Supporting Information

Highly Selective Ammonia Sensing at Room Temperature with DC Plasma Modified MoS_2 Nanoflowers

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Raman Spectra of MoS_2 with different nitrogen plasma treatment times:

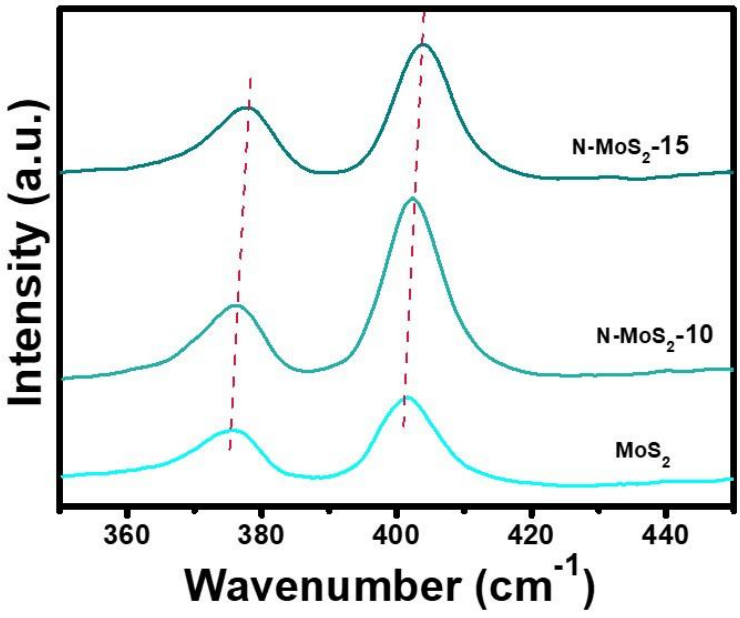


Figure S1: Raman spectra of the prepared N-MoS_2 and pristine MoS_2 nanosheets.

Figure S1 shows the Raman spectra of MoS_2 nanosheets with nitrogen-treated MoS_2 nanosheets for two different times. N-MoS_2-10 and N-MoS_2-15 represent the MoS_2 samples with 10- and 15-min nitrogen plasma treatment. As shown in the figure, the two characteristic peaks of E^1_{2g} and A^1_g appeared with slightly blue shifting of the peaks which is attributed to nitrogen incorporation on the MoS_2 [1].

XRD patterns of bulk MoS_2 and synthesized MoS_2 nanoflower:

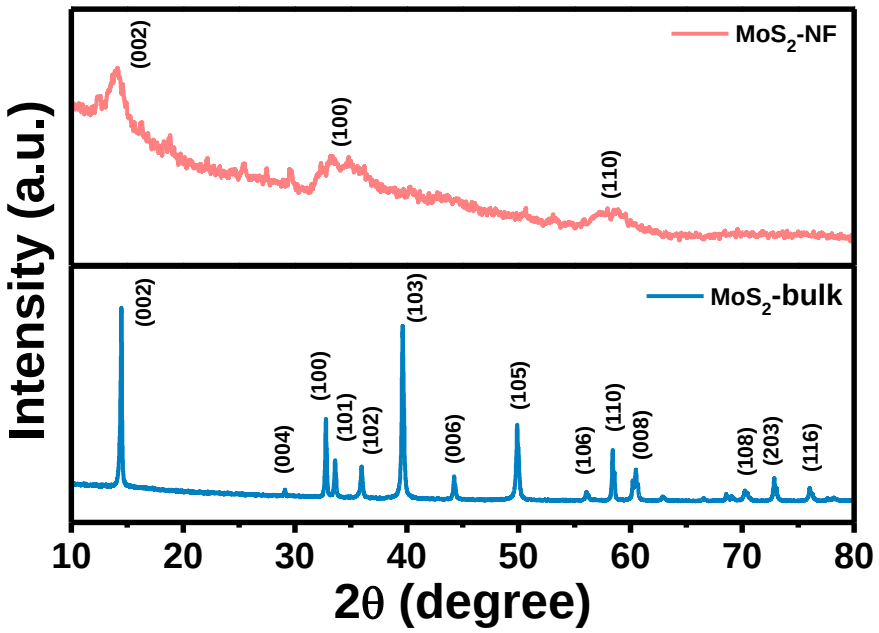


Figure S2: XRD patterns of bulk MoS_2 (MoS_2-bulk) and the synthesized MoS_2 nanoflower (MoS_2-NF) structure.

The XRD patterns in Figure S2 indicates single phase MoS_2 nanoflowers with hexagonal crystal structure and no impurities (ICDD card no. 77-1716) [2]. An X-ray pattern of bulk MoS_2 powder was provided for comparison with the conventional XRD pattern of the MoS_2 nanoflower sample. MoS_2 nanoflower sample exhibited peaks at 33.69° and 59.5°, corresponding to the (100) and (110) planes. The broadness of the peak at 14.2° corresponds to (002) planes in comparison to bulk MoS_2 crystals indicate that the produced products are few layered MoS_2.

