

Supplementary Information

Phosphorene-Derived Ni₂P/NiO Lateral Heterostructure for Highly Sensitive and Selective H₂S Gas Detection

Shutong He,^a Lei Li,^{*a} Yaoda Liu,^a Jie Su,^a Yudong Sun^{*b} and Zhengfei Dai^{*a}

^a State Key Laboratory of Porous Metal Materials, Xi'an Jiaotong University, Xi'an 710049, China; E-mail: sensdai@mail.xjtu.edu.cn (Z.D.); xjlilei@stu.xjtu.edu.cn (L.L).

^b Department of Vascular Surgery, Department of General Surgery, Ruijin Hospital, Shanghai Jiao Tong University School of Medicine, Shanghai 200025, China; E-mail: sunyudong@smmu.edu.cn (Y. S.).

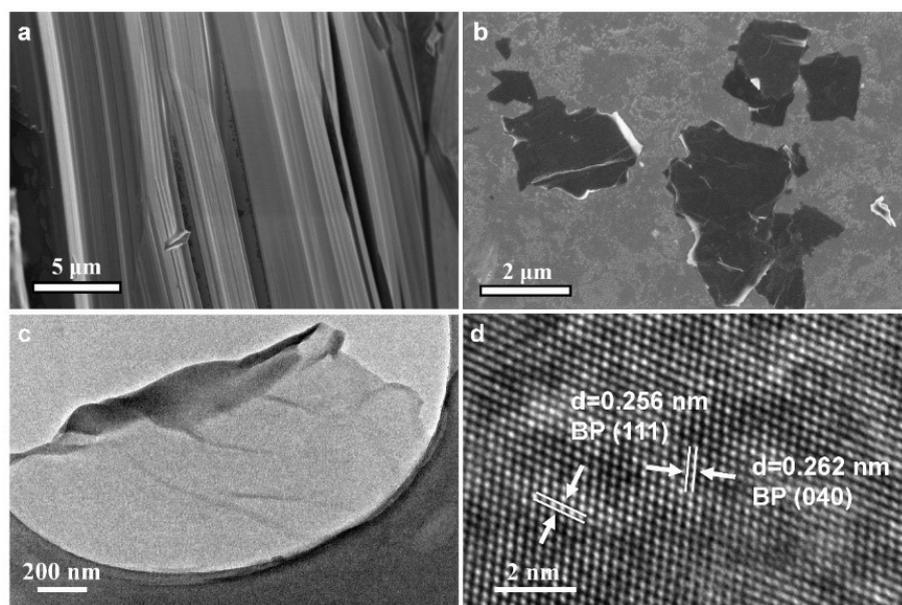


Fig. S1 (a) SEM image of BP bulk. (b) SEM image, (c) TEM image, and (d) HRTEM image of BP nanosheets.

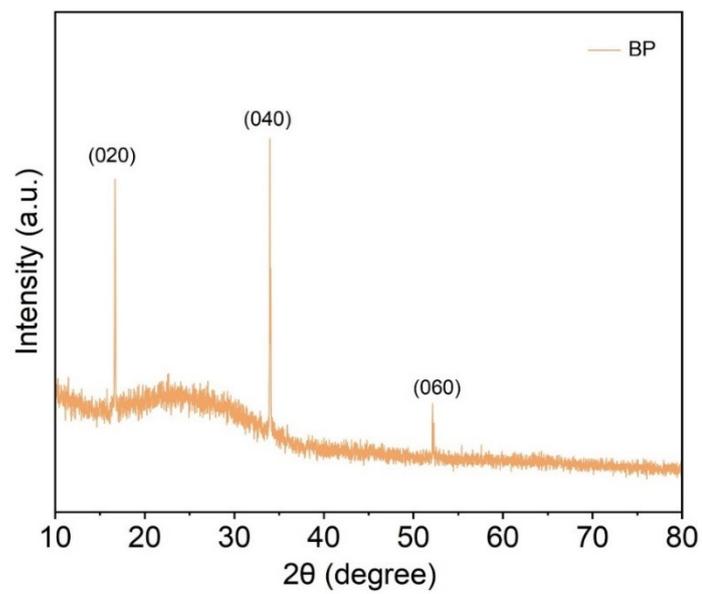


Fig. S2 XRD pattern of BP.

