Supporting Information

Boosted Interfacial Charge Transfer in $SnO_2/SnSe_2$ Heterostructures: Toward Ultrasensitive Room-temperature H_2S Detection

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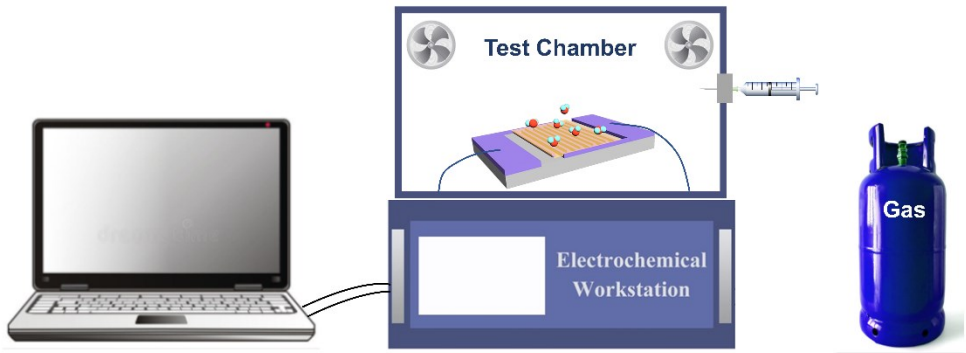

Fig. S1 Schematic diagram of the sensor measurement.

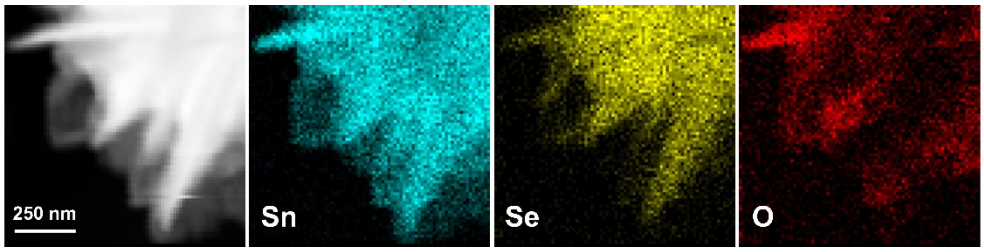

Fig. S2 EDX elemental mapping of $SnO_2/SnSe_2$-4h.

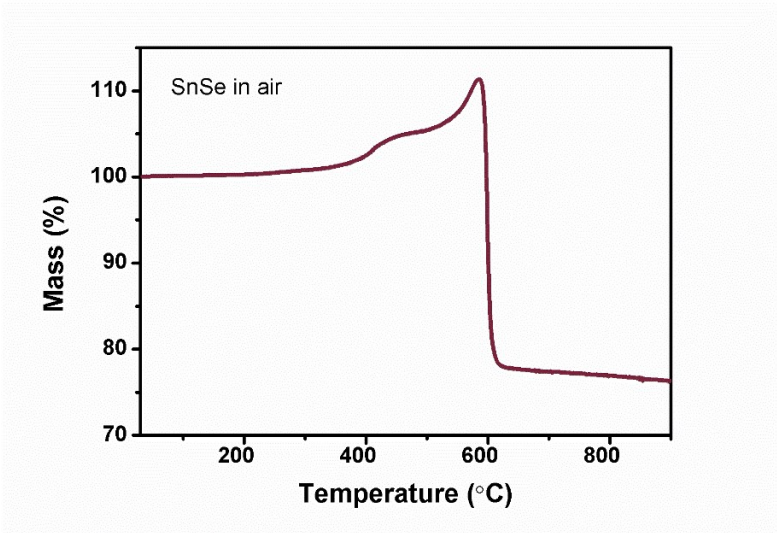

Fig. S3 TGA curves of SnSe from room temperature to 900 ℃ in air.

