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Supplementary Materials

CTAB Enhanced Room-Temperature Detection of NO_2 Based on MoS_2-Reduced Graphene Oxide Nanohybrid

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S1. The details about optimisation and XRD graph.

In this study, we studied the effects of different concentrations of CTAB on molybdenum disulfide. XRD characterization of CTAB-MoS_2 with different concentrations (0, 1.5, 3, 6 mg/mL) of CTAB were shown as following. The following Figure S1 suggested that the main crystal faces of CTAB-MoS_2 in different concentrations could match the standard card of MoS_2, which could indicate that the prepared material was MoS_2.

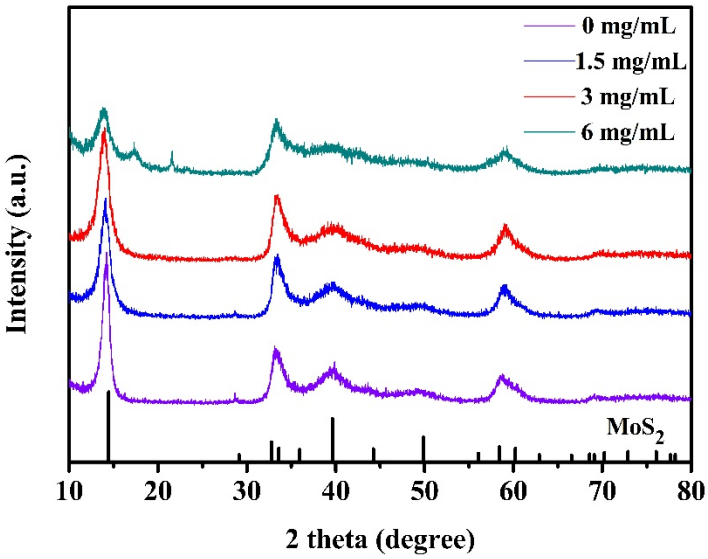

Figure S1. XRD of different concentrations of CTAB-MoS_2.

In order to achieve a better gas sensitivity of the NO_2 sensor with CTAB, four nanohybrid materials with the concentration of CTAB of 0 mg/mL (a), 1.5 mg/mL (b), 3 mg/mL (c), and 6 mg/mL (d) were farbricated and characterized by SEM. In Figure S2a, the size of MoS_2 without CTAB was about 6.5 μm, and the MoS_2 microspheres were agglomerated together. It is possible that large size might reduce the specific surface area, and severe agglomeration was not beneficial to the adsorption of the gas on the surface of the material to probably reduce the gas sensitivity. In Figure S2b, MoS_2 agglomeration seemed to be more severe when the concentration of CTAB was 1.5 mg/mL, and there was no clear spherical MoS_2. In Figure S2c, when the concentration of CTAB was 3 mg/mL, it was clear

that MoS_2 presented a spherical structure with visible nanosheets on the surface, and the size of MoS_2 microsphere was about 3 μm. In Figure S2d, when the concentration of CTAB was increased to 6 mg/mL, some unsphered flaky MoS_2 emerged without good dispersion. Based on SEM analysis, the CTAB concentration of 3 mg/mL was selected as the preferred concentration for the following experiments.

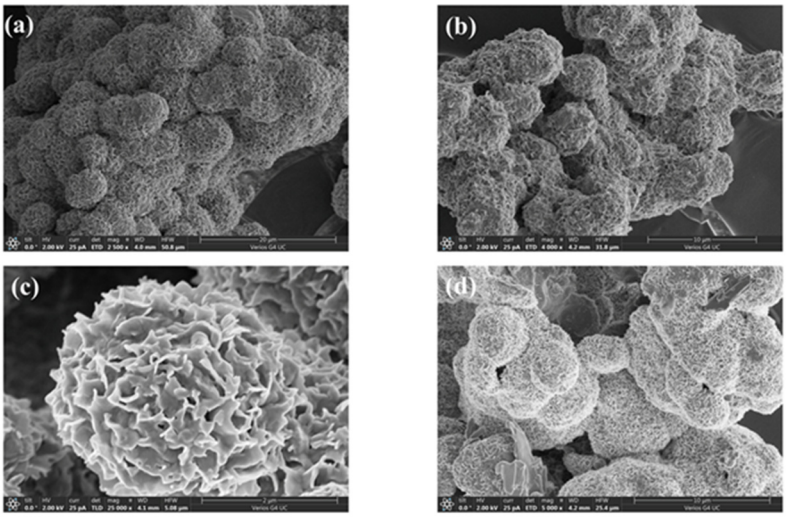

Figure S2. SEM images of CTAB-MoS_2; (**a**) 0 mg/mL (**b**) 1.5 mg/mL (**c**) 3 mg/mL (**d**) 6 mg/mL.

