

# Supporting Information

## **P-N Heterointerface-determined Acetone Sensing Characteristics in $\alpha$ -MoO<sub>3</sub>@NiO Core@Shell Nanobelts**

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## 1. EXPERIMENTATION

### 1.1. Synthesis of 1D $\alpha$ -MoO<sub>3</sub> nanobelts.

All of the reagents used in the experiment were of analytical reagent grade, which were preceded without further purification. The 1D  $\alpha$ -MoO<sub>3</sub> nanobelts were synthesized by a hydrothermal treatment according to previous studies<sup>1</sup>. In a typical procedure, 0.96 g of Mo powder was added in a mixture solution consisted of 20 mL of 30 wt. % H<sub>2</sub>O<sub>2</sub> and 20 mL of H<sub>2</sub>O. The mixed solution was stirred for 12 h at 25 °C. After that, a transparent yellow solution was obtained and poured into a Teflon-lined stainless-steel autoclave followed by a hydrothermal treatment at 180 °C for 24 h. And then the white precipitate was collected by vacuum filtration which was then washed repeatedly at least seven times.

### 1.2. Synthesis of $\alpha$ -MoO<sub>3</sub>@NiO nanobelts.

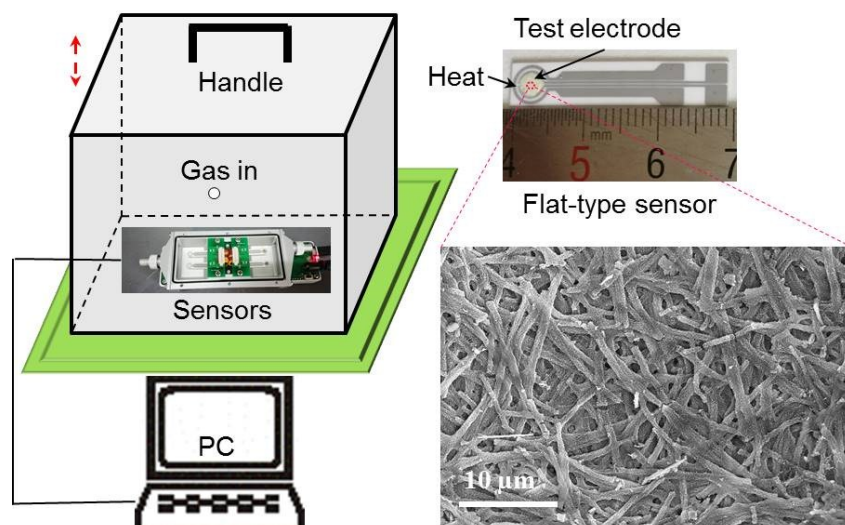
$\alpha$ -MoO<sub>3</sub>@NiO nanobelts were obtained by a facile method without any surfactant, which was also achieved by a hydrothermal and subsequently sintering treatment. Typically, 50 mg of as-prepared 1D  $\alpha$ -MoO<sub>3</sub> nanobelt powder was added in to 30 ml ethanol solution by the assistance of ultrasonication. Then, a certain amount of Ni(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O and hexamethylenetetramine (HMT) was added. This as-obtained solution was then poured into a Teflon-lined stainless-steel autoclave. After hydrothermally treated at 120 °C for 4 h, a green precursor was collected by vacuum filtration which was then washed repeatedly at least seven times. The added amount of Ni(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O and HMT was 54 and 210 mg, 72.7 and 280 mg, respectively, whose final products were named as  $\alpha$ -MoO<sub>3</sub>@NiO-1 and  $\alpha$ -MoO<sub>3</sub>@NiO-2, respectively. Finally, the  $\alpha$ -MoO<sub>3</sub>@NiO nanobelts were obtained by annealing the precursor at 500 °C for 2h in air. For comparison, pristine  $\alpha$ -MoO<sub>3</sub> nanobelts and NiO nanospheres prepared during these processes were obtained which named as  $\alpha$ -MoO<sub>3</sub> and NiO, respectively.

