

Supporting Information

Carbon-Doping Induced Energy Band Modification and Vacancy in SnS₂ Nanosheets for Room-temperature ppb-Level NO₂ Detection

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Fig. S1 Homemade chemical gas sensing analysis system. The gas test box is placed in a cyclic damp heat test instrument (left) with the controllable temperature and relative humidity.

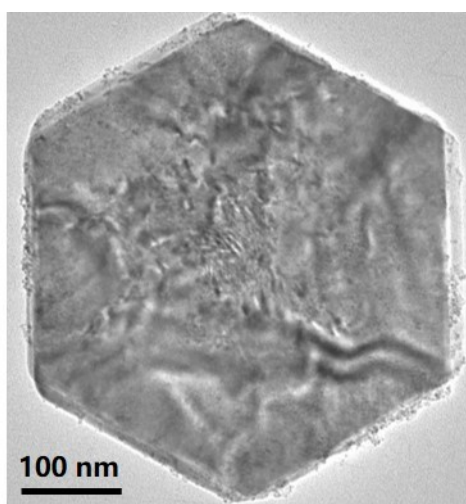


Fig. S2 TEM image of pristine SnS₂. The morphology of pristine SnS₂ showed hexagonal plate-like structure with uniform lateral size of ~400 nm.

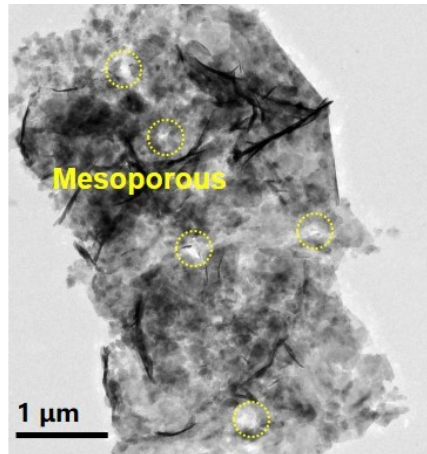


Fig. S3 TEM image of the C-SnS₂-32 sample. It indicates the obvious mesoporous nanostructures in the C-SnS₂-32 nanosheets.

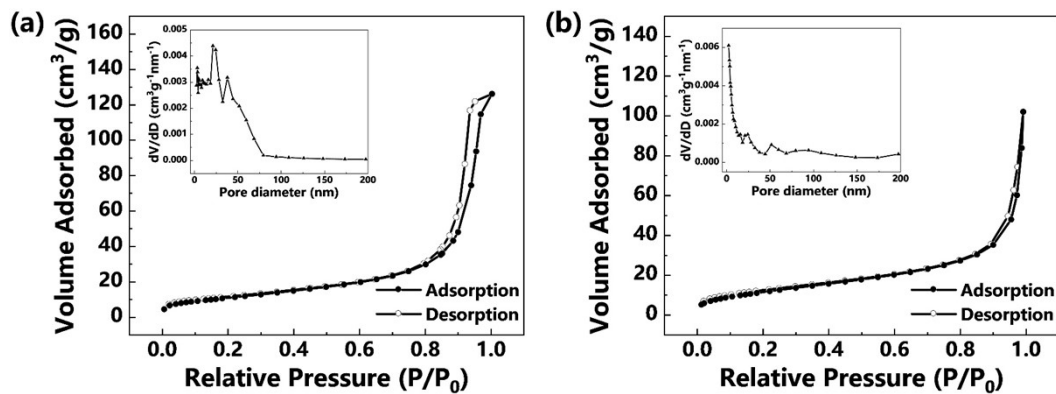


Fig. S4 N₂ sorption isotherms at 77 K of (a) C-SnS₂-32 and (b) pristine SnS₂. The BET surface area of C-SnS₂-32 nanosheets was measured to be 26.6 m²g⁻¹, which was 2.5 times larger than that of pristine SnS₂ (10.7 m²g⁻¹), which indicates that the adsorption capacity of NO₂ is improved on the C-doped SnS₂ surface.

