Supplementary Information

Chemiresistive NH_3 detection at sub-zero temperatures by polypyrrole loaded $Sn_{1-x}Sb_xO_2$ nanocubes

Nirman Chakraborty and Swastik Mondal*

CSIR Central Glass and Ceramic Research Institute, 196, Raja S. C. Mullick Road, Jadavpur, Kolkata-700032, India

Corresponding author: swastik_mondal@cgcri.res.in

Table 1: Lattice parameters from Le'Bail refinement

Sample	ATO_0.05	ATO_0.05_PPY
Space group	$P4_2/mnm$	$P4_2/mnm$
a(Å), c(Å) α(degrees)	4.740(2), 3.190(2) 90	4.740(2), 3.189(2) 90

Table 2: Hall coefficient and carrier mobility values of all samples.

Sample	n/p type		Carrier mobility (m^2/V.s)
	200K	250K	
ATO_0.05	n type	n type	3.370×10^{-3} (electrons)
PPY	p type	p type	1.51210^{-3} (holes)
ATO_0.05_PPY	(p type) Hall coefficient 0.00115 ΩmT^{-1}	(p type) Hall coefficient 0.00413 ΩmT^{-1}	1.370×10^{-3}(electrons)(~2 times more than ATO_0.05) 3.512×10^{-3} (holes) (~2 times more than PPY)

Table 3: Sensor composition from ICP analysis.

Sample	Sb:Sn
ATO_0.03	0.025
ATO_0.05	0.048

Table 4: Sensor coating details.

Sensor	Average coating thickness (µm)
ATO_0.03_PPY	32
ATO_0.05_PPY	35

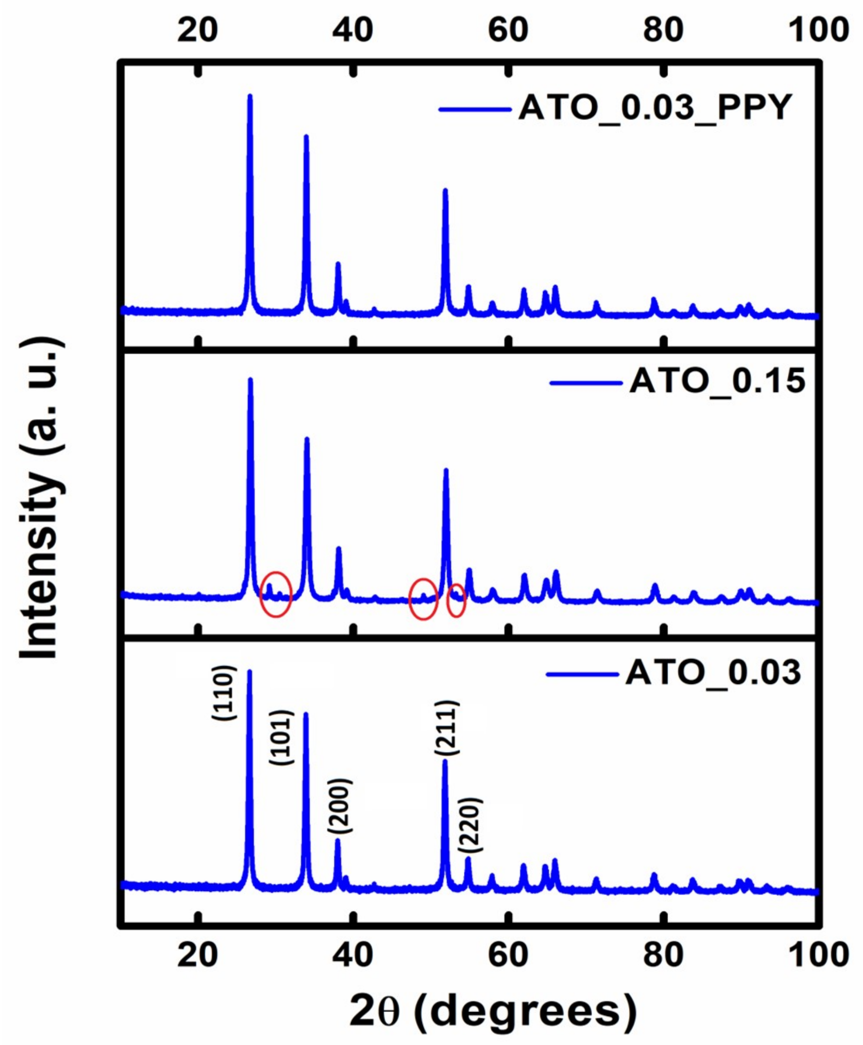

Figure S1: Room temperature powder X-ray diffractograms of antimony doped tin oxide samples (ATO_0.03 and ATO_0.15) and polypyrrole loaded antimony doped tin oxide (ATO_0.03_PPY) sample. Formation of unwanted phases in ATO_0.15 has been shown by red circling the peaks related to that phase.

Figure S2: Arrangement for low temperature ammonia sensing.

Figure S3: Low temperature enclosure for where the sensor has been placed.

Figure S4: Temperature detection during cooling of sensor enclosure.

