

## Supporting Information

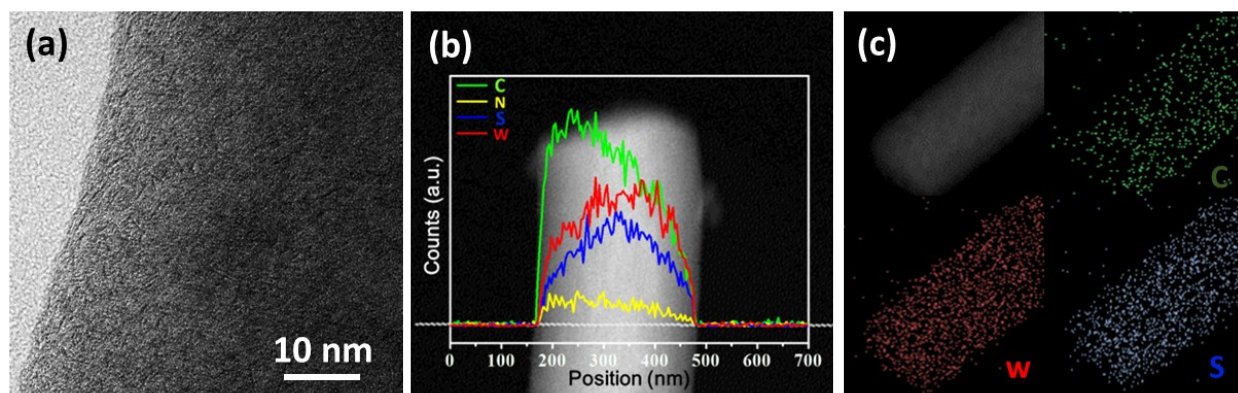
# 2D WS<sub>2</sub>-Edge Functionalized Multi-Channel Carbon Nanofibers: Effect of WS<sub>2</sub> Edge-Abundant Structure on Room-Temperature NO<sub>2</sub> Sensing

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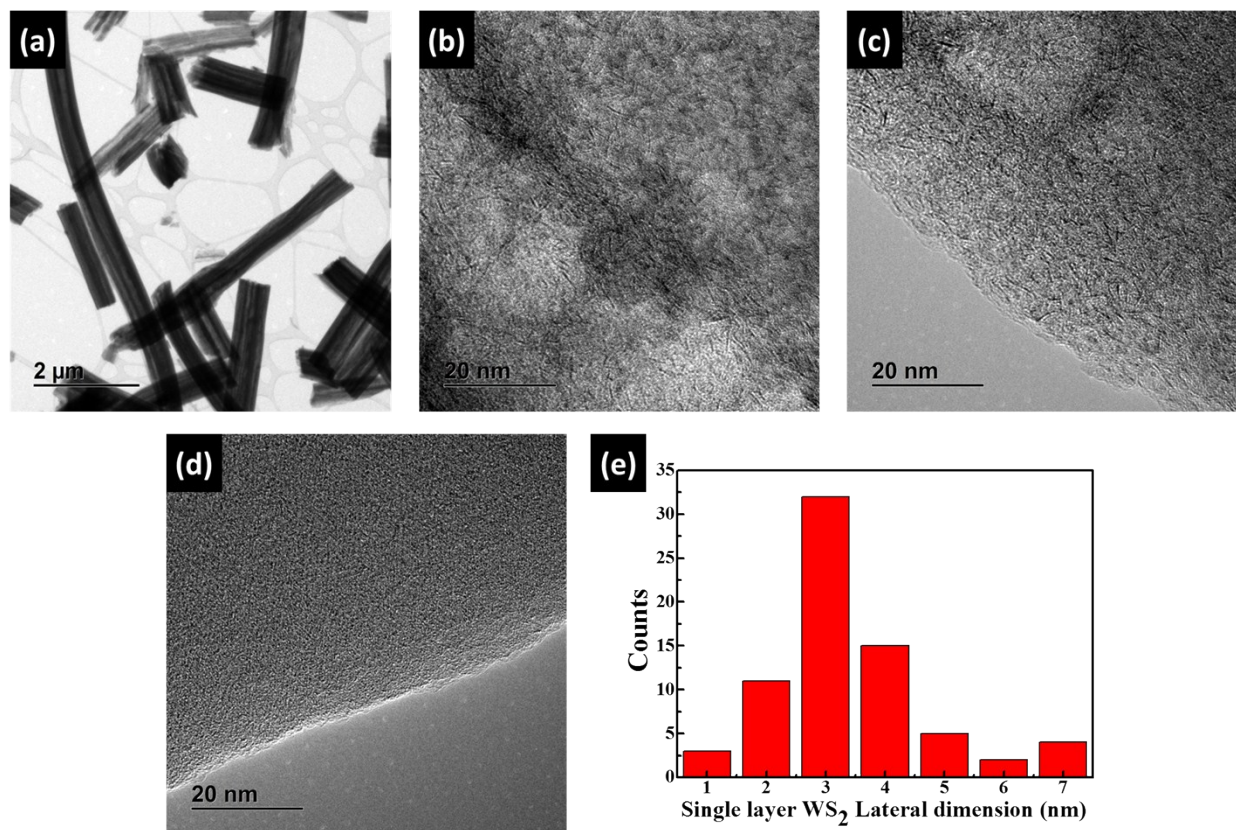
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## S1. WS<sub>2</sub>@CNFs