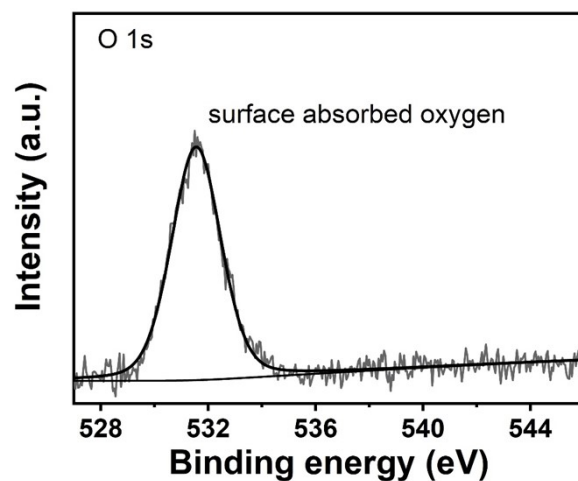


Fig. S5 High-resolution O 1s XPS spectra for the C-SnS₂-32. The peak centred at 531.9 eV is assigned to the surface adsorbed oxygen.^[1,2]

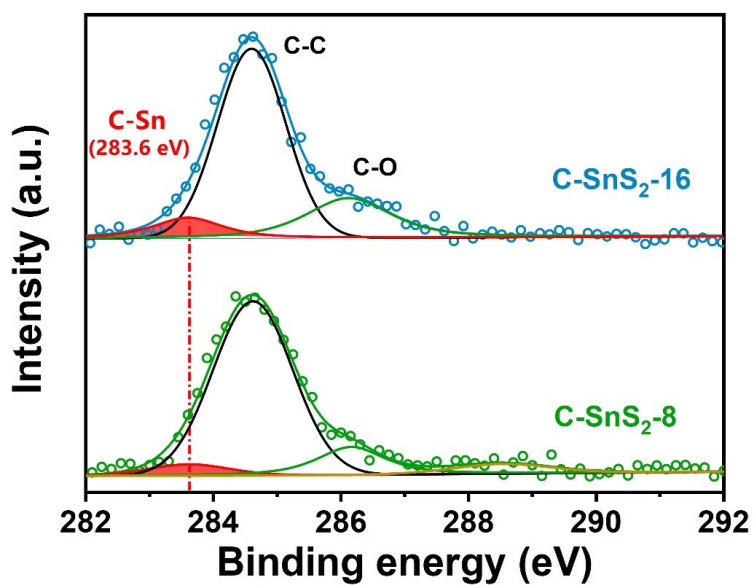


Fig. S6 High-resolution C 1s XPS spectra for C-SnS₂-8 and C-SnS₂-16. The clear signal of C-Sn bond is also found in both of C-SnS₂-8 and C-SnS₂-16, confirming the presence

of C doping in SnS₂.

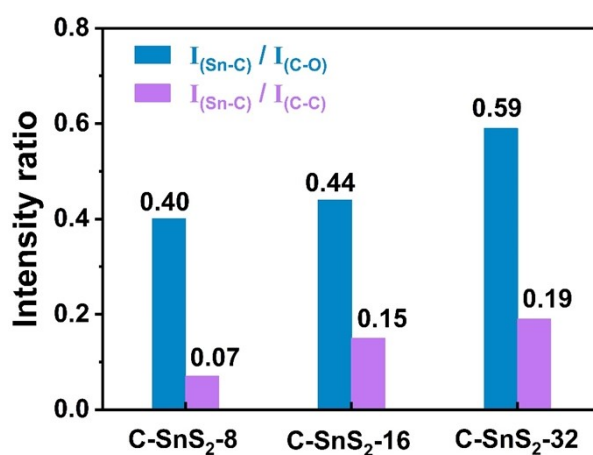


Fig. S7 The peak intensity ratios of Sn-C with C-O and C-C for C-doped SnS₂. The peak intensity ratios of the Sn-C/C-C and the Sn-C/C-O increase from C-SnS₂-8 to C-SnS₂-32, indicating the content of Sn-C bond increases with C dopants concentration while the C-C and C-O peaks does not change.

