Electronic Supplementary Information

Two-dimensional NbS₂ Gas Sensors for Selective and Reversible NO₂ Detection at Room Temperature

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Figure S1. Raman spectra of NbS$_2$ and NbO$_2$ samples from different growth temperatures.

Figure S2. (a) XPS Survey scan and (b) EDS spectrum of 2D NbS$_2$ nanosheets.
Figure S3. (a) Optical microscopic image of as-synthesized NbS$_2$ nanosheets on SiO$_2$ substrate. The inset shows as-synthesized NbS$_2$ nanosheets and a clean SiO$_2$ substrates before transfer process. (b) Photographic image of transferred NbS$_2$ nanosheets on SiO$_2$ substrate. (c) AFM image of transferred NbS$_2$ nanosheets.

Figure S4. (a) Resistance response curve and (b) a response curve of NbS$_2$ nanosheets upon exposure to 5 ppm NO$_2$. 
Figure S5. Response curves of NbS$_2$ nanosheets to 5 ppm NO$_2$ (a) 15 and 90 days later and (b) in different relative humidity from 10 to 50%.

Figure S6. Response curves of NbS$_2$ nanosheets to 50 ppm NO$_2$, NH$_3$, C$_2$H$_5$OH, CH$_3$OHCH$_3$, C$_6$H$_6$, and 3% CO$_2$ at room temperature.
Figure S7. Linear fit of the responses as a function of NO₂ concentration at room temperature.

Figure S8. Adsorption energy of the NO₂ molecule on a clean surface at 300 K and 10 ppm NO₂.
Figure S9. Density of states of NO$_2$ adsorbed S-edge (black line) and bare S-edge (grey line) in Nb-rich condition.
Figure S10. Atomic structure of O$_2$ adsorbed S-edge in Nb-rich condition in (a) isolated limit and (b) saturated limit. Atomic structure of NO$_2$ and O$_2$ adsorbed S-edge with coverage of (a) 25% NO$_2$ and 75% O$_2$, and (b) 50% NO$_2$ and 50% O$_2$. (e) Sum of spin-up DOS and spin-down DOS for various coverage of adsorbed O$_2$ and NO$_2$ at S-edge.