Electronic Supplementary Information

Two-dimensional NbS_2 Gas Sensors for Selective and Reversible NO_2 Detection at Room Temperature

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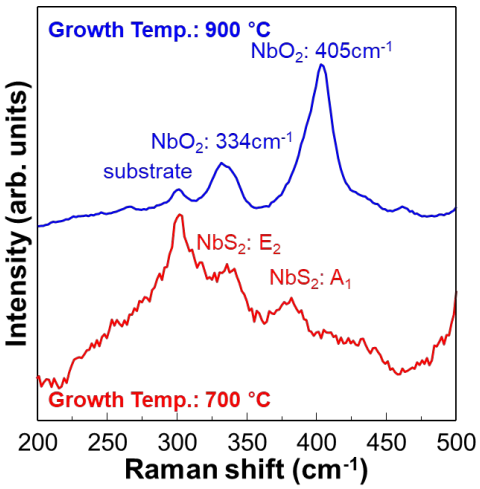

Figure S1. Raman spectra of NbS_2 and NbO_2 samples from different growth temperatures.

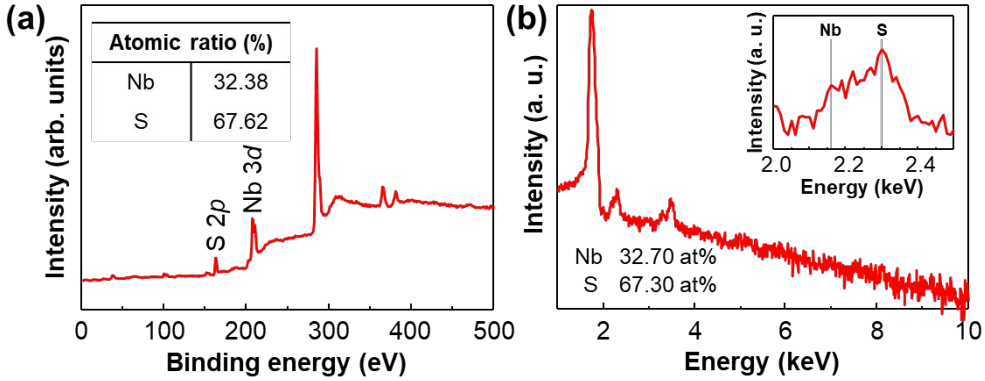

Figure S2. (a) XPS Survey scan and (b) EDS spectrum of 2D NbS_2 nanosheets.

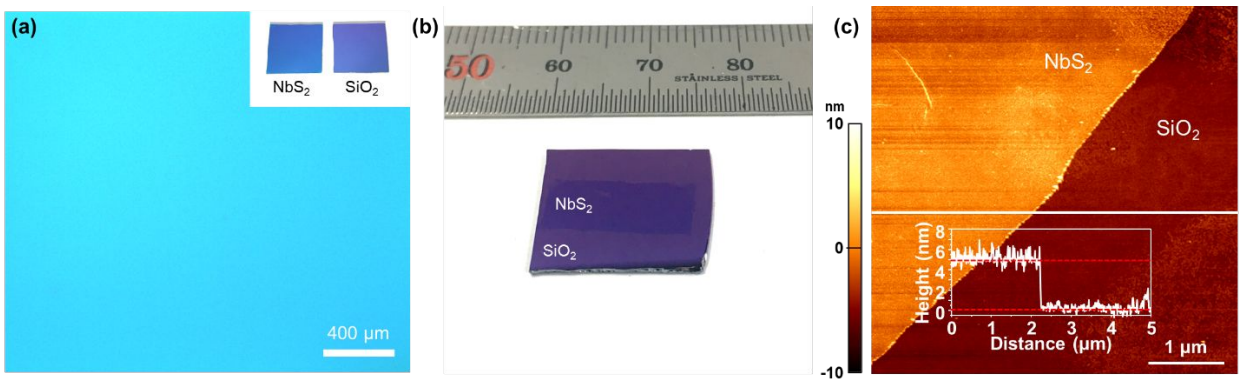

Figure S3. (a) Optical microscopic image of as-synthesized NbS_2 nanosheets on SiO_2 substrate. The inset shows as-synthesized NbS_2 nanosheets and a clean SiO_2 substrates before transfer process. (b) Photographic image of transferred NbS_2 nanosheets on SiO_2 substrate. (c) AFM image of transferred NbS_2 nanosheets.

