

## High-Performance NO<sub>2</sub> Gas Sensing of Ultra-Small ZnFe<sub>2</sub>O<sub>4</sub> nanoparticles

### Based on Surface Charge Transfer

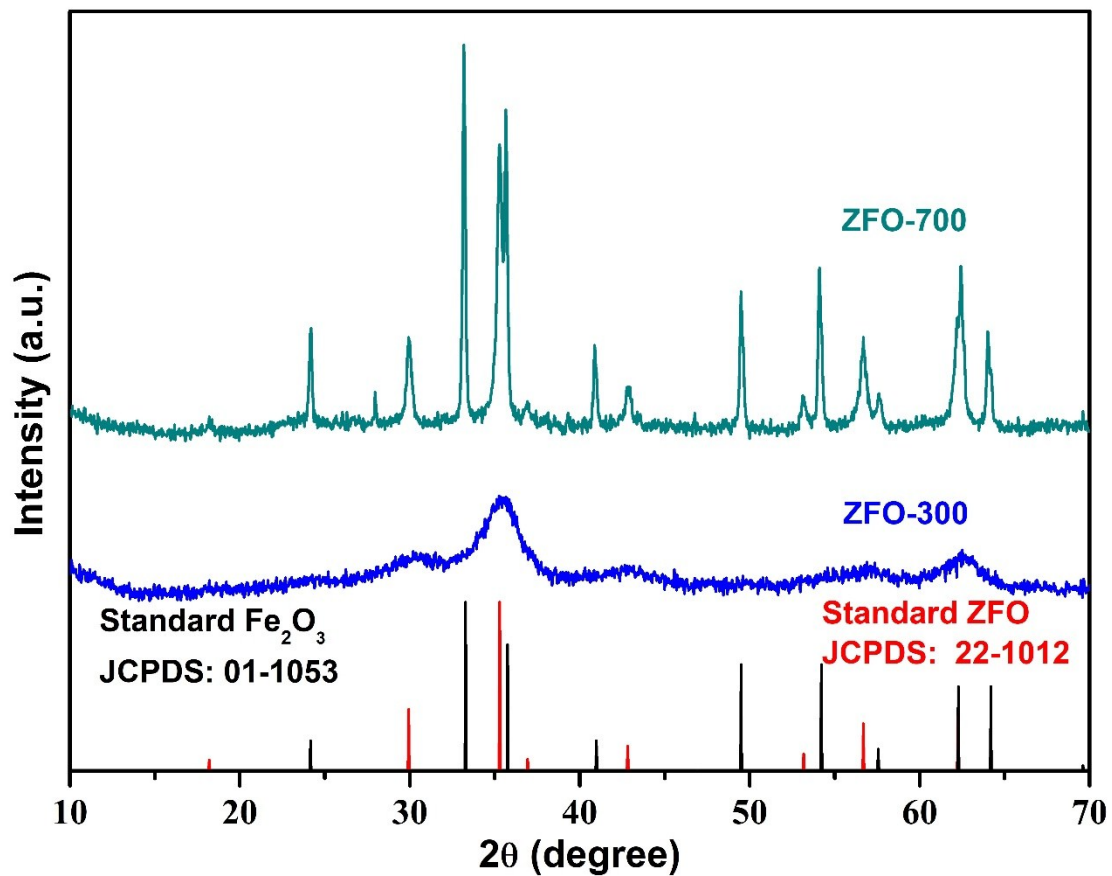