As can be seen from Fig. S3, a weight gain process between 400 to 600 ℃ along with a significant weight loss around 600 ℃ are observed. The weight change is the combination of weight gain due to oxygen pickup from air to form the oxides and weight loss due to sublimation of Se and Se-containing oxides.

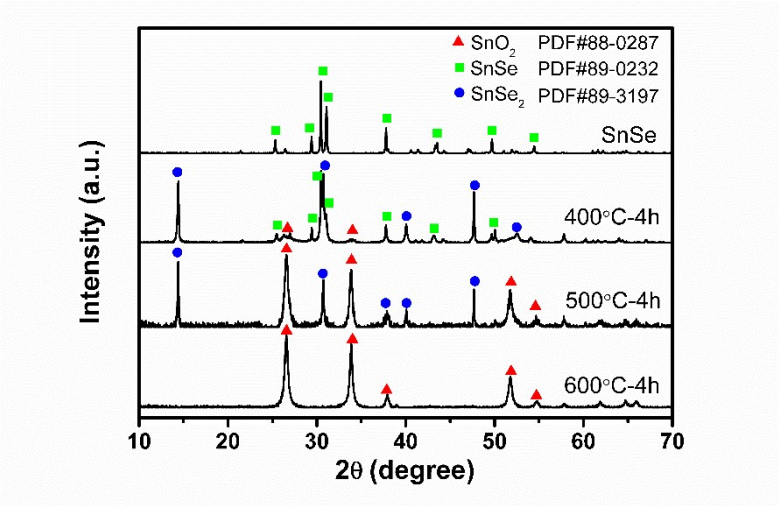

Fig. S4 XRD patterns of pristine SnSe and the obtained samples after thermal oxidation at 400 ℃, 500 ℃, and 600 ℃ for 4 h.

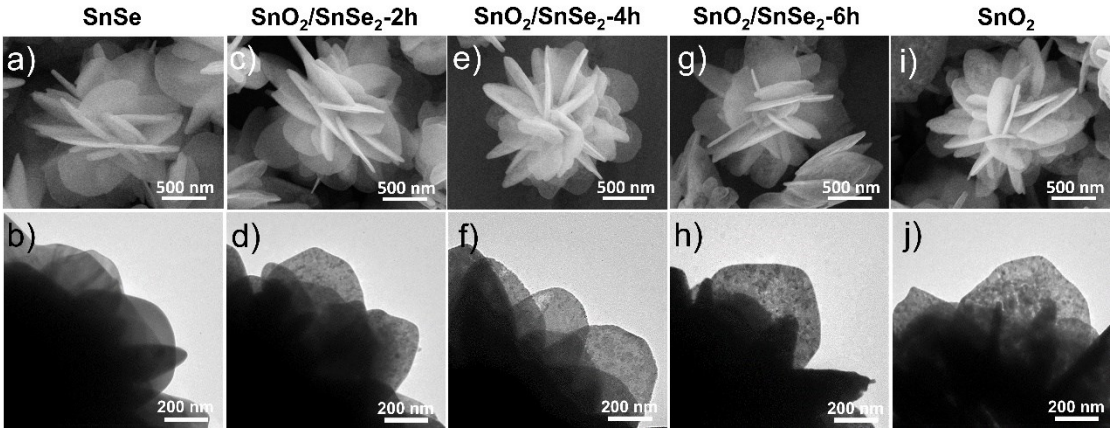

Fig. S5 SEM and TEM images of (a, b) pristine SnSe, (c, d) $SnO_2/SnSe_2$-2h, (e, f) $SnO_2/SnSe_2$-4h, (g, h) $SnO_2/SnSe_2$-6h, (i, j) SnO_2.