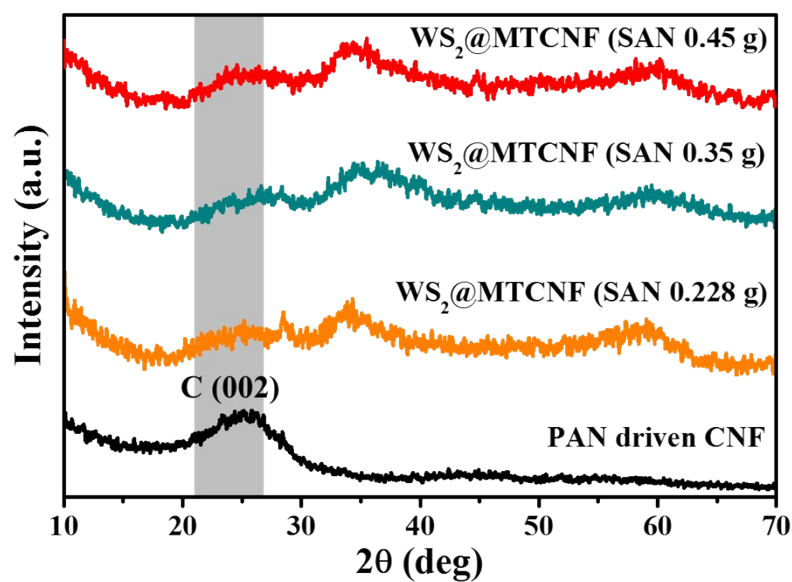
**Figure S1.** (a) HRTEM image of WS<sub>2</sub>@CNFs. (b) STEM image of WS<sub>2</sub>@CNFs on which EDS line-scan profile of W, S, N, and C is presented. (c) STEM image and STEM-EDS mapping image of WS<sub>2</sub>@CNFs: W (red), S (sky-blue), and C (green).

## S2. TEM images of WS<sub>2</sub>@MTCNFs and CNFs



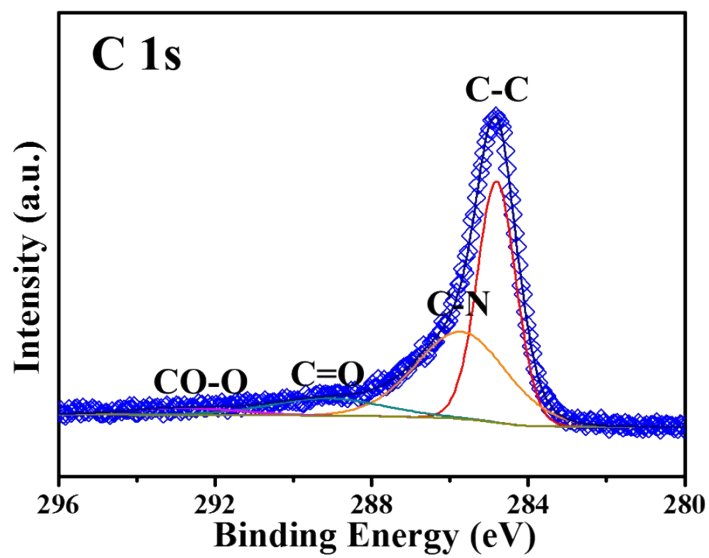
**Figure S2.** (a) TEM image of WS<sub>2</sub>@MTCNFs. HRTEM images of (b-c) WS<sub>2</sub>@MTCNFs and (d) CNFs. (e) Lateral dimension size distribution histogram of single layer WS<sub>2</sub> in MTCNFs.

