Supplementary Information

Indium-Doping-Induced Selenium Vacancy Engineering of Layered Tin Diselenide for Improving Room-Temperature Sulfur Dioxide Gas Sensing

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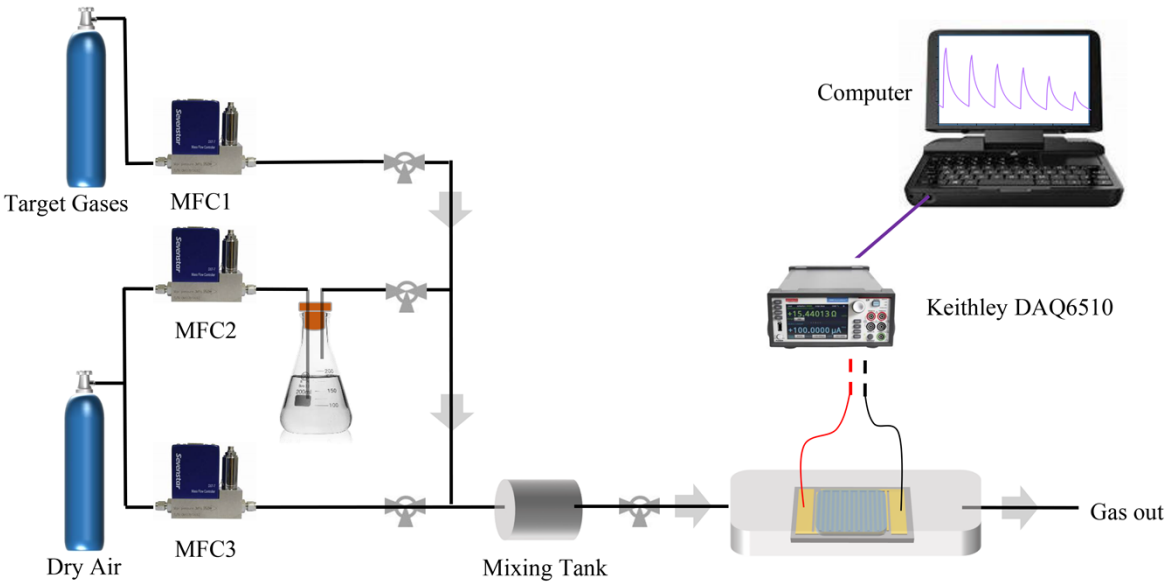

Figure S1. Schematic diagram of gas-sensing procedure.

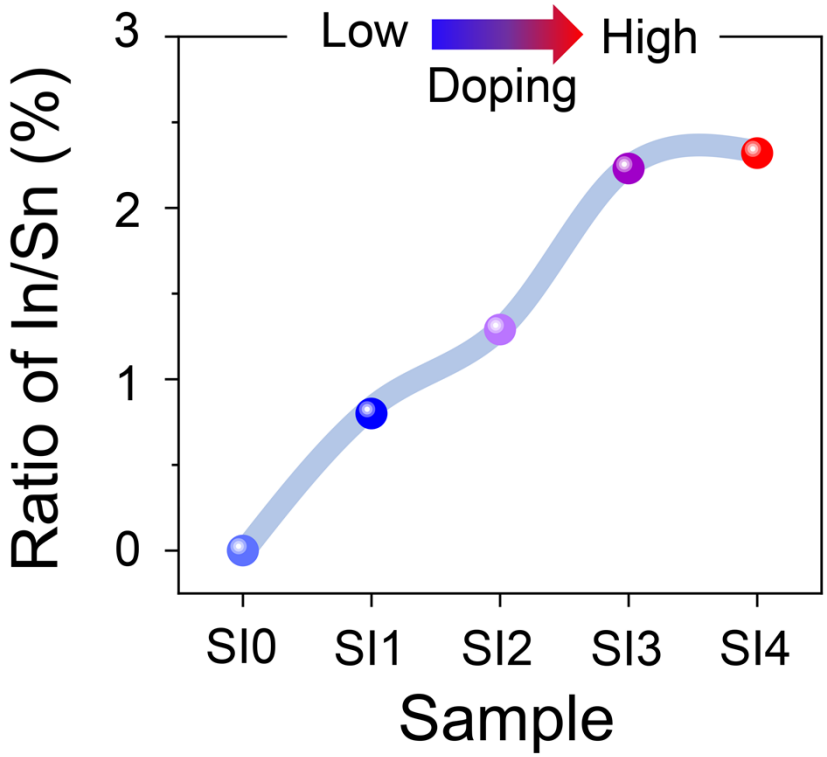

Figure S2. The relationship between In/Sn and the doping samples from ICP-MS.