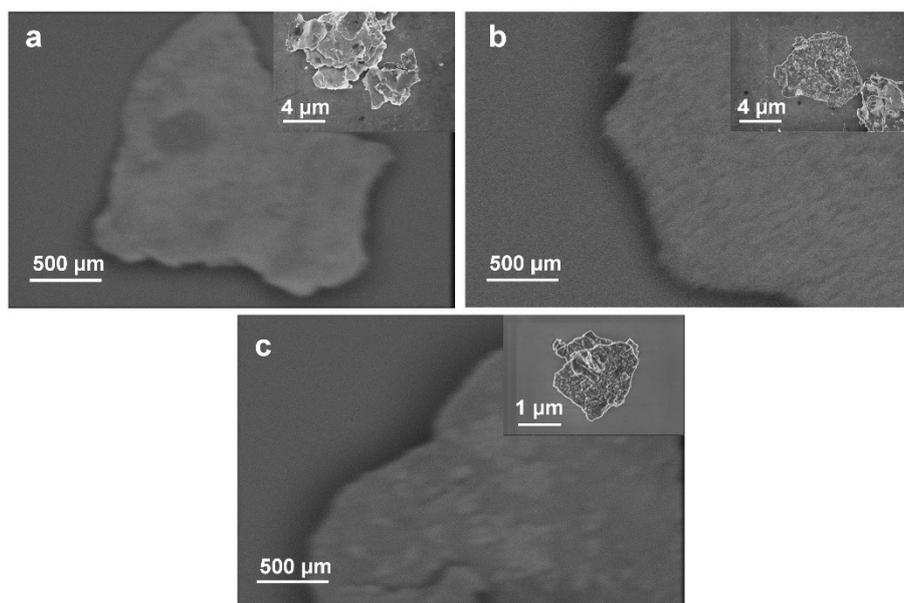


Fig. S3 SEM image of (a) $\text{Ni}_2\text{P}/\text{Ni}_{12}\text{P}_5$, (b) $\text{Ni}_2\text{P}/\text{NiO-4h}$, and (c) $\text{Ni}_2\text{P}/\text{NiO-16h}$.

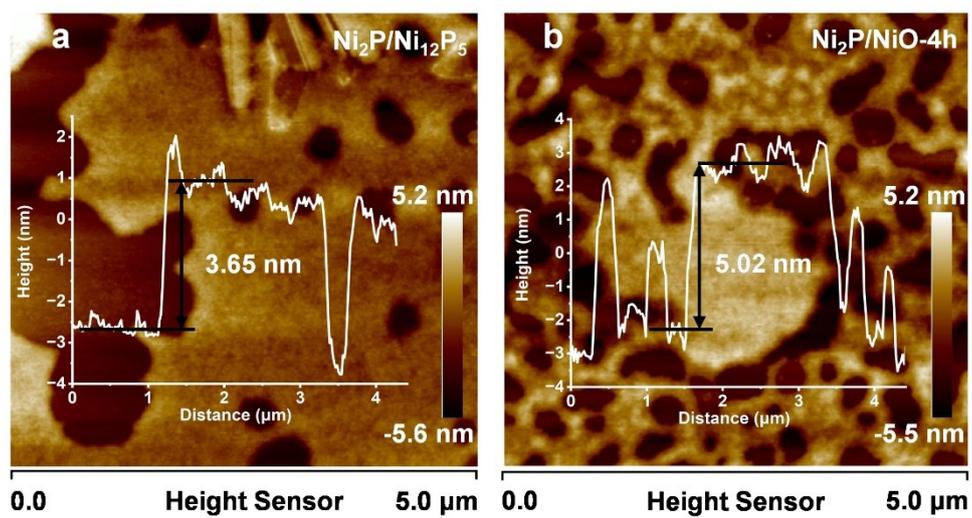


Fig. S4 AFM analysis of (a) $\text{Ni}_2\text{P}/\text{Ni}_{12}\text{P}_5$ and (b) $\text{Ni}_2\text{P}/\text{NiO-4h}$.

