

Supplementary Information

Bifunctional gas sensor based on Bi₂S₃/SnS₂ heterostructures with improved selectivity through visible light modulation

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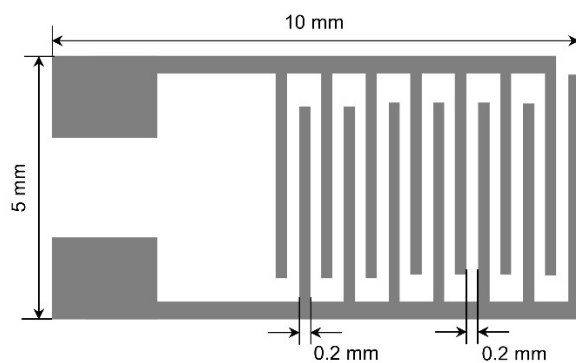


Fig. S1 Schematic diagram of the Au interdigital electrode.

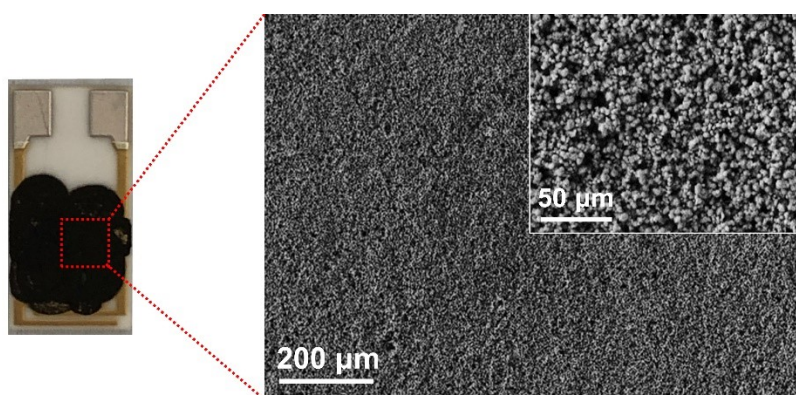


Fig. S2 SEM images of $\text{Bi}_2\text{S}_3/\text{SnS}_2$ dispersed on the interdigitated electrode.

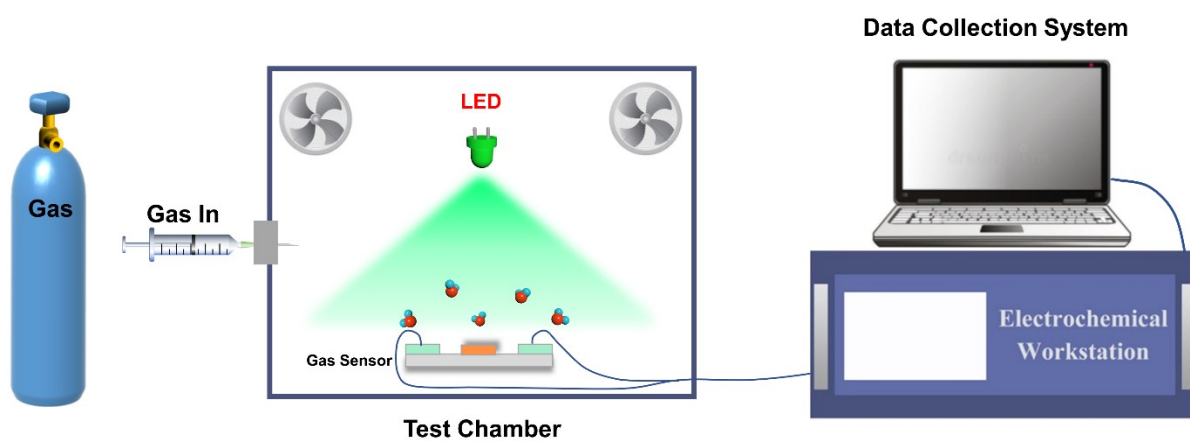


Fig. S3 Schematic diagram of the sensor measurement.

