

Supporting Information

In-Doped ZnO Nanofibers with *Acharia stimulea*-inspired Morphology: A Promising Sensing Platform for Highly Rapid and Sensitive Detection of *Listeria* Biomarker 3-Hydroxy-2-Butanone

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Text S1. Material characterization methods

Necessary techniques were utilized to characterize the as-prepared samples. Mineral composition and crystal structure of all samples were carefully investigated using DX-2000 X-ray diffractometer (XRD, target material is Cu, $\lambda = 0.154184$ nm, tube voltage and tube current are 30 kV and 25 mA respectively, scanning speed was 0.01 deg./s, scanning range is 30°-70°). Microstructure and morphology were studied using a transmission electron microscopy (TEM, FEI Talos F200X, the acceleration voltage is 200 kV, point resolution is 0.25 nm) and a scanning electron microscopy (SEM, TESCAN MIRA LMS, the resolution of the secondary electron image is 0.9 nm, and the resolution of the backscattered electron image is 2 nm. The acceleration voltage is 200 V-30 kV and the probe beam current is 1 pA-100 nA). Chemical constituents were analyzed using Thermo escalab 250XI (XPS, the excitation source is Al K α ray ($h\nu = 1486.6$ eV), the beam spot is 650 μm , the power is 150W, the acceleration voltage is 14.8 kV, and the filament current is 1.6 A. Charge correction was performed using contaminated carbon C1s = 284.8 eV) and energy dispersion X-ray energy spectrometry (EDS, JED-2300T). The pore structure and specific surface area of the materials were characterized by JW-BK200C. The optical band gap width of the sample was tested using an ultraviolet-visible landscape photometer (UV-2600).

Text S2. Gas sensor testing

Gas-sensing measurements were performed using a CGS-8 gas sensing analysis system (Beijing Elite Technology Co.). The sensor under test was placed in a cylindrical test chamber, and it was equipped with a temperature-controlled heating stage to adjust the different operating temperatures. All gas-sensing measurements were conducted under a relative humidity condition of 30% RH. For humidity-specific tests on the gas-sensing devices, an air humidifier was used to precisely set and maintain the required humidity levels within the chamber. In addition, a syringe was used to inject a precise volume of volatile gases into the chamber through a rubber septum. The concentration of gases in the test chamber was calculated using Eq. (1) [1, 2]:

$$C = 22.4 \times \varphi \times \rho \times V_1 \times 1000 / (M \times V_2) \quad (1)$$

Where C (*ppm*) is the target gas concentration, φ is expressed as the purity of the liquid

(%), ρ (g/mL) is the liquid density of the target gas, V_1 (μL) is the fluid volume of the target gas, M (g/mol) is the molecular weight of the target gas and V_2 (L) is the volume of the chamber. The response (R) of the sensors was calculated on the basis of the relative change in sensor resistance from air (R_a) to target gas (R_g), using the following formula [3]:

$$R = R_a/R_g \quad (2)$$

Moreover, the response (τ_{res}) and recovery times (τ_{rec}) were determined as the time taken to reach 90% of the final equilibrium value.

