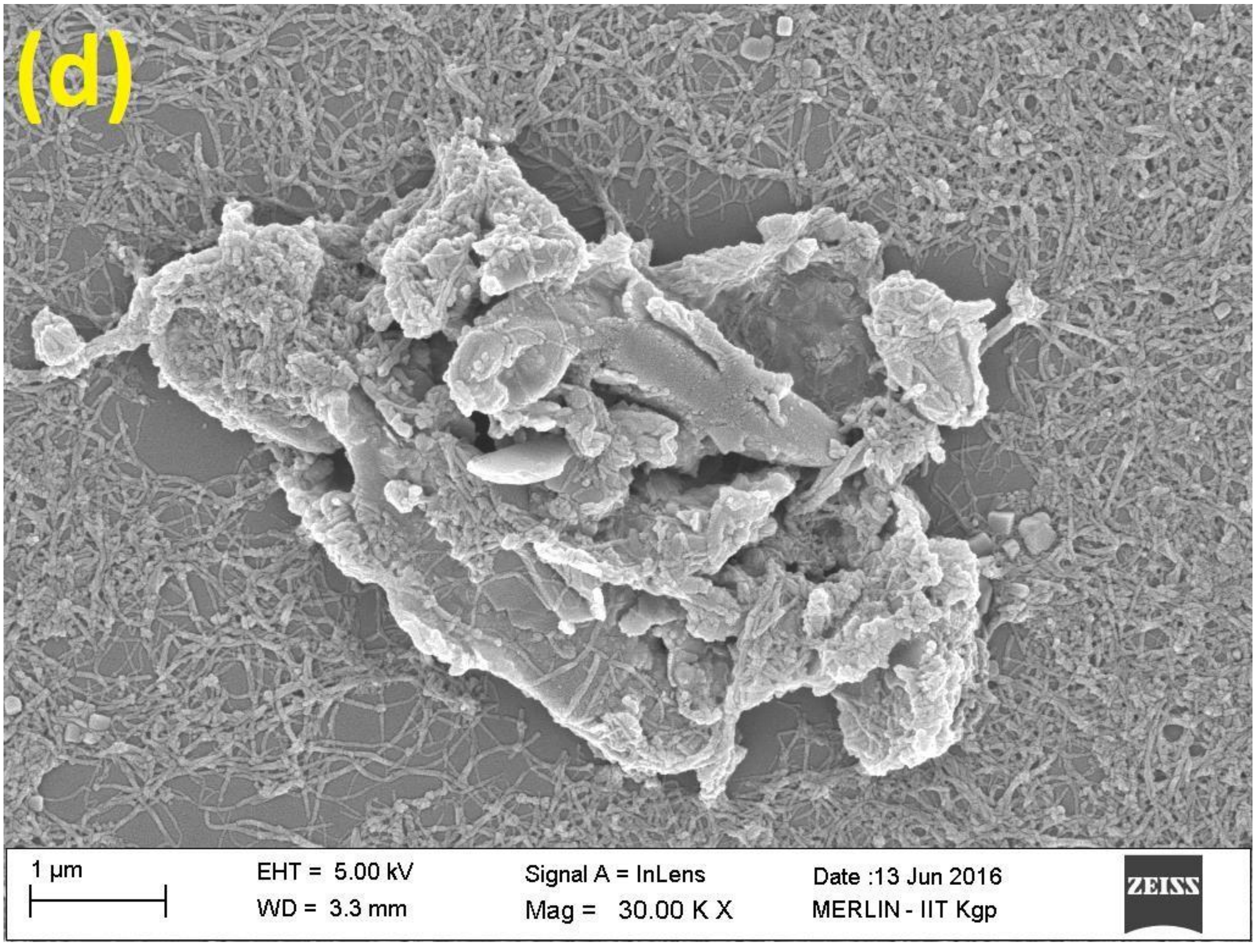
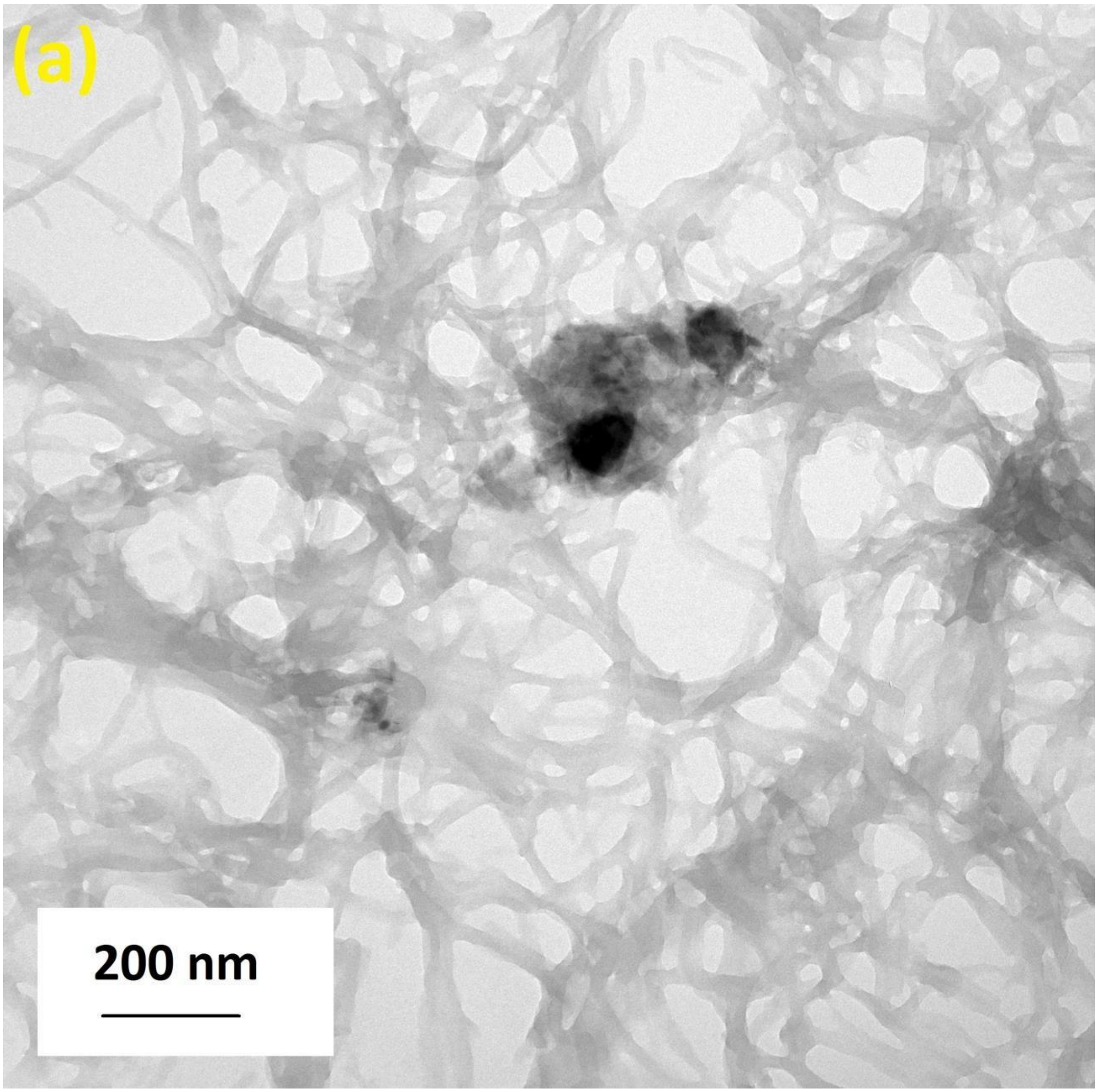
