

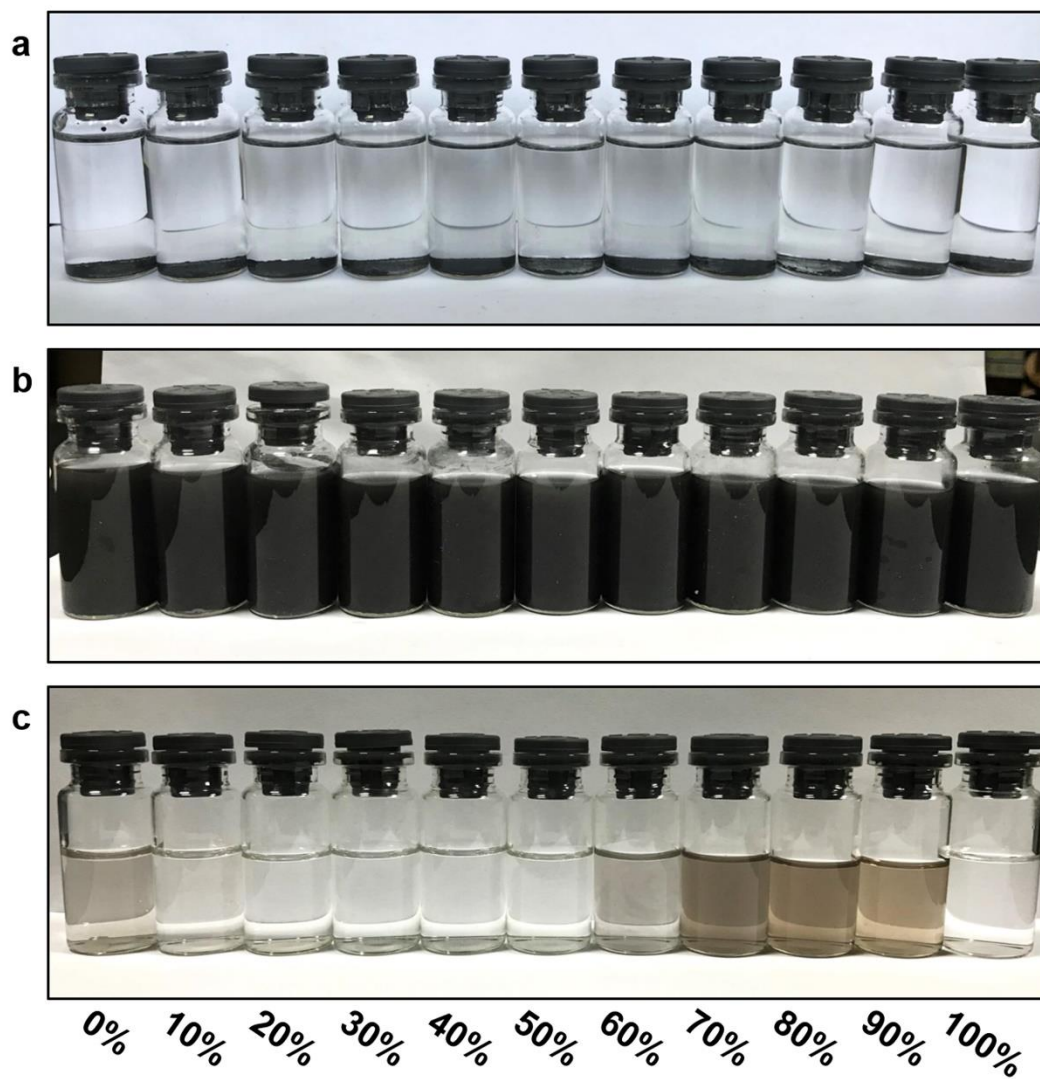
# **A novel artificial neuron-like gas sensor constructed from CuS quantum dots/Bi<sub>2</sub>S<sub>3</sub> nanosheets**

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Zhou<sup>1</sup>, Zhi Yang<sup>1\*</sup>, Yafei Zhang<sup>1\*</sup>

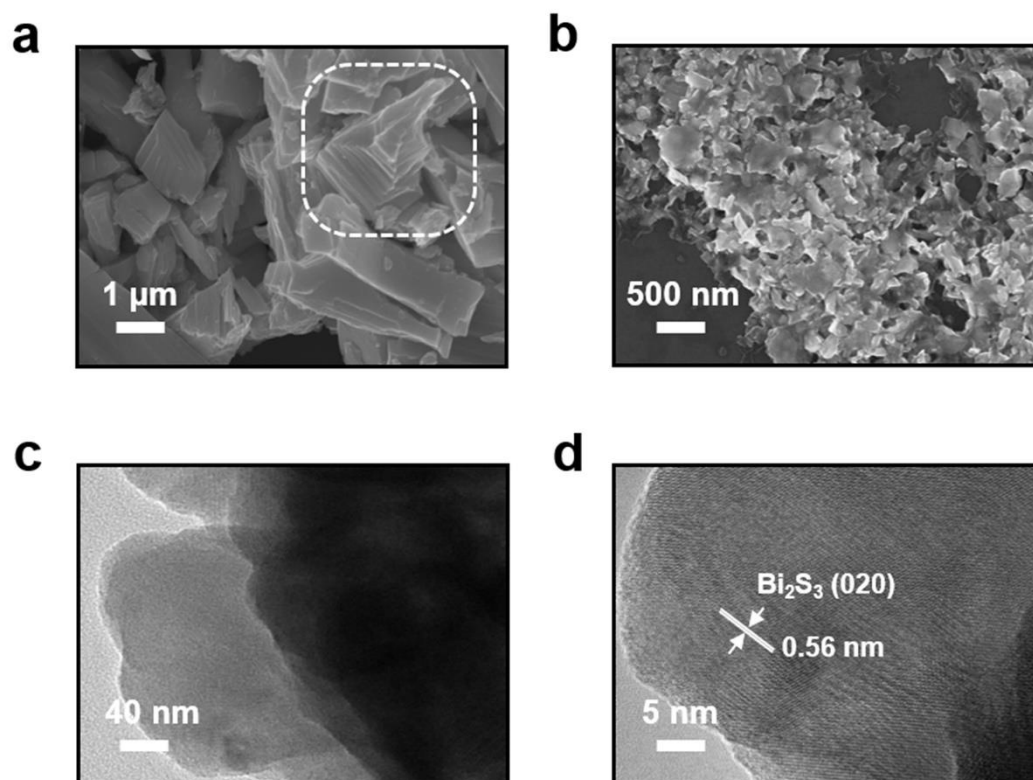
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**Fig. S1** Photographs of  $\text{Bi}_2\text{S}_3$  dispersions in various ethanol/water mixtures: **a** Before and **b** after ultrasonication treatment for 8 h. **c** Supernatant collection by centrifugation at 3000 rpm.