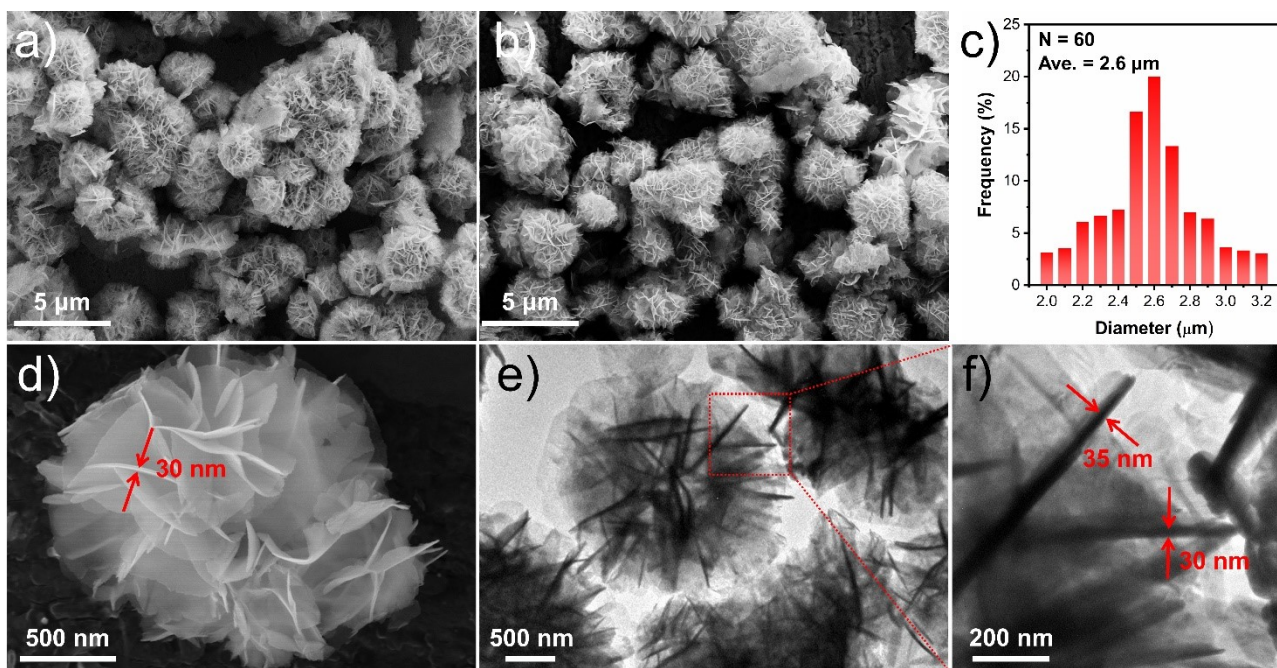


Fig. S4 (a, b, d) SEM and (e, f) TEM image of pure SnS₂; (c) The diameter distribution of the hierarchical SnS₂.

The size of hierarchical SnS₂ is in the range of 2.0-3.2 μm, and the diameter of the majority of nanoflowers are between 2.5 and 2.7 μm, with an average diameter of 2.6 μm. The thickness of constituting nanosheets is about 30-35 nm.

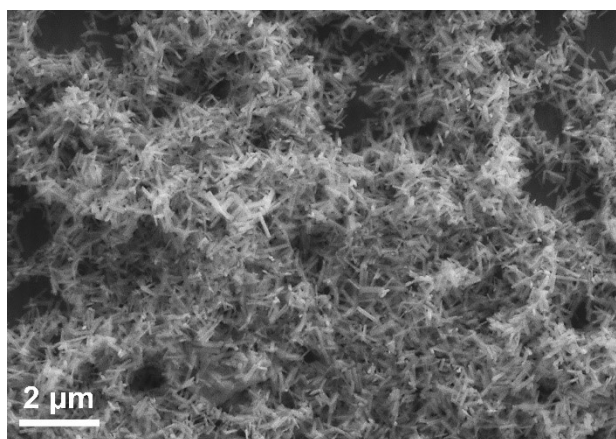


Fig. S5 SEM image of pure Bi₂S₃.