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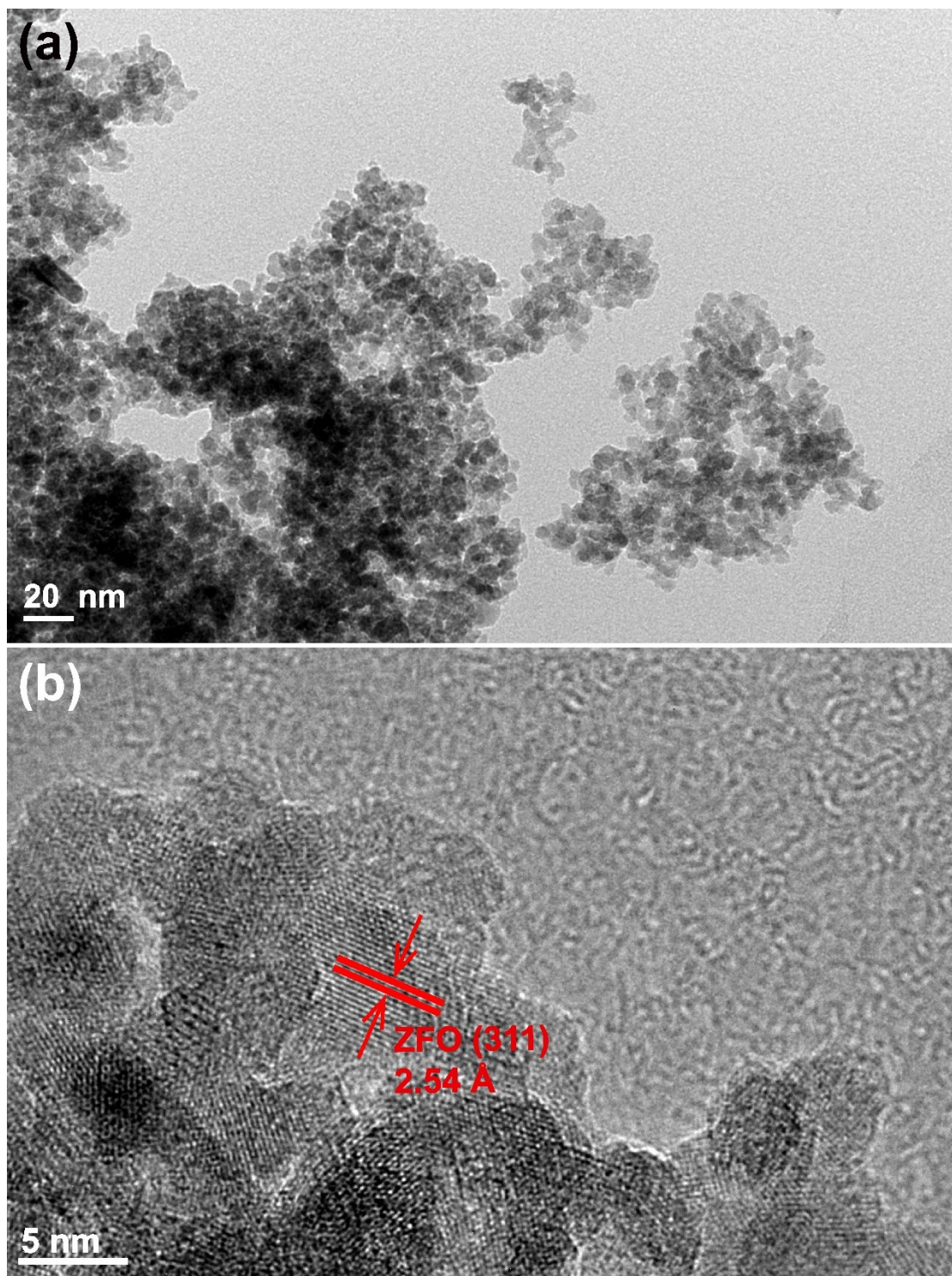
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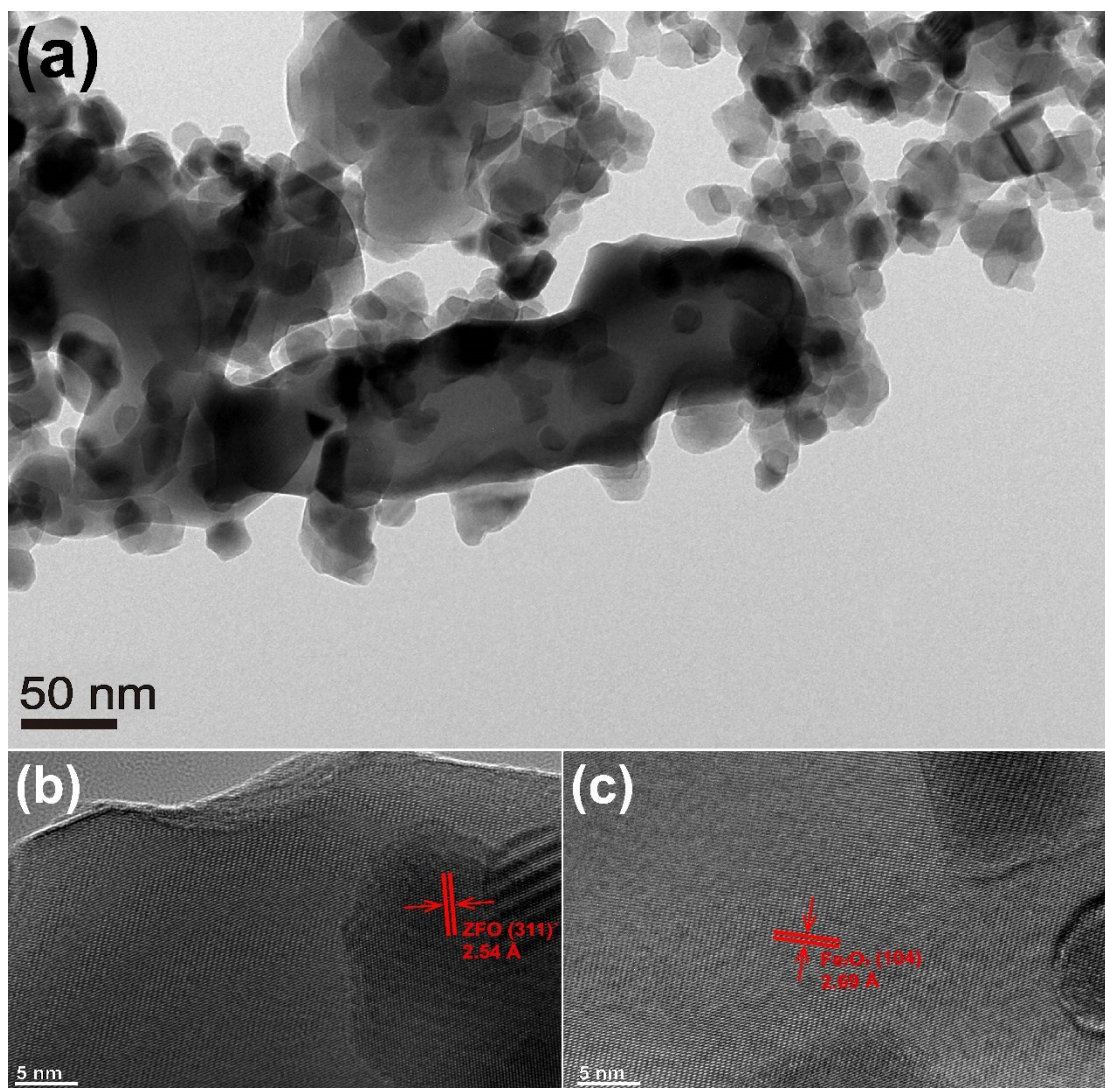
\*Email: yyluo@issp.ac.cn, duangt@hust.edu.cn



