

Supporting Information

ZnO Nanocluster-Functionalised Single-Walled Carbon Nanotubes Synthesized by Microwave Irradiation for Highly Sensitive NO₂ detection at Room Temperature

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- **Calculation of detection limit (DL)**^{equation S1, S2}

1. As shown in Fig. S1(a), the slope value (~ 0.552) and the value of goodness-of-fit (R^2 , ~ 0.98) were derived from the response values versus NO_2 concentration of the fabricated sensor.
2. Before NO_2 gas injected in the gas chamber, we have taken resistance points of $N = 11$ at the base line.
3. As shown in Fig. S1(b), We have plotted the data (resistance value versus time) and then a 5th order polynomial fit is performed within data-point range (see Table S1).
4. To obtain the theoretical detection limit (DL), the root-mean squared deviation (RMS_{noise}) has been calculated as follows,

$$RMS_{noise}(\text{ppm}^{-1}) = \sqrt{\frac{V_{x^2}}{(N - 1)}}, \text{ where } V_{x^2} = \sum(Y_i - Y)^2 \quad (\text{equation S1})$$

Where Y_i is the measured resistance value and Y is the corresponding value calculated from the curve-fitting equation. The DL value could be finally calculated using the following equation.

$$\text{Detection limit (DL)} = 3 \times \frac{RMS_{noise}}{\text{slope}} \quad (\text{equation S2})$$

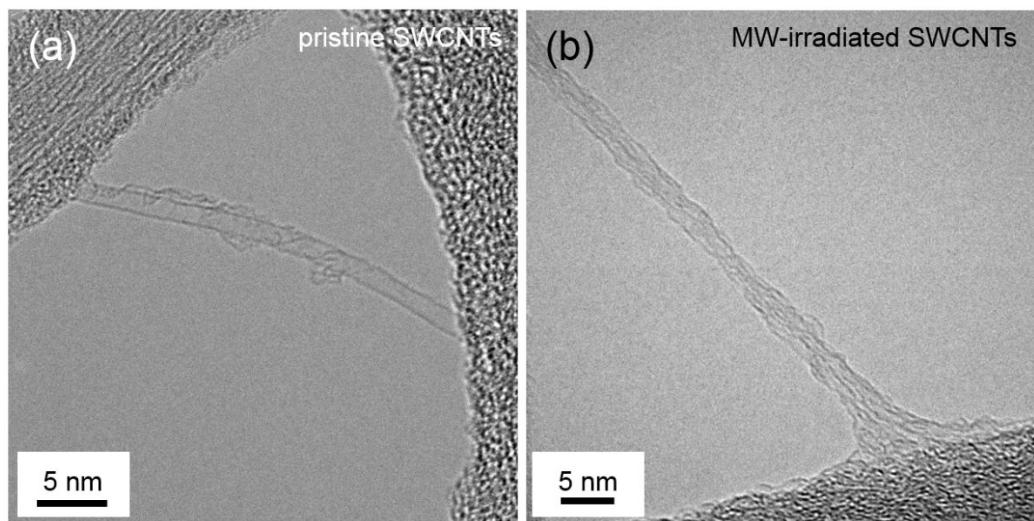


Figure S1. High-resolution TEM images of (a) pristine and (b) MW-irradiated SWCNTs.

