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Highly Sensitive, Selective and Stable NO_2 Gas Sensors with PPb-Level Detection Limit on 2D-Platinum Diselenide Films †

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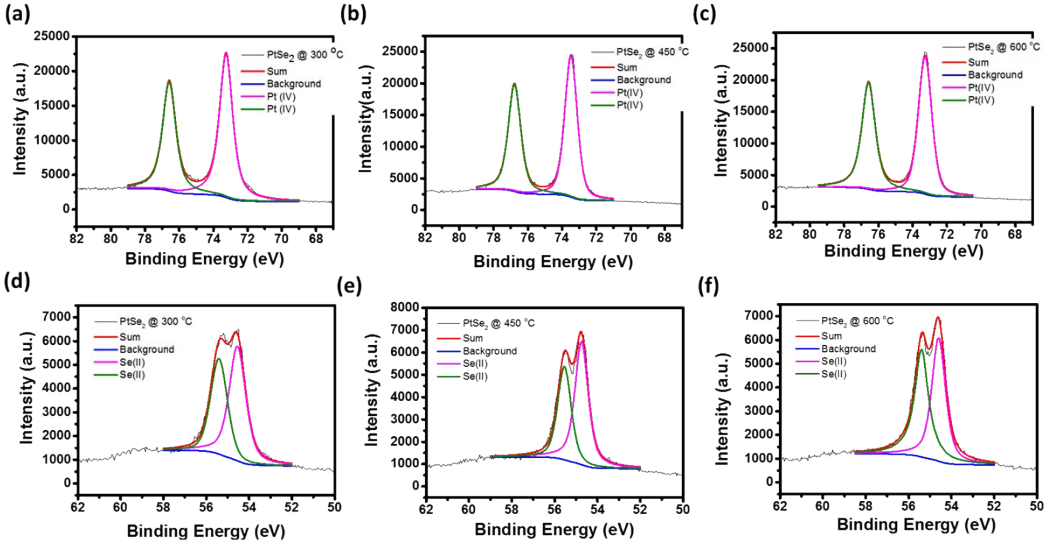

Figure S1 XPS result of 300 °C, 450 °C and 600 °C. Pt 4f spectra for (a) 300 °C (b) 450 °C and (c) 600 °C. and Se 3d spectra (d) 300 °C (e) 450 °C and (f) 600 °C.

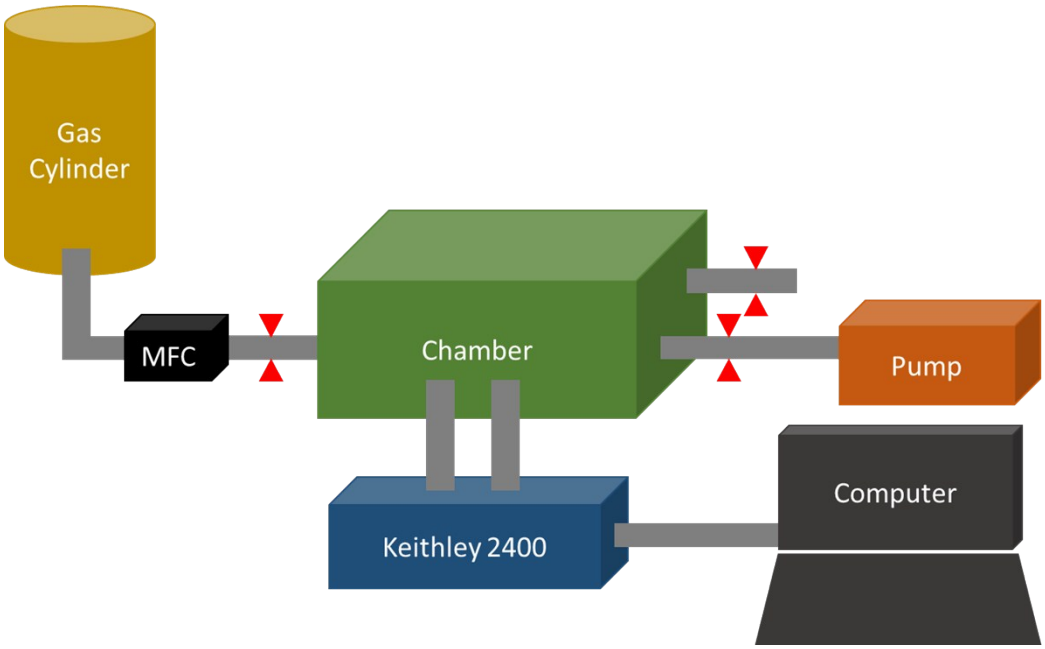

Figure S2. Schematic setup of gas sensing measurement system.