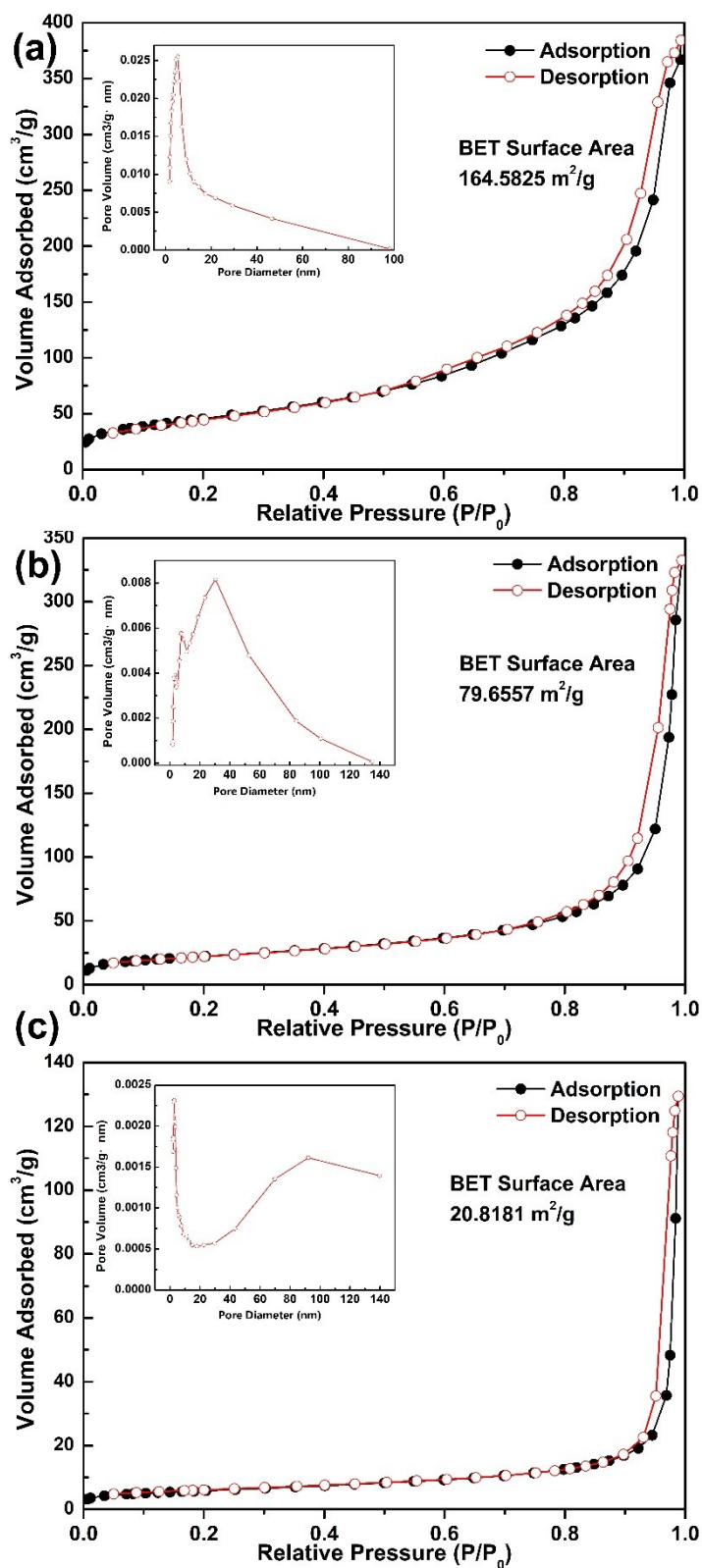
**Figure S1.** The X-ray diffraction patterns of ZFO nanoparticles acquired after calcining ZnFe-nitrate precursor at 700 °C (Green line) and 300 °C (Blue line) for 2 h, respectively.