**Fig. S2** SEM image of Bi<sub>2</sub>S<sub>3</sub> samples before **a** and after **b** Liquid phase stripping. **c** and **d** TEM and HR-TEM images of Bi<sub>2</sub>S<sub>3</sub> NSs.

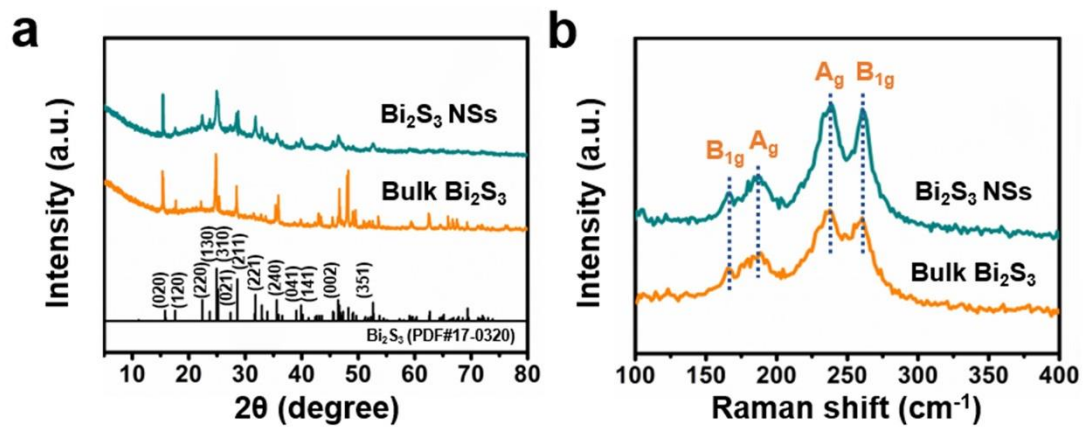
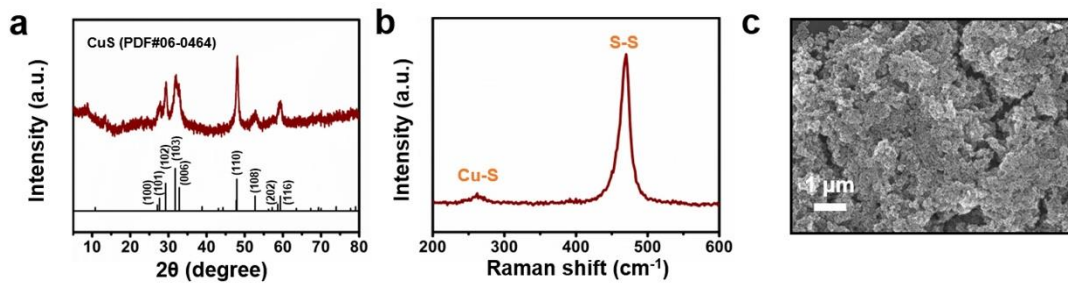


Fig. S3 XRD patterns **a** and Raman spectra **b** of bulk Bi<sub>2</sub>S<sub>3</sub> and Bi<sub>2</sub>S<sub>3</sub> NSs.