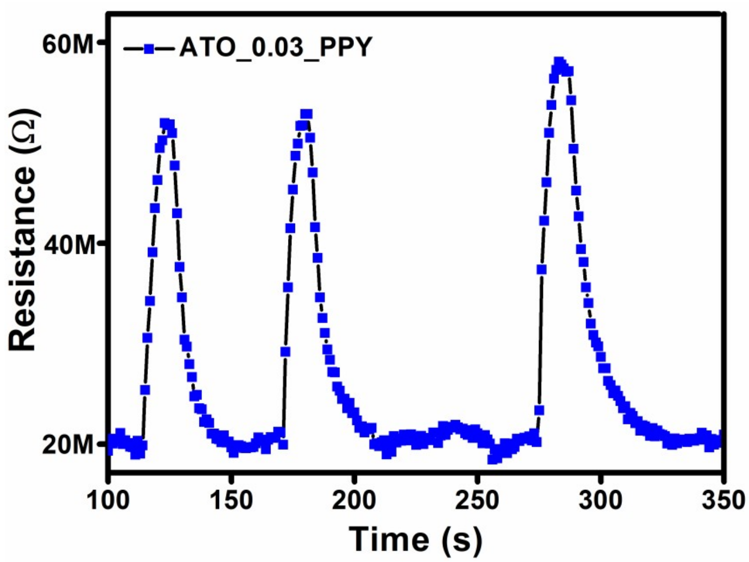

Figure S5: 20 ppm ammonia sensing responses of ATO_0.03_PPY sample at -21°C.

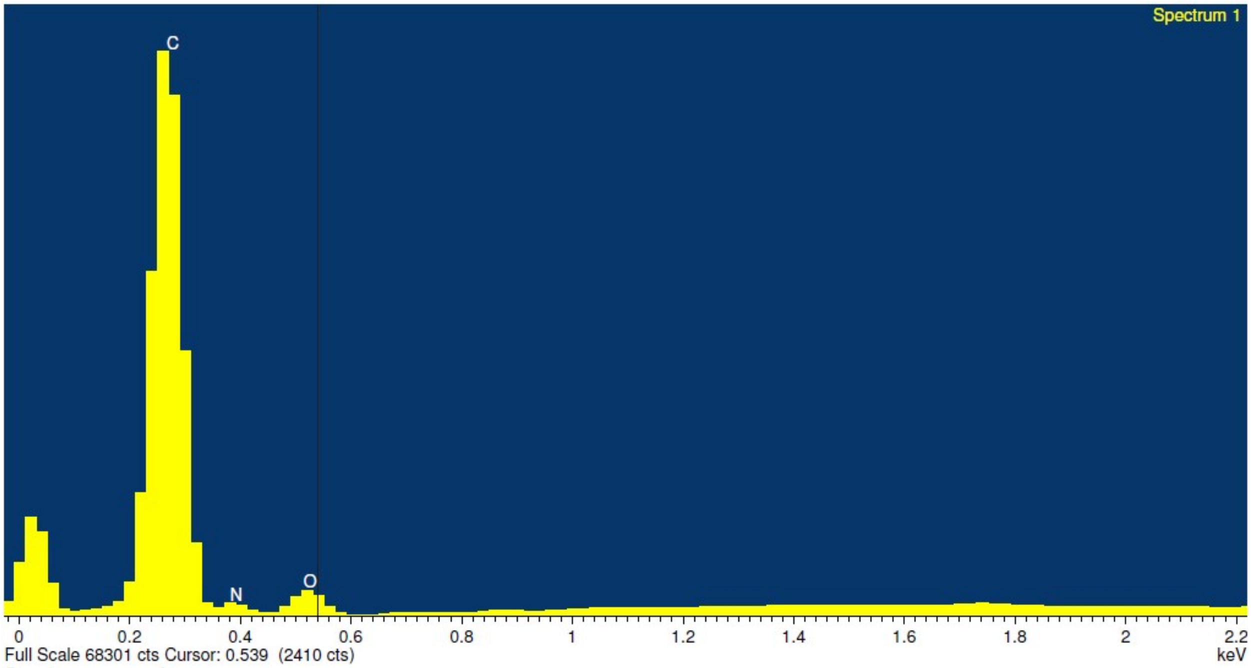

Figure S6: Surface EDX spectrum of polypyrrole (PPY) sample.