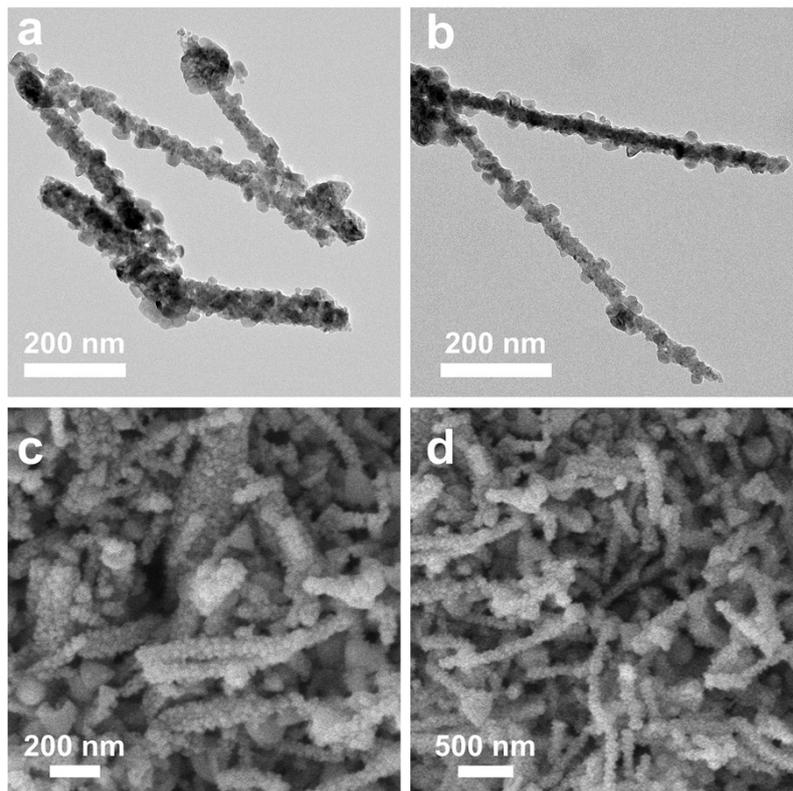


Fig. S1. (a-b) SEM and (c-d) HRTEM images of the IZ4 nanofibers.

LOD calculation:

According to literature reports, the calculation equation for the theoretical detection limit (LOD) is typically used and is shown below [4]:

$$LOD (ppm) = 3 \times \frac{S_{noise}}{b} \quad (3)$$

In Eq. (3), b is the slope value obtained by linearly fitting the response value and 3H-2B concentration curve. Take $N = 10$ data points (Y_i) from the baseline of response versus time curves before 3H-2B exposure (Fig. S2). Then, calculate the regular residual ($Y_i - Y$) of the polynomial fit and determine the root-mean-squared deviation (S_{noise}) using Eq. (4) and Eq. (5) [5]. Here, Y_i represents the measured data point and Y represents the corresponding value calculated from the curve-fitting equation (see Table S1):

$$V_x^2 = \sum_{i=1}^N (Y_i - Y)^2 \quad (4)$$

$$S_{noise} = \sqrt{\frac{V_x^2}{N-1}} \quad (5)$$

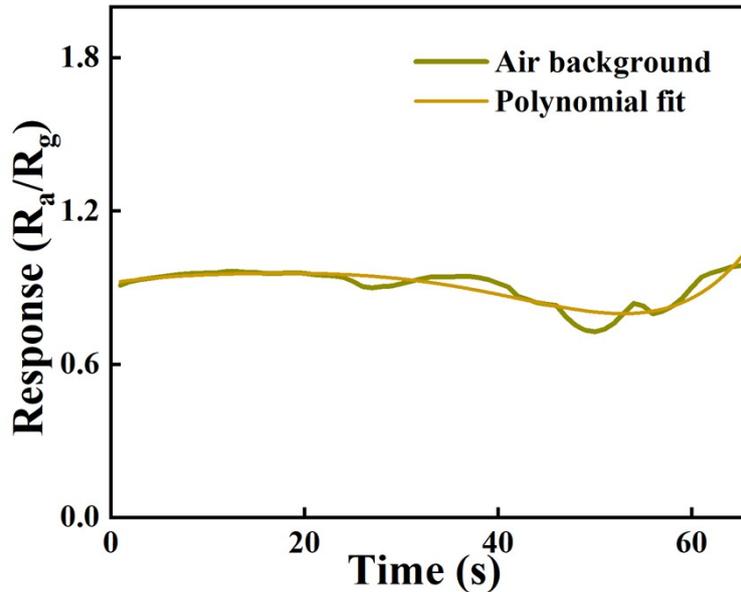


Fig. S2. The 5th order polynomial fitted response of the 3% In-ZnO sensor versus time at the baseline before 3H-2B exposure.

Table S1. 5th order polynomial fitting data for the 3% In-ZnO sensor.