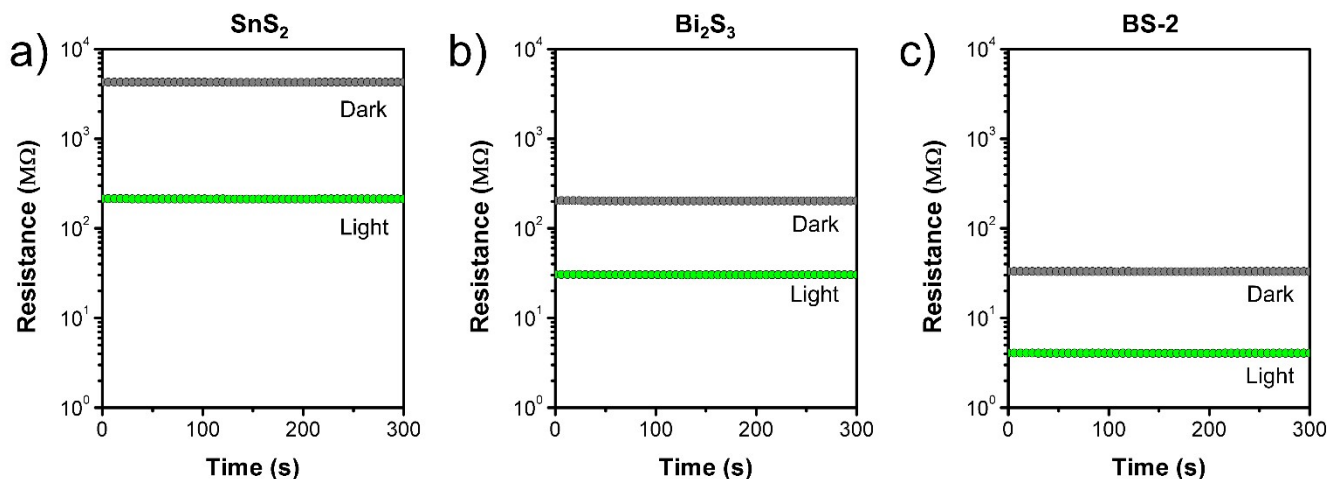


Fig. S6 The baseline curves of devices based on (a) SnS₂, (b) Bi₂S₃, and (c) BS-2 before and after light irradiation.

Table S1 Response value and response/recovery time of SnS₂, Bi₂S₃, and BS-2 sensors toward 500 ppb NO₂ and 500 ppb H₂S in dark and under light illumination, respectively.

Sensing materials	500 ppb NO ₂				500 ppb H ₂ S			
	Dark		Light		Dark		Light	
	Response (R _g /R _a)	t _{res} /t _{rec} (s/s)	Response (R _g /R _a)	t _{res} /t _{rec} (s/s)	Response (R _a /R _g)	t _{res} /t _{rec} (s/s)	Response (R _a /R _g)	t _{res} /t _{rec} (s/s)
SnS ₂	—	—	2.1	26/150	—	—	—	—
Bi ₂ S ₃	2.5	42/400	3.0	35/350	3.5	265/300	1.8	140/130
BS-2	4.0	55/120	14.0	38/80	12.3	175/225	2.1	130/180

t_{res}/t_{rec}: response/recovery time

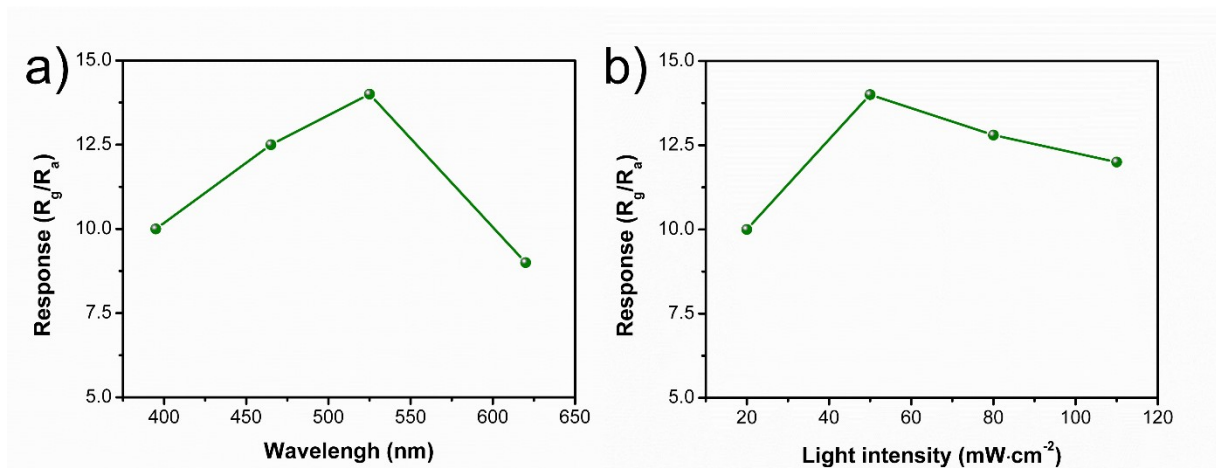


Fig. S7 Influence of (a) light wavelength and (b) light intensity on the sensing response of BS-2 sensor toward 500 ppb NO₂.