S2. The diagram of homemade gas-sensing investigation system.

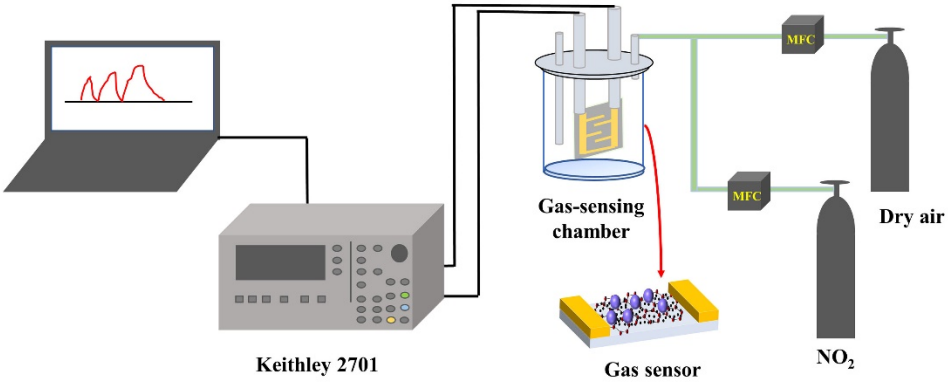

Figure S3. Schematic image of the gas sensor measurement system.

S3. The calculation of the detection limit

More details about the calculation of the detection limit of the CTAB-MoS_2/rGO NO_2 sensor is presented as following:

1. The noise of the sensor is calculated by root mean square deviation (rmsd) using the change of relative conductivity at baseline. 10 data points were collected at baseline before NO_2 exposure. After plotting the data, a fifth order polynomial fitting is carried out in the range of data points.

In eq 1, yi is the measured data point and y is the corresponding value calculated from the curve-fitting equation.

$$V_{X^2} = \sum (y_i - y)^2 \quad (1)$$

Table S1. A fifth order polynomial fitting result.

Time (s)	yi	y	yi−y	(yi−y)²
250	4.24×10^{-4}	-3.29×10^{-4}	7.53×10^{-4}	5.67×10^{-7}
260	1.49×10^{-3}	4.49×10^{-3}	-3.00×10^{-3}	9.00×10^{-6}
270	8.31×10^{-3}	5.04×10^{-3}	3.27×10^{-3}	1.07×10^{-5}
280	5.34×10^{-3}	3.96×10^{-3}	1.38×10^{-3}	1.92×10^{-6}
290	-1.41×10^{-3}	2.84×10^{-3}	-4.24×10^{-3}	1.79×10^{-5}
300	2.91×10^{-3}	2.40×10^{-3}	5.13×10^{-4}	2.63×10^{-7}
310	5.03×10^{-3}	2.65×10^{-3}	2.38×10^{-3}	5.66×10^{-6}
320	2.36×10^{-3}	3.07×10^{-3}	-7.06×10^{-4}	4.98×10^{-7}
330	2.09×10^{-3}	2.76×10^{-3}	-6.62×10^{-4}	4.38×10^{-7}
340	9.56×10^{-4}	6.58×10^{-4}	2.96×10^{-4}	8.78×10^{-8}

2. The blank noise is calculated as

$$RMS_{noise} = \sqrt{\frac{V_{X^2}}{N}} \quad (2)$$

In eq 2, RMS_{noise} is the blank noise, and N is the number of data points collected at baseline. The CTAB-MoS_2/rGO sensor blank noise is calculated as 4.71×10^{-6}.

3. Based on the above data and according to the definition of detection limit (DL) calculation equation (Equation 3), the theoretical detection limit (DL) of CTAB-MoS_2/rGO sensor is calculated to be 26.55 ppb.

$$LOD = 3\frac{RMS_{noise}}{Slope} \quad (3)$$