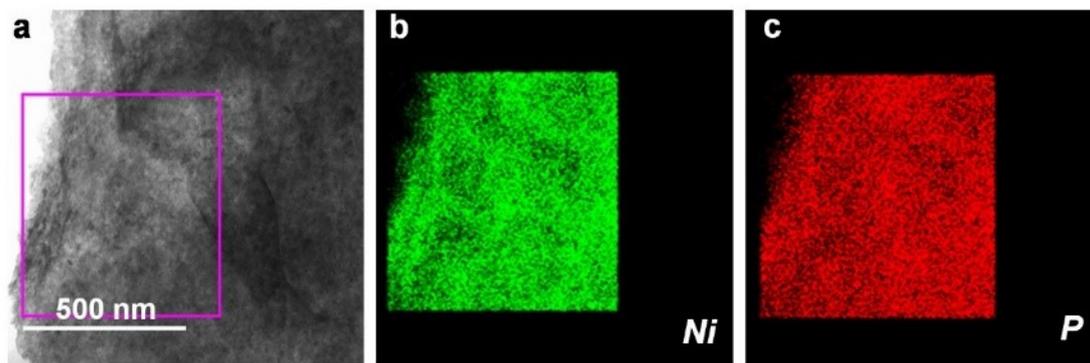


Fig. S5 (a) TEM image and (b-c) elemental mapping images of $\text{Ni}_2\text{P}/\text{Ni}_{12}\text{P}_5$.

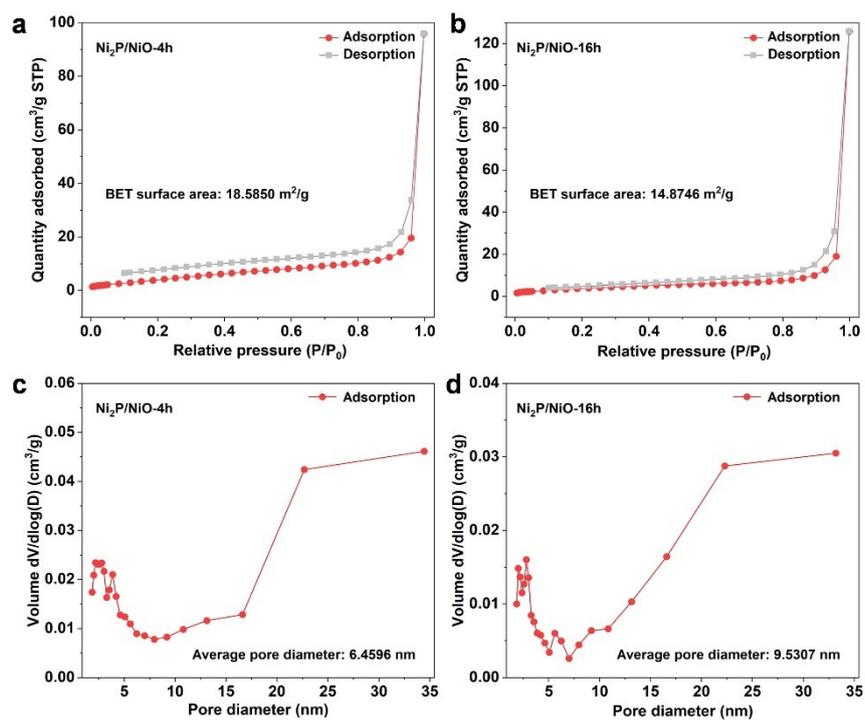


Fig. S6 (a) N₂ adsorption-desorption curve of the Ni₂P/NiO-4h and (b) Ni₂P/NiO-16h.

(c) The BJH pore size distribution of Ni₂P/NiO-4h and (d) Ni₂P/NiO-16h.