With the decrease of light wavelength or increase of light intensity, the response first increases and then decreases. One possible reason is that when the light energy is too strong, the number of photogenerated carriers participating during the sensing process will decrease.^{1,2} Another possible cause is that the desorption reaction tends to dominate under excessively intensive light irradiation.^{3,4} The highest response value is achieved under 525 nm light illumination with the optimal intensity of 50 mW/cm^2 .

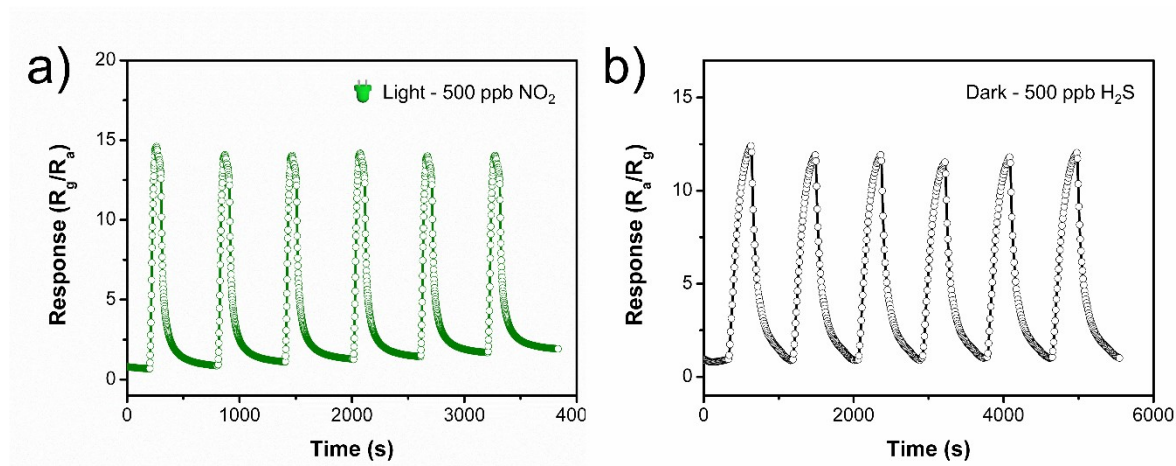


Fig. S8 Repeatability measurement of BS-2 sensor: six successive sensing cycles to (a) 500 ppb NO₂ under light and (b) 500 ppb H₂S in dark.

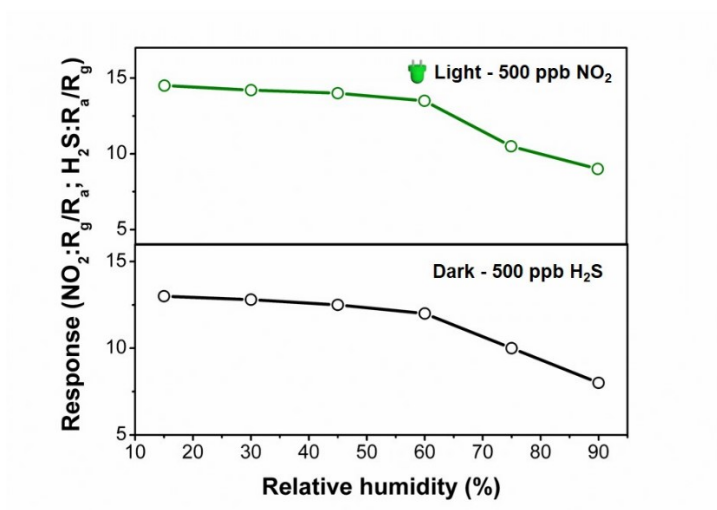


Fig. S9 Effects of humidity on the sensing responses of the BS-2 towards 500 ppb NO₂ under light and 500 ppb H₂S in dark.