### S3. XRD patterns of WS<sub>2</sub>@MTCNFs



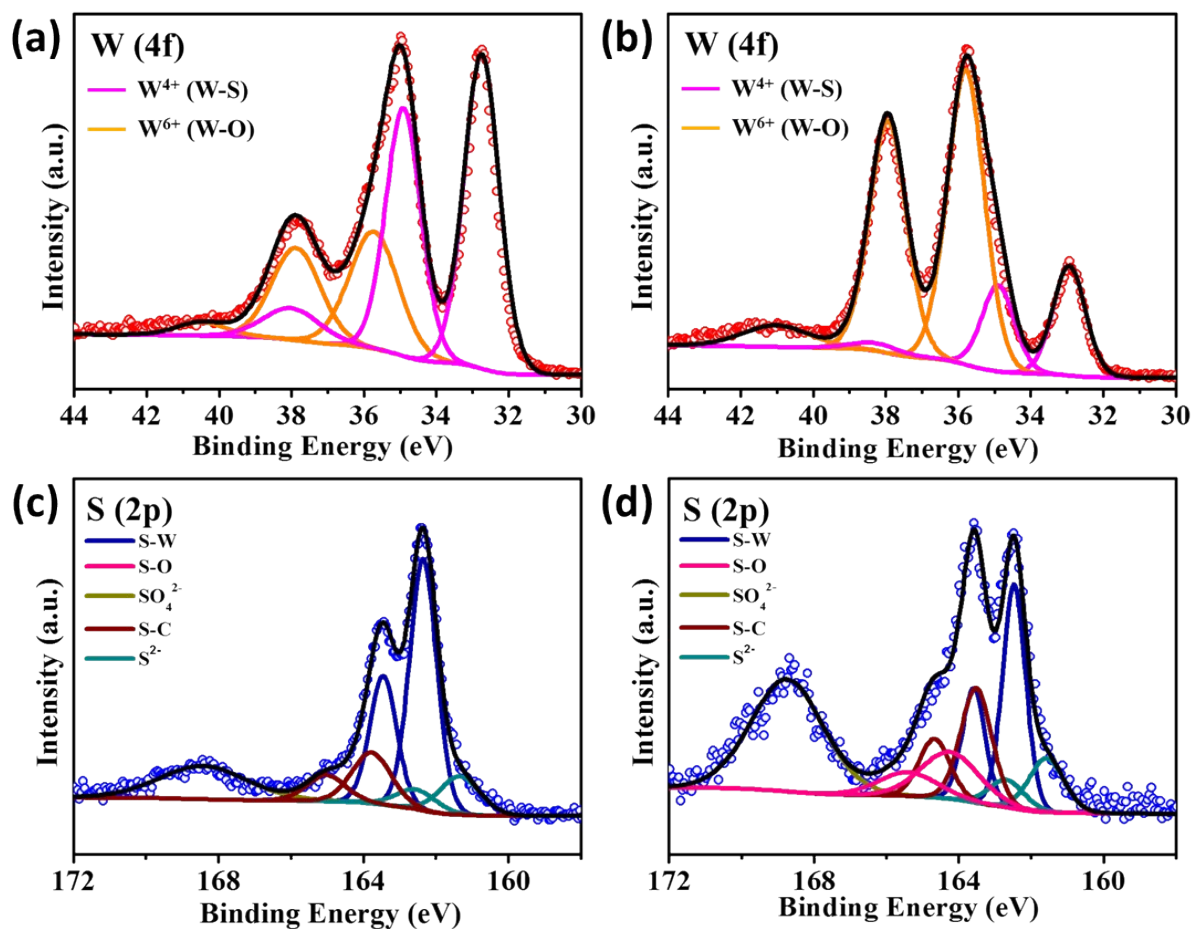
**Figure S3.** XRD patterns of WS<sub>2</sub>@MTCNFs with SAN 0.450 g, SAN 0.350 g, and SAN 0.228 g and PAN-driven CNFs, respectively.