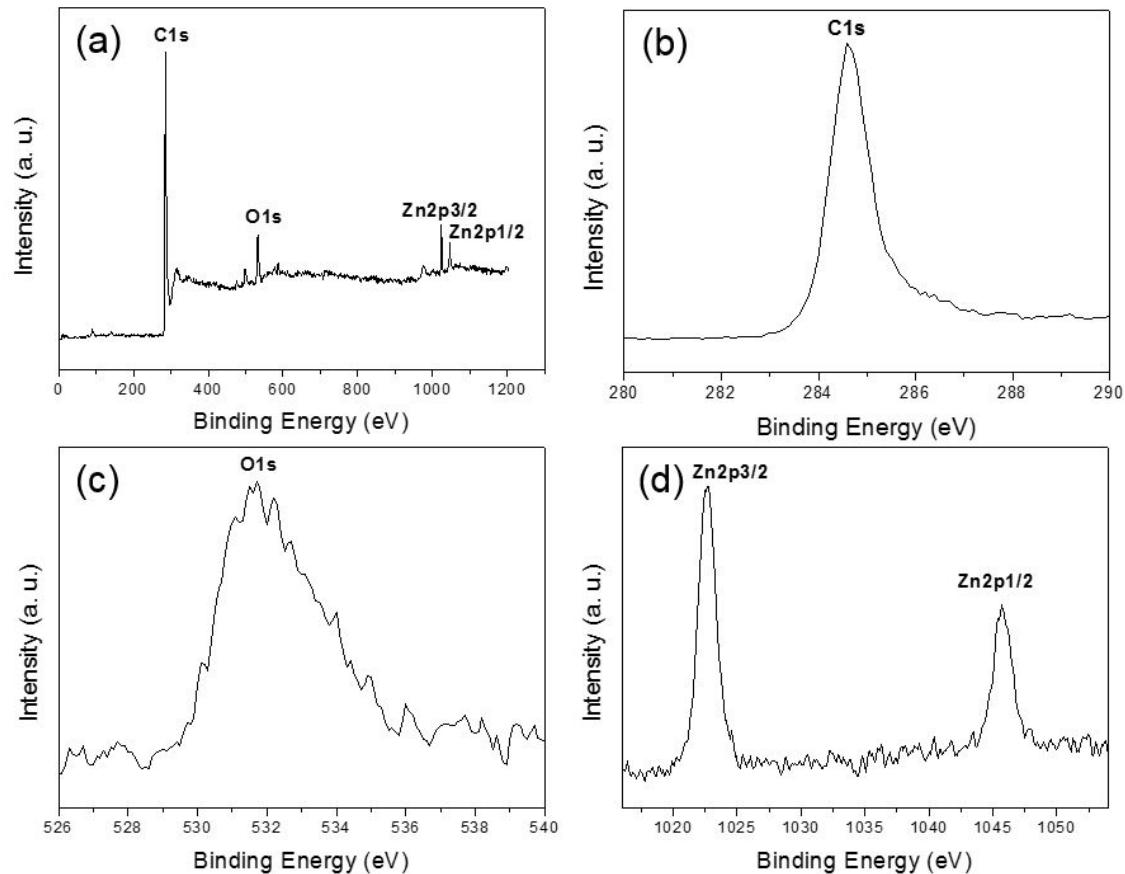


Figure S2. XPS results of the Z-SWCNTs: (a) survey-scanned XPS spectrum of Z-SWCNTs, core level XPS spectra of (b) C 1s, (c) O 1s and (d) Zn 2p.