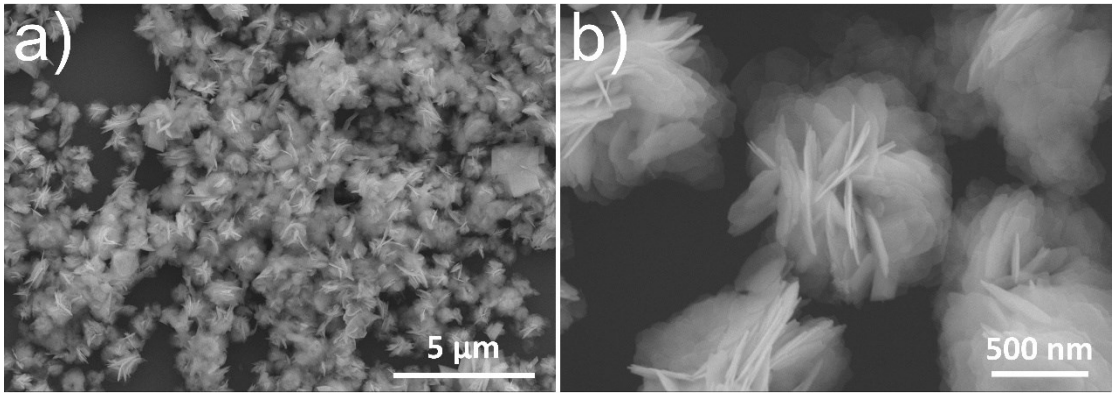

Fig. S6 (a, b) SEM images of pristine $SnSe_2$.

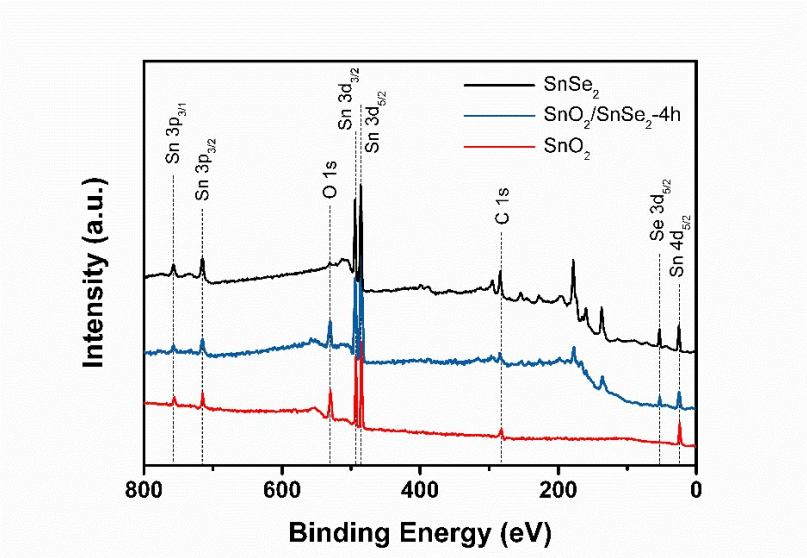

Fig. S7 The survey XPS curves of $SnSe_2$, $SnO_2/SnSe_2$-4h, and SnO_2.