#### S4. XPS spectra of the WS<sub>2</sub>@MTCNFs : C 1s peaks



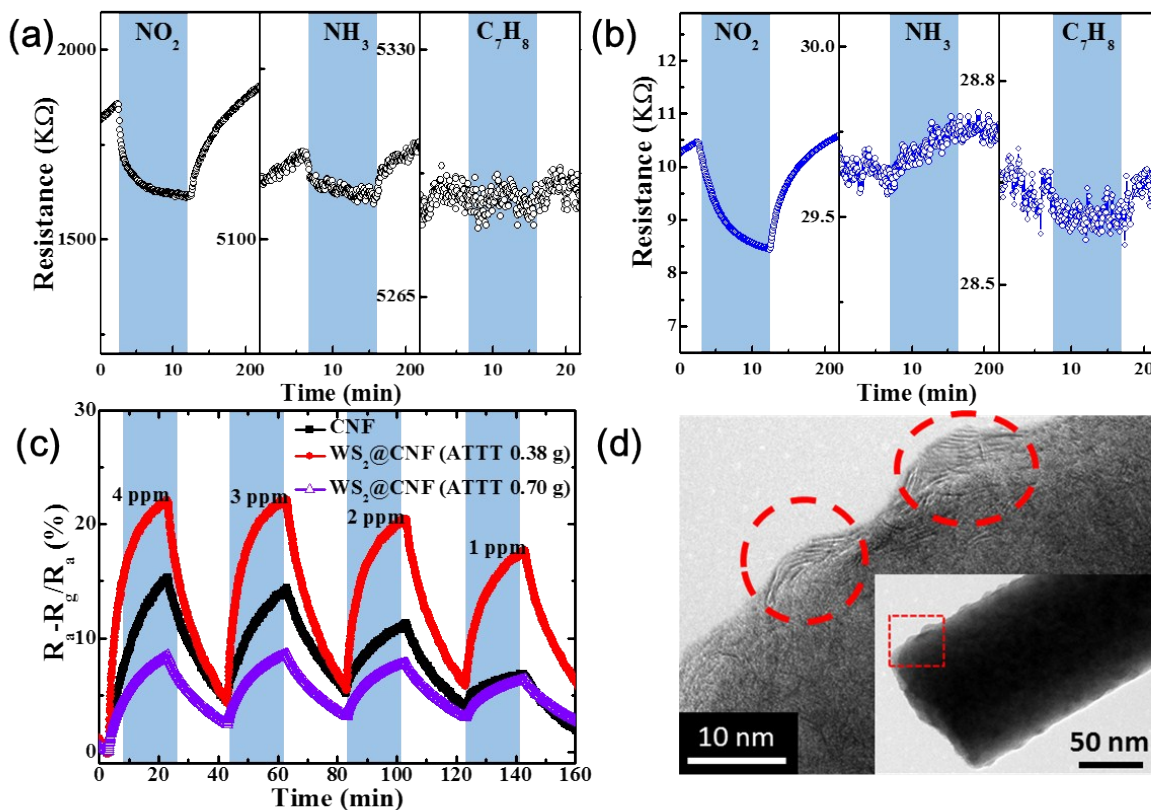
**Figure S4.** XPS spectra of the WS<sub>2</sub>@MTCNFs : C 1s peaks

## S5. Ex-situ XPS analysis in humid condition



**Figure S5.** Ex-situ XPS analysis with  $\text{WS}_2@\text{MTCNFs}$ : W 4f spectra (a) before and (b) after exposure to  $\text{NO}_2$  in humid condition. S 2p spectra (c) before and (d) after exposure to  $\text{NO}_2$  in humid condition.