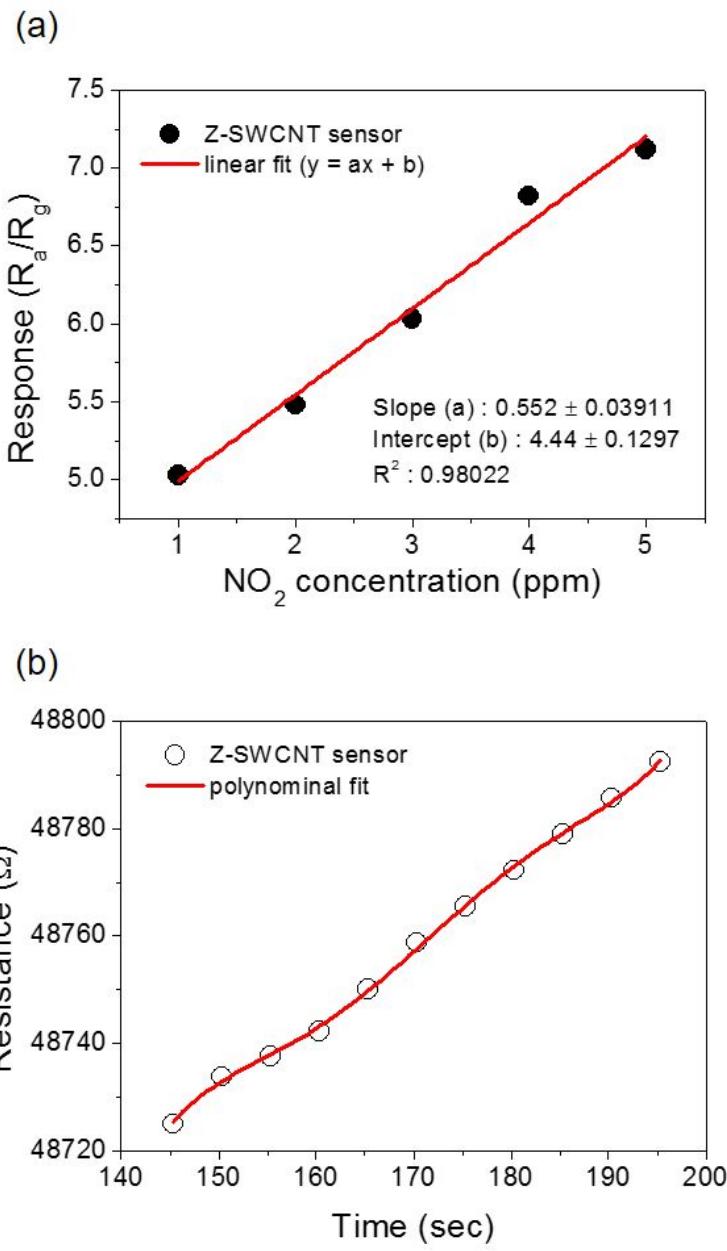


Figure S3. Fitting plots of Z-SWCNT sensor: (a) linear fitting, (b) 5th order polynomial fitting.