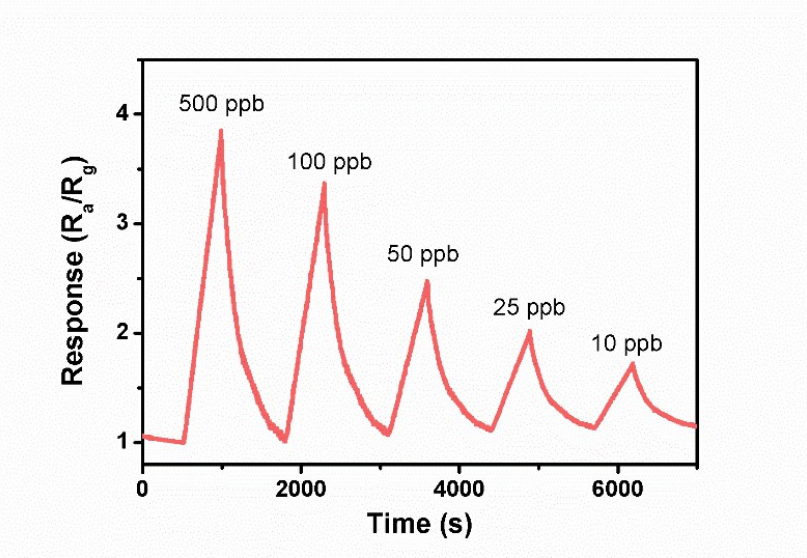

Fig. S8 Dynamic response of the $SnO_2/SnSe_2$-4h sensor with ppb-level H_2S concentrations ranging from 500 to 10 ppb.

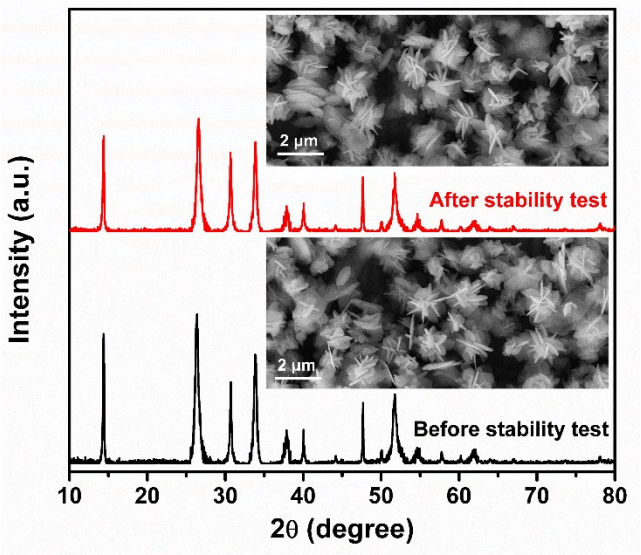

Fig. S9 XRD patterns and SEM images of $SnO_2/SnSe_2$ sensing materials before and after the stability test.

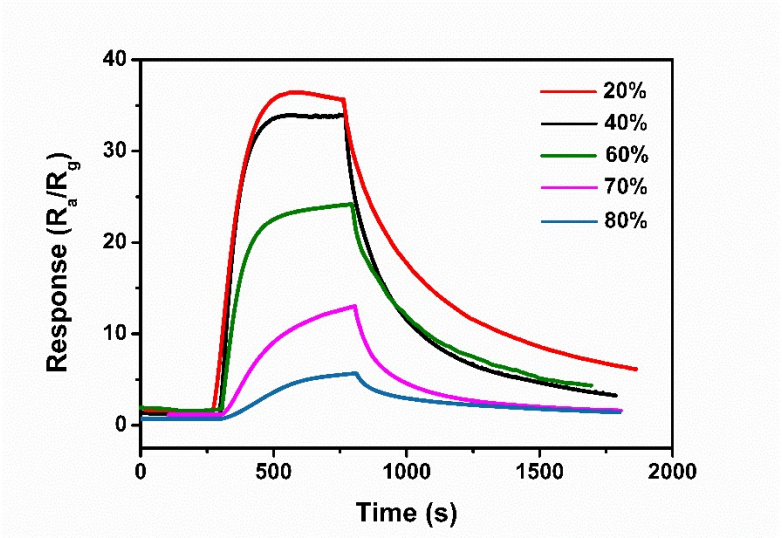

Fig. S10 The sensing behavior of $SnO_2/SnSe_2$-4h sensor to 10 ppm H_2S in different humidity at room-temperature.