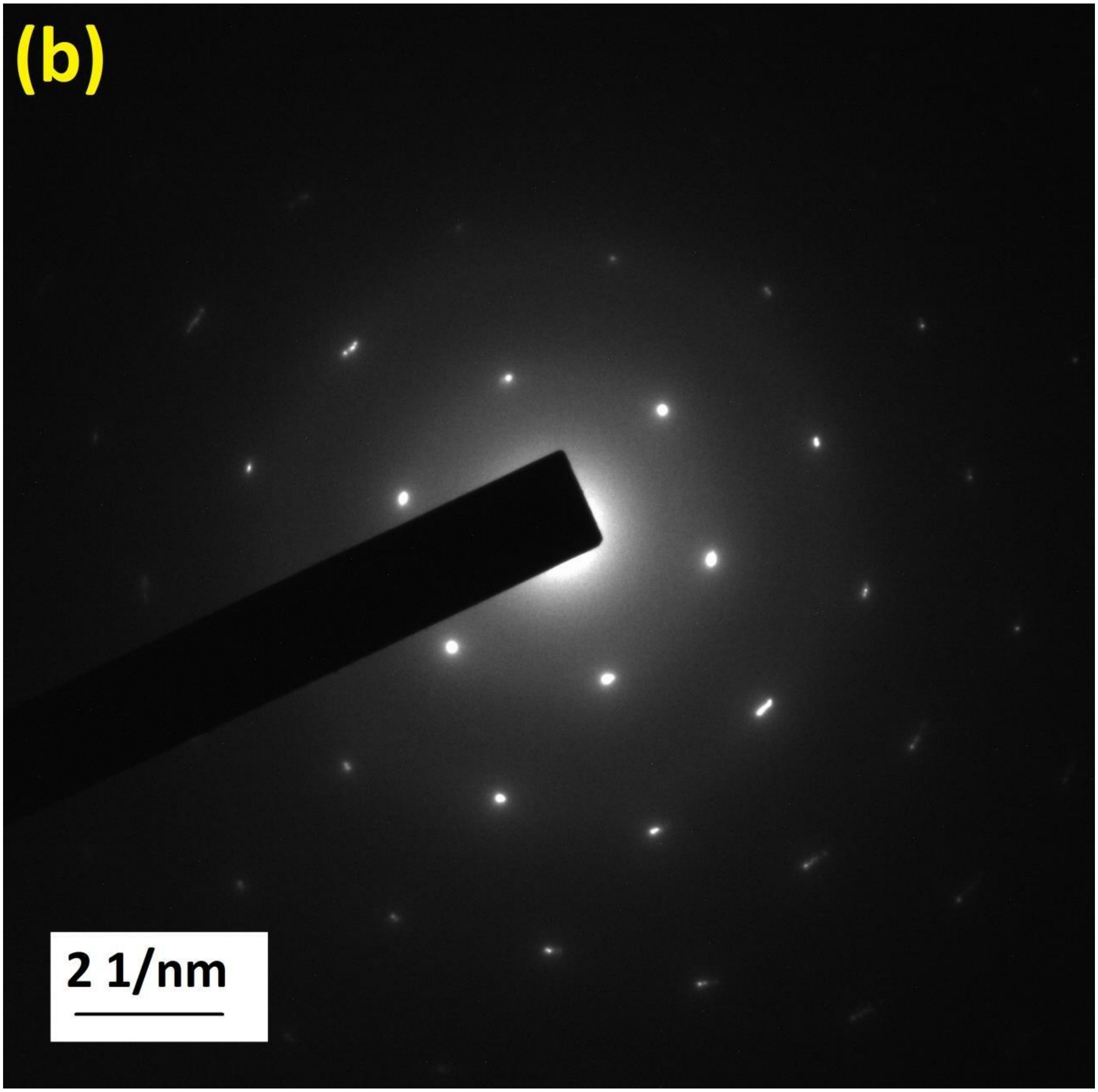
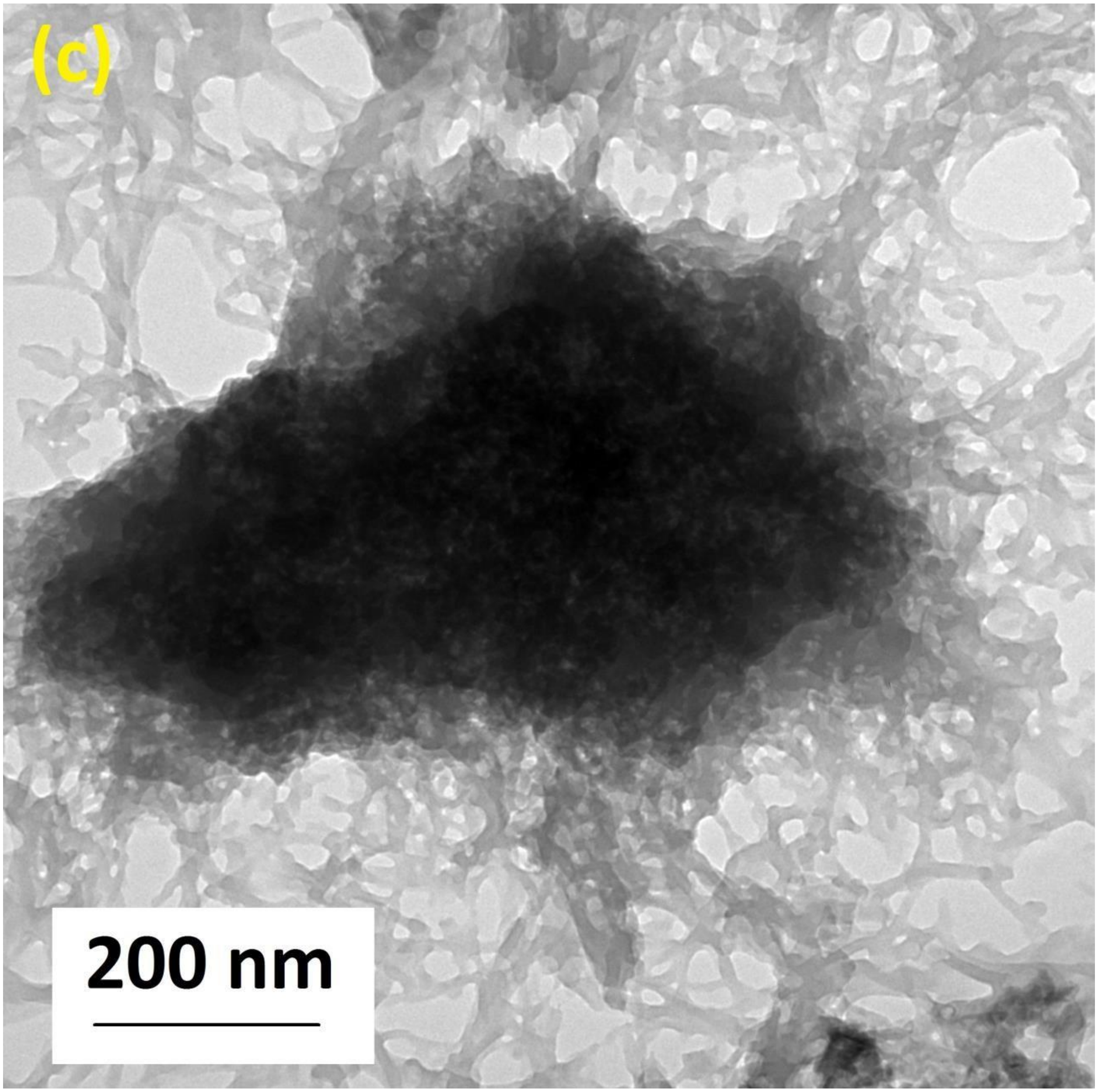