**Fig. S4** **a** XRD pattern **b** Raman spectra and **c** SEM image of CuS sample.

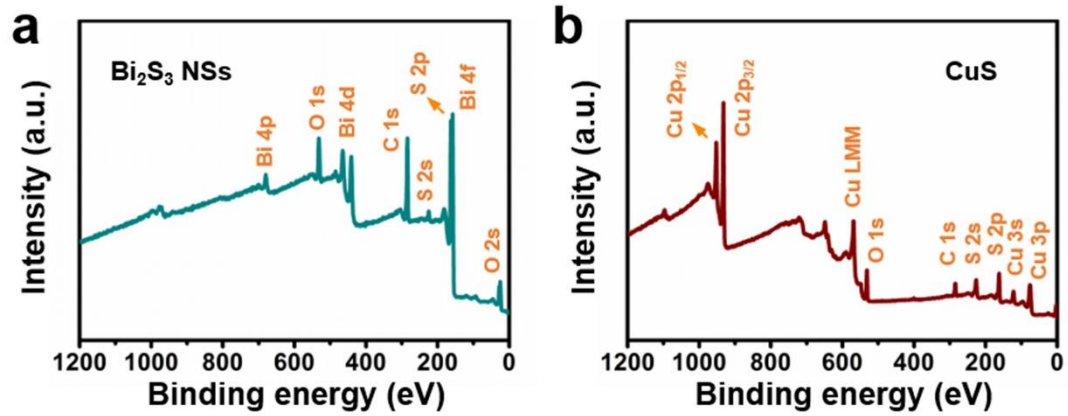
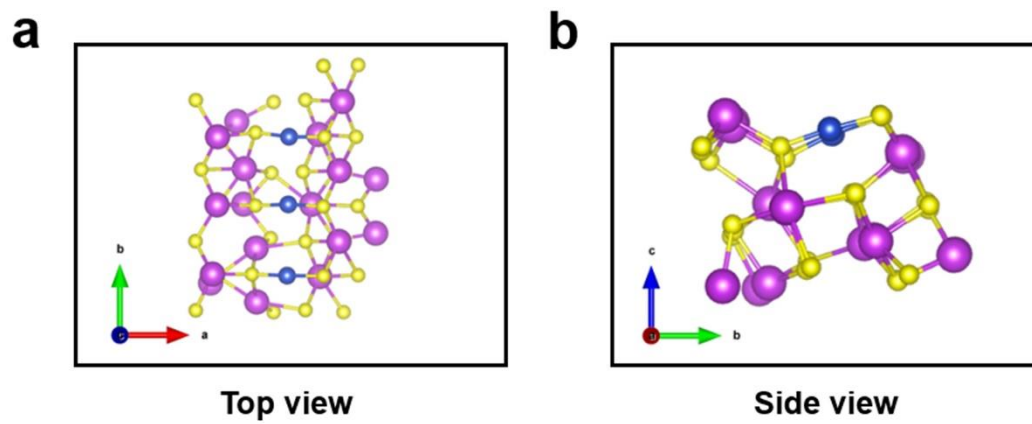
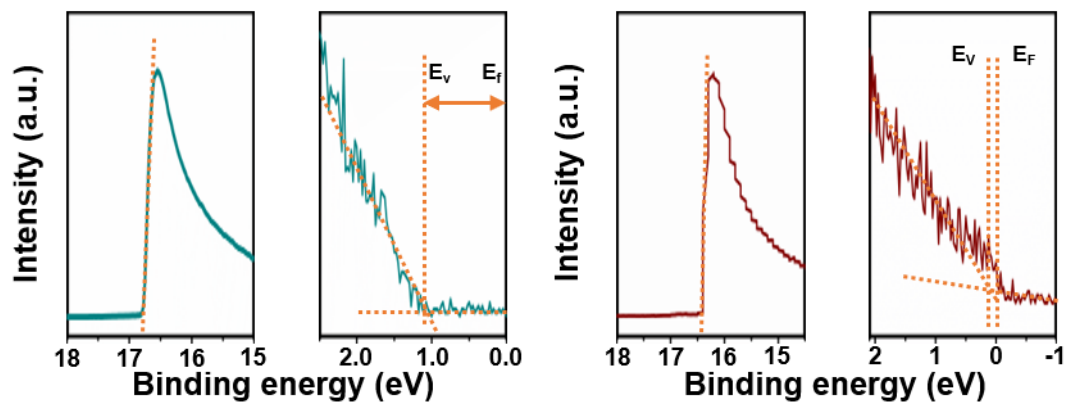


Fig. S5 Full XPS survey spectrums of **a**  $\text{Bi}_2\text{S}_3$  NSs and **b** CuS.