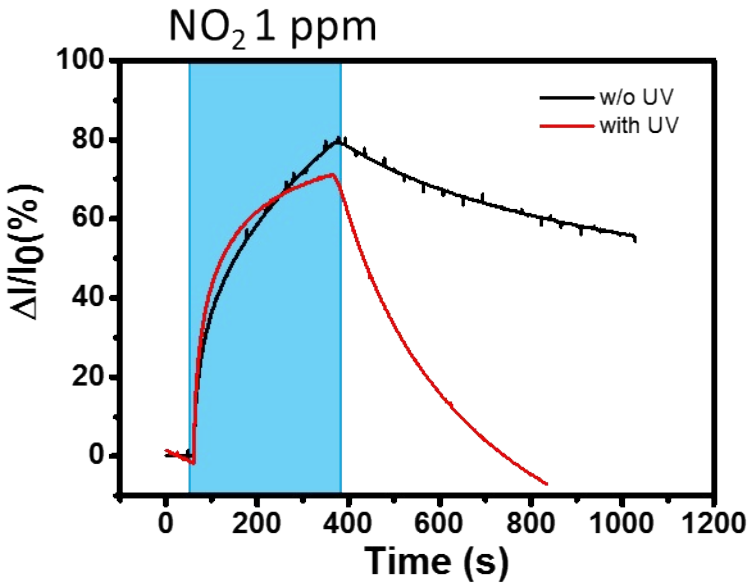

Figure S3. The gas sensing response of $PtSe_2$ fabricated at 450 ^oC with and without UV illumination.

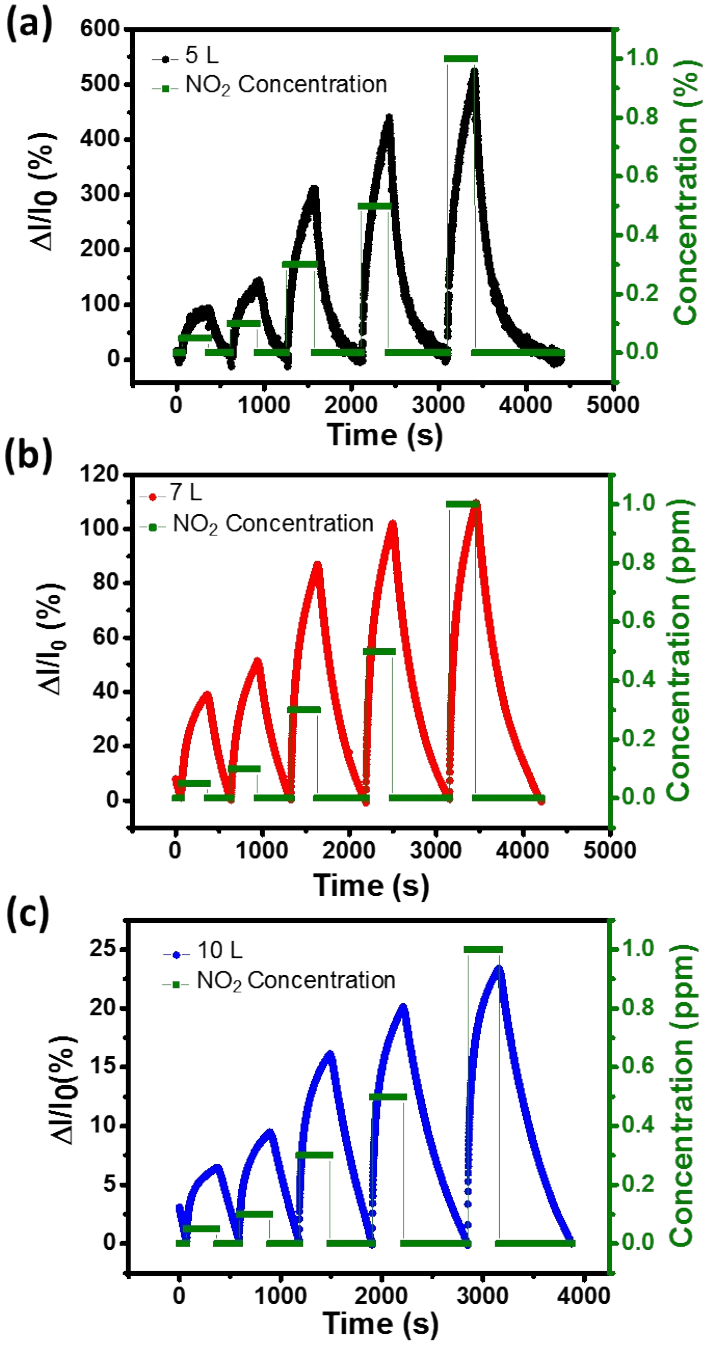

Figure S4 Real time NO_2 response of $PtSe_2$ fabricated at 450 °C and the NO_2 concentration ranged from 50 ppb to 1 ppm at (a) 5 L, (b) 7 L, and (c) 10 L.