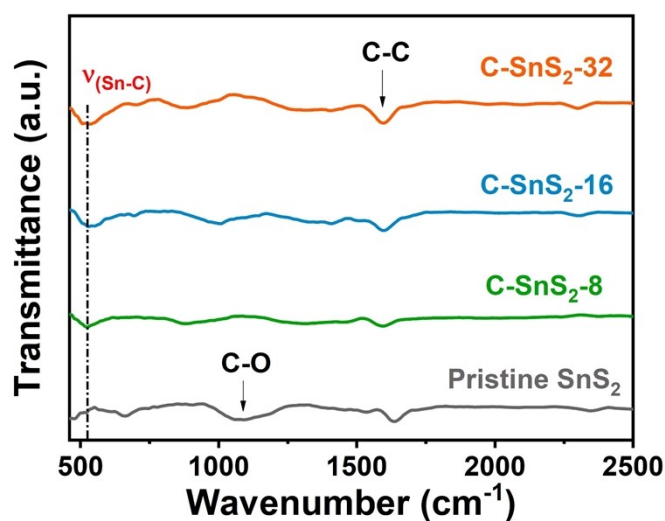


Fig. S8 FT-IR spectra of pristine SnS₂, C-SnS₂-8, C-SnS₂-16, and C-SnS₂-32. The peak at ~520 cm⁻¹ for C-doped SnS₂ is assigned to the Sn-C stretching, which is absent in pristine SnS₂, supporting that C is doping into SnS₂ crystals.

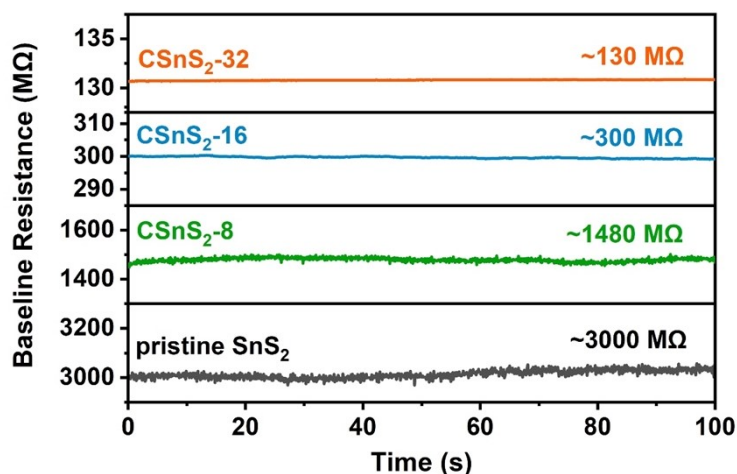


Fig. S9 Baseline resistance of pristine SnS₂, C-SnS₂-8, C-SnS₂-16, and C-SnS₂-32. The baseline resistance sharply declined after C doping, from ~3000 MΩ of pristine SnS₂ to ~130 MΩ of C-SnS₂-32, indicating that the C doping dramatically enhanced the electron concentration and the conductivity of SnS₂.

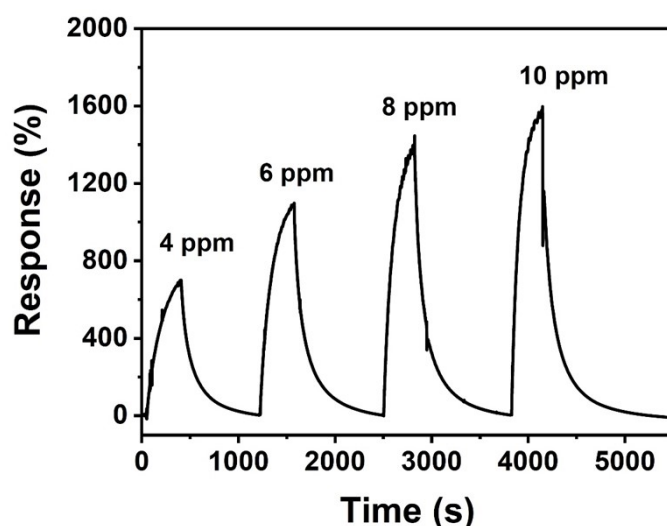


Fig. S10 Dynamic response-recovery curve of C-SnS₂-32 to diverse NO₂ concentrations from 4 ppm to 10 ppm. The result indicates that the response value of C-SnS₂-32 sensor increases with increasing NO₂ concentration and the signal completely returns to initial state after NO₂ release.