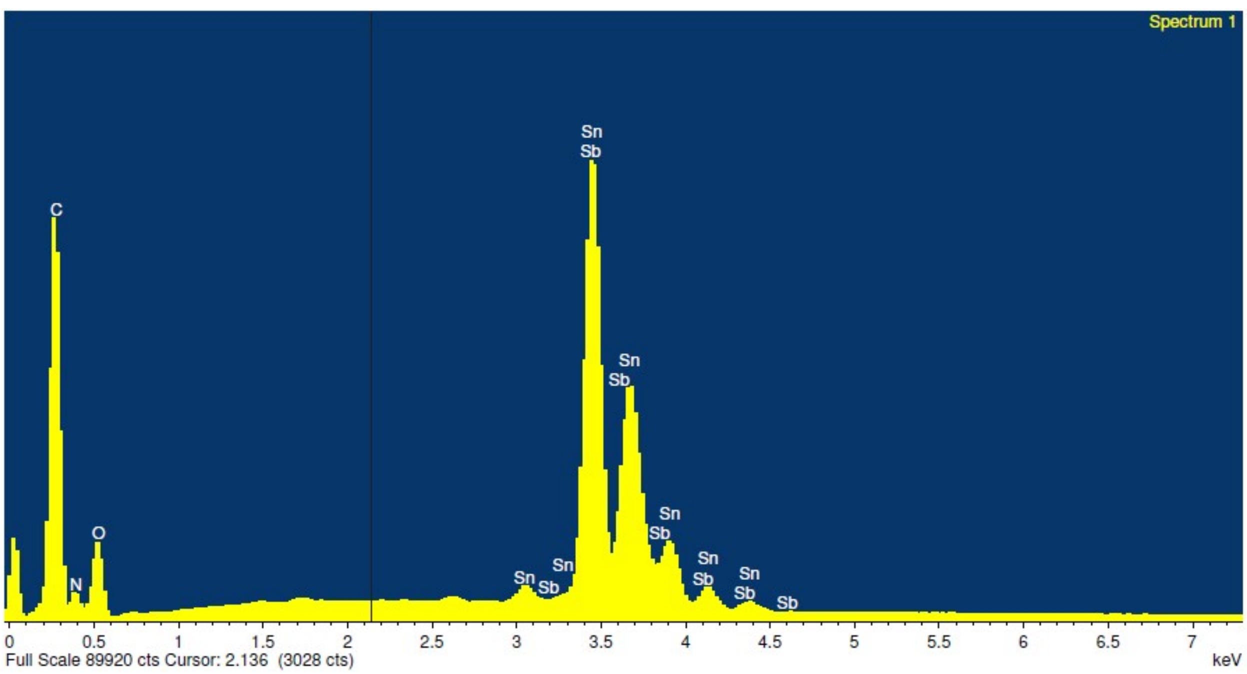

Figure S7: Surface EDX spectrum of polypyrrole loaded antimony doped tin oxide (ATO_0.05_PPY) sample.

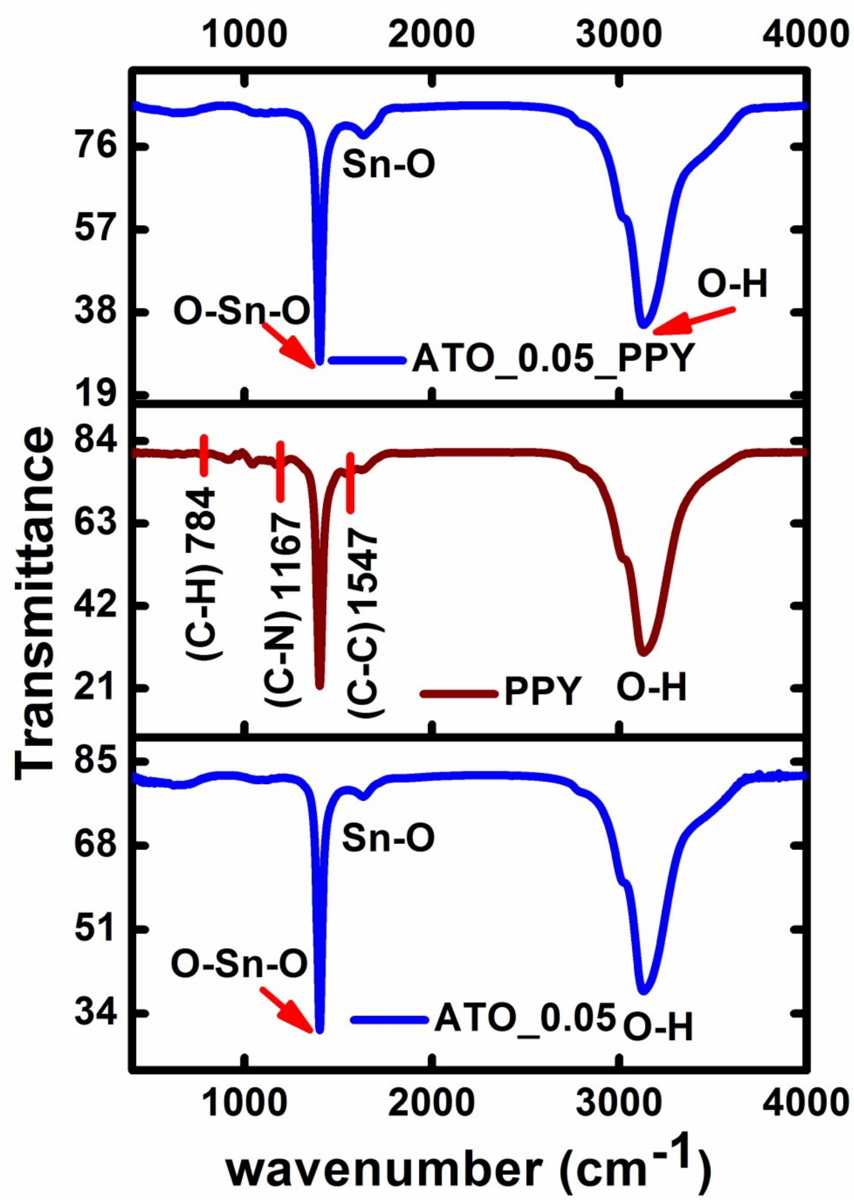

Figure S8: Room temperature FTIR spectra of antimony doped tin oxide (ATO_0.05), polypyrrole (PPY) and polypyrrole loaded antimony doped tin oxide (ATO_0.05_PPY) samples.