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 (5^{th} 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.

RMS (ppm^{-1}) $=\sqrt{V_i^2/(N-1)}$, where $V_i=\sum(Y_i - Y_{fit})$

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

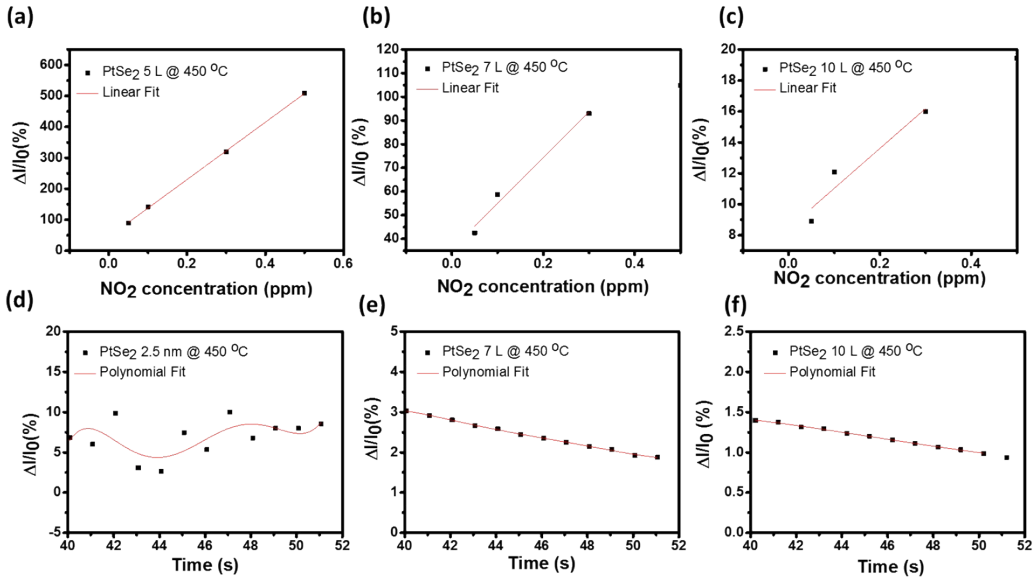

Figure S5 (a) to (c) the linear fit of the plot of the response versus concentration with 5, 7 and 10 layers. (d) to (f) 5^{th} order polynomial fit of 11 points before gas purging in with 5, 7 and 10 layers.

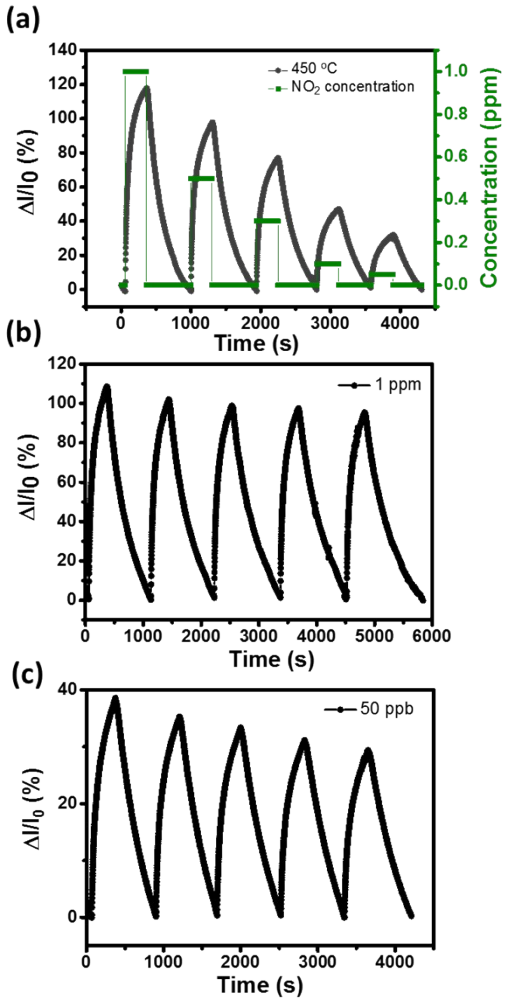

Figure S6 (a) Real time NO_2 response of $PtSe_2$ fabricated at 450 °C with 7 layers and the NO_2 concentration ranged from 1 ppm to 50 ppb. (b) and (c) the cycling response of 1 ppm and 50 ppb with 5 cycles.