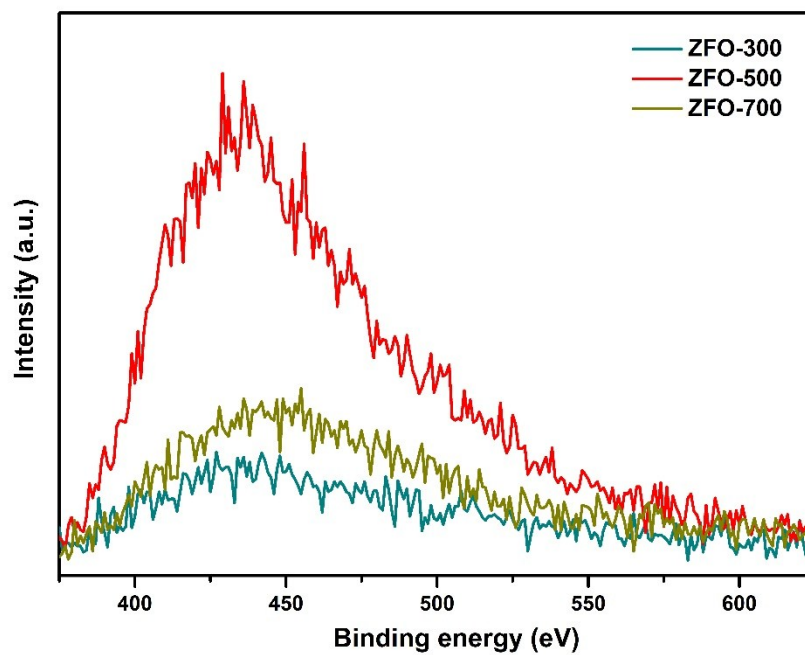
**Figure S2.** (a) TEM image of the ZFO-300 nanoparticles. (b) HRTEM of ZFO-700 nanoparticles.