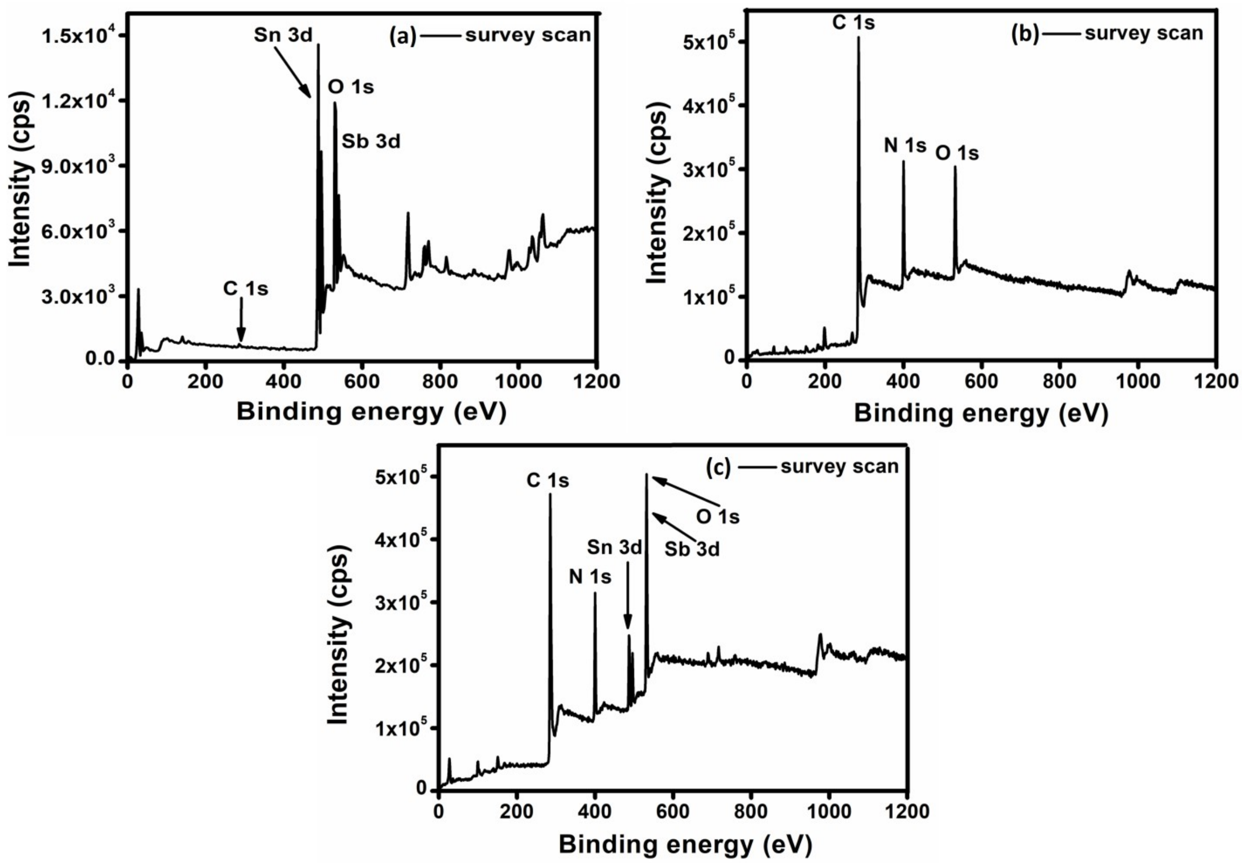

Figure S9: XPS survey scan of (a) antimony doped tin oxide (ATO_0.05) (b) polypyrrole (PPY) and (c) polypyrrole loaded antimony doped tin oxide (ATO_0.05_PPY) samples respectively.

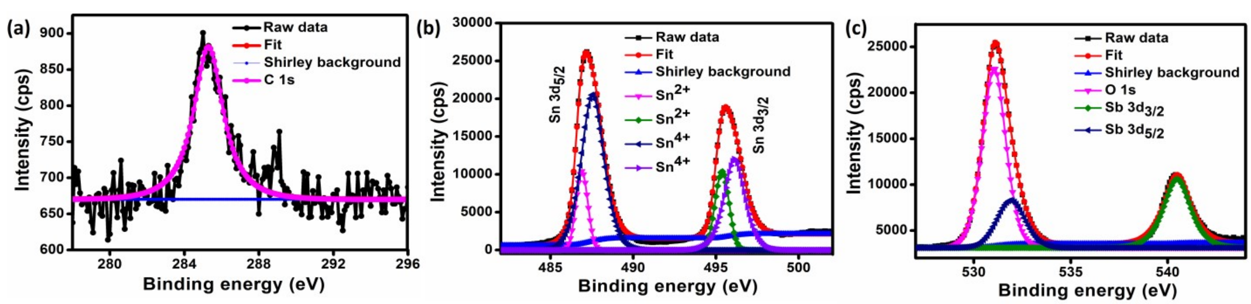

Figure S10: XPS core level (a) C 1s (b) Sn 3d (c) O1s and Sb 3d spectra of antimony doped tin oxide (ATO_0.05) sample.