**1.3. Sensor fabrication and measurements.** The sensor fabrication processes were similar to our previous work<sup>2, 3</sup>. In a typical process, 5 mg precursor was uniformly dispersed in ethanol in a weight ratio of 5:1 by ultrasonication for 15 min to form a paste. Then, a ceramic flat placed with Pt interdigitated electrodes and Pt

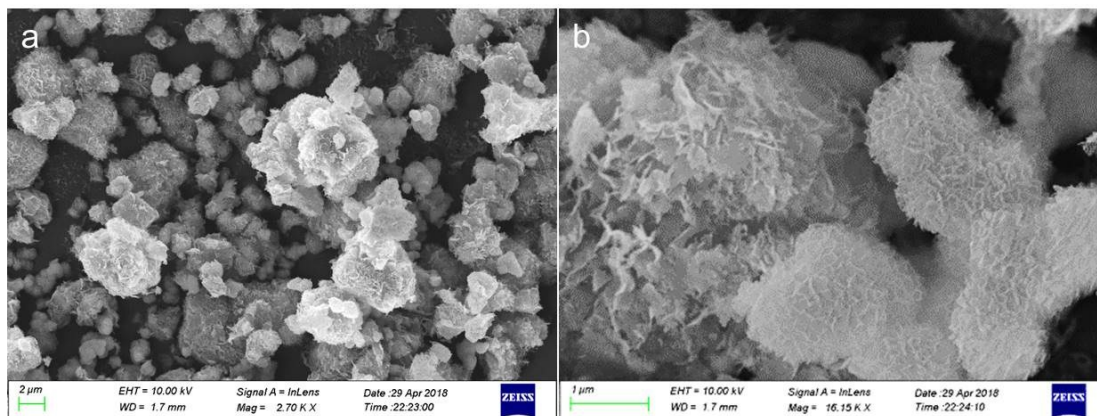
heater was chosen as substrate. The as-prepared paste was coated uniformly onto the substrate. Before gas-sensing measurements, the as-obtained gas sensor was annealed at 500 °C for 2 h and stabilized at 300 °C for 3 days in air. Then, gas-sensing measurements were carried out on a static gas-sensing analysis system (Wuhan Hua Chuang Rui Ke Co. Ltd., China). This system contains a test chamber (30 L in volume) and a personal computer as shown in Fig. S1. During the gas-sensing tests, the as-prepared sensors were mounted in the chamber. A given amount of target gas was introduced into this chamber by injecting their corresponding liquid using a microsyringe which was rapidly vaporized by a heater. After a few minutes, the ambient air (humidity: 18~22 %) was introduced again to restore base resistance by lifting the sealed chamber. During these processes, the resistance of the sensors was continuously recorded by the personal computer. Based on a regular basis, the gas-sensing response was defined as  $R_g/R_a$  or  $R_a/R_g$ , where  $R_g$  is the resistance of sensors in the presence of detecting gases and  $R_a$  is the resistance in air.

**1.4. Characterization.** The prepared products were characterized by means of the X-ray diffraction (XRD) (Philips X'pert X-ray diffractometer with Cu  $K_{\alpha 1}$  radiation). The structure was characterized by the field emission scanning electron microscopy (ZEISS EVO) and transmission electron microscopy (JEM-2100 microscope), which was operated at an acceleration voltage of 20 kV and 200 kV, respectively. With a probe size of 0.2 nm, Energy Dispersive X-ray Spectroscopy (EDS) was performed. The pore-size-distribution and Brunauer–Emmett–Teller (BET) surface area of these samples were analyzed by  $N_2$  adsorption/desorption isotherms (BELSORP-mini II) at 77 K.