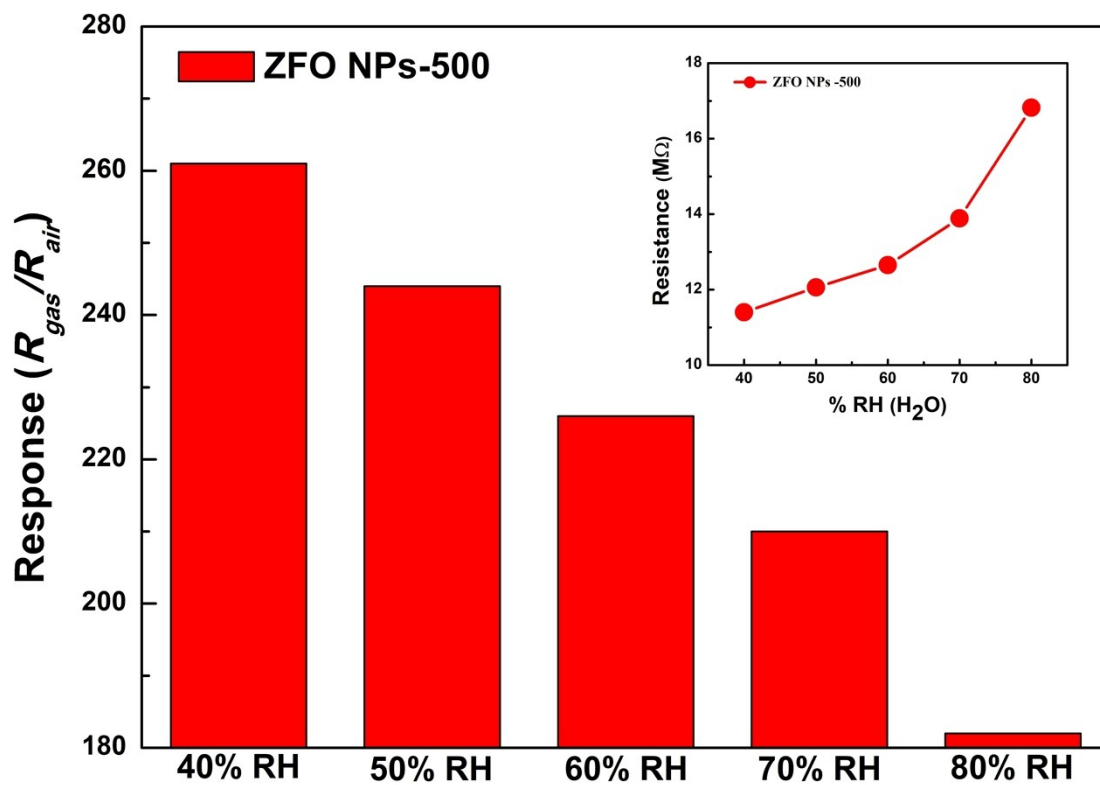
**Figure S3.** (a) TEM image of the ZFO-700 nanoparticles. (b~c) HRTEM of ZFO-700 nanoparticles.