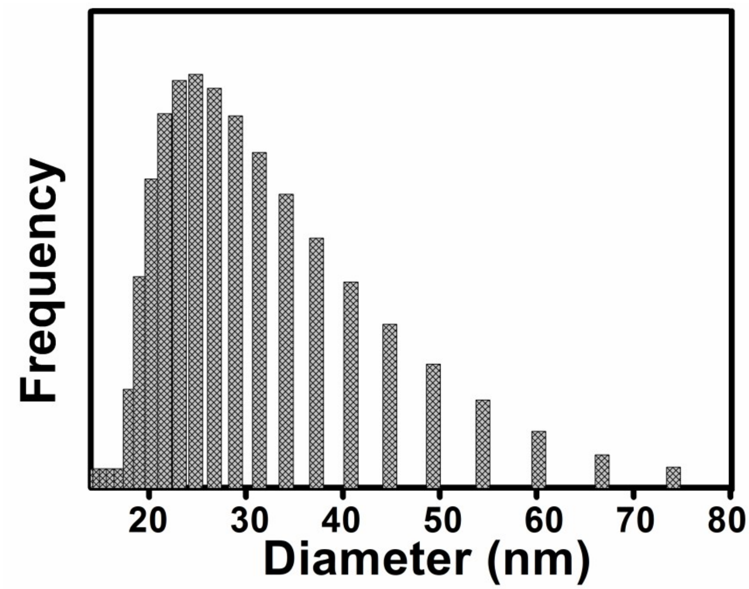

Figure S11: DLS pattern of antimony doped tin oxide (ATO_0.05) sample.

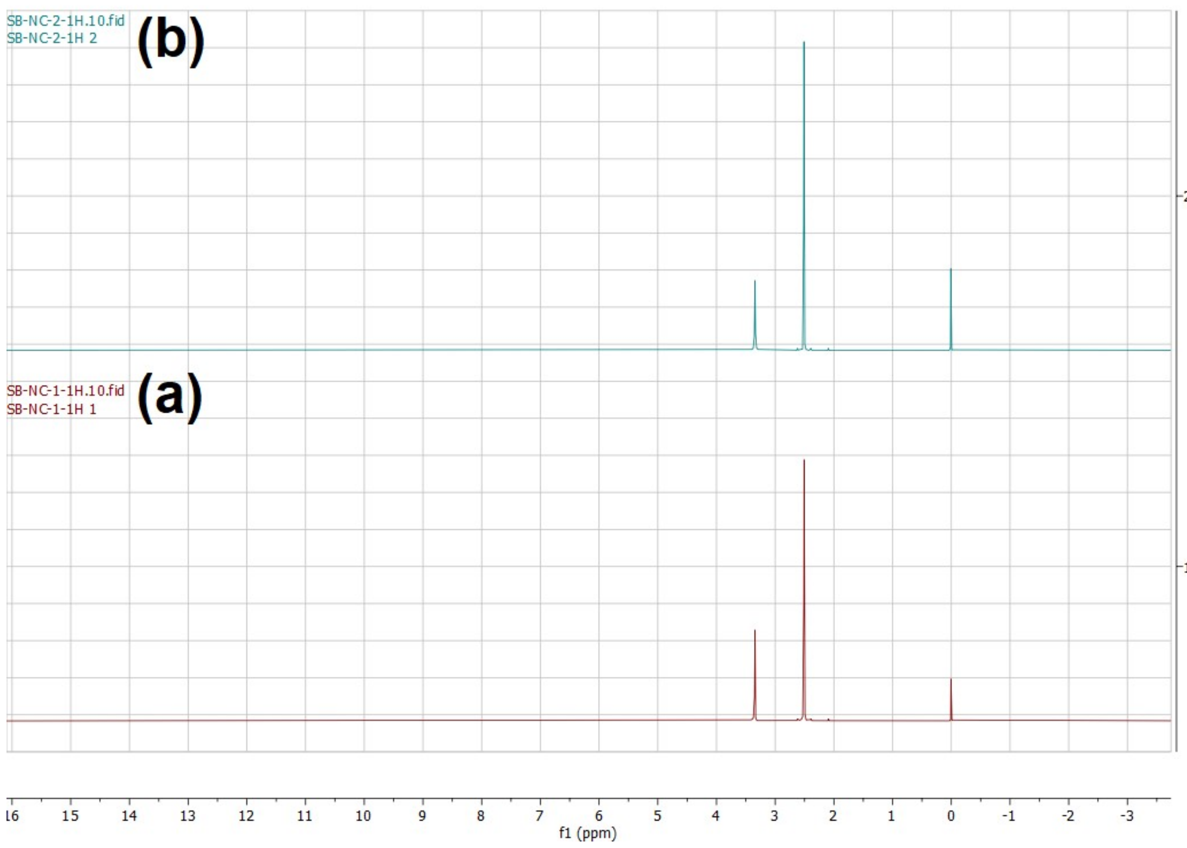

Figure S12: NMR spectra of (a) polypyrrole sample (PPY) and (b) polypyrrole loaded antimony doped tin oxide (ATO_0.05_PPY) sample.

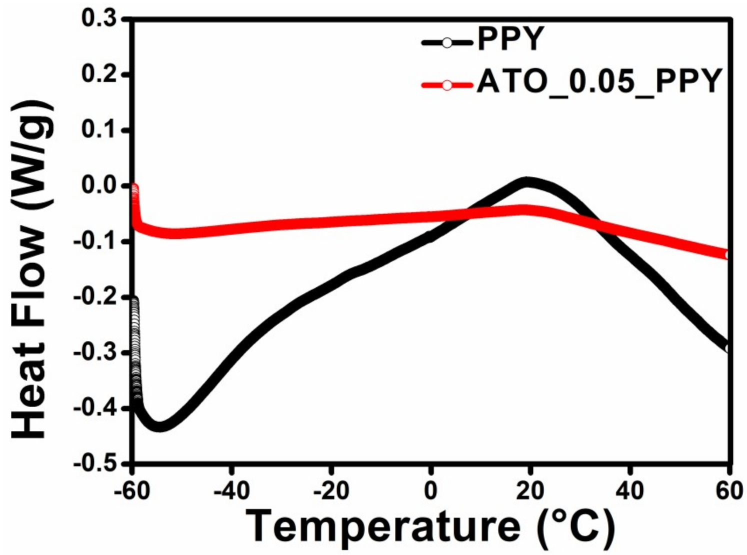

Figure S13: Low temperature DSC curves of polypyrrole (PPY) and polypyrrole loaded antimony doped tin oxide (ATO_0.05_PPY) samples.