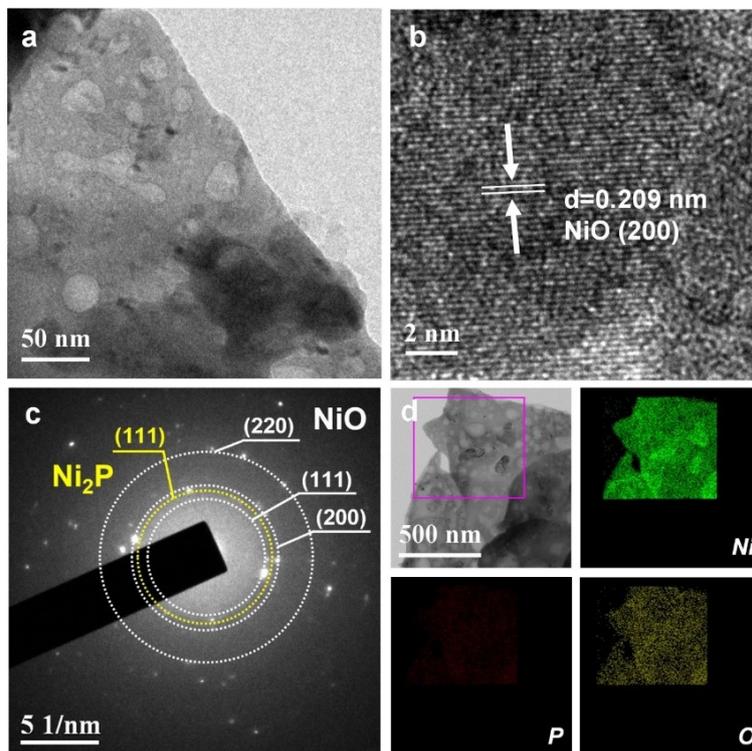


Fig. S7 (a) TEM image, (b) HRTEM image, (c) SAED pattern, and (d) elemental mapping images of Ni₂P/NiO-16h.

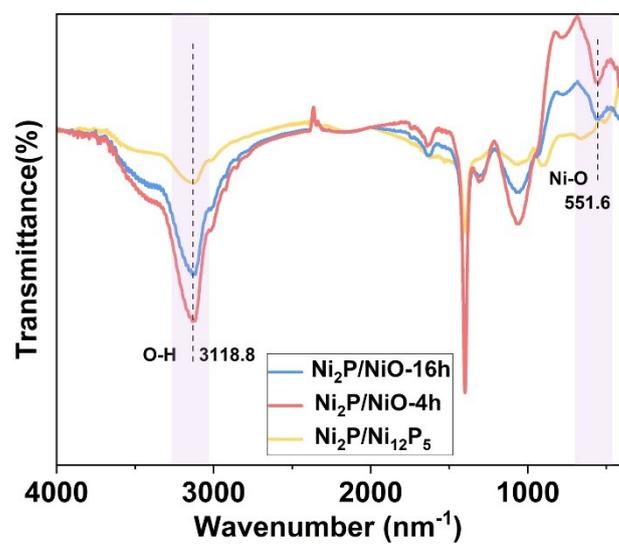


Fig. S8 FTIR spectra of $\text{Ni}_2\text{P}/\text{Ni}_{12}\text{P}_5$, $\text{Ni}_2\text{P}/\text{NiO}-4\text{h}$, and $\text{Ni}_2\text{P}/\text{NiO}-16\text{h}$.

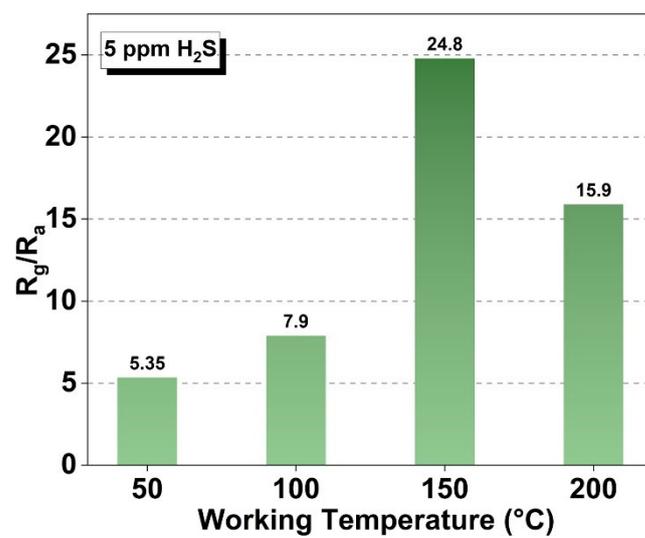


Fig. S9 Response values of Ni₂P/NiO-4h to 5 ppm H₂S at different temperatures.