Times of measurement	Y_i	Y	(Y_i-Y)	$(Y_i-Y)^2$
1	0.9468	0.9027	0.0441	1.9448E-3
2	0.9411	0.9044	0.0367	1.3469E-3
3	0.9004	0.9445	-0.0441	1.9448E-3
4	0.8857	0.9372	-0.0515	2.6522E-3
5	0.8121	0.7385	0.0736	5.4169E-3
6	0.8008	0.9493	-0.1485	2.2052E-2
7	0.7991	0.8432	-0.0441	1.9448E-3
8	0.8574	0.8942	-0.0368	1.3542E-3
9	0.8783	0.9372	-0.0589	3.4692E-3
10	1.040	0.9887	0.0513	2.6317E-3

Table S2. Calculation of slope, S_{noise} and LOD.

Sensing Material	b (ppm ⁻¹)	V_x^2	S_{noise}	LOD (ppm)
3% In-ZnO	8.0619	4.4758E-2	7.05E-2	0.0262

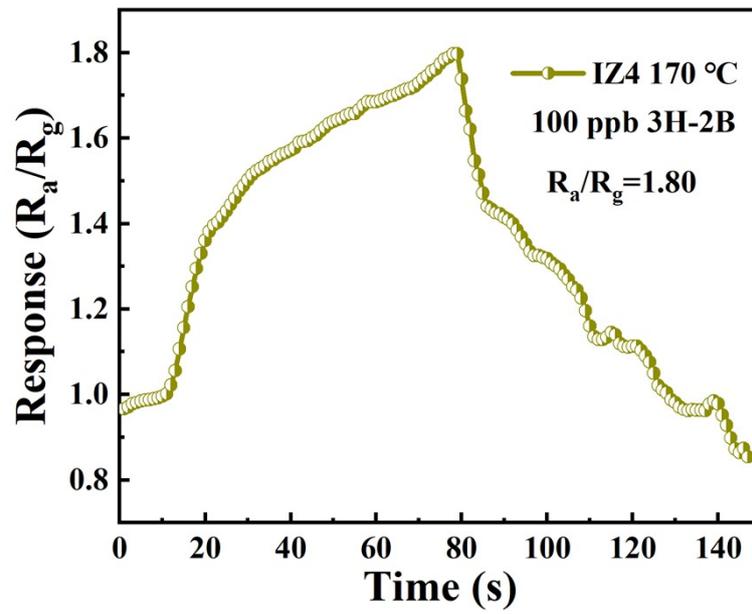


Fig. S3. Response curve of the IZ4 sensor toward 100 ppb 3H-2B.

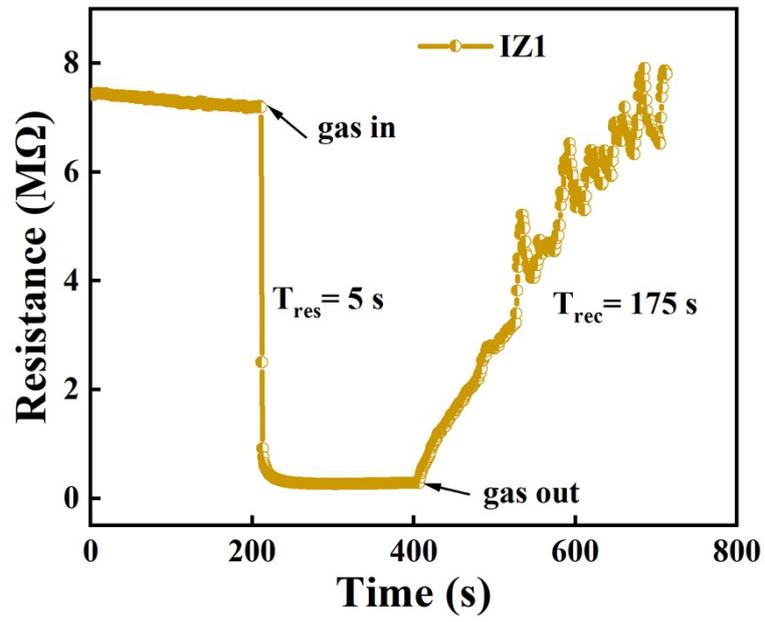


Fig. S4. Response-recovery time curves of the IZ1 sensor toward 100 ppm 3H-2B.