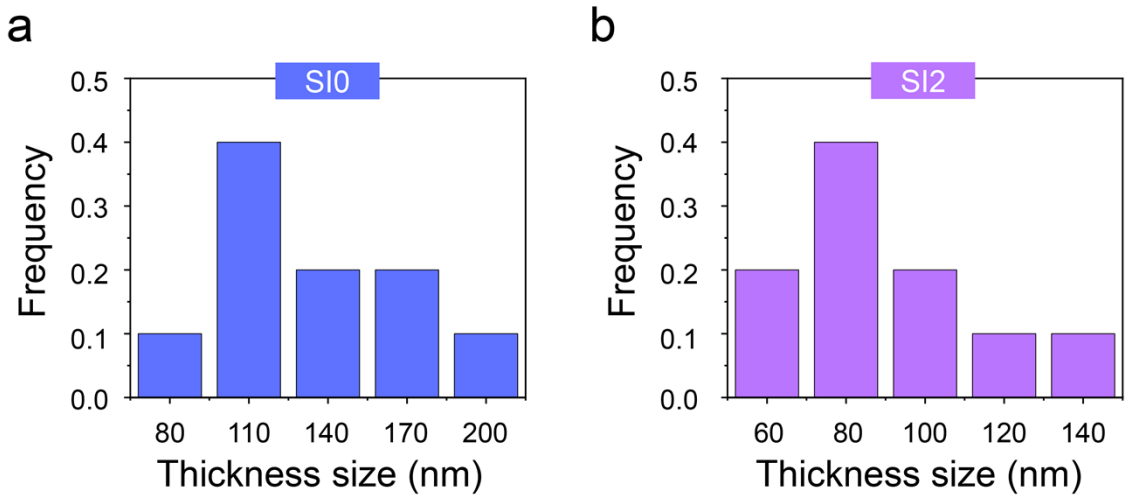

Figure S3. The thickness distribution statistics of (a) SI0 and (b) SI2 samples.

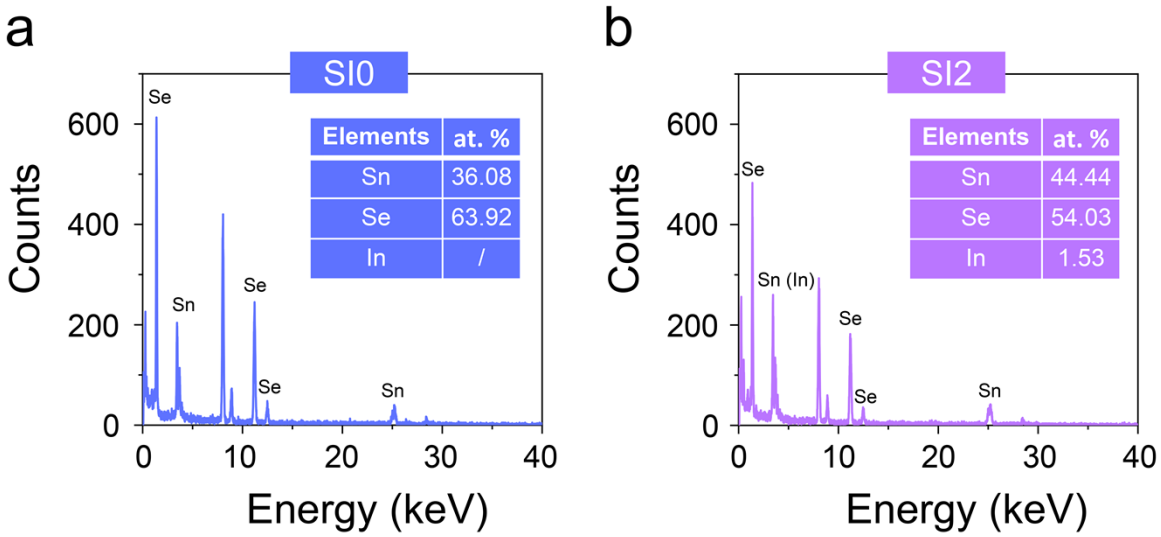

Figure S4. EDS elemental estimations for the (a) SI0 and (b) SI2 samples.

Table S1. The results of the ratio of the integrated area under each peak in XPS.