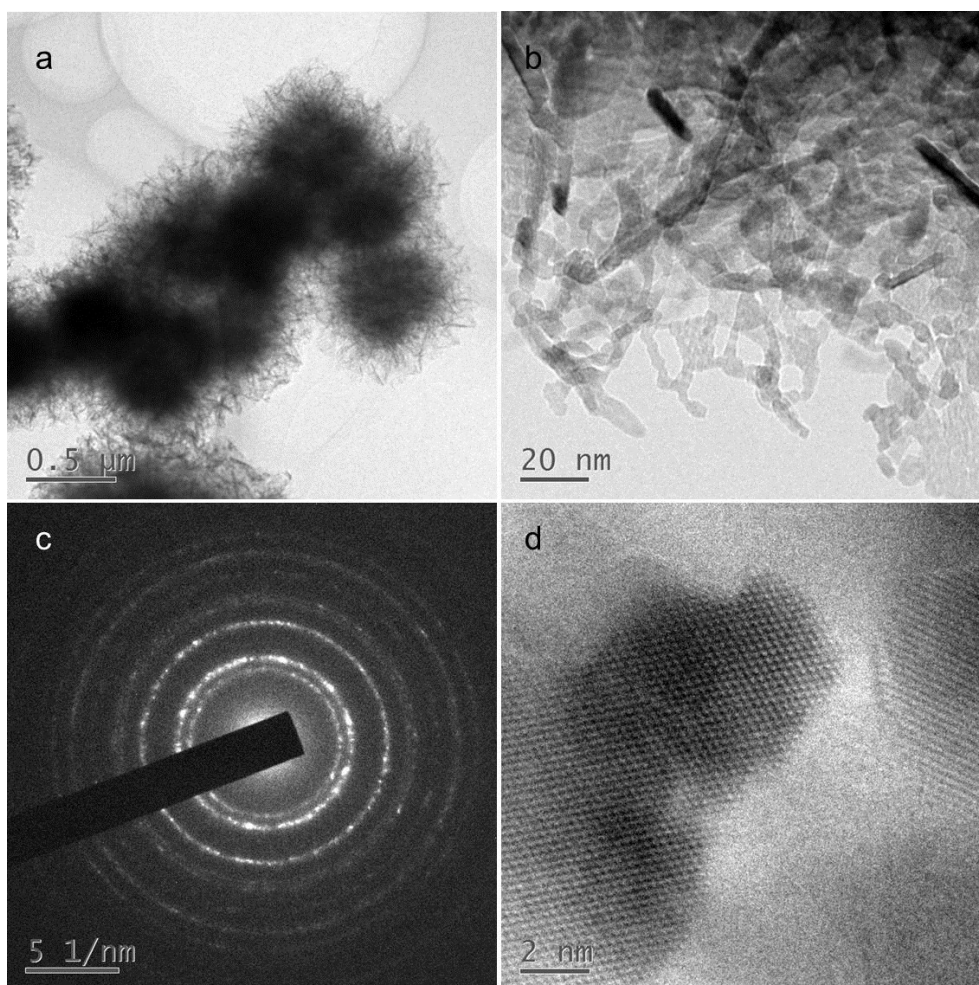
## 2. FIGURES



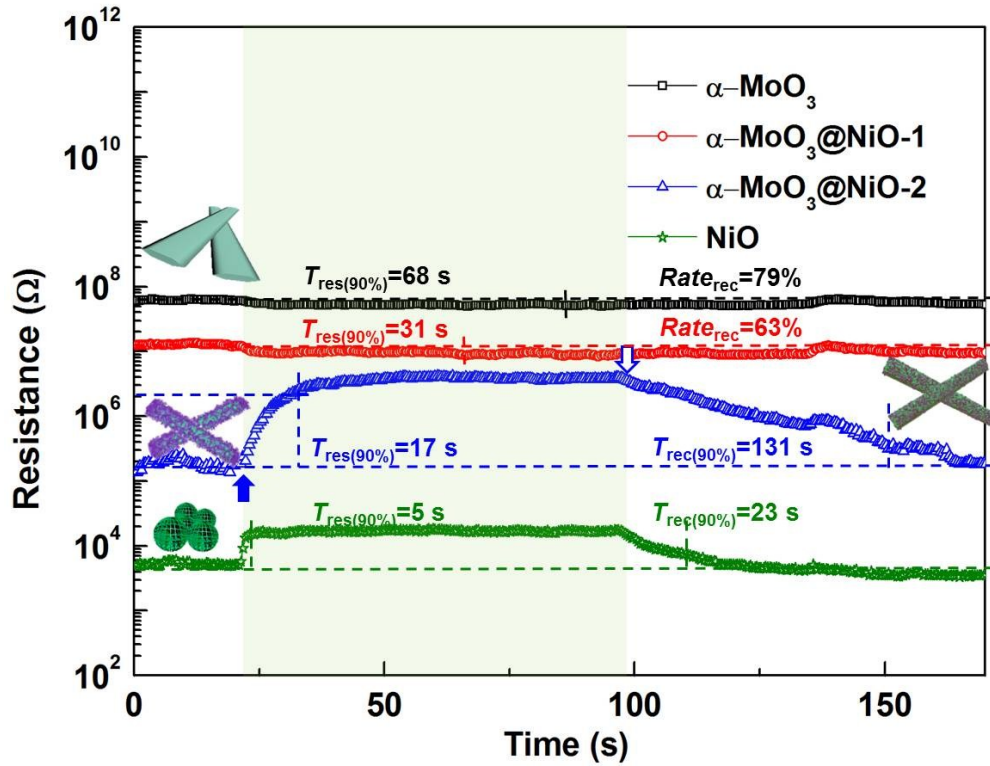
**Figure S1.** Schematic diagram of the applied gas-sensing measurement system. The right is the structure of the sensor and the morphology of sensing film ( $\text{NiO}@ \alpha\text{-MoO}_3\text{-2}$ ) on the surface of sensor.



**Figure S2.** SEM images of pristine NiO.



**Figure S3.** (a-b) Low-resolution TEM images of pristine NiO, (c) the corresponding SAED pattern, (d) High-resolution TEM image.



**Figure S4.** Typical response and recovery curve of  $\alpha$ - $\text{MoO}_3$ ,  $\alpha$ - $\text{MoO}_3$ @NiO-1,  $\alpha$ - $\text{MoO}_3$ @NiO-2 and NiO to 100 ppm acetone at their optimal operating temperatures.