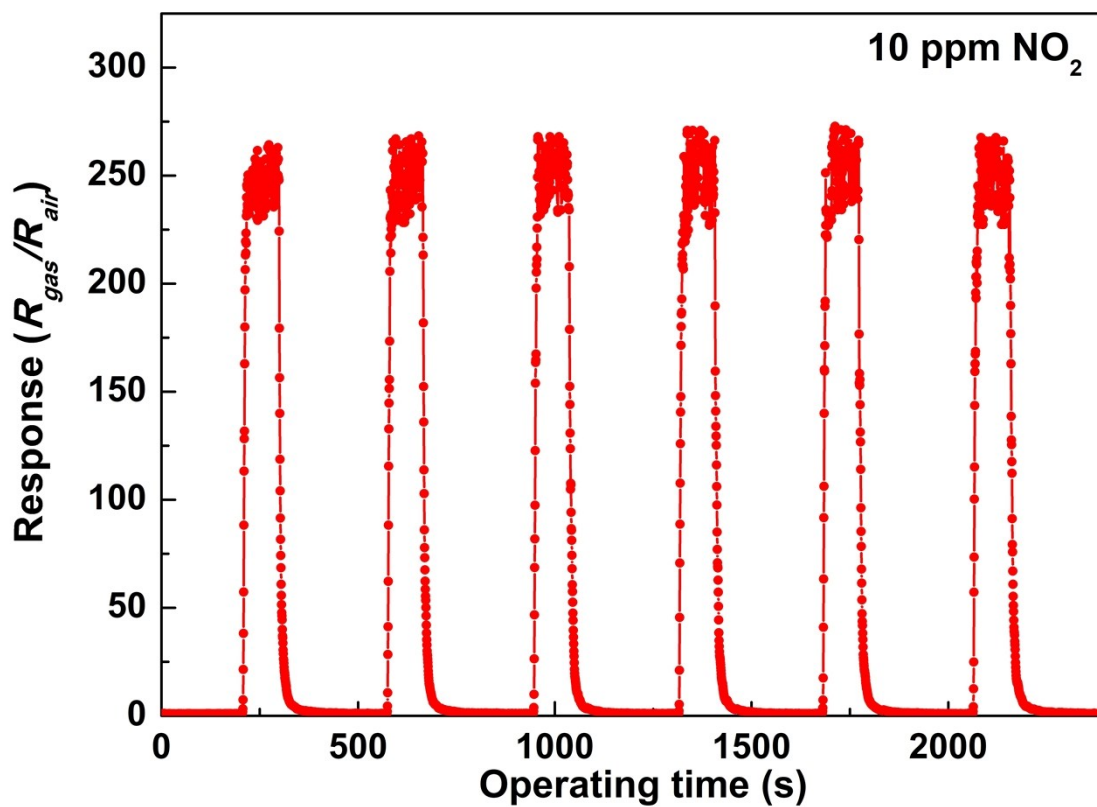
**Figure S4.**  $N_2$  adsorption-desorption isotherms and the pore size distributions(inset) of ZFO nanoparticles obtained after calcination at 300(a), 500(b) and 700(c) °C, respectively.



**Figure S5.** Photoluminescence spectrum of ZFO-300, ZFO-500 and ZFO-700 obtained after using a 400 nm optical filter at xenon lamp with excitation wavelength of 350 nm.