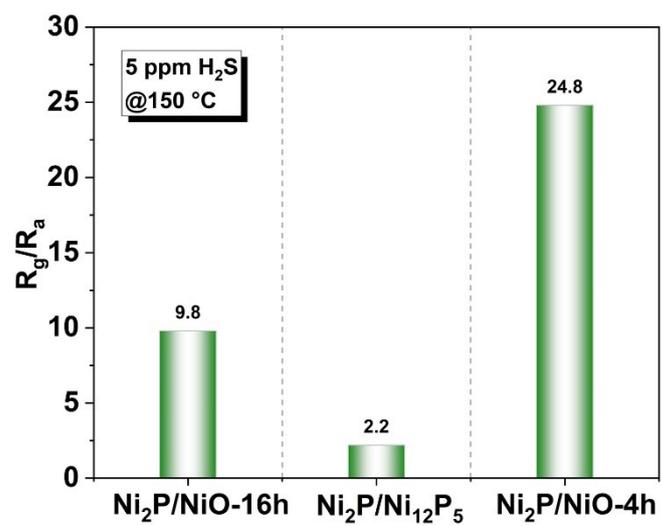


Fig. S10 Response values of $Ni_2P/Ni_{12}P_5$, $Ni_2P/NiO-4h$, and $Ni_2P/NiO-16h$ to 5 ppm H_2S at 150 °C.

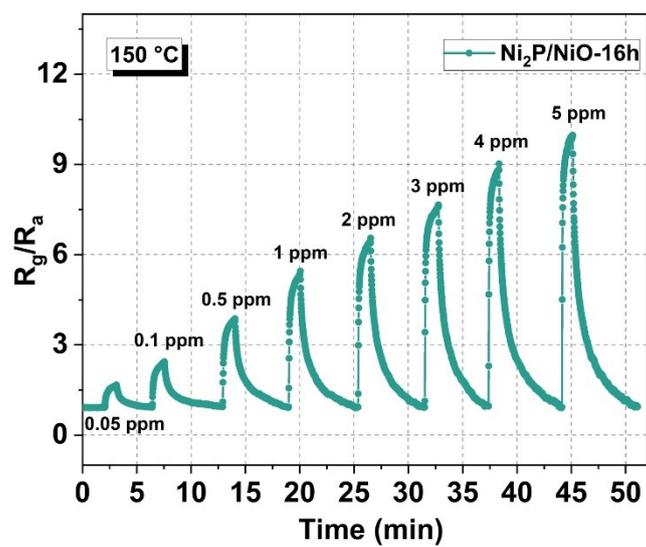


Fig. S11 Ni₂P/NiO-16h sensor response curve to 0.05-5 ppm H₂S at 150 °C.

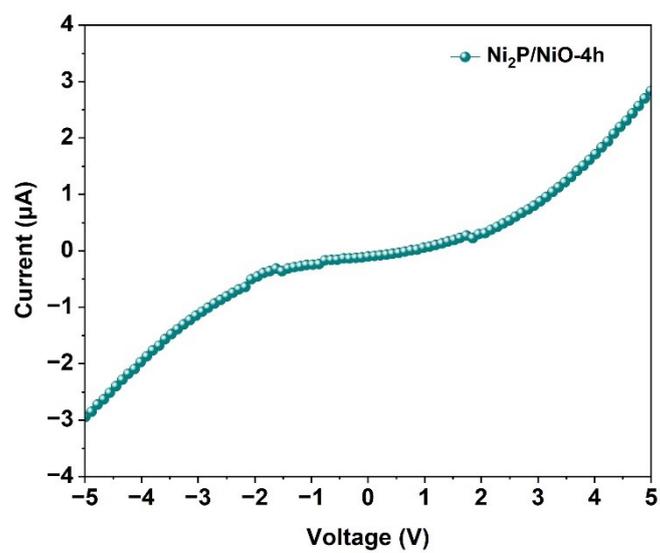


Fig. S12 I-V characteristics of Ni₂P/NiO-4h gas sensor.