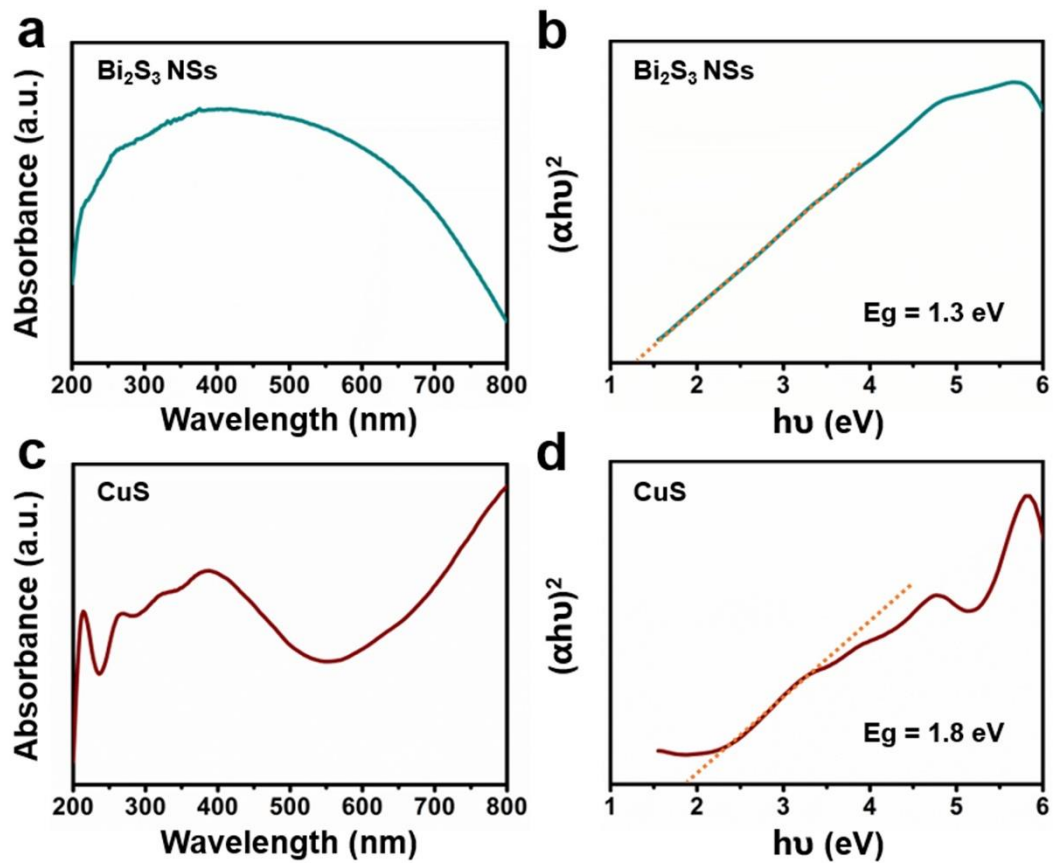


**Fig. S6** The atomic structure of  $\text{CuS-Bi}_2\text{S}_3$ .

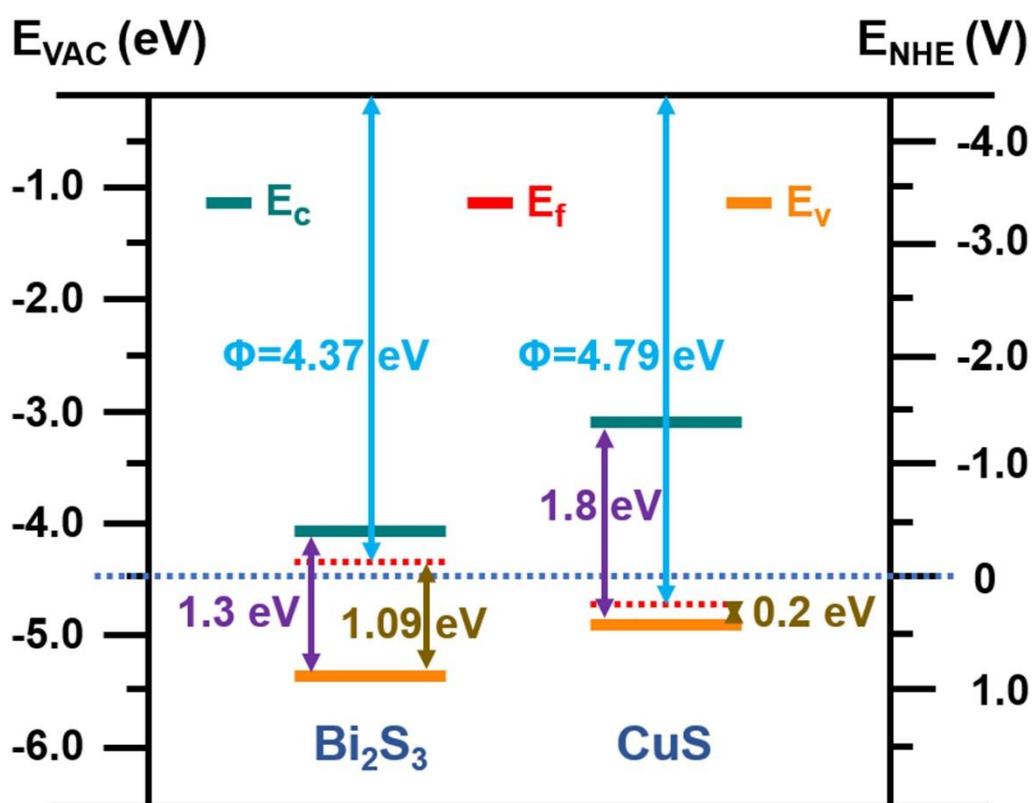


**Fig. S7** UPS spectra of **a**  $\text{Bi}_2\text{S}_3$  and **b**  $\text{CuS}$ : the secondary electron cut-off energy region (left) and low binding energy region (right) of each.

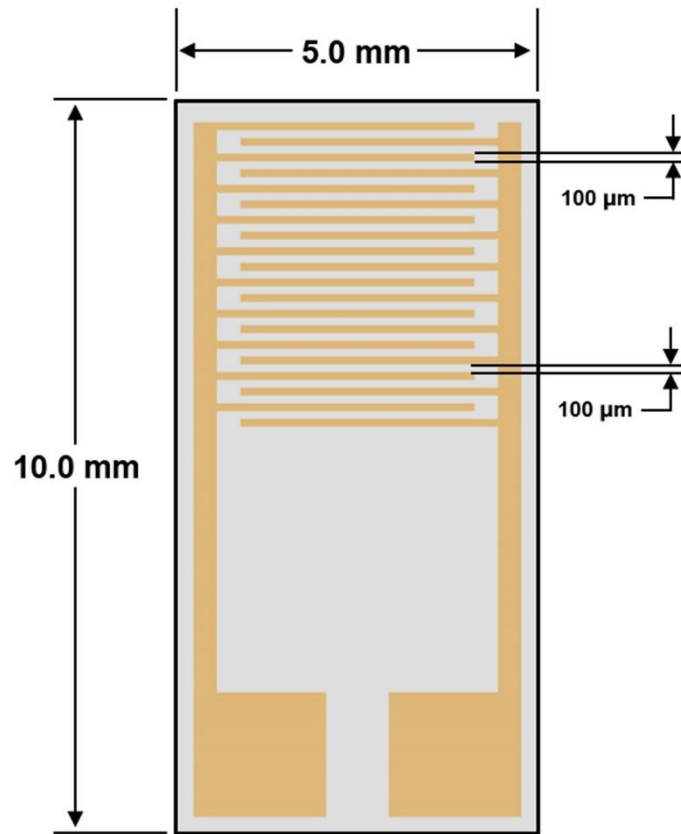




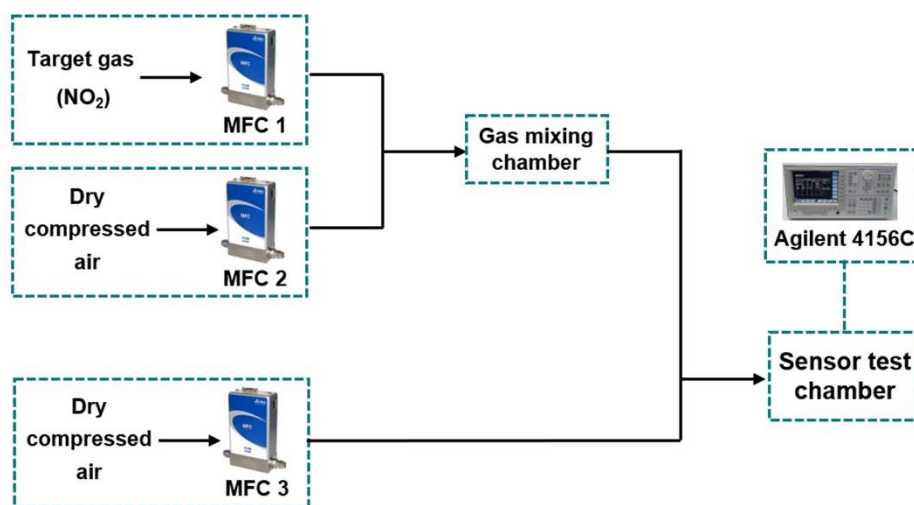
**Fig. S8** UV-vis diffuse reflectance spectra of **a** Bi<sub>2</sub>S<sub>3</sub> NSs and **c** CuS.  $(\alpha h\nu)^2$  v.s.  $h\nu$  curve of **b** Bi<sub>2</sub>S<sub>3</sub> NSs and **d** CuS.