## S6. Sensing characteristics of CNFs and WS<sub>2</sub>@MTCNFs



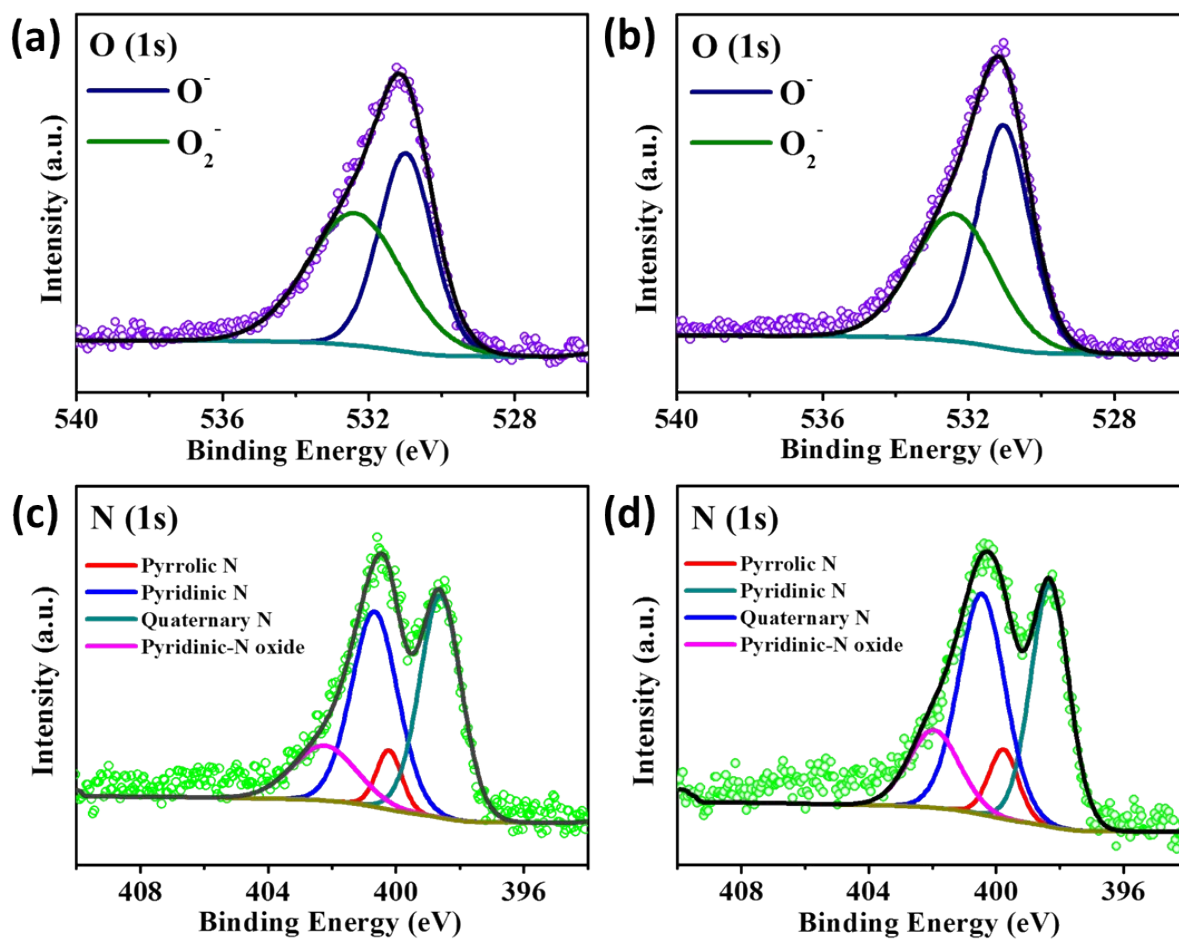
**Figure S6.** (a) Dynamic resistance transition characteristics of CNFs toward 5 ppm of NO<sub>2</sub>, NH<sub>3</sub>, and C<sub>7</sub>H<sub>8</sub>. (b) Dynamic resistance transition characteristics of WS<sub>2</sub>@MTCNFs toward 5 ppm of NO<sub>2</sub>, NH<sub>3</sub>, and C<sub>7</sub>H<sub>8</sub>. (c) Dynamic response transients of CNFs, WS<sub>2</sub>@CNFs (ATTT 0.38 g), and WS<sub>2</sub>@CNFs (ATTT 0.7 g) toward NO<sub>2</sub> in the concentration range of 4-1 ppm at room temperature. (d) TEM image and HRTEM image of WS<sub>2</sub>@CNFs (ATTT 0.7 g)