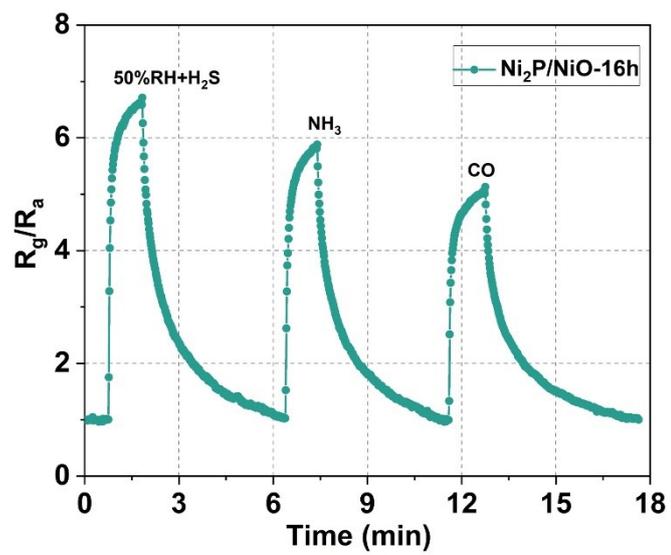


Fig. S13 $\text{Ni}_2\text{P}/\text{NiO}-16\text{h}$ gas sensor responses to 50%RH+H₂S, NH₃, and CO.

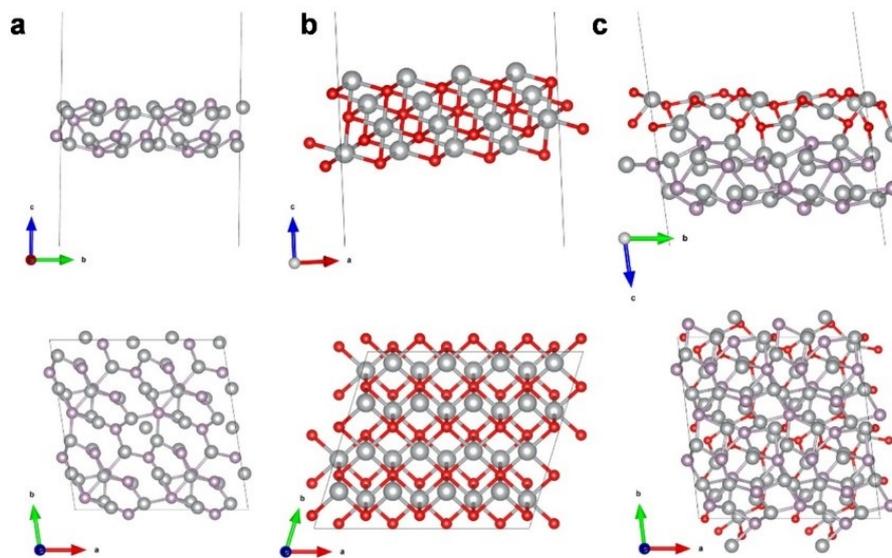


Fig. S14 Theoretical structural model of (a) Ni_2P , (b) NiO , and (c) $\text{Ni}_2\text{P}/\text{NiO}$ heterostructure (Atoms are colored as follows: Ni, gray; P, purple; O, red).

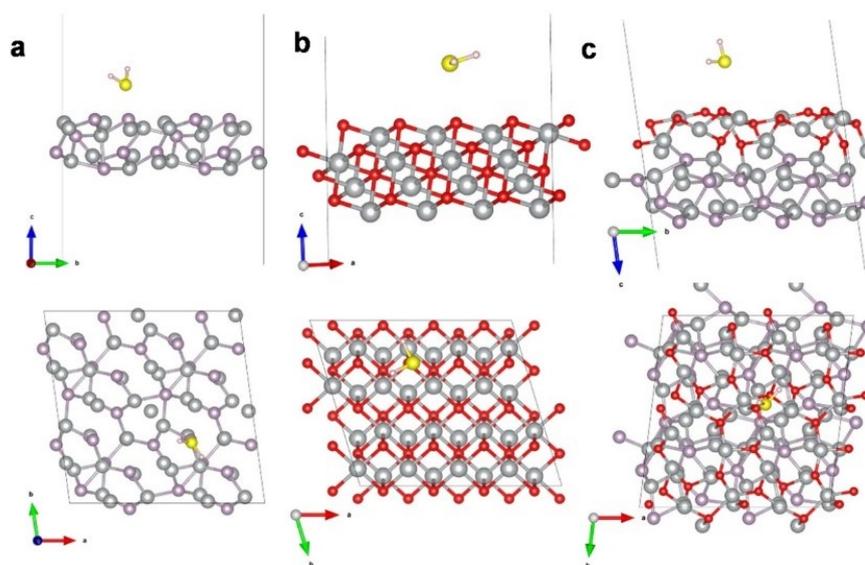


Fig. S15 Theoretical structural model for H_2S molecular adsorption of (a) Ni_2P , (b) NiO , and (c) $\text{Ni}_2\text{P}/\text{NiO}$ heterostructure (Atoms are colored as follows: Ni, gray; P, purple; O, red; S, yellow; H, pink).