A commercial damp-heat chamber (CK-80G, Kingjo) was used to control the relative humidity (RH) during the sensing test. The result shows a decrease in sensing response toward 10 ppm H_2S from 37 to 5 with the increase of RH from 20 to 80%. The possible reason for this phenomenon is that the adsorption of water molecules may occupy a part of active sites for the attraction of target gas. Besides, water molecules would prevent the adsorption of oxygen molecules in the high-humidity environment, which leads to

a lower adsorption concentration of ionized oxygen involved in the sensing reaction, and thus a decreased sensing response. [1-3]

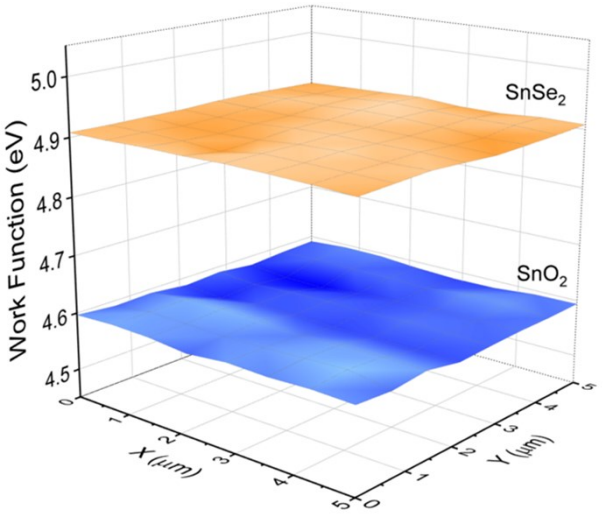

Fig. S11 Work functions of $SnSe_2$ (4.9 eV) and SnO_2 (4.6 eV) measured by the Kelvin probe based on 256 data points.

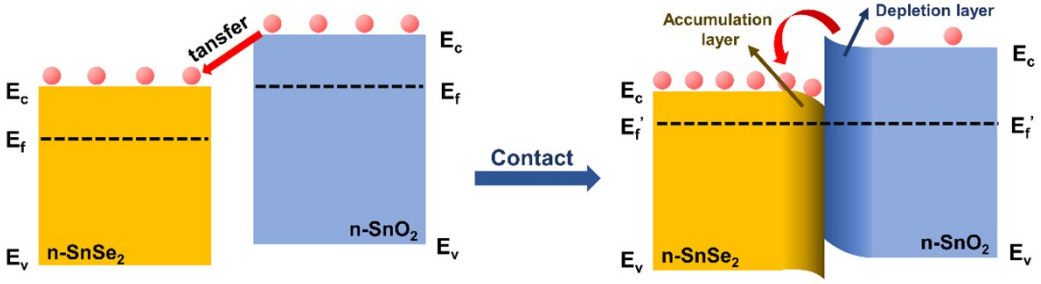

Fig. S12 The schematic and band diagrams of $SnO_2/SnSe_2$ heterostructures before and after equilibrium (E_c = conduction band edge energy; E_v = valence band edge energy; E_f= Fermi level).

As SnO_2 has a higher Fermi energy level than that of $SnSe_2$, the electrons will transfer from SnO_2 to $SnSe_2$ and form an interface depletion layer at SnO_2 as well as an accumulation layer at $SnSe_2$ when the $SnO_2/SnSe_2$ heterojunction is formed.

References

[1]. L. Liu, Y. Wang, Y. Dai, G. Li, S. Wang, T. Li, T. Zhang and S. Qin, In Situ Growth of NiO@SnO_2 Hierarchical Nanostructures for High Performance H_2S Sensing, *ACS Appl. Mater. Interfaces*, 2019, **11**, 44829-44836.

[2]. B. Y. Song, M. Zhang, Y. Teng, X. F. Zhang, Z. P. Deng, L. H. Huo and S. Gao, Highly selective ppb-level H_2S sensor for spendable detection of exhaled biomarker and pork freshness at low temperature: Mesoporous SnO_2 hierarchical architectures derived from waste scallion root, *Sens. Actuators, B*, 2020, **307**, 127662.

[3]. A. Mirzaei, S. S. Kim and H. W. Kim, Resistance-based H_2S gas sensors using metal oxide nanostructures: A review of recent advances, *J Hazard. Mater.*, 2018, **357**, 314-331.