The sensing tendency of the dense CNFs and WS<sub>2</sub>@MTCNFs toward NH<sub>3</sub> based on resistance might be further supported by edge effects exerted by WS<sub>2</sub> nanoflakes distributed on the surface. During exposure to NH<sub>3</sub>, the resistance of the dense CNFs decreases due to the electron

donating property of  $\text{NH}_3$  molecules. According to previous studies, carbon-based gas sensors such as carbon nanotubes and graphene exhibiting n-type sensing behavior against reducing gases even though carbon nanofibers exhibit a p-type response in oxidizing gases.<sup>1-2</sup> In the present study, the resistance of  $\text{WS}_2$ -edge functionalized CNFs ( $\text{WS}_2@\text{MTCNFs}$ ) is increased with no recovery when  $\text{NH}_3$  gas was injected, which is identical in sensing tendency toward  $\text{NH}_3$  of layered  $\text{MoS}_2$ .<sup>3-4</sup>

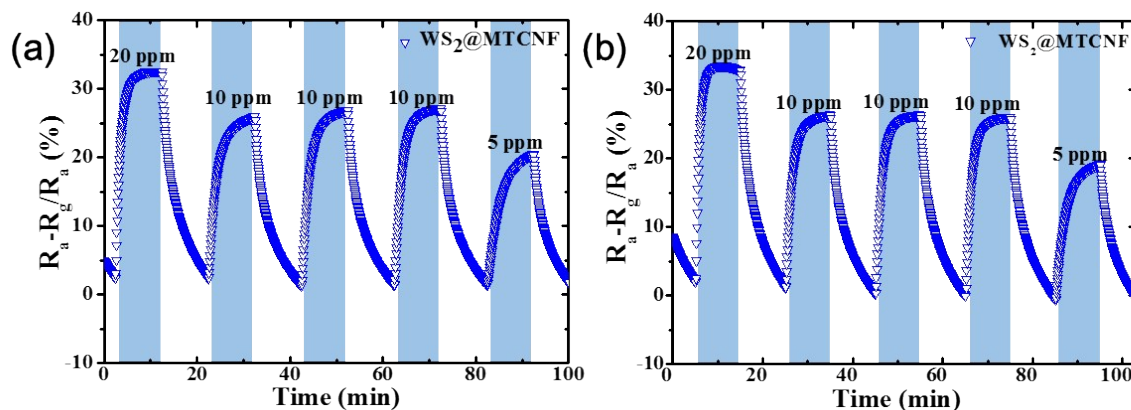


## S7. Ex-situ XPS analysis in dry condition



**Figure S7.** Ex-situ XPS analysis with  $\text{WS}_2@\text{MTCNFs}$ : O 1s spectra (a) before and (b) after exposure to  $\text{NO}_2$  in dry air. N 1s spectra (c) before and (d) after exposure to  $\text{NO}_2$  in dry air.

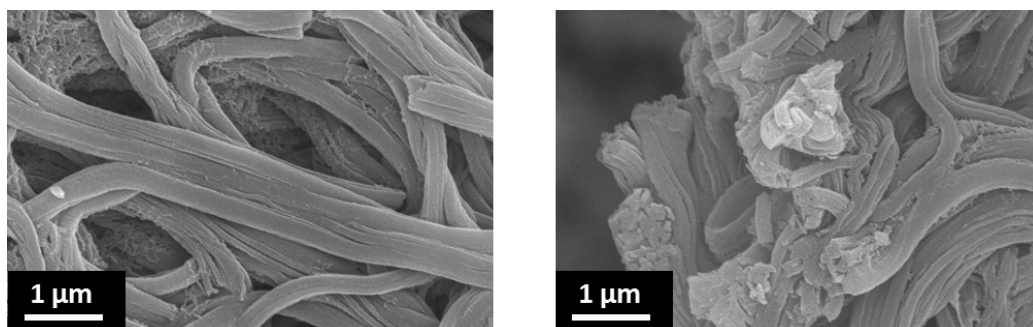
## S8. Temperature dependency of sensing characteristics of WS<sub>2</sub>@MTCNFs



**Figure S8.** Dynamic response transients of WS<sub>2</sub>@MTCNFs toward NO<sub>2</sub> in the concentration range of 20-5 ppm at (a) 25 °C and (b) 80 °C.