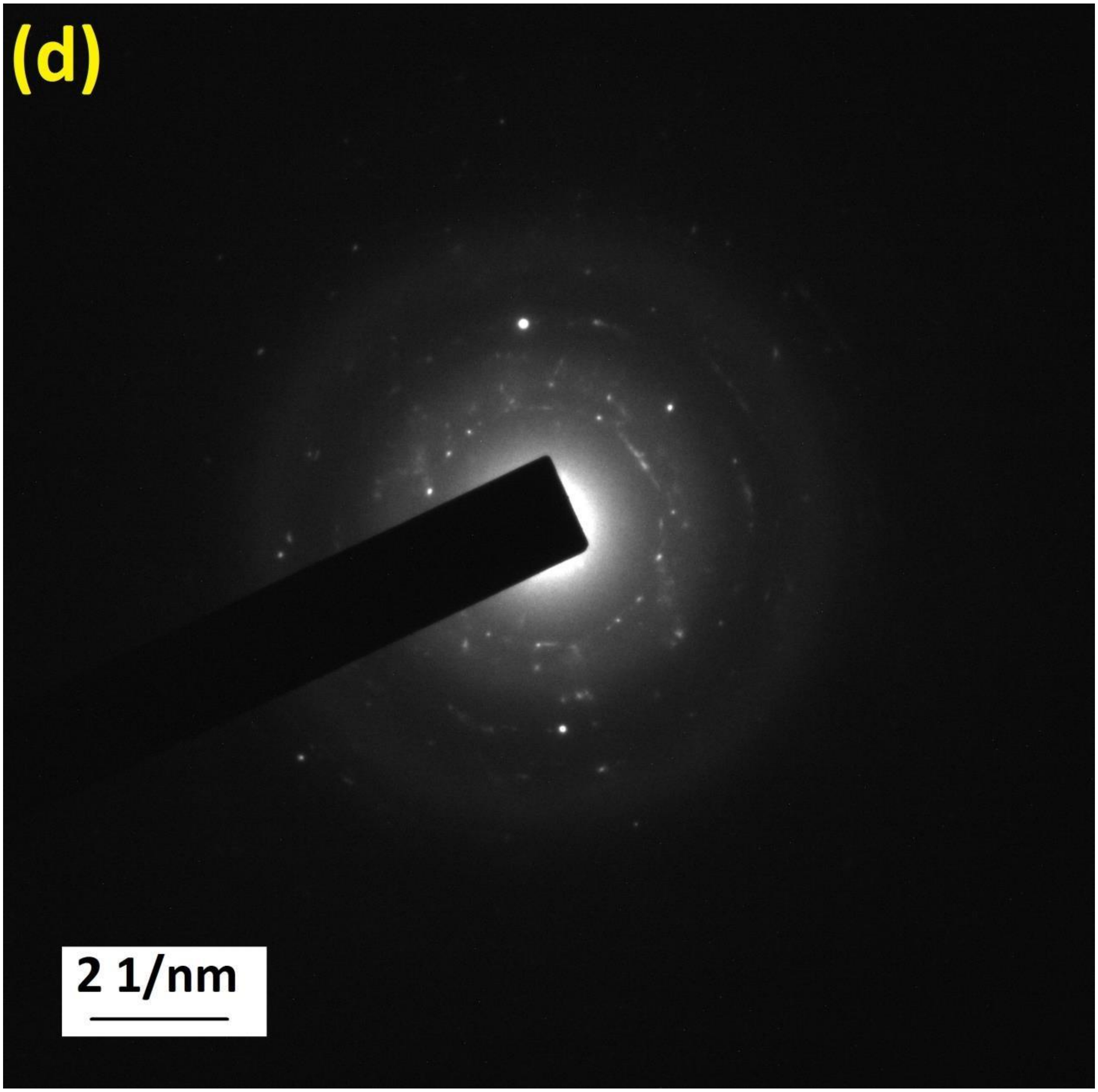
Fig. S1. FESEM image of (a) Pure PANI (b) PANI/WS_2 (5 wt.%) (c) PANI/WS_2 (20 wt.%) (d) PANI/WS_2 (30 wt.%).