Vapour phase detection The concentration of VOCs injected inside the chamber has been calculated using the following Equation [3,4]:

$$C_{ppm} = \frac{V_{\mu L} D_{gmL^{-1}}}{M_{g\ mol^{-1}} V_{mL}} \times 2.24 \times 10^7 \quad \text{…….. S1}$$

where C_{ppm} = the required vapor concentration,

$V_{\mu L}$ = volume of the liquid analyte,

$D_{gmL^{-1}}$ = density of the liquid,

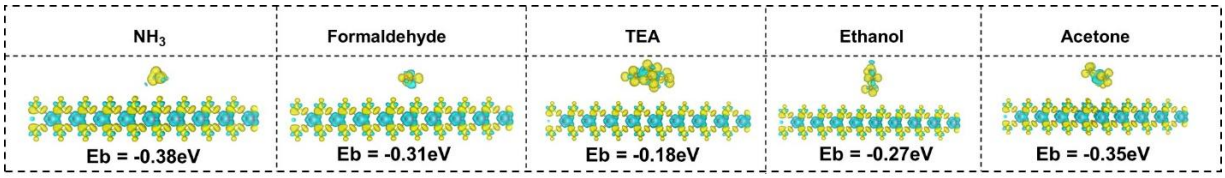
V_{mL} = volume of the test chamber

$M_{g\ mol^{-1}}$ = molecular weight of the liquid analyte.

The subscripts are the corresponding units of the measuring quantities.

Optimised configuration structures of MoS_2 and N-MoS_2 without S vacancy:

(a)



(b)

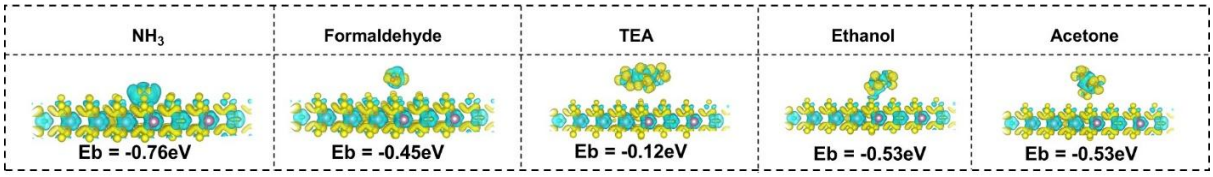


Figure S3: Optimized configuration structures with electron charge density differences (EDDs) (Δρ) of (a) MoS_2 and (b) N-MoS_2 system without S vacancy with various VOCs. The yellow colour corresponds to charge accumulations, and the cyan colour corresponds to charge depletion.

Current vs. Voltage plot of MoS_2 and N-MoS_2 sensors:

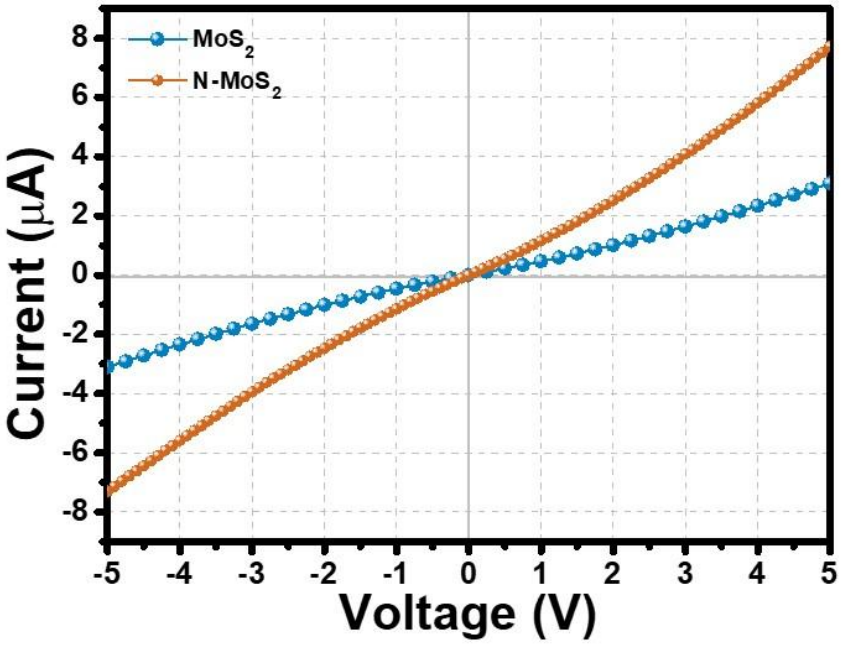


Figure S4. Current vs. Voltage (I-V) plot of MoS_2 and N-MoS_2 sensors.

References:

(1) Wu, R.; Hao, J.; Zheng, S.; Sun, Q.; Wang, T.; Zhang, D.; Zhang, H.; Wang, Y.; Zhou, X. N Dopants Triggered New Active Sites and Fast Charge Transfer in MoS2 Nanosheets for Full Response-Recovery NO2 Detection at Room Temperature. *Appl. Surf. Sci.* **2022**, *571*, 151162. https://doi.org/10.1016/J.APSUSC.2021.151162.

(2) Sathiyan, S.; Ahmad, H.; Chong, W. Y.; Lee, S. H.; Sivabalan, S. Evolution of the Polarizing Effect of MoS2. *IEEE Photonics J.* **2015**, *7* (6). https://doi.org/10.1109/JPHOT.2015.2499543.

(3) Kashyap, A.; Sarma, H.; Chakraborty, B.; Kalita, H. Selective and Sensitive Detection of Ammonia at Room Temperature by the WS2-PANI Nanocomposite on a Flexible Paper-Based Sensor with Cost-Effective Chemically Expanded Graphite Ink Electrodes. *ACS Appl. Electron. Mater.* **2024**. https://doi.org/10.1021/ACSAELM.4C01273/

(4) Kashyap, A.; Chakraborty, B.; Siddiqui, M. S.; Tyagi, H.; Kalita, H. Selective and Sensitive Detection of Formaldehyde at Room Temperature by Tin Oxide Nanoparticles/Reduced Graphene Oxide Composite. *ACS Appl. Nano Mater.* **2023**, *6* (9), 7948–7959. https://doi.org/10.1021/ACSANM.3C01183