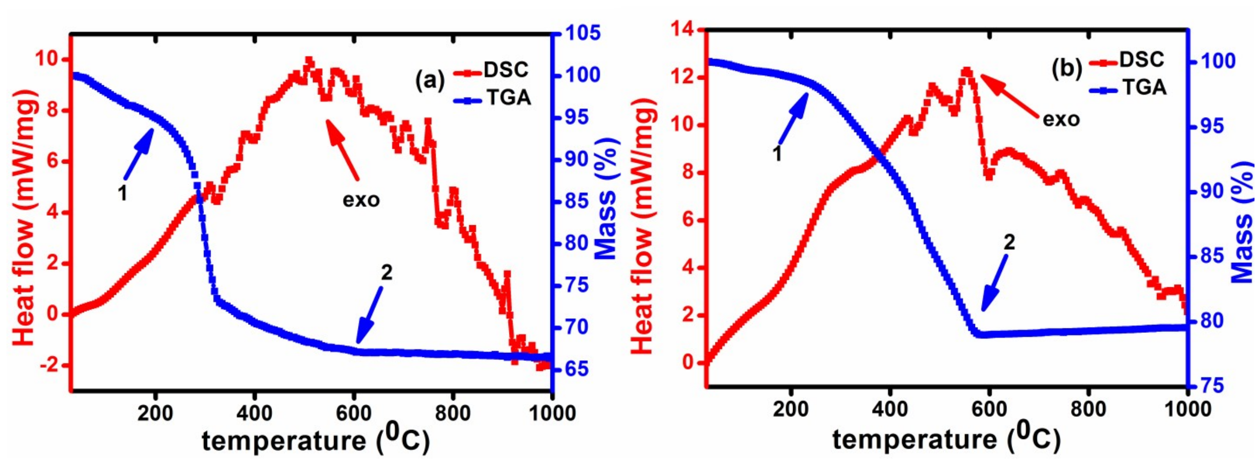

Figure S14: Simultaneous TGA and DSC plots (room temperature to 1000°C) of (a) polypyrrole (PPY) ["1" represents onset of polymer decomposition and "2" represents formation of decomposition products] and (b) polypyrrole loaded antimony doped tin oxide (ATO_0.05_PPY) ["1" represents onset of polymer decomposition and "2" represents pure ATO_0.05 sample with no polymeric remains] in air medium.

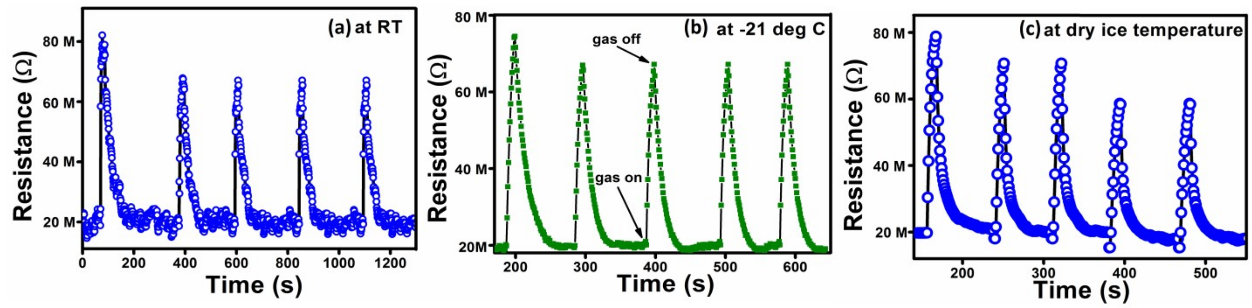

Figure S15: Dynamic sensing response curves (showing repeatability upto 5 cycles) of ATO_0.05_PPY sensor at different temperature to 20 ppm ammonia gas. The best results have been achieved for sensing at -21°C.

