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Supplementary Information For

Bifunctional role of PDMS membrane in designing humiditytolerant H₂S chemiresistors with high selectivity

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Experimental Section

1.1 Synthesis of Pt-anchored CuCrO₂ nanoparticles

Pt anchored CCO nanoparticles were prepared by glycine-nitrate solution combustion route. Copper nitrate (Cu(NO₃)₂·3H₂O), chromium nitrate (Cr(NO₃)₂·9H₂O), glycine (C₂H₅NO₂) and chloroplatinic acid hexahydrate (H₂PtCl₆·6H₂O) were from Sinopharm Chemical Reagent Co., Ltd. Firstly, 5 mmol Cu(NO₃)₂·3H₂O, 5 mmol Cr(NO₃)₂·9H₂O and 7 mmol C₂H₅NO₂ were sequentially dissolved in 50 mL deionized water, then 1.39 weight percentages of Pt precursor was gradually dropped in the above Cu-Cr precursor. After stirring at 80 °C for 2 h, the precursor was heated at 100 °C in an oven to dry the water solvent and then auto ignited at 200 °C to generate porous gray-black powder. Finally, the powder was repeatedly washed 3 times with dilute hydrochloric acid, deionized water, and absolute ethanol, respectively, and then dried in an oven at 80 °C for 24 h.

1.2 Synthesis of PDMS

Dow SYLGARD[™] 184 Silicone Elastomer Base (prepolymer, 12.0 g) and Curing Agent (crosslinking agent, 1.2 g) were mixed in glassware at a ratio of 10:1 for 10 minutes, and then were put into a vacuum chamber, and pumped for 5 minutes and release air for 5 minutes, and repeated the operation until the bubbles of the mixture disappear completely. Finally, it was placed in an oven at 60 °C for 10 hours to obtain PDMS.

1.3 Synthesis of PDMS-coated Pt-anchored CuCrO₂ nanoparticles

To synthesize PDMS-coated Pt-anchored CuCrO₂, pristine Pt-anchored CuCrO₂ devices were placed in sealed glassware, and PDMS pieces (5 mm \times 5 mm) were placed on the devices respectively as shown in Fig.S3. The glassware was placed in an oven at 200 °C for 30 min, 60 min, 90 min, and 120 min, respectively to get PDMS-coated Pt-anchored CuCrO₂.

1.4 Characterization

To demonstrate the successful coating of PDMS, samples were characterized by X-ray powder diffraction (XRD, Rigaku Smartlab 9 kW), high-angle annular dark-field scanning transmission microscopy (HAADF-STEM, JEM ARM-200F) equipped with energy dispersive spectrometer (EDS), scanning electron microscope (SEM, TESCAN VEGA3) and X-ray photoelectron spectroscopy (XPS, Escalab-250Xi).

1.5 Gas sensing test

Gas sensing tests were investigated in the SD101 (Hua Chuang Rui Ke Technology Co., Ltd.) testing system. The concentration of H₂S was adjusted by diluting the H₂S standard gas with dry air (controlled by two mass flow controllers), and the total gas flow was kept to 500 sccm during the measurement. The response of the chemiresistor was defined as R_g/R_a , where R_g was the resistance in the presence of target gas and R_a was the resistance in air, respectively. The operating temperature of 100 °C was controlled by a heating voltage of 2.5V.



Fig.S1 HAADF-STEM image of Pt-anchored CCO (squares represent the PtO_x clusters and the circles represent the Pt single atoms).



Fig.S2 XPS spectra of (a) Si 2p, (b) O 1s, (c) Cu 2p, (d) Cr 2p, and (e) Pt 4f for Pristine, PDMS-90 and PDMS-120. (f) Pt 4f XPS spectrum of PDMS-90.



Fig.S3 Schematic diagram of PDMS coating onto the chemiresistor devices by thermal evaporation.



Fig.S4 SEM images of (a) Pristine, (b) PDMS-90. (c-d) Elemental line-scanning profile of a single layer of PDMS-90 along cross section direction.



Fig.S5 The variation of contact angle and the net PDMS film (deposited onto a flat surface alumina substrate) thicknesses of Pristine, PDMS-30, PDMS-60, PDMS-90, and PDMS-120 with PDMS deposition time. Note that the contact angle was measured on the chemiresistor surface (porous CCO sensing layer on the alumina sensing substrate).



Fig.S6 Cross-sectional SEM image of (a) PDMS-90 and (c) PDMS-120. Si element mapping of (b) PDMS-90 and (d) PDMS-120. Note that the porous CCO sensing layer was coated on the alumina substrate.



Fig.S7 The contact angle of (a) PDMS-30 and (b) PDMS-60. (Note that the contact angle was measured on the porous CCO sensing layer on the alumina substrate.).



Fig.S8 (a) The resistance and (b) response of PDMS-30, PDMS-60, and PDMS-120 to 5 ppm H_2S under different relative humidity levels.



Fig.S9 Response of PDMS-90 versus (a) 100–1000 ppb and (b) 3–10 ppm H_2S at an operation temperature of 100 °C at RH 50%.



Fig.S10 Response curve of PDMS-90 to different vapors at an operation temperature of 100 °C at RH 50%.



Fig.S11 Response curve of Pristine, PDMS-90 and PDMS-120 to 5 ppm H_2S at an operation temperature of 100 °C at RH 50% after 235 days.