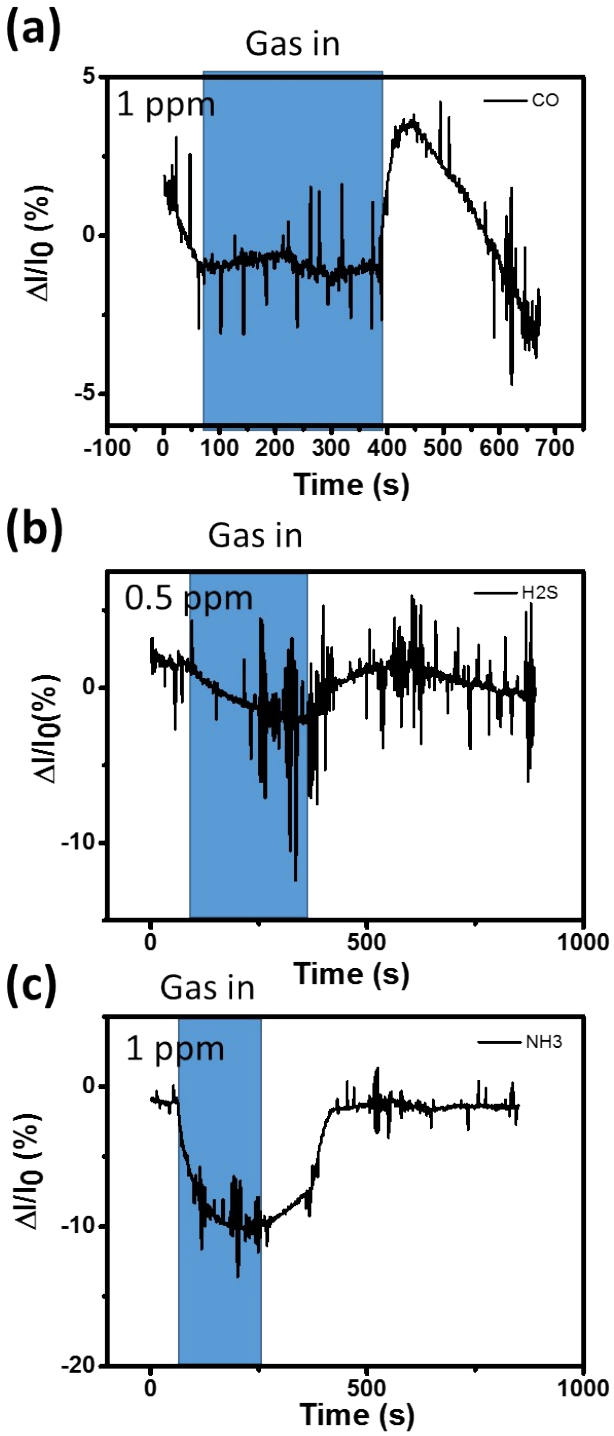

Figure S7. $PtSe_2$ sensing performance with (a) CO in 1 ppm (b) H_2S in 0.5 ppm, and (c) NH_3 in 1 ppm