XPS – Se 3d	SI0	SI2
Se $3d_{5/2}$	38115.54	28031.93
Se $3d_{3/2}$	30140.31	26793.88
Se vacancies	2397.61	5027.21

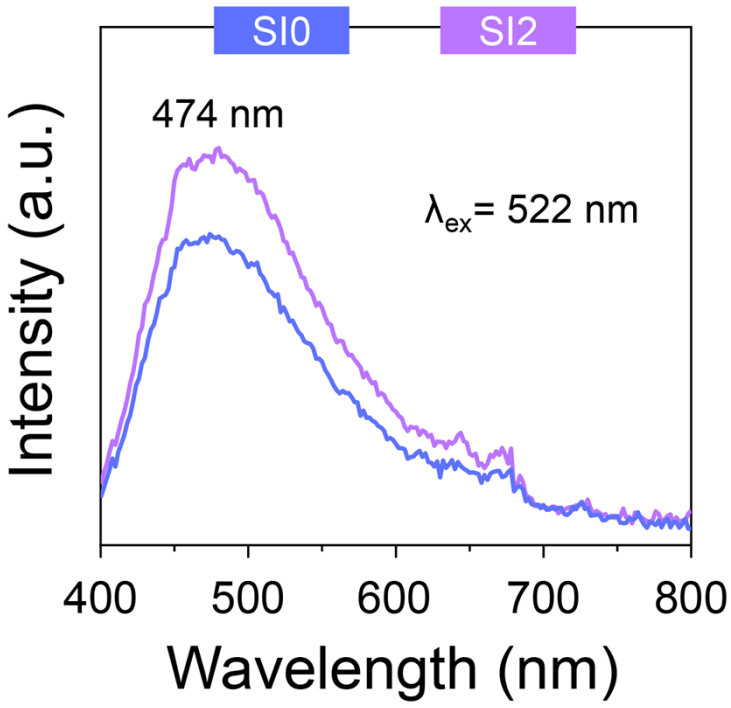

Figure S5. PL spectra of the SI0 and SI2 samples.