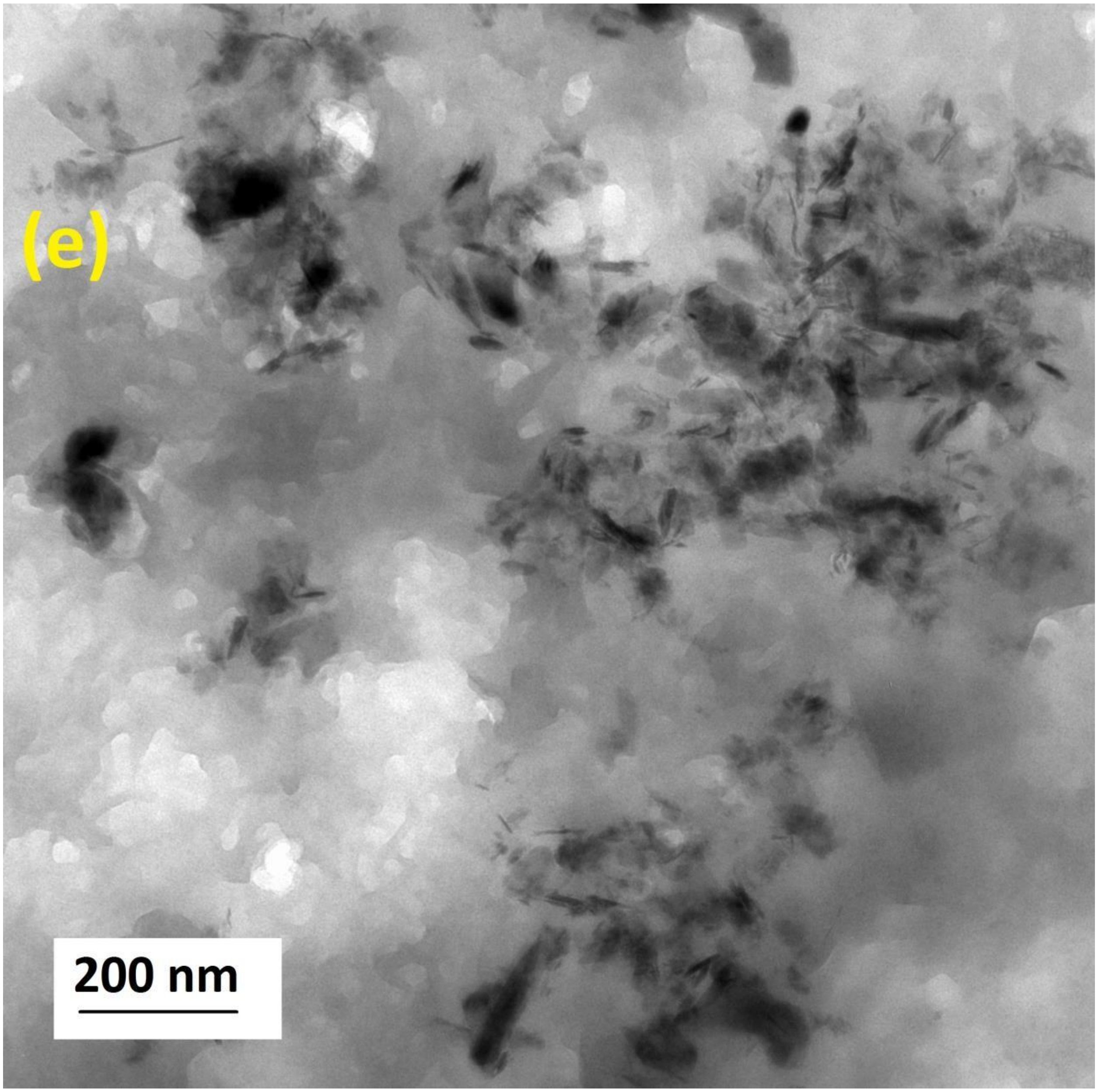
2. TEM images




(b)
2 1/nm


(c)
200 nm


(d)
2 1/nm


(e)
200 nm

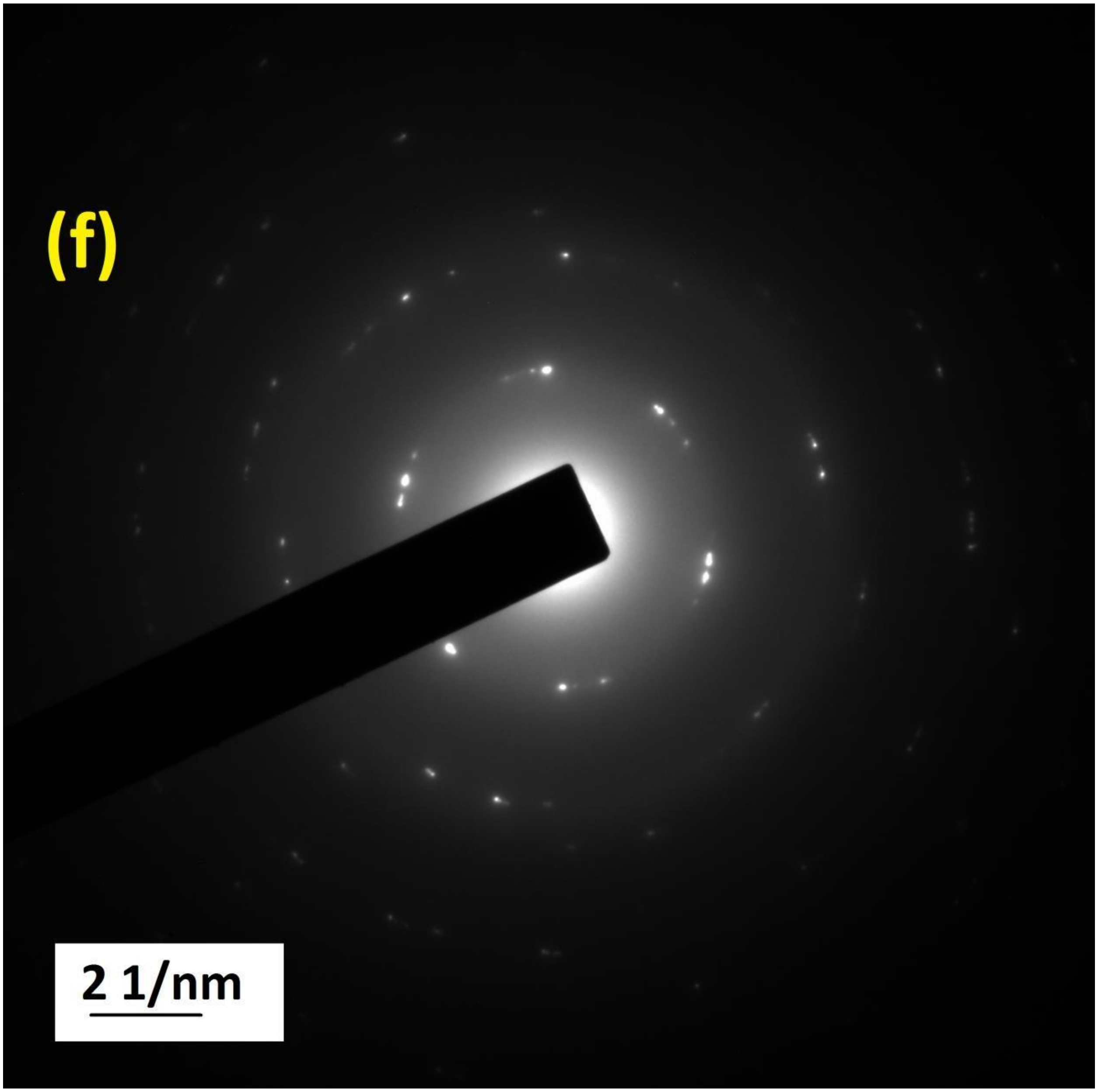


Fig. S2. (a) TEM image of PANI/WS_2 (5 wt%) nanocomposite and (b) its SAED pattern (c) TEM image of PANI/WS_2 (20 wt%) nanocomposite and (d) its SAED pattern (e)TEM image of PANI/WS_2 (30 wt%) nanocomposite and (f) its SAED pattern.