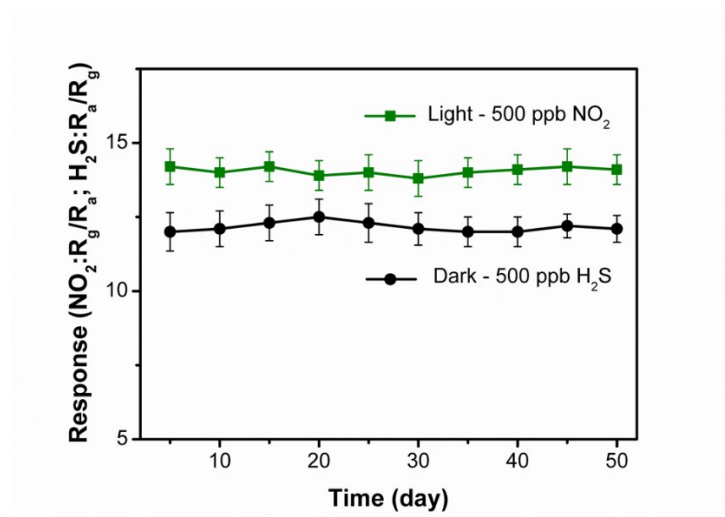


Fig. S10 Long-term stability of BS-2 sensor within 50 days to 500 ppb NO₂ under light and 500 ppb H₂S in dark.

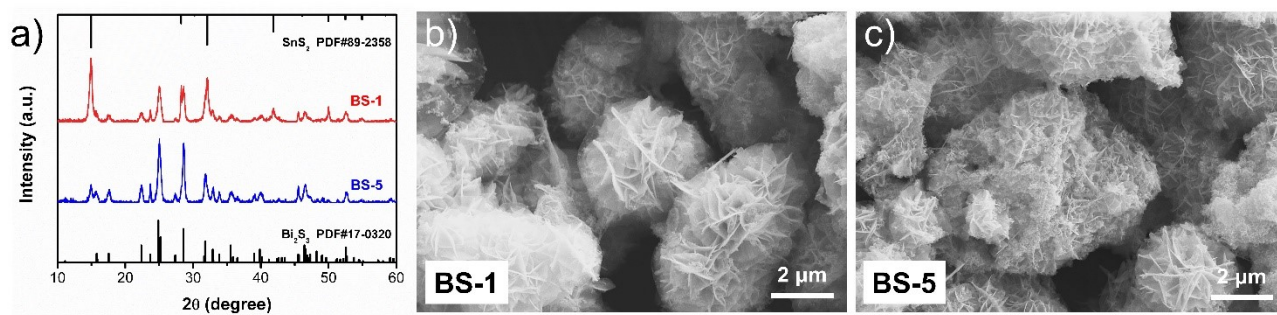


Fig. S11 (a) XRD patterns and (b-c) SEM images of BS-1 and BS-5 samples.

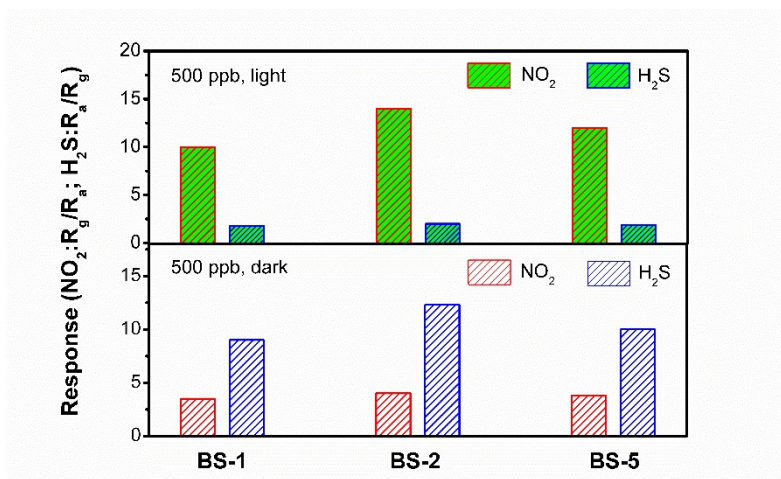


Fig. S12 The gas sensing responses of BS-1, BS-2, and BS-5 to 500 ppb NO₂ and 500 ppb H₂S under light and dark, respectively.