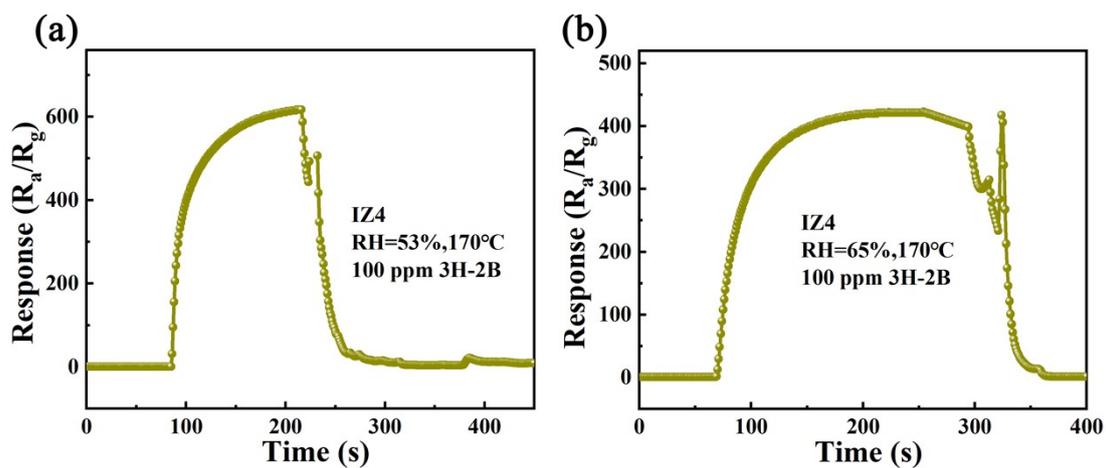


Fig. S5. Dynamic response-recovery curves of the IZ4 sensor toward 100 ppm 3H-2B at RH values of 53% and 65%

References

- [1] Y. Luo, A. Ly, D. Lahem, J.D.M. Martin, A.-C. Romain, C. Zhang, M. Debliquy, Role of cobalt in Co-ZnO nanoflower gas sensors for the detection of low concentration of VOCs, *Sensors and Actuators B: Chemical*, 360 (2022). <https://doi.org/10.1016/j.snb.2022.131674>.
- [2] C. Sun, J. Shao, G. Pan, X. Yang, Triethylamine gas sensor based on Zn₂SnO₄ polyhedron decorated with Au nanoparticles and density functional theory investigation, *Sensors and Actuators B: Chemical*, 408 (2024). <https://doi.org/10.1016/j.snb.2024.135510>
- [3] Y. Zhang, M. Wang, X. San, L. Zhang, N. Wang, G. Wang, D. Meng, Y. Shen, Highly selective gas sensors for formaldehyde detection based on ZnO@ZIF-8 core-shell heterostructures, *Sensors and Actuators B: Chemical*, 398 (2024). <https://doi.org/10.1016/j.snb.2023.134689>.
- [4] X. Shao, D. Zhang, M. Tang, H. Zhang, Z. Wang, P. Jia, J. Zhai, Amorphous Ag catalytic layer-SnO₂ sensitive layer-graphite carbon nitride electron supply layer synergistically enhanced hydrogen gas sensor, *Chemical Engineering Journal*, 495 (2024). <https://doi.org/10.1016/j.cej.2024.153676>.
- [5] T. Murugesan, R.R. Kumar, A. Ranjan, M.-Y. Lu, H.-N. Lin, Fabrication of large-area Au nanoparticle decorated ZnO@ZIF-8 core-shell heterostructure nanorods for ppb-level NO₂ gas sensing at room temperature, *Sensors and Actuators B: Chemical*, 402 (2024). <https://doi.org/10.1016/j.snb.2023.135106>.