3. XRD

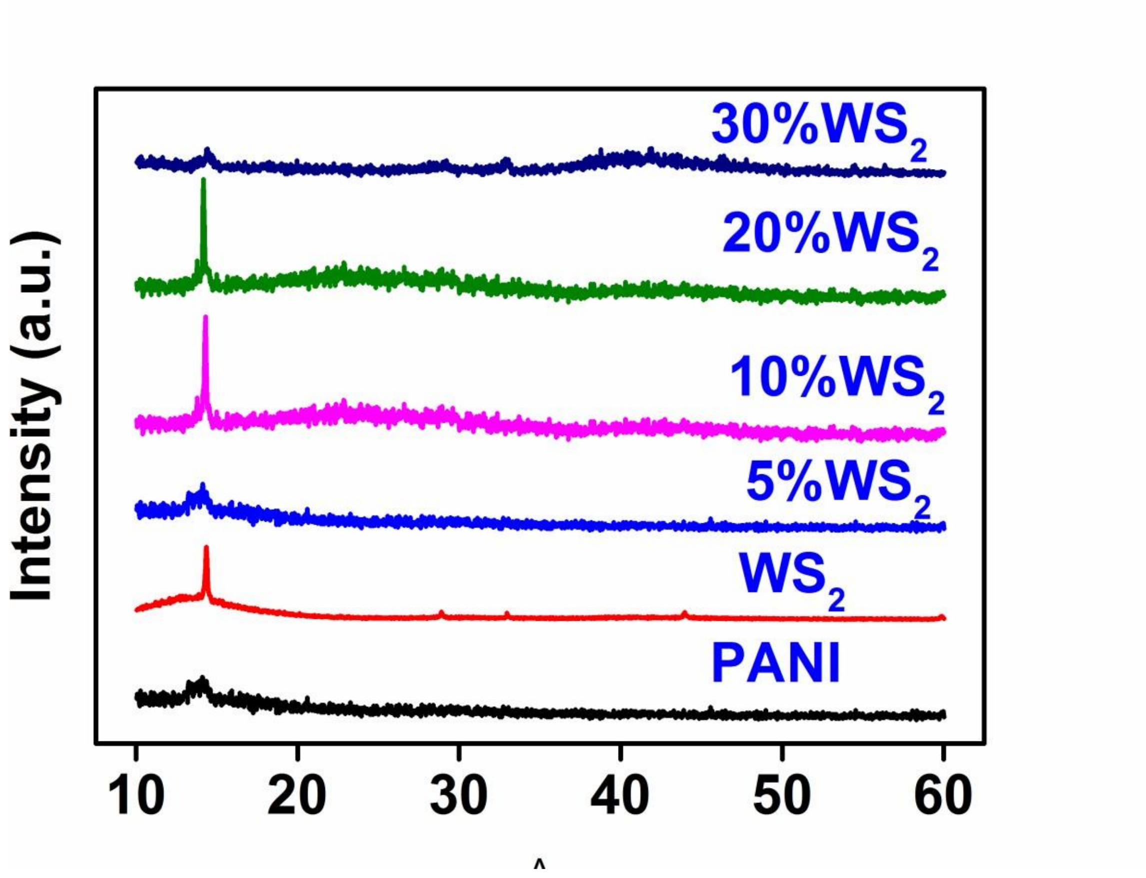


Fig. S3. XRD pattern of nanocomposites and nanomaterials.

4. Raman Spectra

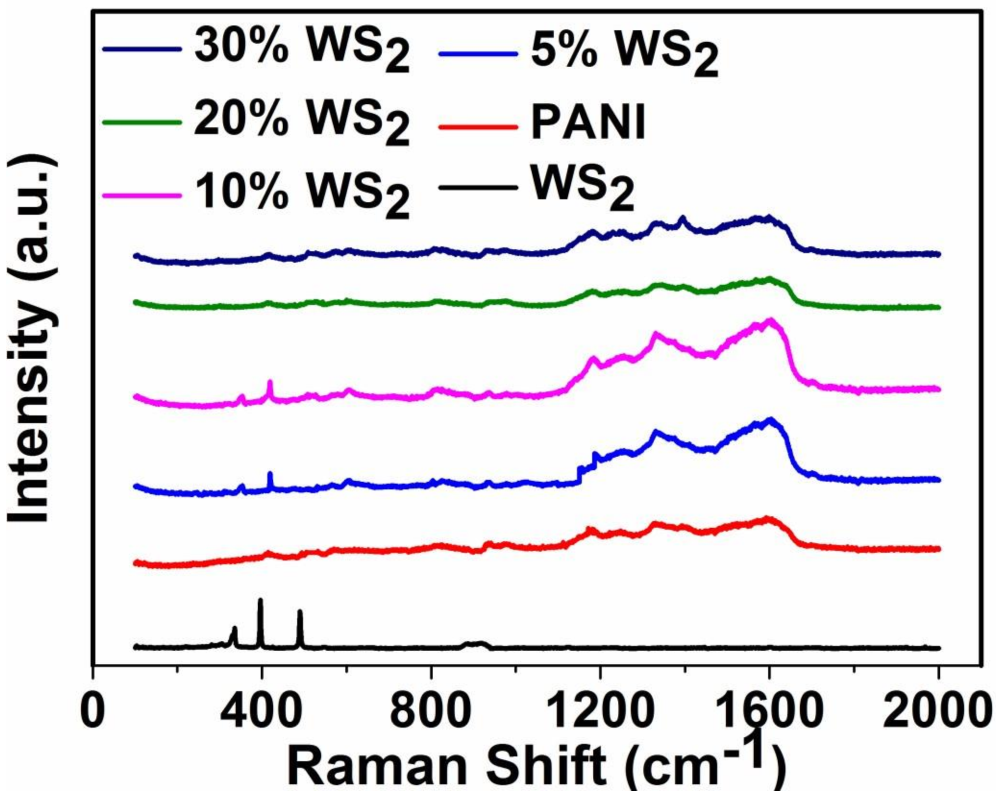


Fig. S4. Raman Spectra of different nanostructured materials synthesized in this work.