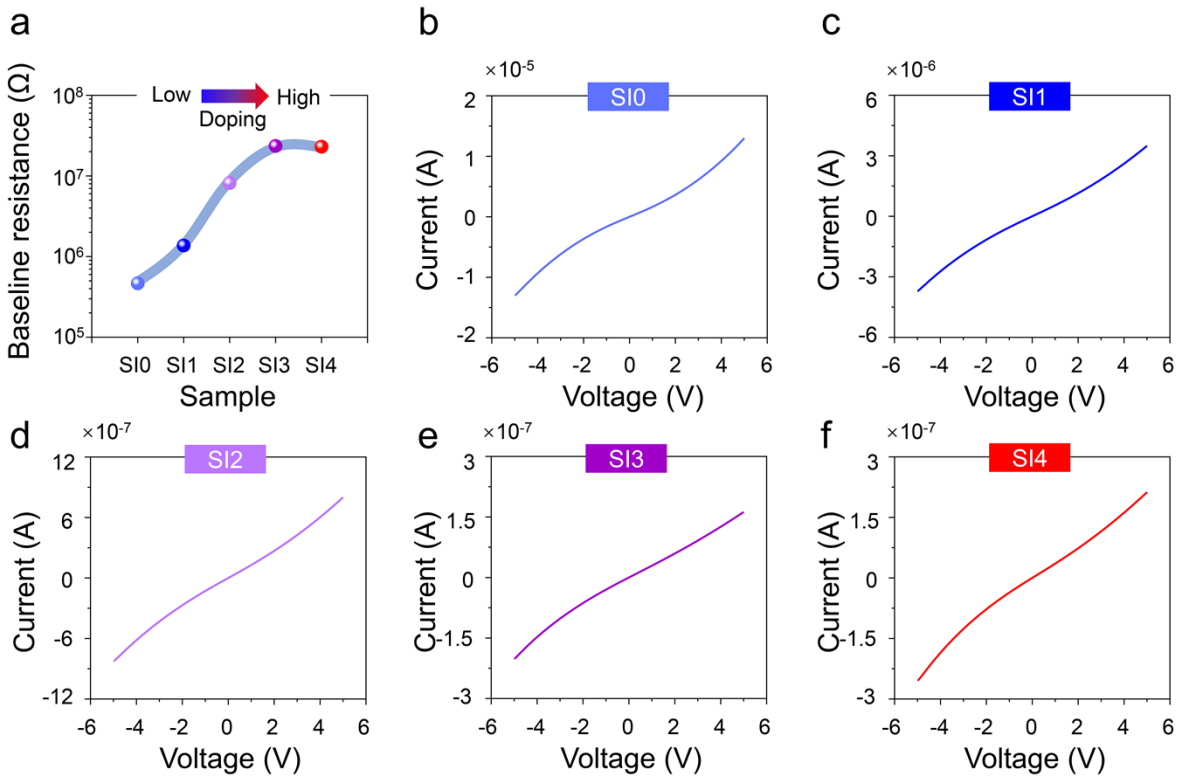

Figure S6. (a) The relationship between baseline resistance and the doping samples. The I-V curves of the (b) SI0, (c) SI1, (d) SI2, (e) SI3, and (f) SI4 samples.

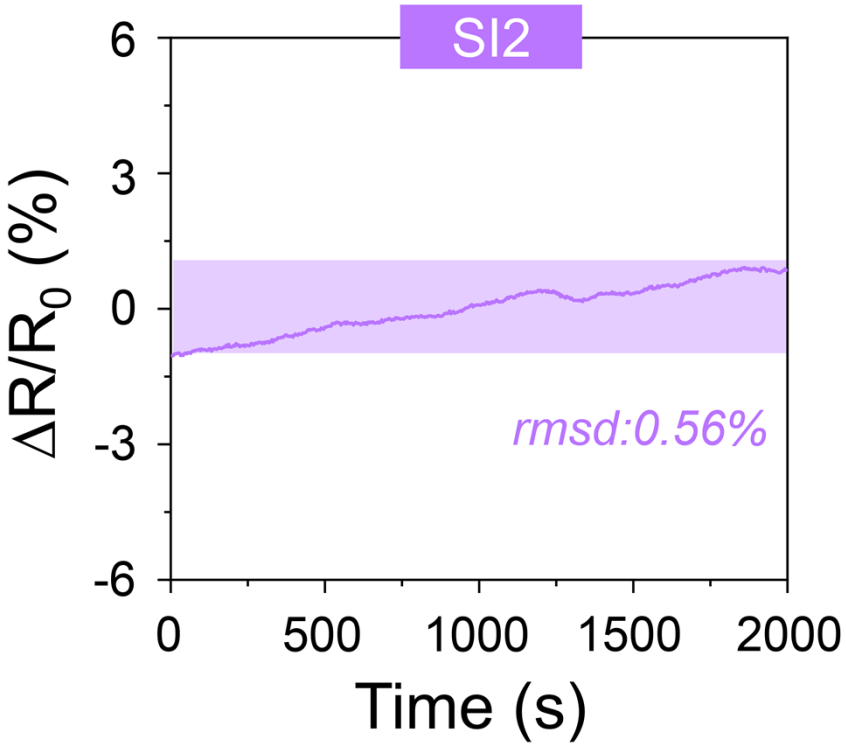

Figure S7. The root-mean-squared deviation noise (rmsd) of the SI2 sensor.

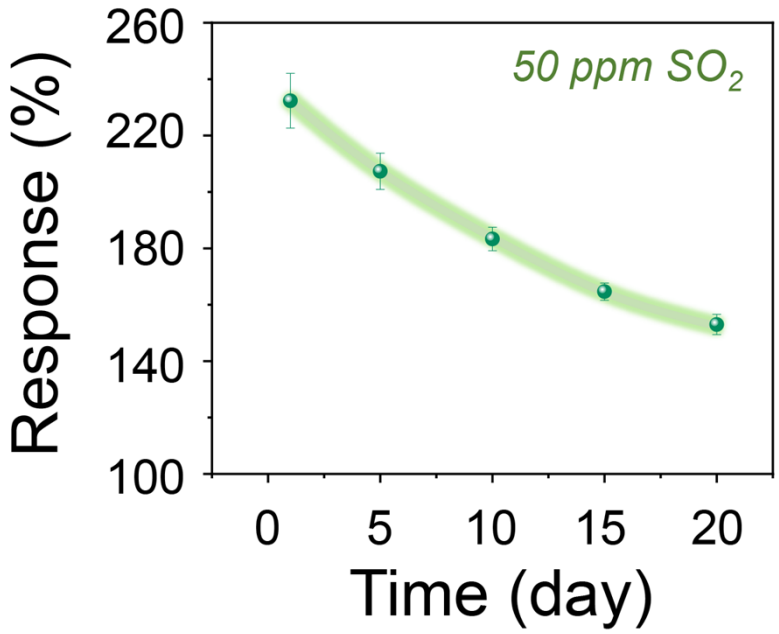

Figure S8. The stability of the SI2 sensor to 50 ppm SO_2.