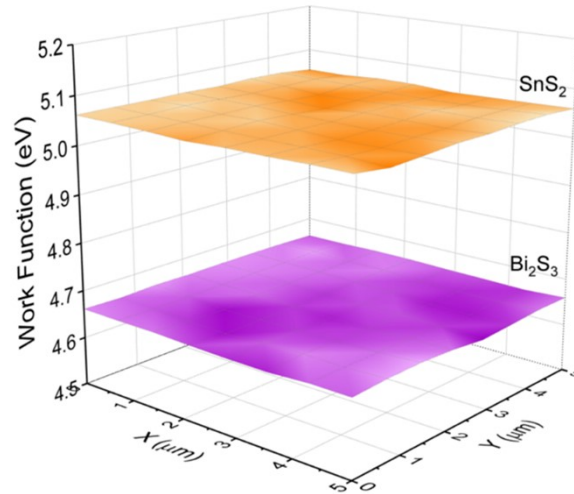


Fig. S13 Work functions of SnS₂ (5.05 eV) and Bi₂S₃ (4.65 eV) measured by the Kelvin probe based on 256 data points.

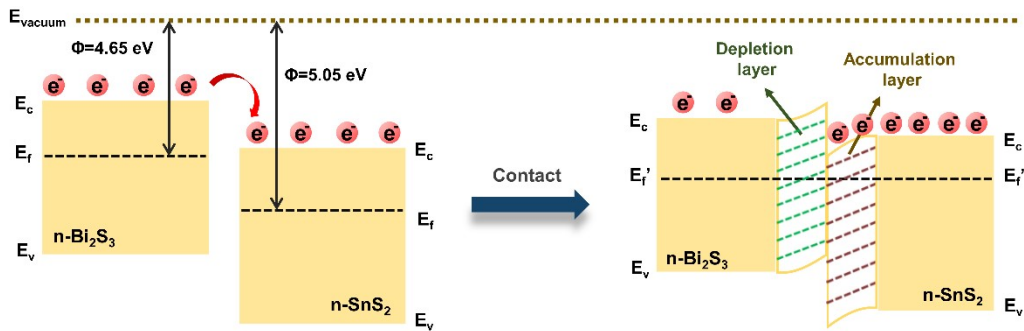


Fig. S14 Energy band diagram of Bi₂S₃/SnS₂ heterostructure before and after equilibrium.

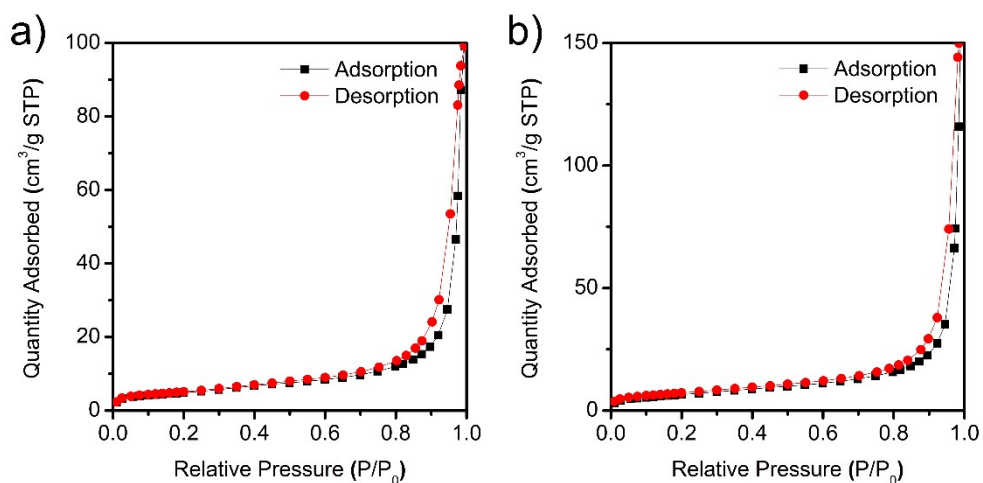


Fig. S15 Nitrogen adsorption/desorption isotherms of (a) SnS₂ and (b) BS-2 samples.

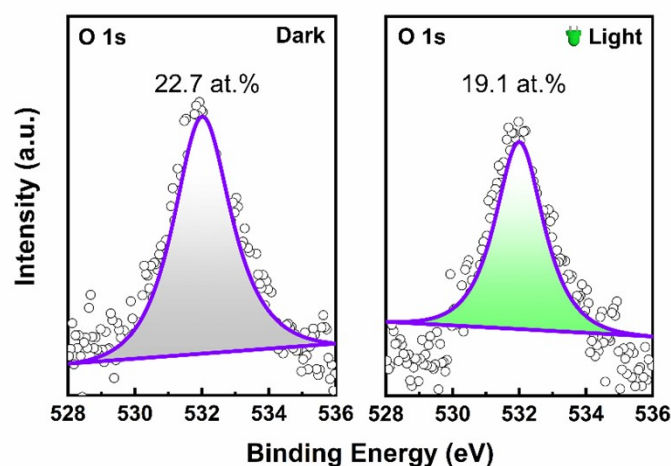


Fig. S16 The in-situ O 1s XPS spectra of Bi₂S₃/SnS₂ heterostructure: (a) in dark and (b) under 525 nm light illumination.