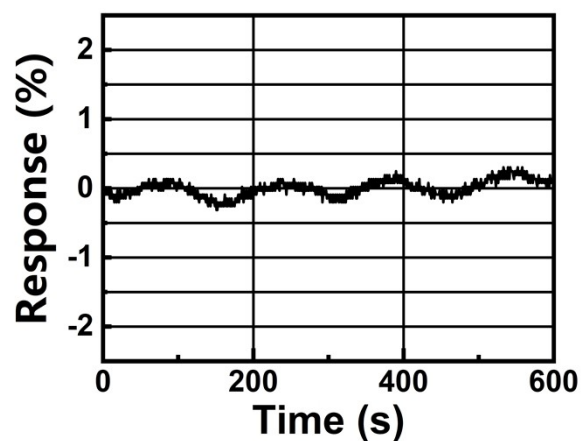


Fig. S11 A temporal trace of experimentally recorded noise of response for the sample C-SnS₂-32. The result indicates that the root-mean-square value of response noise is approximate ~0.12%.

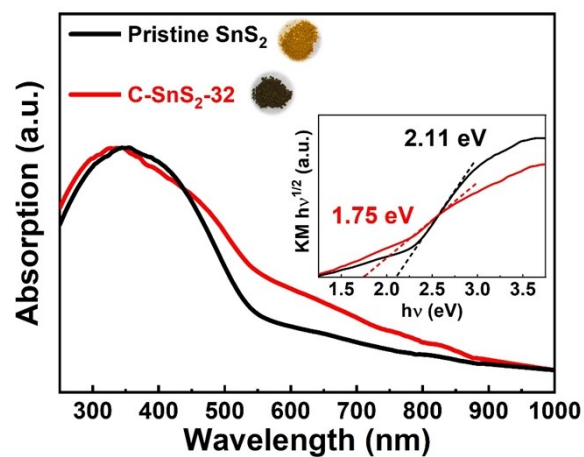


Fig. S12 UV-Vis diffuse reflectance spectroscopy of the C-SnS₂-32 and pristine SnS₂. The inset is Tauc plot with indirect bandgap fitting. The characterization of UV-Vis diffuse reflectance spectroscopy indicates the conspicuously narrowed bandgap structure from 2.11 to 1.75 eV after C doping.

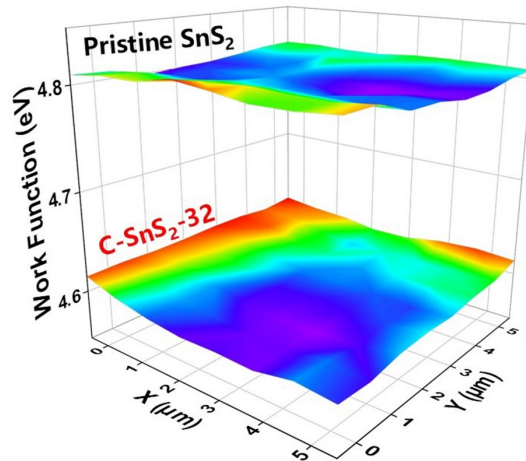


Fig. S13 KPFM measured work function area scans of the C-SnS₂-32 and pristine SnS₂. The measurement of KPFM indicates the elevation of Fermi energy level from 4.81 to 4.61 eV after C doping.

References

- [1] H. Chen, Y. Zhao, L. Shi, G.-D. Li, L. Sun and X. Zou, Revealing the relationship between energy level and gas sensing performance in heteroatom-doped semiconducting nanostructures, *ACS Appl. Mater. Interfaces*, 2018, **10**, 29795-29804.
- [2] Q. Yang, Y. Wang, J. Liu, J. Liu, Y. Gao, P. Sun, Z. Jie, T. Zhang, Y. Wang and G. Lu, Enhanced sensing response towards NO₂ based on ordered mesoporous Zr-doped In₂O₃ with low operating temperature, *Sens. Actuators, B*, 2017, **241**, 806-813.