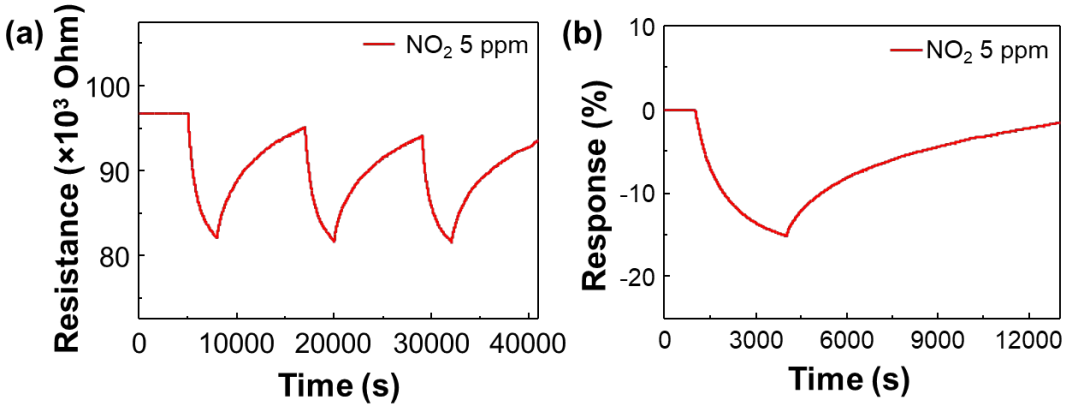

Figure S4. (a) Resistance response curve and (b) a response curve of NbS_2 nanosheets upon exposure to 5 ppm NO_2.

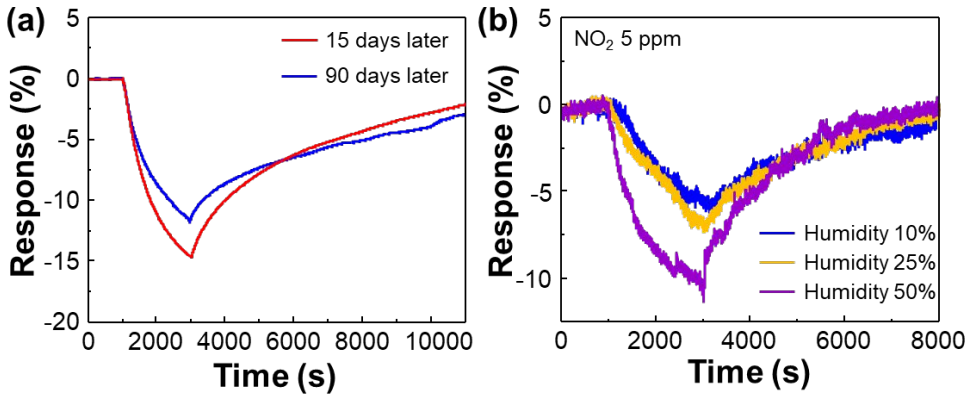

Figure S5. Response curves of NbS_2 nanosheets to 5 ppm NO_2 (a) 15 and 90 days later and (b) in different relative humidity from 10 to 50%.