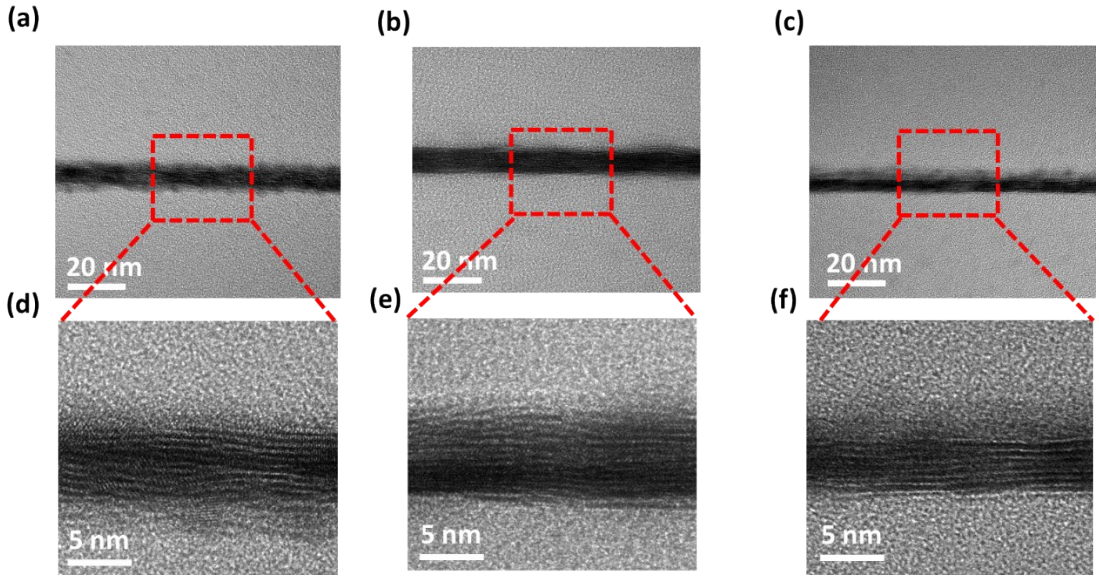

Figure S8. The cross section TEM image of $PtSe_2$ fabricated at 300 °C, 450 °C and 600 °C in low and high magnification. (a) and (d) are 300 °C, (b) and (e) are 450 °C, (d) and (f) are 600 °C.

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 (α) through –log (absorption (%))/thickness
3. According to the formula: $(\alpha h\nu)^{1/n} = A(h\nu - E_g)$, where the value n is 2 for indirect band, we can extrapolate the linear region of abscissa.

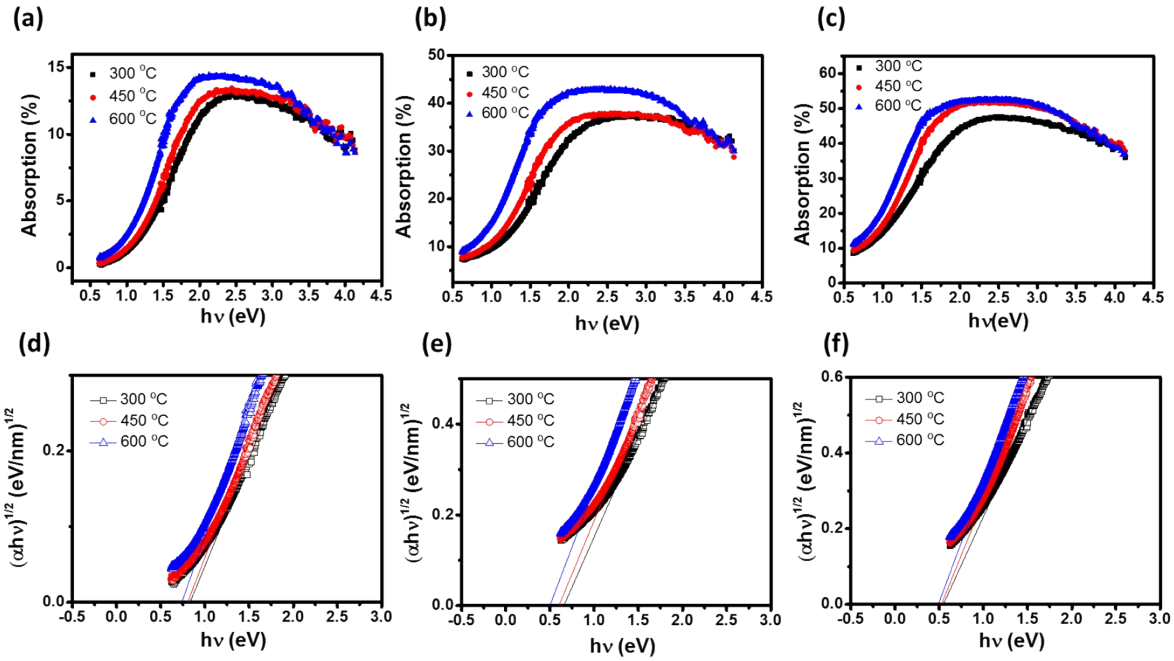

Figure S9. The absorption spectrum of $PtSe_2$ with different growth temperature in (a) 5 L, (b) 7 L, and (c) 10 L. The Tauc plot of abscissa of $PtSe_2$ with different temperature in (d) 5 L, (e) 7L and (f) 10 L.