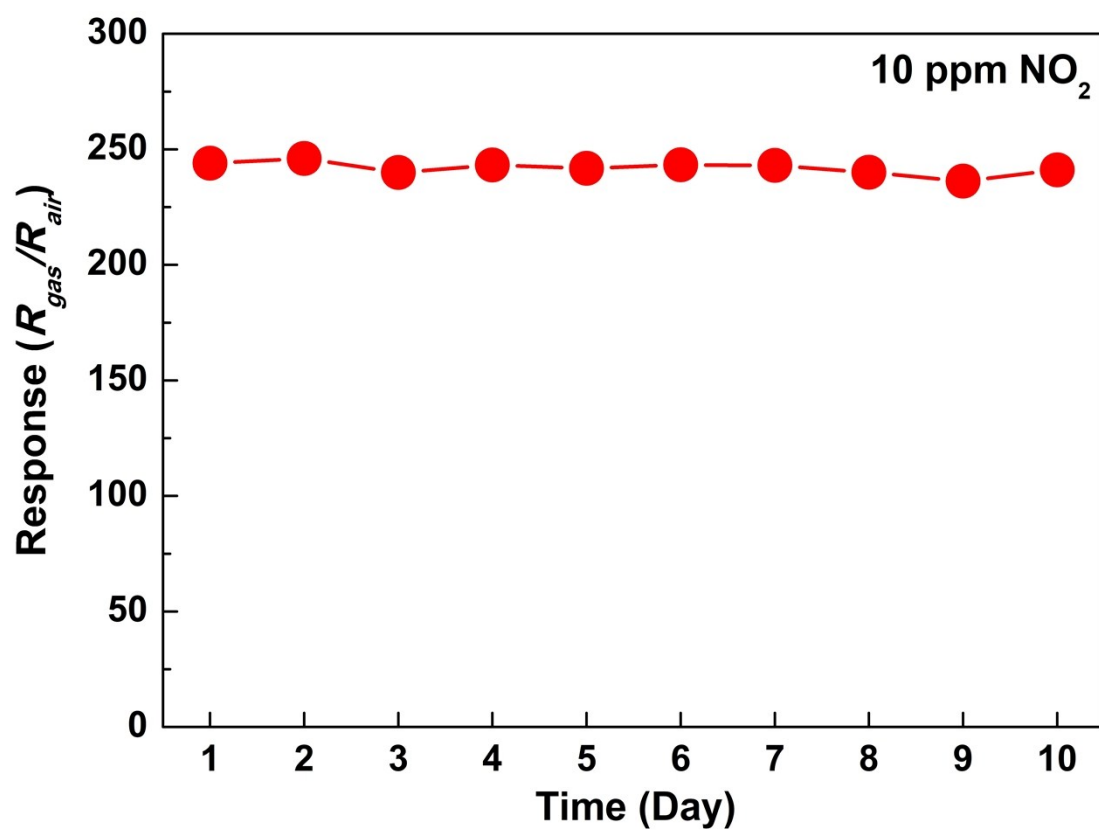


**Figure S6.** The gas response and initial resistance (inset) of ZFO NPs based sensor upon exposure into 10 ppm NO<sub>2</sub> under different humidity at the temperature of 125°C.

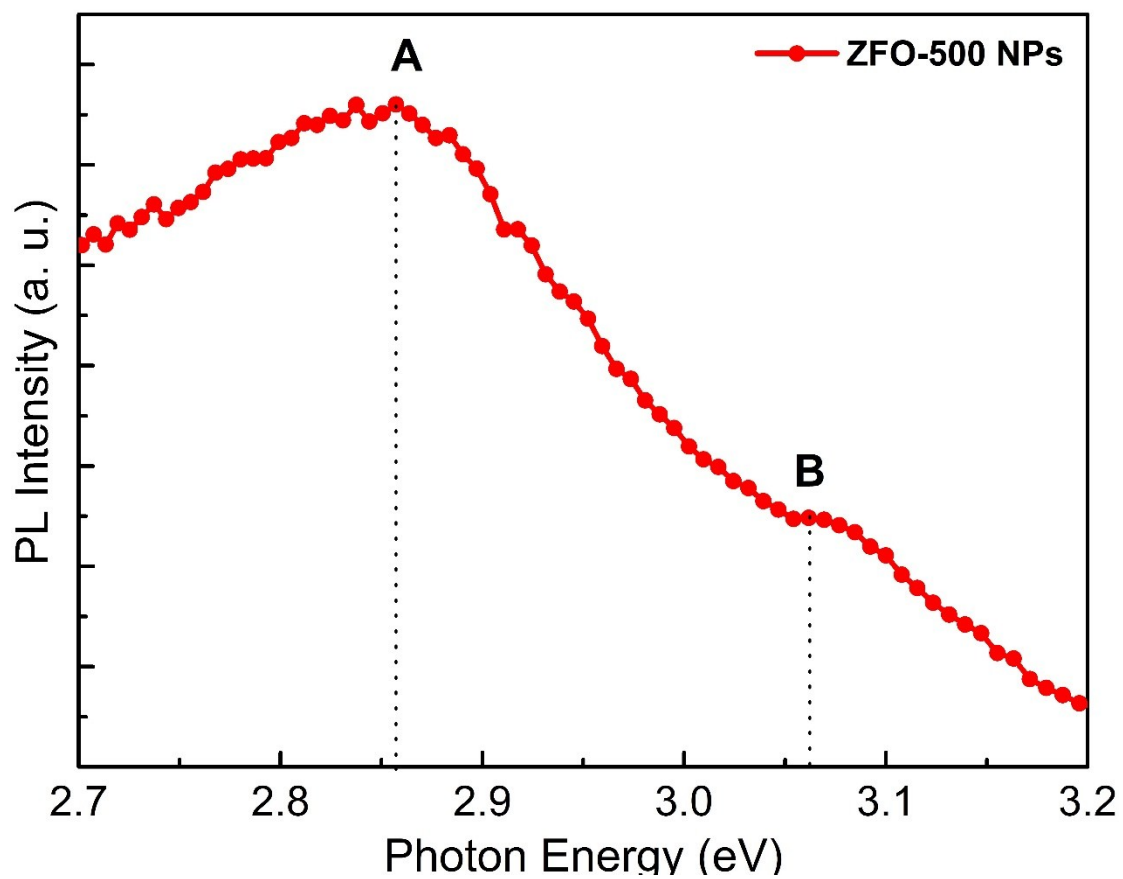


**Figure S7.** The cycling stability of ZFO NPs based sensor, which placed three months, upon exposure into 10 ppm NO<sub>2</sub> at the temperature of 125°C.