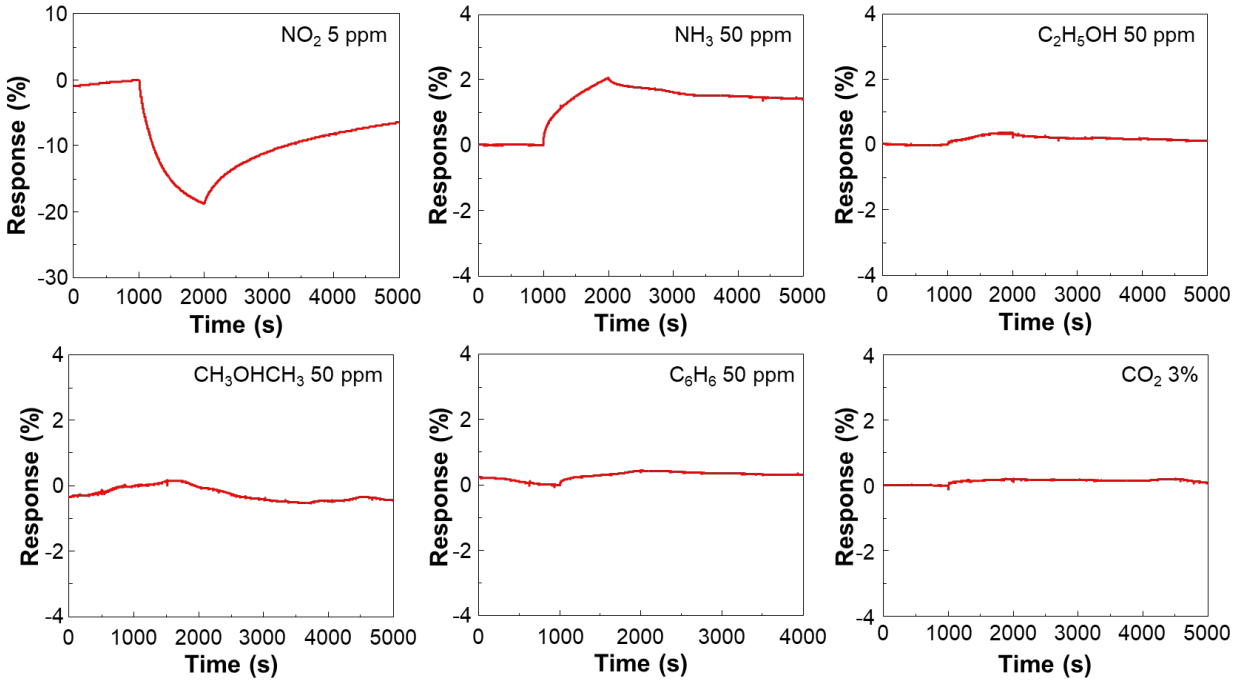

Figure S6. Response curves of NbS_2 nanosheets to 50 ppm NO_2, NH_3, C_2H_5OH, CH_3OHCH_3, C_6H_6, and 3% CO_2 at room temperature.

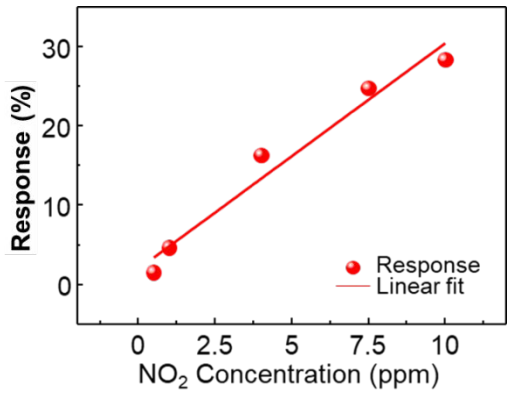

Figure S7. Linear fit of the responses as a function of NO_2 concentration at room temperature.

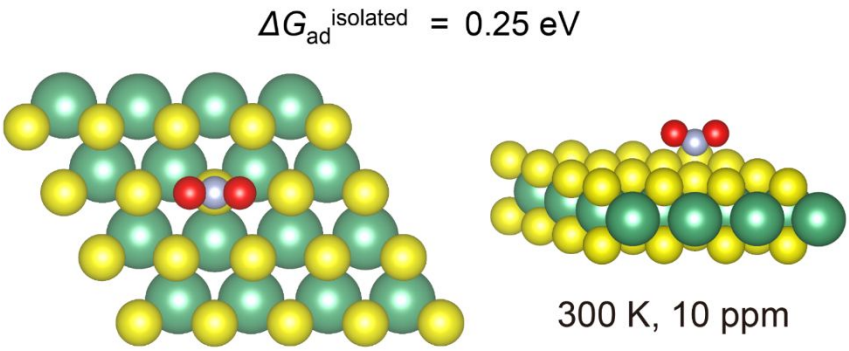

Figure S8. Adsorption energy of the NO_2 molecule on a clean surface at 300 K and 10 ppm NO_2.

