Highly Sensitive, Selective and Stable NO$_2$ Gas Sensors with PPb-Level Detection Limit on 2D-Platinum Diselenide Films †

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Figure S1 XPS result of 300 °C, 450 °C and 600 °C. Pt 4f spectra for (a) 300 °C (b) 450 °C and (c) 600 °C. and Se 3d spectra (d) 300 °C (e) 450 °C and (f) 600 °C.
Figure S2. Schematic setup of gas sensing measurement system.
Figure S3. The gas sensing response of PtSe$_2$ fabricated at 450 °C with and without UV illumination.
Figure S4 Real time NO$_2$ response of PtSe$_2$ fabricated at 450 ºC and the NO$_2$ concentration ranged from 50 ppb to 1 ppm at (a) 5 L, (b) 7 L, and (c) 10 L.
Calculation of noise level (RMS) and limit of detection (LOD)
1. Execute the linear fitting for plot of response versus NO$_2$ concentration and then extract the slope (sensitivity) and standard error in the linear region shown in figure S4(a) to (c)
2. Take 11 data points at the baseline before NO$_2$ response and execute the polynomial fit (5th order) shown in figure S4(d) to (f).
3. Take the regular residual of $(Y_i-Y_{fit})$ of polynomial fit and calculate the root-mean squared deviation (RMS) and the LOD with the equation S1 and S2.

$$\text{RMS (ppm}^{-1}) = \sqrt{\frac{\sum V_i}{N-1}}$$

where $V_i = \sum (Y_i - Y_{fit})$

Limit of detection (ppm) = 3RMS/slope(sensitivity).

Figure S5 (a) to (c) the linear fit of the plot of the response versus concentration with 5, 7 and 10 layers. (d) to (f) 5th order polynomial fit of 11 points before gas purging in with 5, 7 and 10 layers.
Figure S6 (a) Real time NO$_2$ response of PtSe$_2$ fabricated at 450 °C with 7 layers and the NO$_2$ concentration ranged from 1 ppm to 50 ppb. (b) and (c) the cycling response of 1 ppm and 50 ppb with 5 cycles.
Figure S7. PtSe$_2$ sensing performance with (a) CO in 1 ppm (b) H$_2$S in 0.5 ppm, and (c) NH$_3$ in 1 ppm.
Figure S8. The cross section TEM image of PtSe$_2$ fabricated at 300 °C, 450 °C and 600 °C in low and high magnification. (a) and (d) are 300 °C, (b) and (e) are 450 °C, (d) and (f) are 600 °C.
Band gap calculation through absorption spectrum and Tauc plot.

1. We can directly measure the absorption spectrum by fabricating PtSe$_2$ on quartz substrate.
2. Calculation the absorptance ($\alpha$) through $-\log$ (absorption (%))/thickness
3. According to the formula: $(ah\nu)^{1/n} = A(h\nu - E_g)$, where the value n is 2 for indirect band, we can extrapolate the linear region of abscissa.

Figure S9. The absorption spectrum of PtSe$_2$ with different growth temperature in (a) 5 L, (b) 7 L, and (c) 10 L. The Tauc plot of abscissa of PtSe$_2$ with different temperature in (d) 5 L, (e) 7L and (f) 10 L.