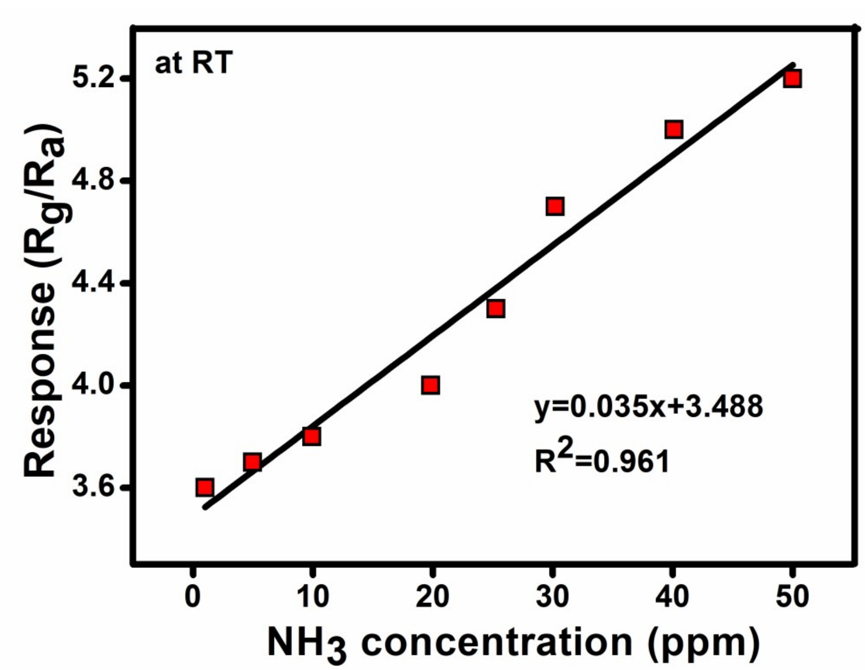

Figure S16: Sensing response vs. ammonia concentration calibration curve for ATO_0.05_PPY sensor at room temperature. The curve shows linear correlation upto 50 ppm ammonia at room temperature.

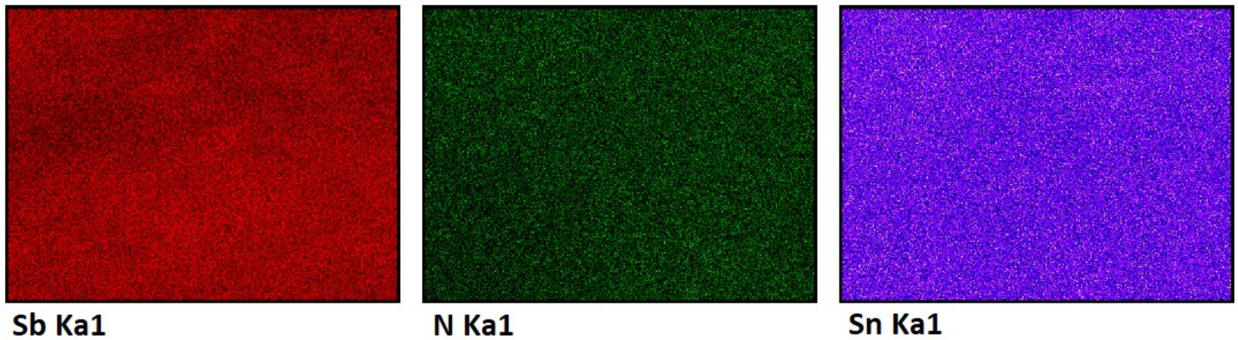

Figure S17: FESEM color mapping of ATO_0.05_PPY sample highlighting distribution of Sn, Sb and N (in an area of 3.43×2.57 μm^2). Elemental mapping is conducted on pellets formed out of powder samples. Sb is shown in red color (black represents other elements). N is shown in green color and Sn is shown in purple color.

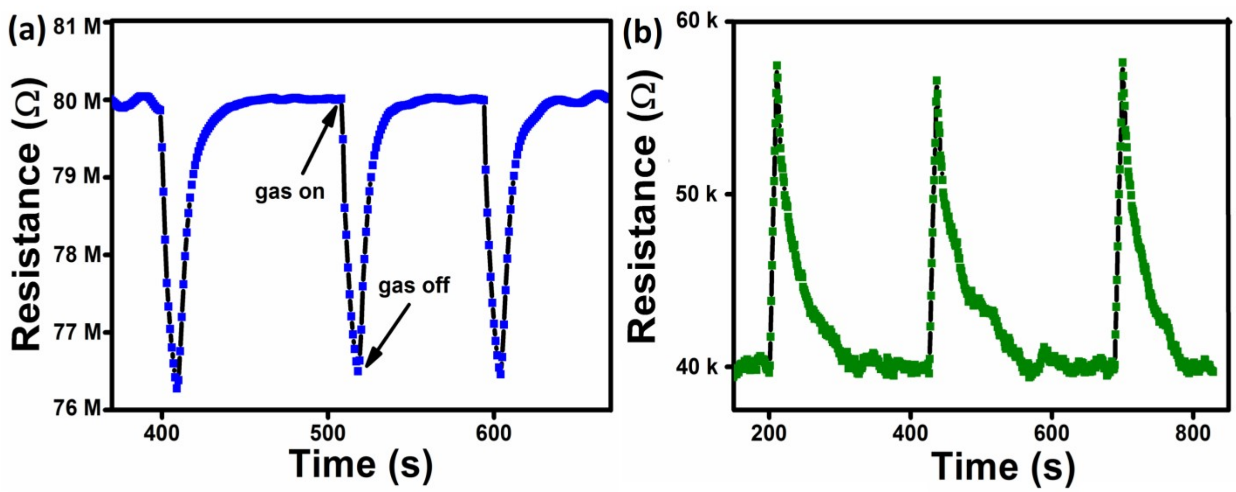

Figure S18: Dynamic sensing responses to 20 ppm ammonia at room temperature by (a) ATO_0.05 sensor (b) PPY based sensor.