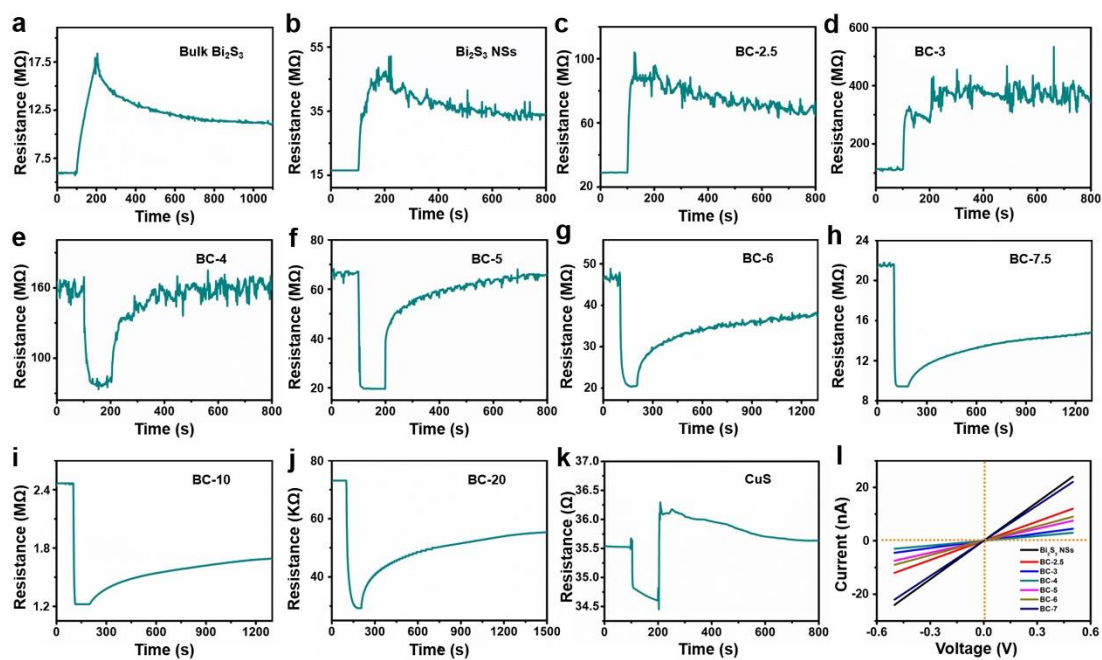
**Fig. S9** Energy level diagram between interfacial materials  $\text{CuS}$  and  $\text{Bi}_2\text{S}_3$  and schematic diagram of the charge transfer process.



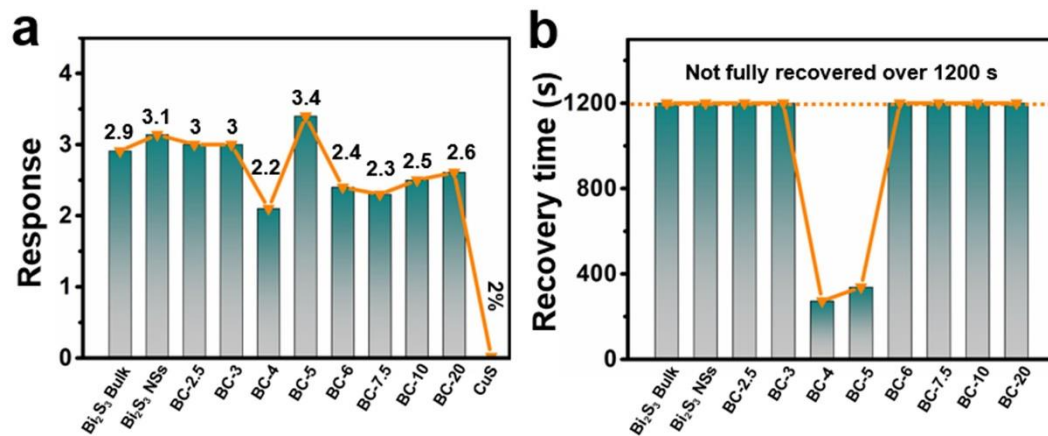
**Fig. S10** Structure diagram of the flexible interdigital electrode.



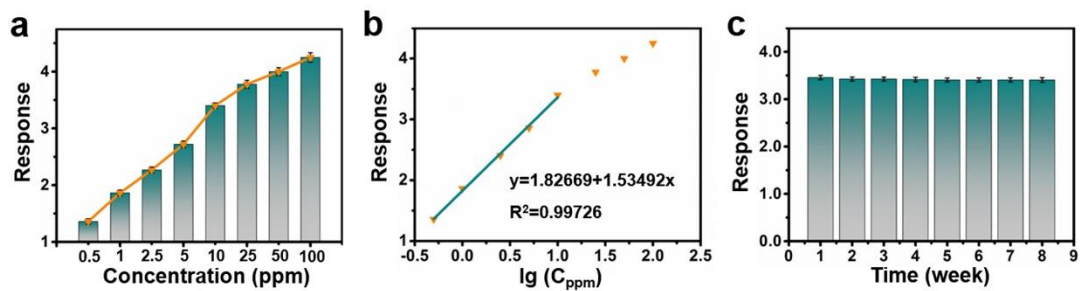
**Fig. S11** Schematic diagram of the homemade gas-control system.