Table. S1 The quantitative composition of Ni, P, and O in the samples by ICP analysis (wt %).

Sample	Ni	P	O
Ni ₂ P/Ni ₁₂ P ₅	74.25	23.32	2.43
Ni ₂ P/NiO-4h	67.85	13.39	18.76
Ni ₂ P/NiO-16h	65.63	5.81	28.56

The mass fraction of P in Ni₂P is 20.87%, and the P element only exists in the Ni₂P part in the Ni₂P/NiO-4h composite. According to the ICP results, the P weight ratio in the Ni₂P/NiO-4h is 13.39%. So, the Ni₂P weight ratio in the Ni₂P/NiO-4h can be calculated as $13.39\%/20.87\%=64.18\%$, and thus the NiO weight ratio is 35.82 wt%.

Table. S2 Comparison of sensing performance based on NiO materials towards H₂S in the previous literatures.

Sensing materials	Working Temperature	Gas concentration	Response (R _g /R _a)	Detection limit	Ref.
ZnO-NiO	250 °C	5 ppm	1.5	1 ppm	[1]
Zn/NiO	270 °C	2 ppm	3.23	0.05 ppm	[2]
Co-NiO@g-C ₃ N ₄ -3	172 °C	20 ppm	45	5 ppm	[3]
α-Fe ₂ O ₃ /NiO	300 °C	20 ppm	239	0.25 ppm	[4]
NiO epitaxial films	300 °C	100 ppm	13.07	0.186 ppm	[5]
NiWO ₄ (5%)-NiO	20 °C	1 ppm	7.36	0.1 ppm	[6]
Fe-NiO _x	270 °C	0.8 ppm	5.24	0.05 ppm	[7]
NiO thin films	350 °C	100 ppm	14.8	3 ppm	[8]
Ni₂P/NiO-4h	150 °C	5 ppm	24.8	0.05 ppm	This work

Reference

1. J. N. O. Amu Darko, S. Hussain, E. Issaka, M. Wang, A. A. Alothman, S. Lei, G. Qiao and G. Liu, *Ceram. Int.*, 2024, **50**, 17681–17690.
2. O. Wang, J. W. Kong, Z. G. Xue, B. L. An, J. Q. Xu and X. H. Wang, *ACS Sensors*, 2024, **9**, 3233–3243.
3. W. J. Du, X. Y. Su, H. Yang, S. H. Dong, L. Chen, J. F. Shang, L. X. Su, S. H. Liu, L. L. Wu and N. N. Wu, *Ceram. Int.*, 2024, **50**, 47939–47948.
4. N. D. Cuong, V. H. Sinh, D. T. Quang, L. T. Hoa, V. V. Tan, H. D. Mai, K. J. Jeon, P. H. Phuoc and N. V. Hieu, *Curr. Appl Phys.*, 2024, **59**, 153–164.
5. L. L. Kuang, T. Xiang, J. X. Li, S. Y. Wu, Y. Q. Dong, Q. Y. He, J. W. Xue, X. Y. Chen, Y. J. Tao, Y. T. Wang, H. Jin, J. X. Yi and Z. L. Luo, *Chin. J. Chem. Phys.*, 2025, **38**, 272–280.
6. J. S. Guo, D. Z. Zhang, J. D. Bian, J. S. Zhai, P. L. Jia and X. Y. Ji, *IEEE Sens. J.*, 2025, **25**, 117–124.
7. Y. Chen, T. W. Yuan, Y. X. Li, B. Shen, W. S. Zhang, J. Q. Xu and M. H. Wu, *Ceram. Int.*, 2024, **50**, 22243–22251.
8. S. Srivastava, A. K. Gangwar, A. Kumar, G. Gupta and P. Singh, *Micro Nanostruct.*, 2023, **184**, 207678.