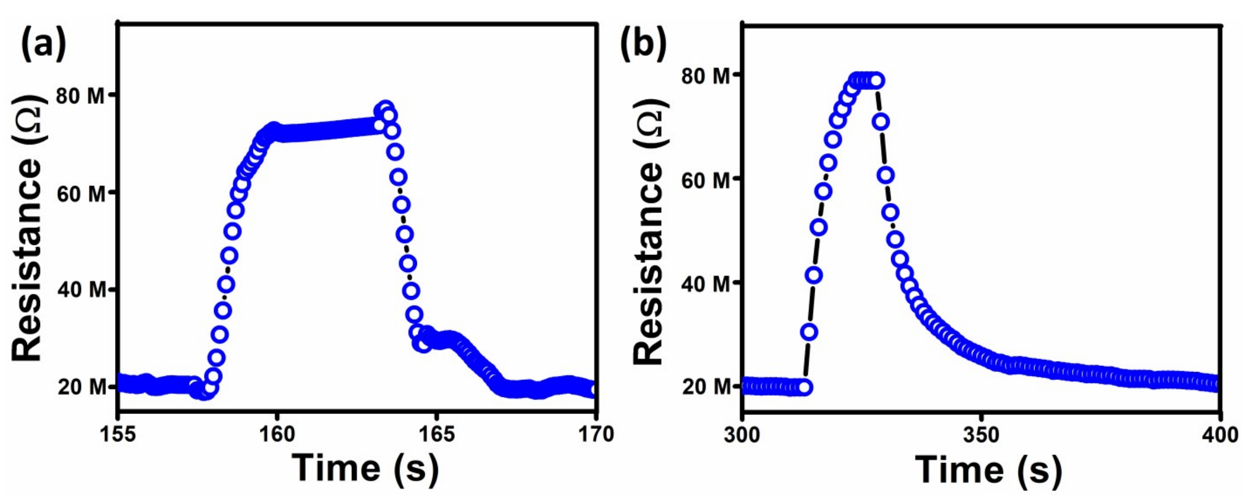

Figure S19: Dynamic sensing responses of ATO_0.05_PPY sensor at (a) room temperature (b) -78°C showing saturation.

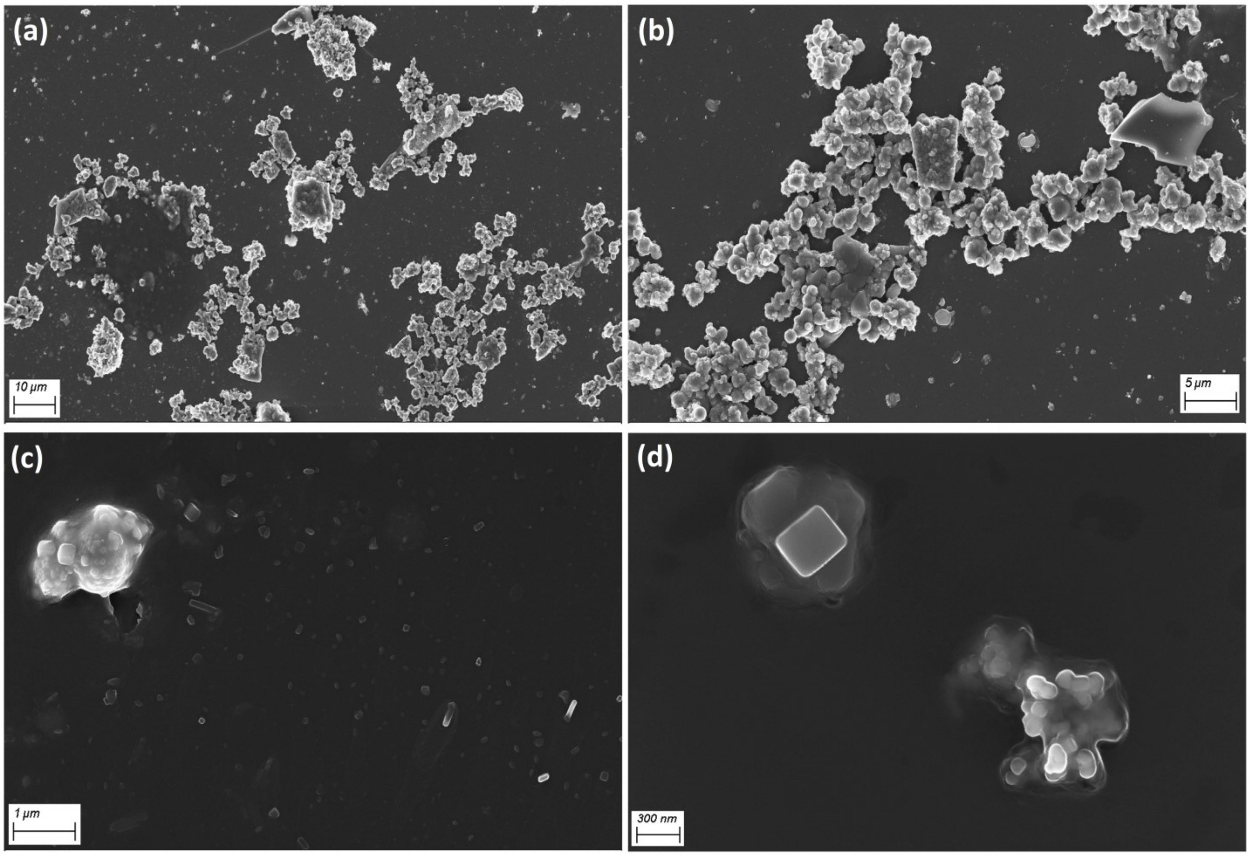

Figure S20: (a-d) FESEM images depicting distribution of Sb doped SnO_2 nanocubes and PPY network in ATO_0.05_PPY sample.