5. Response from as-synthesized PANI nanofibers based ammonia sensors

The response of pure PANI nanofibers based ammonia sensor is shown in Figure S5.

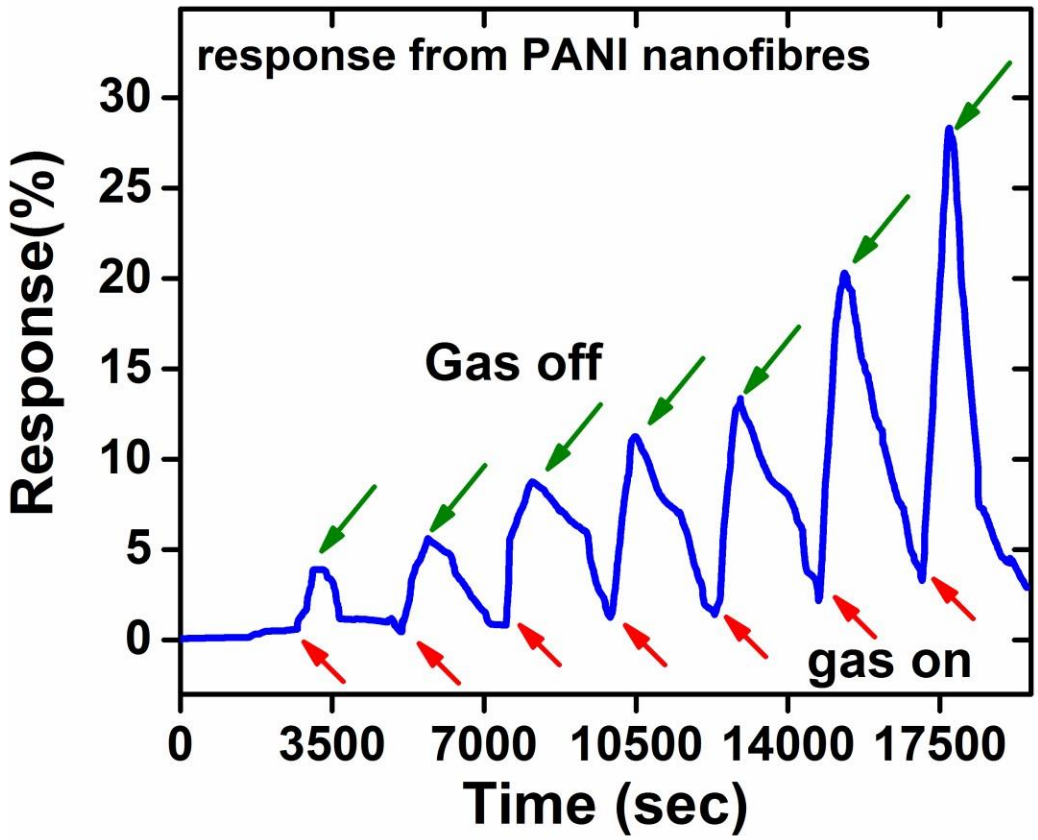


Fig. S5. Response from as-synthesized PANI.

6. I-V Characteristics of sensing devices loaded with different sensing nanomaterials

The current (I)-voltage (V) characteristics of PANI, WS_2, and PANI/WS_2(10%) based devices at room temperature is shown in Figure S6.

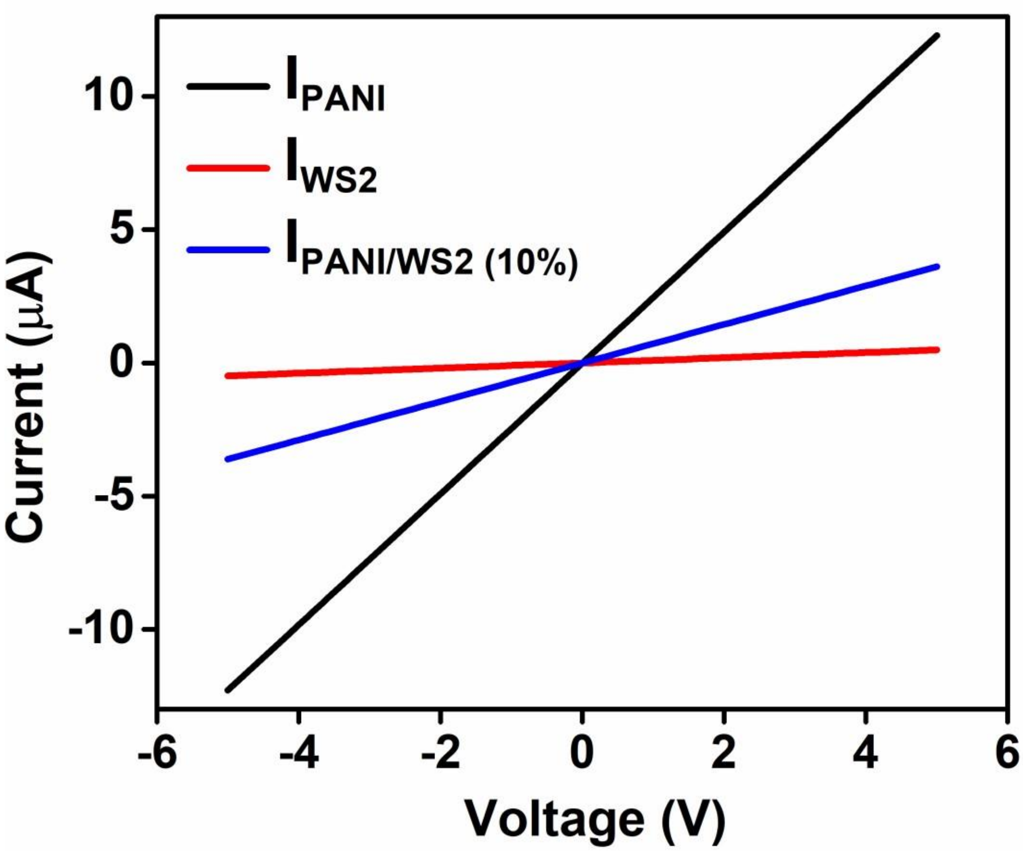


Fig. S6. current (I)-Voltage (V) characteristics of devices loaded with (i)PANI nanofibers (ii) WS_2 (iii) PANI/WS_2 (10%) nanocomposite.

7. Generation of Ammonia vapours from aqueous ammonia solution

We have obtained ammonia vapour from aqueous ammonia solution which has been discussed in the literature as well [1]. Briefly, the calculation is shown below:

We have used a 25% ammonia solution which has a density of 0.91 g/ml.