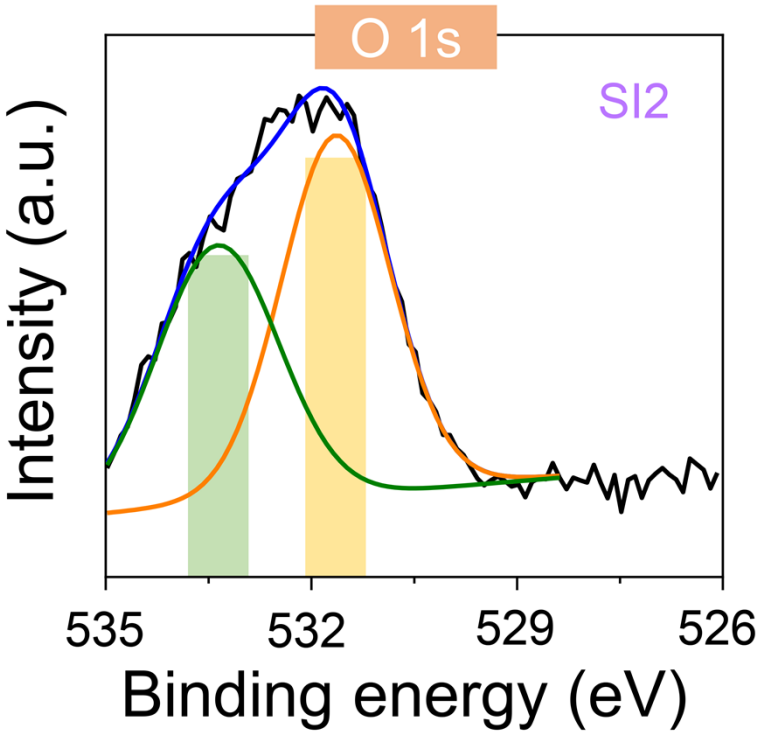

Figure S9. O 1s spectrum of the SI2 sample.

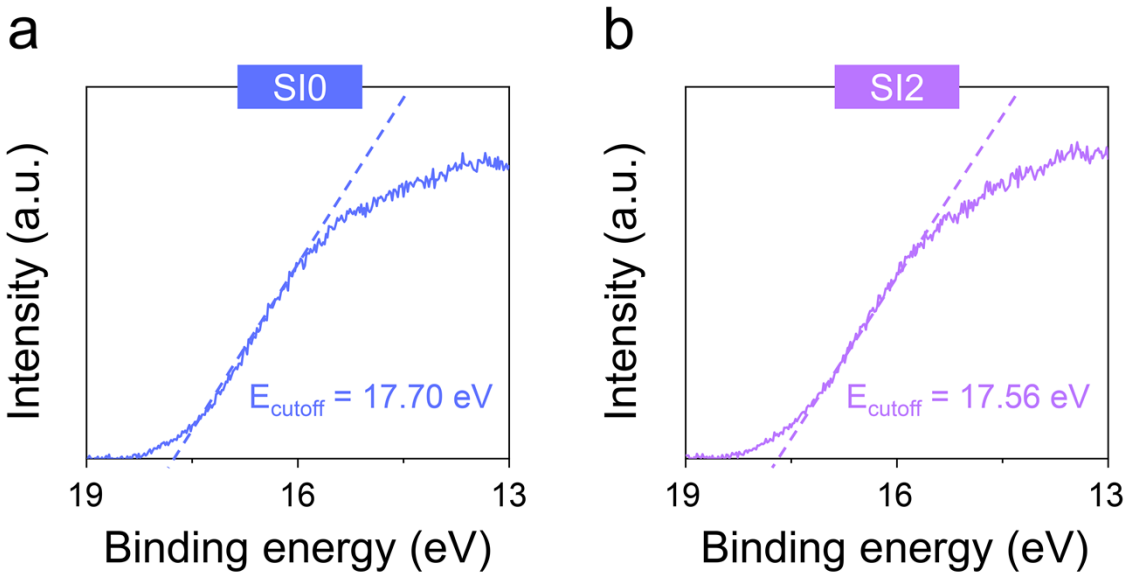

Figure S10. UPS results and the corresponding work functions of (a) SI0 and (b) SI2 samples.