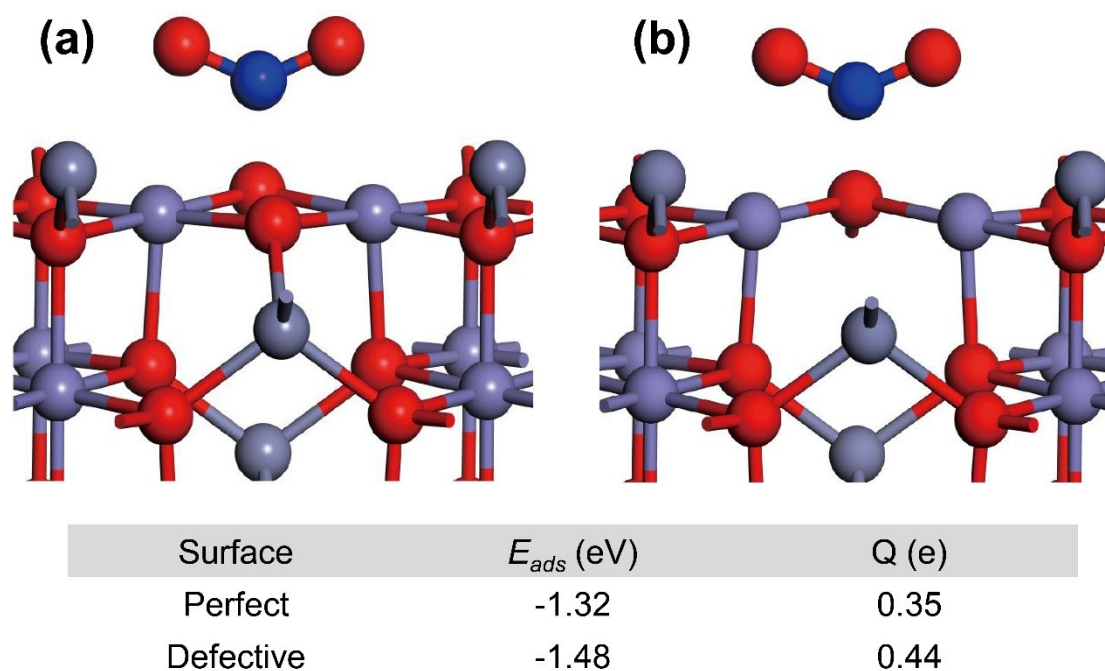




**Figure S8.** The long-term stability of ZFO NPs based sensor, which placed three months, upon exposure into 10 ppm NO<sub>2</sub> at the temperature of 125°C.



**Figure S9.** PL spectra of ZFO-500 NPs (flowed by pure N<sub>2</sub> at the temperature of 125 °C for 2 hours) upon exposure to pure N<sub>2</sub> along.



**Figure S10.** Optimized adsorption geometries for: (a) NO<sub>2</sub> molecule on a perfect ZFO (100) surface, (b) NO<sub>2</sub> molecule on a defective ZFO (100) surface with oxygen vacancy. The adsorption energy ( $E_{ads}$ ) and net charge (Q) for NO<sub>2</sub> molecule on perfect and defective ZFO (100) surface. The red, blue, grey and purple balls indicate oxygen, nitrogen, iron and zinc atoms, respectively.

**Table S1.** The gas-sensing performances (Response  $R_{gas}/R_{air}$ , Response time and Recovery time) of ZFO-500 under different NO<sub>2</sub> concentrations at the operating temperature of 125 °C.

NO <sub>2</sub> concentration (ppm)	Response ( $R_{gas}/R_{air}$ )	Response time (s)	Recovery time (s)
1	5.5	42	15
1.5	31	41	15
2	60	36	14
2.5	68	25	13
5	113	15	14
7.5	212	10	12
10	247.7	6.5	11