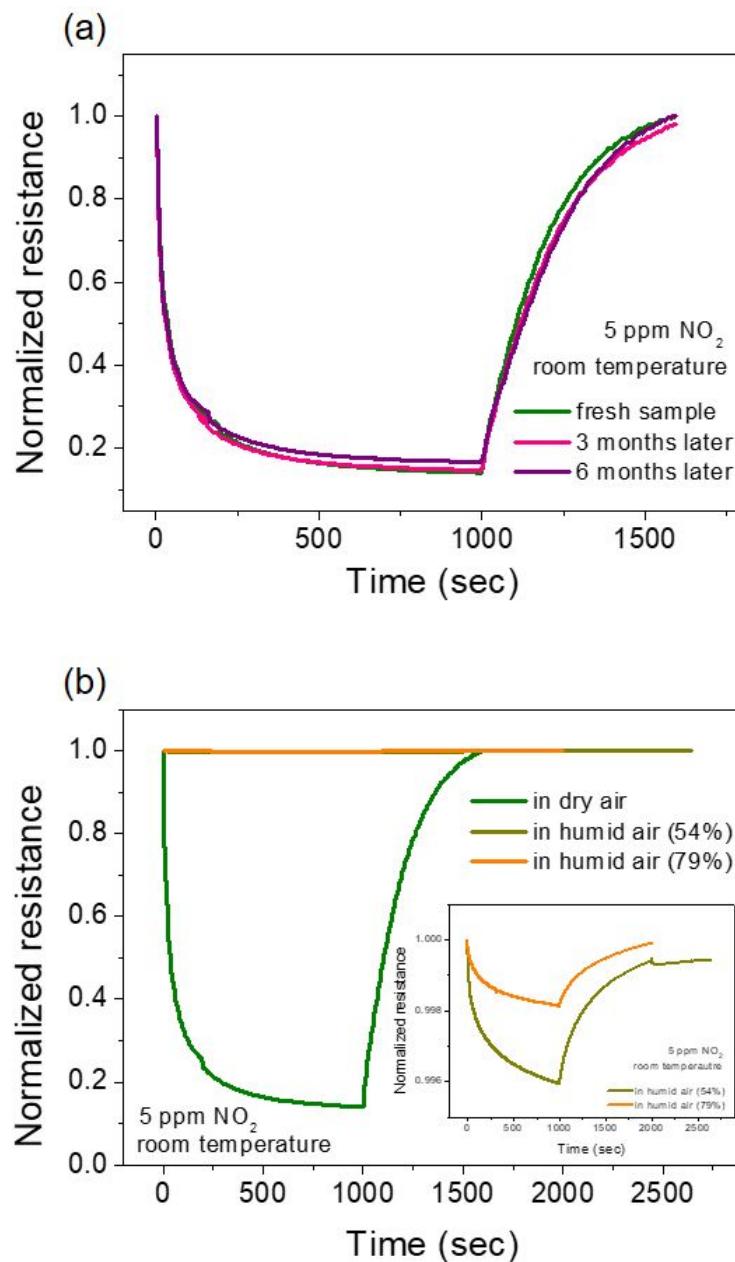


Figure S4. (a) Long-term stability of the Z-SWCNTs, and (b) comparison of the NO_2 response of Z-SWCNTs under dry air, RH 54% and RH 79% humid air, respectively.