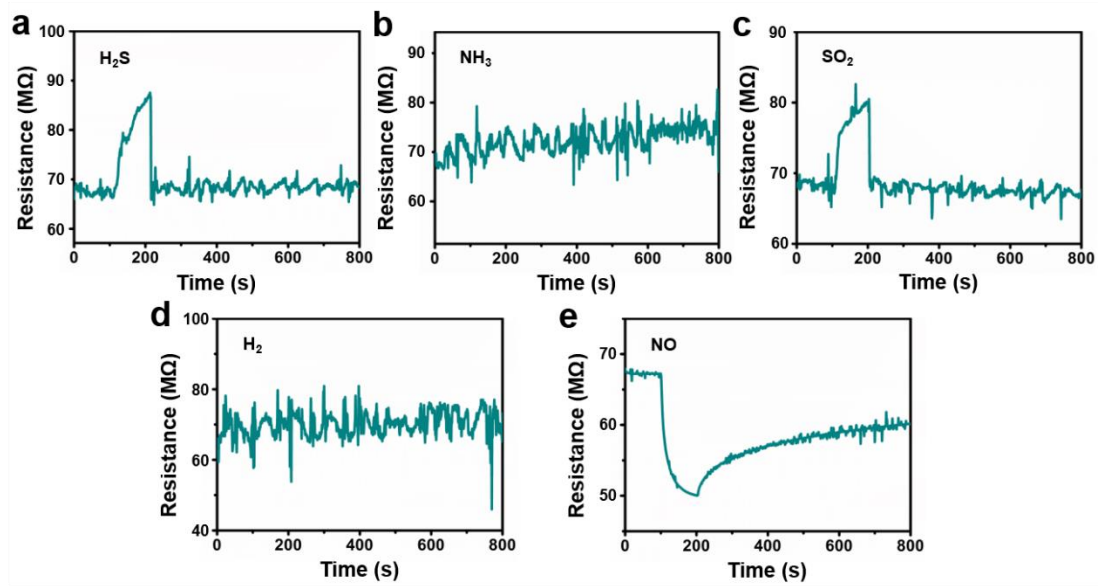
**Fig. S12 a-k** Sensitive response at a concentration to 10 ppm NO<sub>2</sub> through a dynamic gas-sensing room temperature testing for bulk pure Bi<sub>2</sub>S<sub>3</sub>, Bi<sub>2</sub>S<sub>3</sub> NSs, BC-2.5, BC-3, BC-4, BC-5, BC-6, BC-7.5, BC-10, BC-20, and pure CuS. **l** *I-V* curves of Bi<sub>2</sub>S<sub>3</sub>, different content of CuS QDs/Bi<sub>2</sub>S<sub>3</sub> NSs and CuS-based gas sensors.



**Fig. S13 a** Response and **b** recovery performances of Bi<sub>2</sub>S<sub>3</sub>, different content of CuS QDs/Bi<sub>2</sub>S<sub>3</sub> NSs, and CuS-based gas sensors to 10 ppm NO<sub>2</sub>.

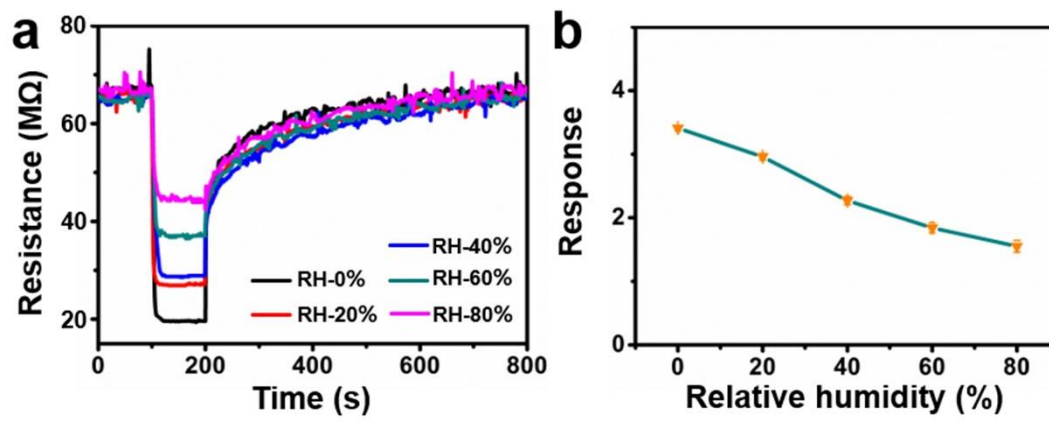


**Fig. S14** **a** The response value of BC-5 sensor to different concentrations of NO<sub>2</sub> and its error bars. **b** The response of BC-5-based sensor as a function of the logarithm of the NO<sub>2</sub> concentration. **c** Long-term stability of BC-5-based sensor.