Since 100 ml of this solution has 25×0.91 g of ammonia

And subsequently, 1 L (1000 ml) of this solution has $25\times 0.91\times 10$ g $=25\times 0.91\times 10^4$ mg

Concentration= $25\times 0.91\times 10^4$ mg/1L=227500 ppm

Different ammonia concentration was prepared by diluting this solution by DI water.

Furthermore, the values were confirmed by calculating ammonia concentration in the chamber by another method. In this method, weight % (wt.%) of ammonia in the aqueous ammonia solution was first calculated as

$$wt.\%\ \left(NH_3\right)=\frac{w_{NH_3}}{w_{NH_3}+w_{H_2O}}\times 100 \quad (1)$$

Further, vapour over aqueous ammonia solution was calculated from wt% of NH_3 vs partial pressure of NH_3 (P_{NH3}) curve as shown below (for 0℃ of NH_3 , this condition is maintained by keeping ammonia solution in ice bath during measurement). This curve was obtained from ammonia data sheet.

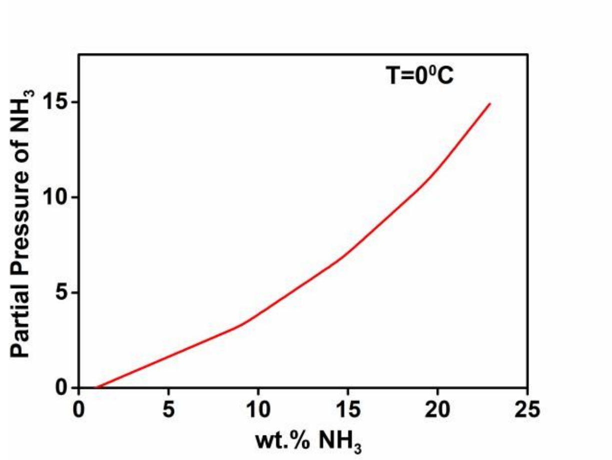


Fig. S7. Vapour over aqueous ammonia solution.

After obtaining P_{NH3} the concentration of ammonia in the chamber is calculated as

$$\text{Total concentration of NH}_3\,(in\ ppm) = \frac{P_{NH_3}}{P_{air}(760mm \text{ of Hg})} \times 10^6 \quad (2)$$

Further, concentration of NH_3 in the chamber was calculated as

$$\text{conc. of NH}_3 \text{ in the chamber } (in\ ppm) = \frac{\text{flow of NH}_3\,(\text{in sccm})}{\text{Total Flow(in sccm)}} \times (\text{total conc. of NH}_3\,(in\ ppm)) \quad (3)$$

8. Humidity Sensing Properties of PANI/WS$_2$ (10%) nanocomposite

We have also tested the capabilities of the sensing device towards humidity sensing. An opposite behavior was observed in the response than ammonia i.e. the current was found to be increasing with relative humidity (RH%) level due to proton conductivity which is an established fact in literature [2]. Therefore we can say that PANI/WS$_2$ nanocomposite based sensor is selective towards ammonia as compared to humidity as the response of our device to even low ammonia concentration is much higher (i.e.81% @ 200 ppm ammonia). However a small change in current for high humidity change from 25% RH (6020 ppm of water molecule) to 80% RH or(20370 ppm of water molecule).

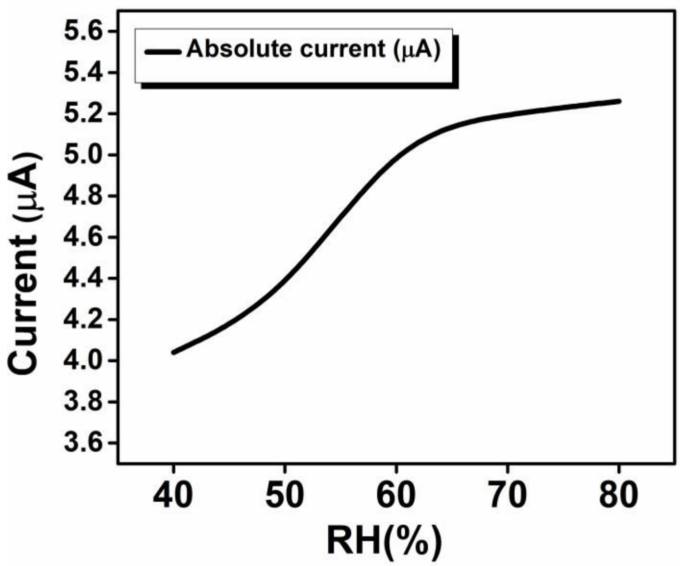


Fig. S8. Variation in Current and Response (%) with RH (%).

9. Effect of Humidity on Ammonia Sensing Properties of PANI/WS_2 (10%) nanocomposite and response of PANI/WS_2 (10%) nanocomposite to dry ammonia gas

Further we measured effect of humidity on ammonia sensing properties of PANI/WS_2(10%) nanocomposite. The comparison of the dynamic responses of the sensor in presence of humidity (here 60% RH) and in absence of this is shown in Figure S9(a). It was found that the overall response decreases by 4-6% in presence of 60% RH. Sorption of H_2O molecule on backbone of PANI nanofibers (by formation of hydrogen bond) is an established fact. Therefore, competitive sorption between H_2O and NH_3 molecules is responsible for this decrement in response [3]. We have also measured response of our sensor towards dry ammonia gas. The response of the sensor to this gas is shown in Figure S9(b). An enhancement in response of 1.5-7% was observed as compared to aqueous ammonia vapours.