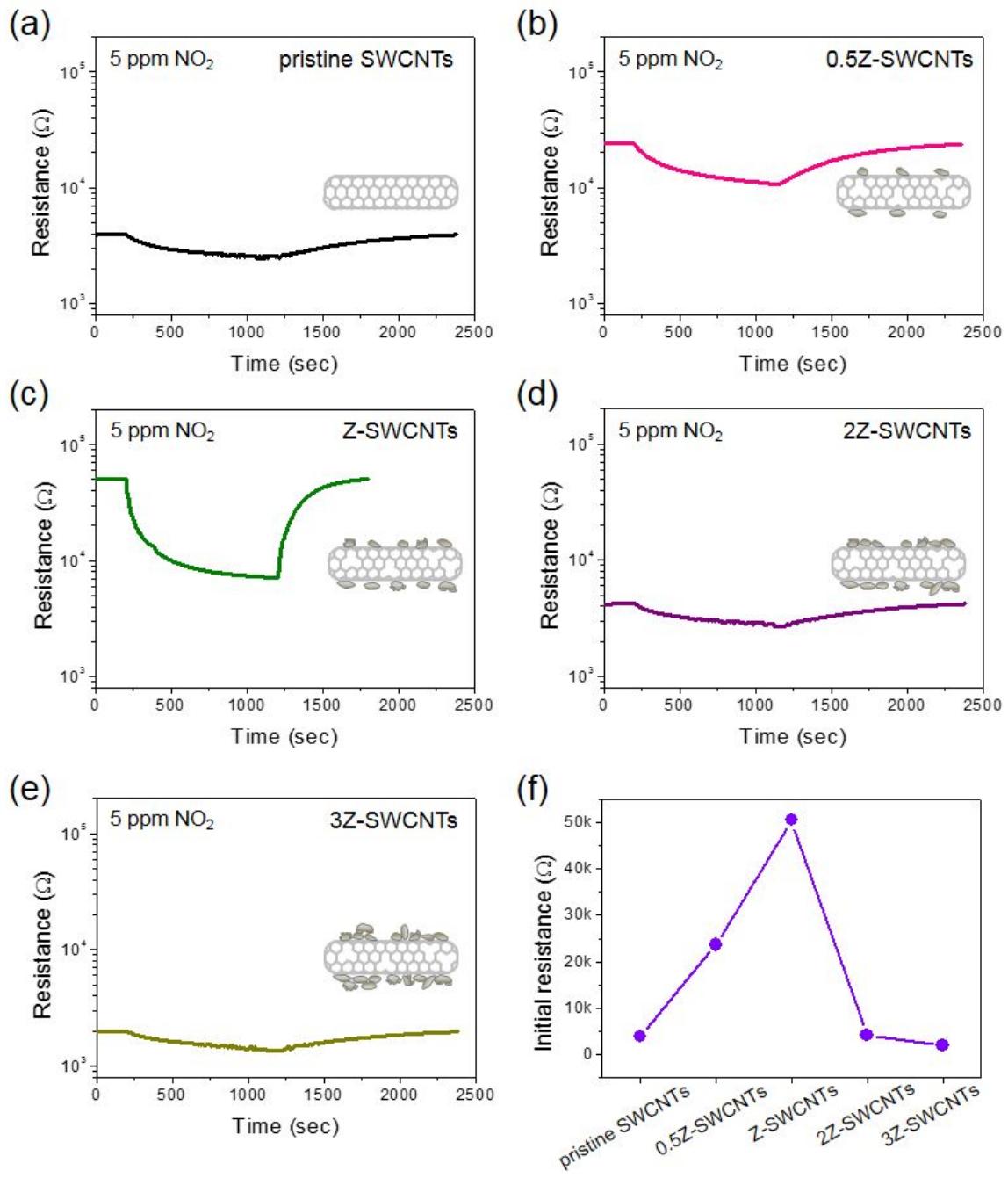


Figure S5. Resistance curves of the n -ZnO NC-functionalised defect-induced SWCNTs: (a) pristine SWCNTs, (b) 0.5Z-SWCNTs, (c) Z-SWCNTs, (d) 2Z-SWCNTs, and (e) 3Z-SWCNTs. (d) Initial resistance values of each sensor. (f) Summary of initial resistance values of the fabricated sensors.

Table S1. Polynomial fitting data of the Z-SWCNT sensor

Time (sec)	$(Y_i - Y)$	$(Y_i - Y)^2$
145	0.0101	0.000102
150	-0.00508	2.58×10^{-5}
155	-0.00616	3.79×10^{-5}
160	-0.00024	5.76×10^{-8}
165	-0.00052	2.7×10^{-7}
170	-0.0496	0.00246
175	-0.00068	4.62×10^{-7}
180	-0.00076	5.78×10^{-7}
185	0.0002	4.8×10^{-8}
190	-2×10^{-5}	4×10^{-10}
195	-1×10^{-5}	1×10^{-10}

Table S2. Comparison of NO₂-response in Z-SWCNT sensor with various types of sensors prepared different sensing materials

Materials	Concentration (ppm)	Temperature (°C)	Gas response (R_a/R_g)	Reference
Z-SWCNTs	1	RT	5.03 (R_a/R_g)	this work
Z-SWCNTs	1	RT	403% $(\Delta R/R_a) \times 100$	this work
Cu ₂ O-conjugated RGO*	2	RT	67.8% $(\Delta I/I_a) \times 100$	1
SnO ₂ -ZnO core-shell NWs	1	RT	238.73% $(\Delta R/R_a) \times 100$	2
Co ₃ O ₄ -intercalated RGO	60	RT	80% $(\Delta R/R_a) \times 100$	3
PPy** thin films	10	RT	12% $(\Delta R/R_a) \times 100$	4
ZnO-RGO hybrid	5	RT	25.6% $(\Delta R/R_a) \times 100$	5
rGO-CNT-SnO ₂ hybrid	5	RT	2.53 (R_a/R_g)	6
Mesoporous NiO nanosheets	5	RT	0.30 $(\Delta G/G_a)$	7
TeO ₂ -SnO ₂ heterostructure	3	RT	9.97 (R_a/R_g)	8
Bi-layer graphene	5	RT	12.87% $(\Delta R/R_a) \times 100$	9

* rGO: Reduced graphene oxide, ** PPy: Polypyrrole,

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