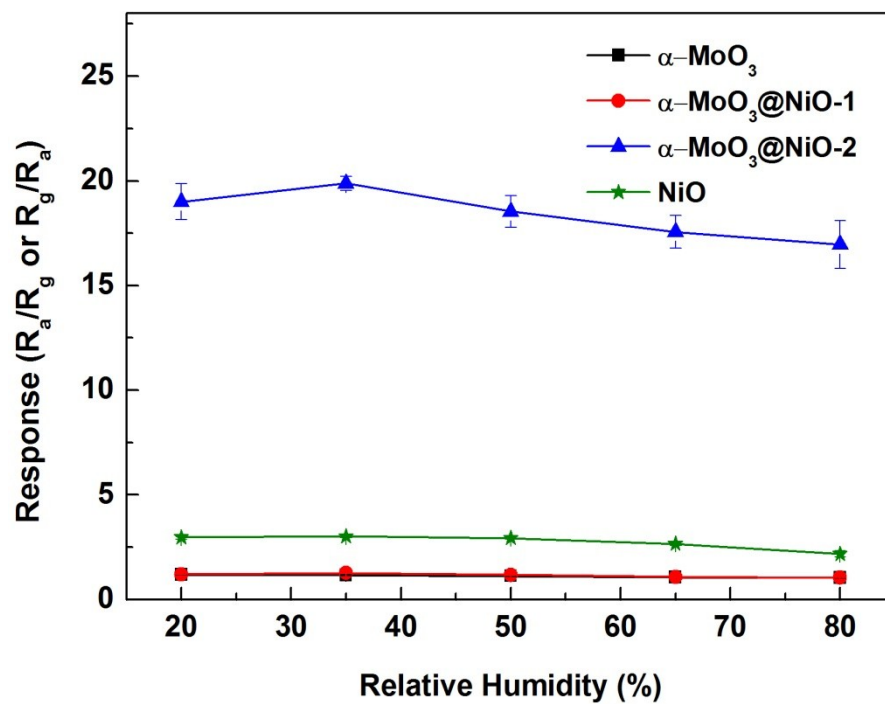
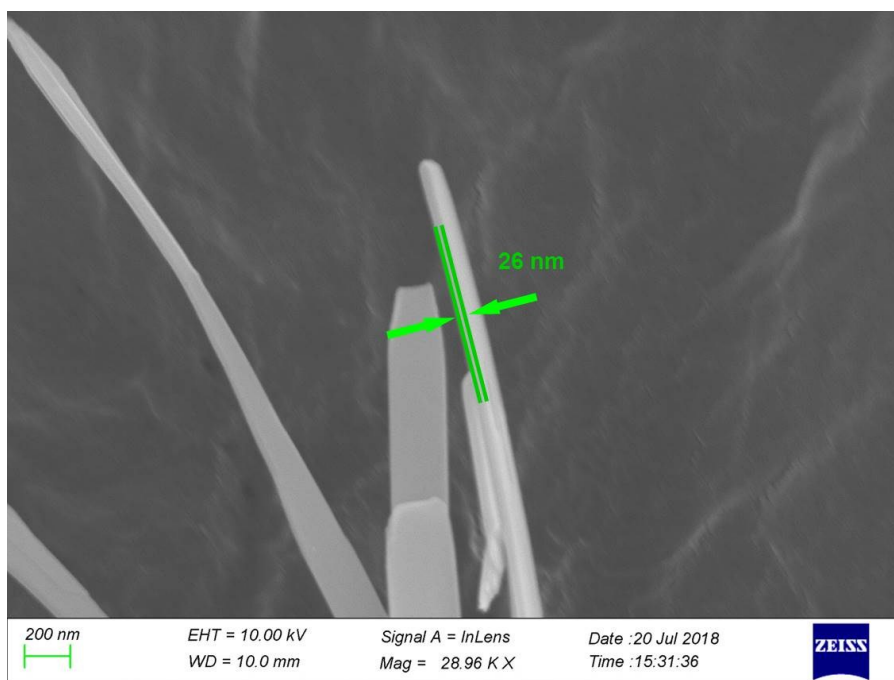


Figure S5. The relationship between relative humidity and response.





**Figure S6.** Thickness measurement of  $\alpha$ -MoO<sub>3</sub> nanobelts.

### 3. Calculations on space charge layers at $\alpha$ -MoO<sub>3</sub>@NiO PN heterointerface.

The width of the space charge layers induced by the PN heterojunctions created between  $\alpha$ -MoO<sub>3</sub> and NiO can be calculated using eqs 1 and 2 respectively,

$$\omega_{MoO_3} = \left\{ \frac{2\varepsilon_{MoO_3} \Delta\varphi}{q} \times \left[ \frac{N_{NiO}}{N_{MoO_3} \times (N_{MoO_3} + N_{NiO})} \right] \right\}^{1/2} \quad (1)$$

$$\omega_{NiO} = \left\{ \frac{2\varepsilon_{NiO} \Delta\varphi}{q} \times \left[ \frac{N_{MoO_3}}{N_{NiO} \times (N_{NiO} + N_{MoO_3})} \right] \right\}^{1/2} \quad (2)$$

where  $\varepsilon_{MoO_3}$  is  $11.2 \times 10^{-10} \text{ F}\cdot\text{m}^{-1}$ .<sup>4</sup>  $\Delta\varphi$  (=2.5 eV) is the contact potential difference between  $\alpha$ -MoO<sub>3</sub> and NiO, and  $N_{MoO_3}$  and  $N_{NiO}$  are the electron and hole concentrations, respectively ( $N_{MoO_3} = 1.5 \times 10^{18}$  and  $N_{NiO} = 2.24 \times 10^{18} \text{ cm}^{-3}$ )<sup>5, 6</sup>. The calculated  $\omega_{MoO_3}$  is 96 nm. Since the width of  $\alpha$ -MoO<sub>3</sub> (=20-30 nm) was less than  $2\omega_{MoO_3}$  (=35 nm), the  $\alpha$ -MoO<sub>3</sub> nanowires could be depleted completely.

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