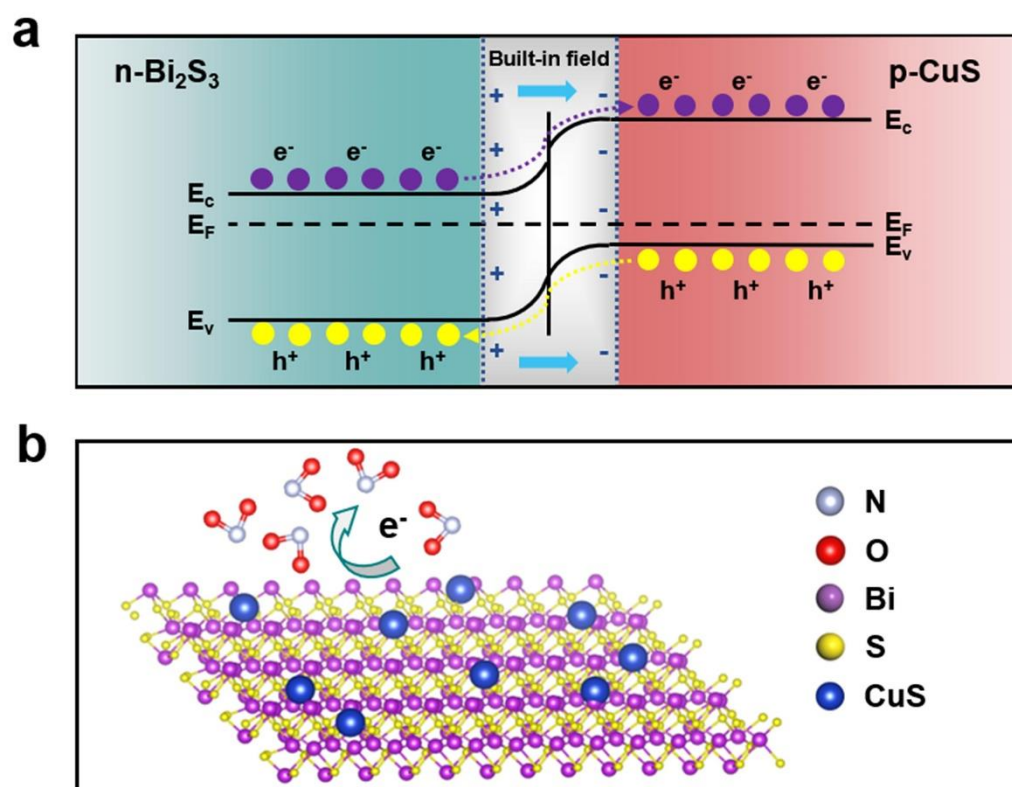


**Fig. S15** The selectivity of the BC-5-based sensor to 10 ppm different target gases of **a** H<sub>2</sub>S, **b** NH<sub>3</sub>, **c** SO<sub>2</sub>, **d** H<sub>2</sub> and **e** NO.

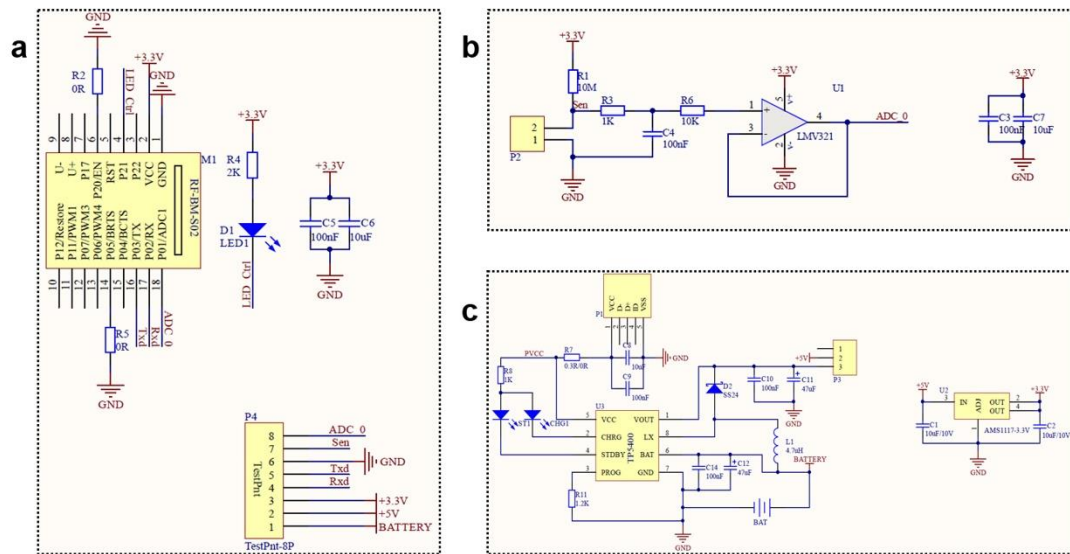




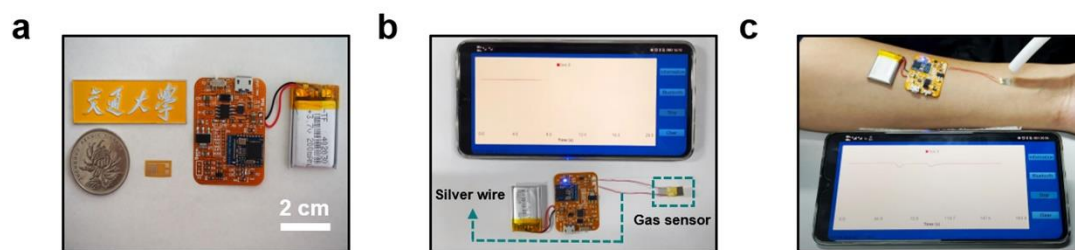
**Fig. S16** Sensing characteristics of the sensor to 10 ppm NO<sub>2</sub> at different humidity levels.



**Fig. S17 a** Energy band structures of CuS QDs/Bi<sub>2</sub>S<sub>3</sub> NSs heterostructure in air. **b** the proposed sensing mechanism of the heterostructure.



**Fig. S18** The schematic circuit diagram of the flexible printed circuit board: **a** Data acquisition and communication circuit. **b** Sensor front-end circuit. **c** USB/Wireless charging circuit.



**Fig. S19** **a** Photograph of the flexible circuit and electrode used in the current work (placed next to a school logo and 1 RMB coin for comparison). **b** Photographs of Bluetooth signal connection of wearable sensor device. **c** Photographs of wireless sensor signal acquisition process of the wearable sensor device.