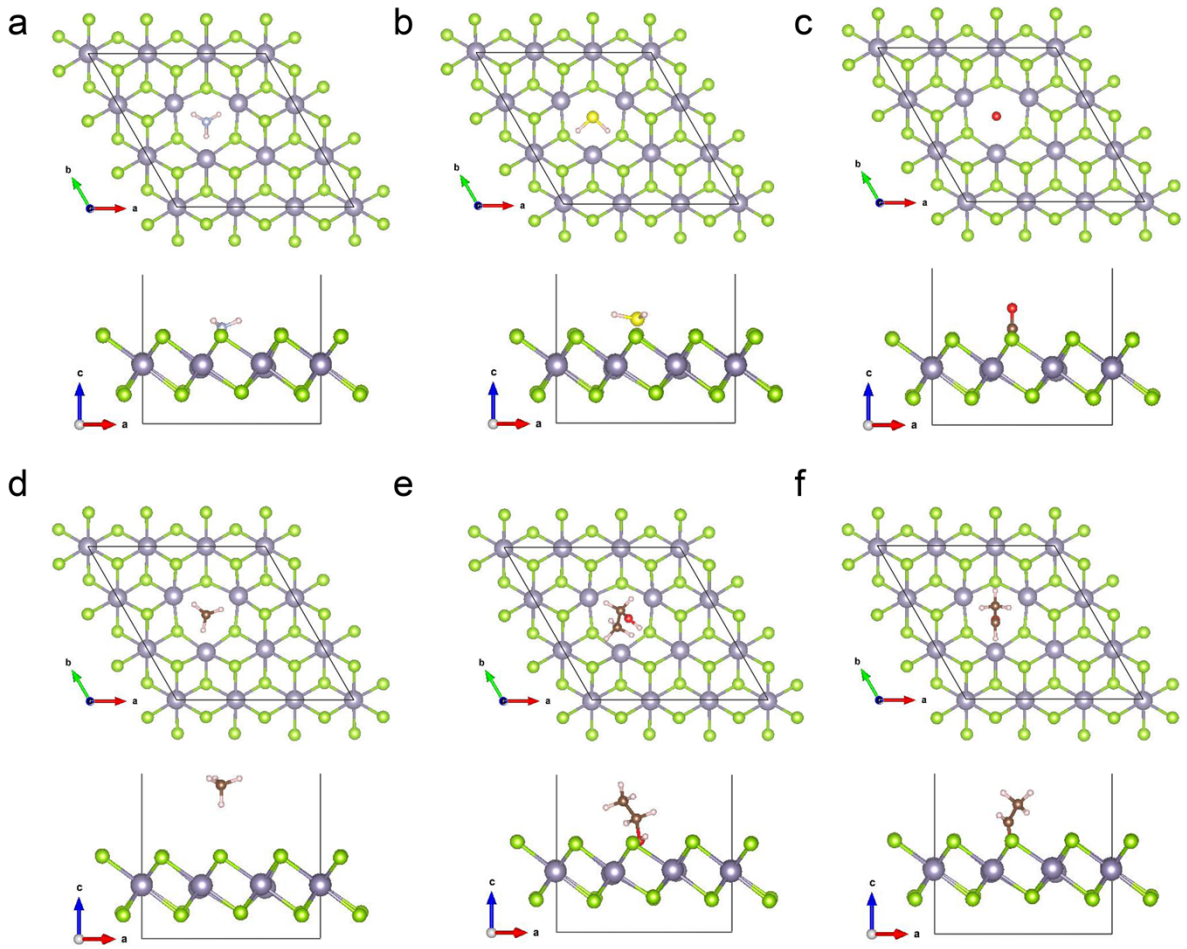

Figure S11. Optimized adsorption models on $SnSe_2$ with Se vacancies to (a) H_2S, (b) NH_3, (c) CO, (d) CH_4, (e) CH_3CH_2OH, and (f) CH_3CHO.

Table S2. Calculated adsorption parameters from different gas molecules to $SnSe_2$ monolayer with Se vacancies system.

$SnSe_2$ system	Gas molecules	E_{ad} (eV)	d (Å)	h (Å)	ΔQ_b (e)
$SnSe_2$ with V_{Se}	SO_2	-0.362	3.122	1.435	-0.149
	NH_3	-0.703	3.035	-0.392	0.008
	H_2S	-0.576	3.100	0.907	0.019
	CO	-0.344	3.376	0.540	-0.050
	CH_4	-0.063	4.847	2.890	-0.002
	CH_3CH_2OH	-0.939	2.695	0.066	-0.009
	CH_3CHO	-1.031	2.620	-0.225	-0.018