The in-situ X-ray photoelectron spectroscopy analysis was performed by the VG Thermo ESCALAB 250 spectrometer with the 525 nm light assistance. Firstly, the chemical states information of the sample without light illumination was recorded. The circumstances were kept under dark during this entire test. Then, 525nm light was shone on the surface of the sample through the observation window of the spectrometer, simultaneously the surface chemical state of the sample with light irradiation was measured and recorded. In addition to the 525 nm light, there is no other light source during this testing process.

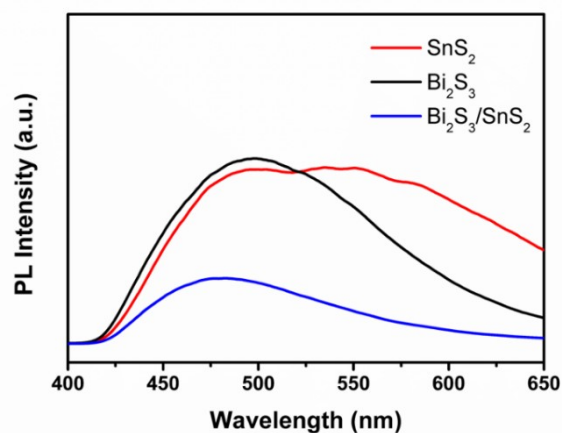


Fig. S17 PL spectra of SnS₂, Bi₂S₃, and BS-2 samples.

The recombination rate of the photo-generated electron-hole pairs is an important factor affecting the light-assisted sensing properties. The PL spectra of the samples were measured to investigate the charge separation capability. As shown, the Bi₂S₃/SnS₂ heterostructure displays a much lower emission peak than that of pure SnS₂ and Bi₂S₃, indicating that the electron-hole recombination is efficiently suppressed by the interfacial charge transfer between Bi₂S₃ and SnS₂, thereby prolonging the carrier lifetime and further boosting the light-activated NO₂ sensing performance.

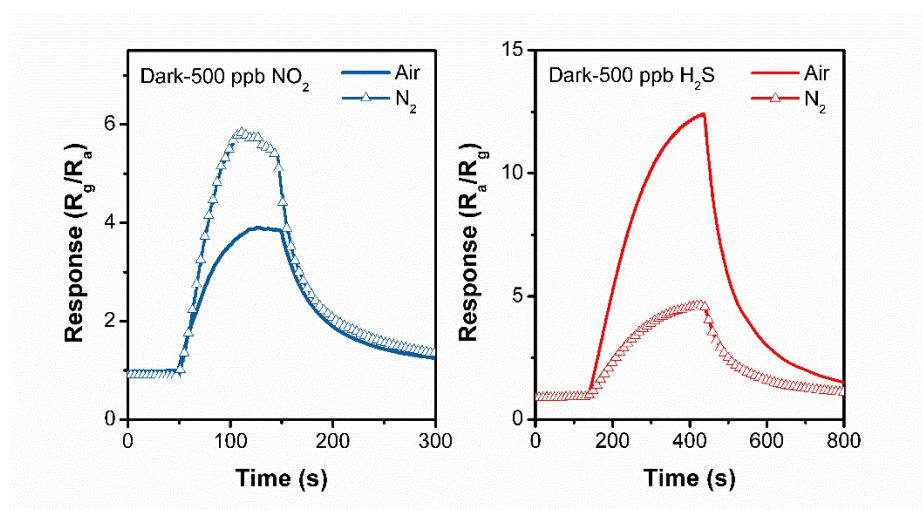


Fig. S18 The response curves of the BS-2 sensor to 500 ppb (a) NO₂ and (b) H₂S in nitrogen/air balance under dark.

References

1. J. M. Suh, T. H. Eom, S. H. Cho, T. Kim and H. W. Jang, *Mater. Adv.*, 2021, **2**, 827-844.
2. Y. Huang, W. Jiao, Z. Chu, X. Nie, R. Wang and X. He, *ACS Appl. Mater. Interfaces*, 2020, **12**, 25178-25188.
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