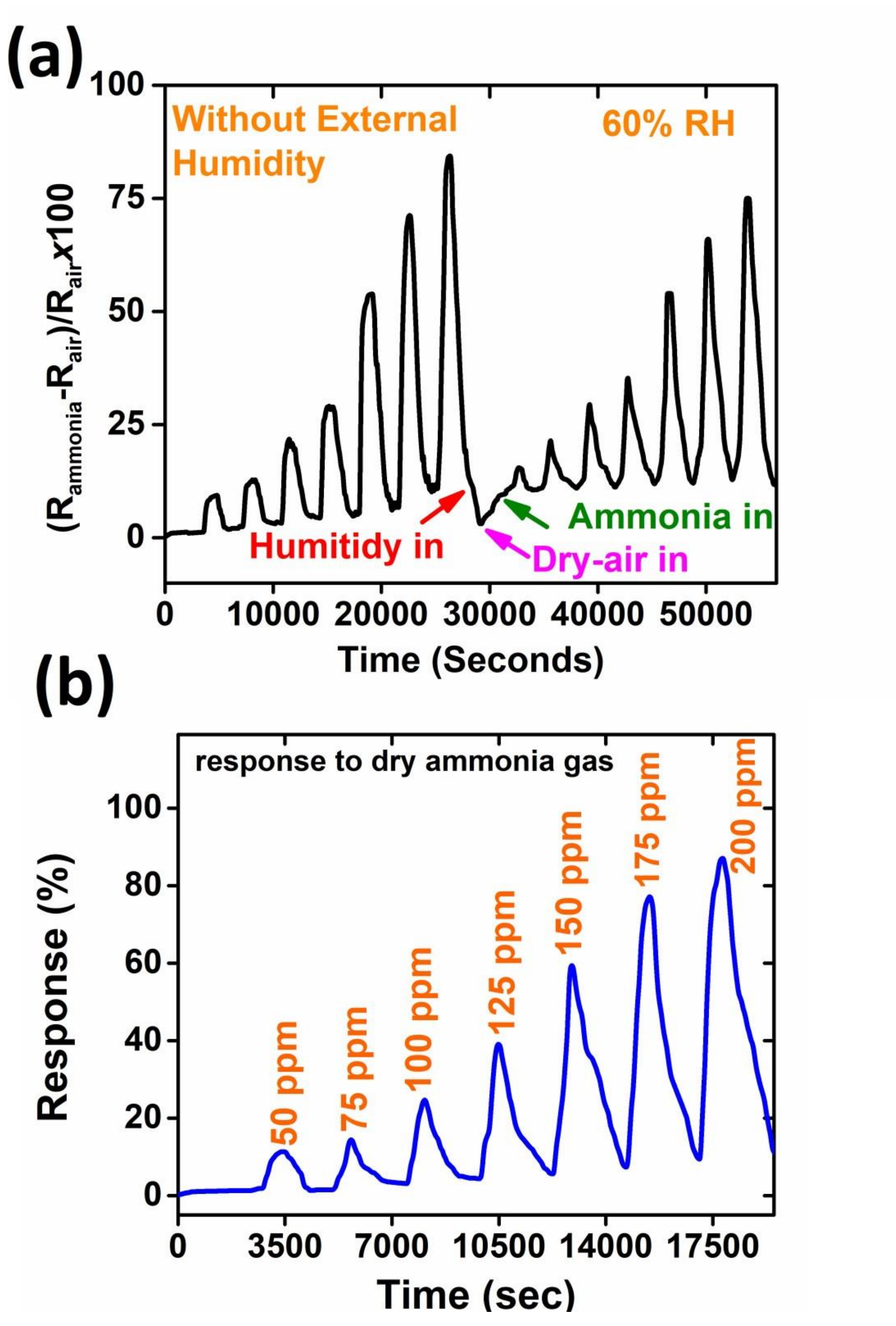


Fig. S9. (a) Response in presence of 60% RH and in absence of humidity (b) And response to dry ammonia gas.

10. Resistance change in PANI/WS_2 (10%) nanocomposite

Figure S10 shows the change in resistance in PANI/WS_2 (10%) nanocomposite . The response is shown in Figure 6 (a) of the main manuscript.

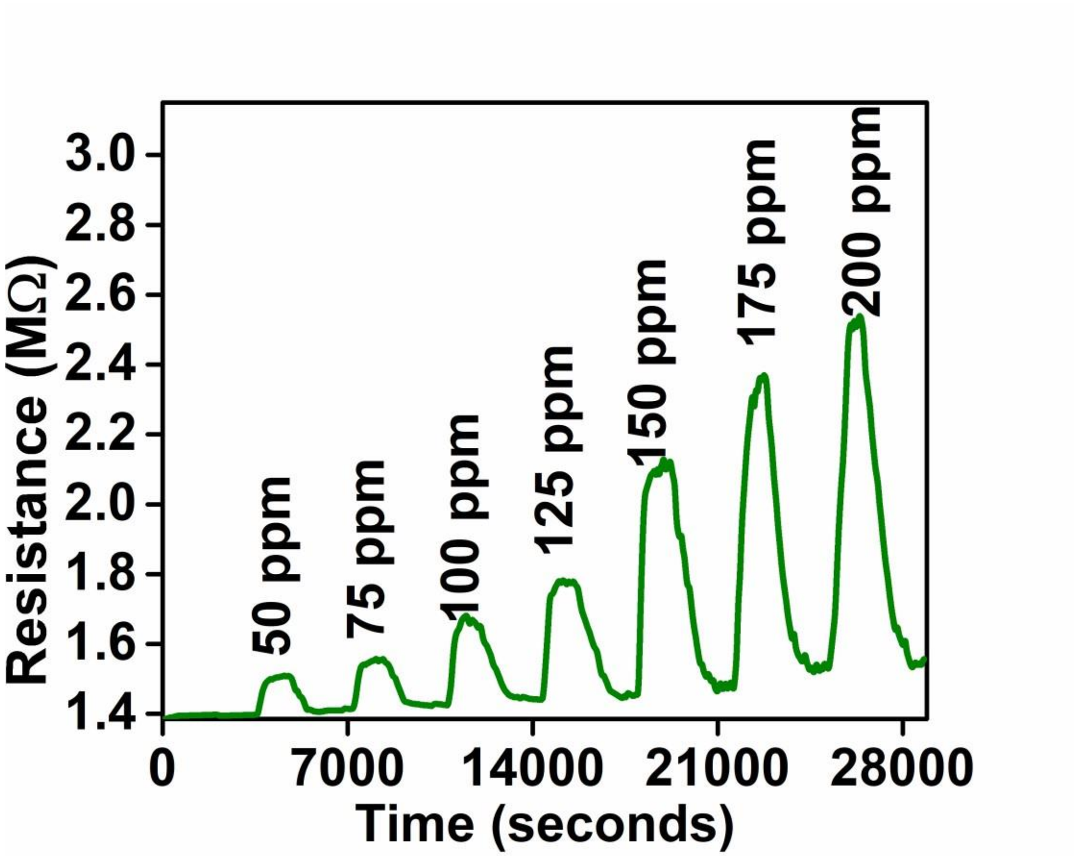


Fig. S10. Variation in Current at different concentration of ammonia in PANI/WS_2(10%) nanocomposite based ammonia sensor and its corresponding response (in inset).

References

[1] S. Pandey, K.K. Nanda, Au Nanocomposite Based Chemiresistive Ammonia Sensor for Health Monitoring, ACS Sensors, 1(2016) 55-62.

[2] Nohria, R.; Khillan, R. K.; Su, Y.; Dikshit, R.; Lvov, Y.; Varahramyan, K., Humidity sensor based on ultrathin polyaniline film deposited using layer-by-layer nano-assembly. *Sensors and Actuators B: Chemical* **2006,** *114* (1), 218-222.

[3] Matsuguchi, M.; Okamoto, A.; Sakai, Y., Effect of humidity on NH3 gas sensitivity of polyaniline blend films. *Sensors and Actuators B: Chemical* **2003,** *94* (1), 46-52.