**Table S1** The bond length of M-O on NO<sub>2</sub>-CuS-Bi<sub>2</sub>S<sub>3</sub> structure.

Binding structure	Atoms	Bond	Length (Å)
n1	N (from NO <sub>2</sub> )	Cu-N	1.978
	Cu (CuS-Bi <sub>2</sub> S <sub>3</sub> )		
n2	O (from NO <sub>2</sub> )	Bi-O	2.025
	Bi (CuS-Bi <sub>2</sub> S <sub>3</sub> )		2.018
n3	O (from NO <sub>2</sub> )	Cu-O	2.396
	Bi/Cu (CuS-Bi <sub>2</sub> S <sub>3</sub> )	Bi-O	2.557
n4	O (from NO <sub>2</sub> )	Cu-O	2.555
	Cu (CuS-Bi <sub>2</sub> S <sub>3</sub> )		2.567

**Table S2** The charge and charge transfer of NO<sub>2</sub> correlated to Fig. 5.

Binding structure	Atoms	Charge	Charge transfer
n2	N	4.4197582	-0.5802418
	O	6.5942103	0.5942103
	O	6.6273451	0.6273451
	Total-NO <sub>2</sub>		0.6413136
n4	N	4.4885298	-0.5114702
	O	6.598587	0.598587
	O	6.6327922	0.6327922
	Total-NO <sub>2</sub>		0.719909

**Table S3** The charge and charge transfer of CuS correlated to Fig. 3d.

Binding structure	Atoms	Charge (e)	Charge transfer (e)
CuS-Bi <sub>2</sub> S <sub>3</sub>	Cu1	10.59286	-0.40714
	Cu2	10.59062	-0.40938
	Cu3	10.58872	-0.41128
	S1	6.800926	0.800926
	S2	6.751016	0.751016
	S3	6.768011	0.768011
	S4	6.763804	0.763804
	S5	6.771819	0.771819
	S6	6.74335	0.74335
	Total-CuS		3.371122

**Table S4** Resistance values of bulk Bi<sub>2</sub>S<sub>3</sub>, Bi<sub>2</sub>S<sub>3</sub> NSs, CuS, and different complex amounts of CuS QDs/Bi<sub>2</sub>S<sub>3</sub> heterostructures.

	<i>R</i>		<i>R</i>
Bulk Bi <sub>2</sub> S <sub>3</sub>	6.4 MΩ	BC-6	48 MΩ
Bi <sub>2</sub> S <sub>3</sub> NSs	17 MΩ	BC-7.5	21.5 MΩ
BC-2.5	30 MΩ	BC-10	2.5 MΩ
BC-3	110 MΩ	BC-20	73 KΩ
BC-4	160 MΩ	CuS	35.5 Ω
BC-5	66 MΩ		



**Table S5** The room-temperature sensing performance comparison of NO<sub>2</sub> flexible gas sensors with different sensing materials.

Materials	Conc. (ppm)	Response	$\tau_{res.}$ (s)	$\tau_{rec.}$ (s)	LOD (ppb)	Ref.
MoSe <sub>2</sub>	10	4 <sup>a</sup>	250	150	10	1
VA-2D MoS <sub>2</sub>	5	380% <sup>b</sup>	500	Can't recover	-	2
SnS <sub>2</sub> /S-rGO	1	75% <sup>c</sup>	600	1200	0.7	3
RGO/Mesoporous ZnO NSs	15	44% <sup>c</sup>	140	630	43.5	4
3D SnS <sub>2</sub> -rGO	5	32.1% <sup>d</sup>	300	Can't recover	2.8	5
CuS QDs/Bi <sub>2</sub> S <sub>3</sub>	10	3.4 <sup>e</sup>	18	338	78	This work

Conc.: Gas concentration; Temp.: Operating temperature;  $\tau_{rec.}$ : Recovery time; RT: Room temperature.

<sup>a</sup>  $I_g/I_a$ .

<sup>b</sup>  $\Delta I/I_0$

<sup>c</sup>  $\Delta R/R_a$ .

<sup>d</sup>  $\Delta G/G$ .

<sup>e</sup>  $R_g/R_a$ .

## References

- [1] S. Guo, D. Yang, S. Zhang, Q. Dong, B. Li, N. Tran, Z. Li, Y. Xiong, M.E. Zaghoul, Development of a cloud-based epidermal MoSe<sub>2</sub> device for hazardous gas sensing. *Adv. Funct. Mater.* **29**, 1900138 (2019). <https://doi.org/10.1002/adfm.201900138>
- [2] M.A. Islam, H. Li, S. Moon, S.S. Han, H.-S. Chung, J. Ma, C. Yoo, T.-J. Ko, K.H. Oh, Y.J. Jung, Y.W. Jung, Vertically aligned 2D MoS<sub>2</sub> layers with strain-engineered serpentine patterns for high-performance stretchable gas sensors: experimental and theoretical demonstration. *ACS Appl. Mater. Interfaces* **12**(47), 53174–53183 (2020). <https://doi.org/10.1021/acsami.0c17540>
- [3] Y. Huang, W. Jiao, Z. Chu, S. Wang, L. Chen, X. Nie, R. Wang, X. He, High sensitivity, humidity-independent, flexible NO<sub>2</sub> and NH<sub>3</sub> gas sensors based on SnS<sub>2</sub> hybrid functional graphene ink. *ACS Appl. Mater. Interfaces* **12**(1), 997–1004 (2020). <https://doi.org/10.1021/acsami.9b14952>
- [4] W. Li, R. Chen, W. Qi, L. Cai, Y. Sun, M. Sun, C. Li, X. Yang, L. Xiang, D. Xie, T. Ren, Reduced graphene oxide/mesoporous ZnO NSs hybrid fibers for flexible, stretchable, twisted, and wearable NO<sub>2</sub> e-textile gas sensor. *ACS Sens.* **4**(10), 2809–2818 (2019). <https://doi.org/10.1021/acssensors.9b01509>
- [5] J. Wu, Z. Wu, H. Ding, Y. Wei, W. Huang, X. Yang, Z. Li, L. Qiu, X. Wang, Three-dimensional graphene hydrogel decorated with SnO<sub>2</sub> for high-performance NO<sub>2</sub> sensing with enhanced immunity to humidity. *ACS Appl. Mater. Interfaces* **12**(2), 2634–2643 (2020). <https://doi.org/10.1021/acsami.9b18098>