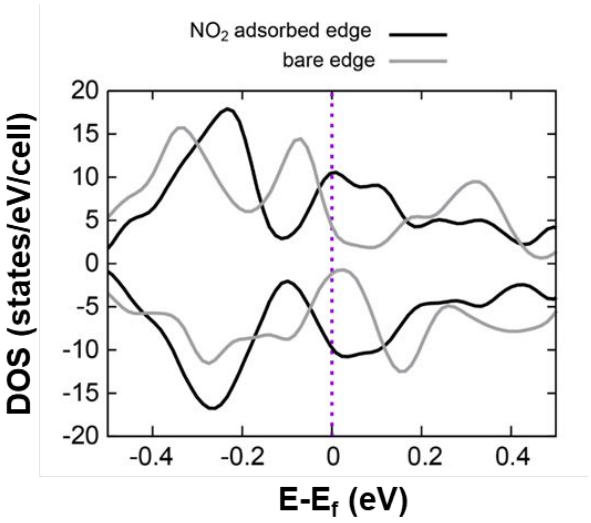

Figure S9. Density of states of NO_2 adsorbed S-edge (black line) and bare S-edge (grey line) in Nb-rich condition.

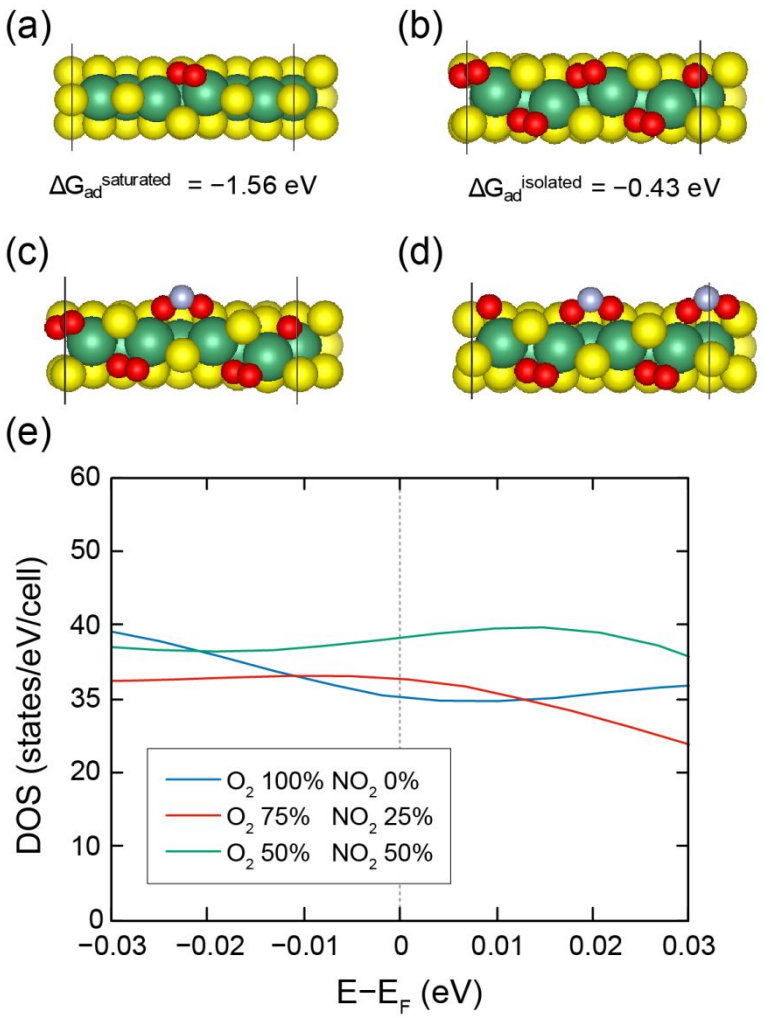

Figure S10. Atomic structure of O_2 adsorbed S-edge in Nb-rich condition in (a) isolated limit and (b) saturated limit. Atomic structure of NO_2 and O_2 adsorbed S-edge with coverage of (a) 25% NO_2 and 75% O_2, and (b) 50% NO_2 and 50% O_2. (e) Sum of spin-up DOS and spin-down DOS for various coverage of adsorbed O_2 and NO_2 at S-edge.