For analysis regarding temperature dependency of the sensing materials, the sensing performance of WS<sub>2</sub>@MTCNFs was characterized at 80 °C in the concentrations of 20, 10, and 5 ppm. As a result, any enhancement in response of the WS<sub>2</sub>@MTCNFs was not observed, showing that the sensing material are not affected much by temperature.

## S9. SEM images



**Figure S9.** SEM images of CNFs obtained from combination of PAN and SAN without ATTT, followed by heat treatment. It shows that the morphology of synthesized products is much different from that of WS<sub>2</sub>@MTCNFs.

## S10. Comparison with other WS<sub>2</sub> gas sensors

**Table S1.** Recent publications on a variety of WS<sub>2</sub> based gas sensors.

Gas species	Materials	Working temperature	Balance gas	Measurement	Response	Exposure time	Detection limit	reference
Various gases	Multilayer WS <sub>2</sub> nanoflakes	Room temp.	Dry	Source drain current	–	~25 s	–	5
Humidity	WS <sub>2</sub> Nanoparticles	Room temp.	Air	Current	–	~200 s	–	6
Methanol	Metallic 1T WS <sub>2</sub>	Room temp.	Humid air	Impedance	–	–	–	7
H <sub>2</sub>	WS <sub>2</sub> -Pd composite film	Room temp.	Dry N <sub>2</sub>	Resistance	380% at 1000 ppm	30 min	10 ppm	8
NH <sub>3</sub>	2nm-WS <sub>2</sub> film	Room temp.	Dry N <sub>2</sub>	Resistance	0.2% at 60 ppm	2 min	1.2 ppm	9
NH <sub>3</sub>	Fluorinated 1L WS <sub>2</sub>	Room temp.	Dry air	PL intensity	–	2 min	–	10
NO <sub>2</sub>	Ag-NW@WS <sub>2</sub> nanosheets	100 °C	Dry air	Current	60% at 25 ppm	5 min	–	11
NO <sub>2</sub>	WS <sub>2</sub> @MTCNFs	Room temp.	Dry air	Resistance	15% at 1 ppm	20 min	10 ppb	This work

# S11. Comparison with other TMD gas sensors for NO<sub>2</sub> sensing

**Table S2.** Recent publications on TMD based gas sensors toward NO<sub>2</sub> sensing.

Gas species	Materials	Working temperature	Balance gas	Measurement	Response	Exposure time	Detection limit	reference
NO <sub>2</sub>	Thin-layered MoS <sub>2</sub>	Room temp.	Dry N <sub>2</sub>	Source drain current	1372% at 1000 ppm	~300 s	–	3
	Atomic-layer MoS <sub>2</sub>	Room temp.	Dry air	Resistance	27% at 20 ppm	2 min	–	4
	CVD Atomic-layer MoS <sub>2</sub>	Room temp.	Dry N <sub>2</sub>	Resistance	150% at 1200 ppb	5 min	120 ppb	12
	Graphene/MoS <sub>2</sub>	100 °C	Dry N <sub>2</sub>	Resistance	3% at 1.2 ppm	5 min	–	13
	Graphene/MoS <sub>2</sub>	150 °C	Dry air	Resistance	3% at 5 ppm	5 min	–	14
	MoS <sub>2</sub> /SnO <sub>2</sub>	Room temp.	Dry air	Conductance	0.6% at 0.5 ppm	~750 s	0.5 ppm	15
	Exfoliated MoS <sub>2</sub> flakes	200 °C	Dry air	Resistance	1.6 at 1 ppm	120 min	20 ppb	16
	Vertically aligned MoS <sub>2</sub>	Room temp.	Dry N <sub>2</sub>	Resistance	4% at 100 ppm	10 min	–	17
	MoS <sub>2</sub> /Graphene hybrid aerogel	200 °C	Dry N <sub>2</sub>	Resistance	9% at 0.5 ppm	10 min	14 ppb	18
	Ag-NW@WS <sub>2</sub> nanosheets	100 °C	Dry air	Current	60% at 25 ppm	5 min	–	11
	WS <sub>2</sub> @MTCNFs	Room temp.	Dry air	Resistance	15% at 1 ppm	20 min	10 ppb	This work

## Note and References

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