Electronic Supplementary Information (ESI)

Ag Nanocrystal as a Promoter for Carbon Nanotube-based Roomtemperature Gas Sensors

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Fig. S1 Schematic setup of SnO₂ nanoparticle synthesis system.



Fig. S2 (a) Low magnification TEM image and SAED pattern (inset) of SnO_2 nanoparticles synthesized at 950 °C. (b) HRTEM image of SnO_2 nanoparticles. 0.335 nm lattice spacing is indexed to (110) plane of rutile SnO_2 .



Fig. S3 Low magnification TEM image (a) and SAED pattern (b) of as-produced Ag NPs. (c), and (d) HRTEM images of Ag NPs, and 0.235 nm lattice spacing is indexed to (111) plane of Ag.



Fig. S4 (a) I-V curve evolution of MWCNTs at different conditions (with and without NP coating). (b) The dependence of current on gate voltage.



Fig. S5 Differential IR absorbance spectra of MWCNT hybrid sensors exposed to100 ppm NO₂ diluted in Ar.



Fig. S6 Upper panel: Perspective views of the SnO_2 (110) surface with the coordination number of different Sn atoms labeled, (a) planar-reduced surface and (b) oxidized surface with oxygen atoms sitting on the bridge sites. Lower panel: Charge density difference upon NO₂ molecule adsorption on the surface. Green and yellow represent electron accumulation and depletion regions, respectively. (c) NO₂ is attracted directly to the Sn4 atom with gain of 0.0576 e⁻. (d) NO₂ forms NO₃^{δ} complex with gain of 0.0069 e⁻. For NH₃ adsorption, it prefers the Sn5 site instead of the bridging oxygen. However, this site is preoccupied by O₂ at room temperature and leads to the reluctance of sensor to NH₃.



Fig. S7 Representative sensing response of $Ag/SnO_2/MWCNTs$ hybrid structures to 100 ppm NO_2 at room temperature.



Fig. S8 Differential IR absorbance spectra of MWCNT hybrid sensors exposed to 1% NH₃ diluted in Ar. Spectra are scaled and offset for clarity. Features at 2,350 cm⁻¹ and 1,400-1,800 cm⁻¹ are due to incomplete cancellation of atmospheric CO₂ and water vapor, respectively. Gas-phase NH₃ rotation-vibration bands are present in the region



900-1,200 cm⁻¹. The MWCNT and MWCNT/SnO₂ spectra are quite similar, with only small difference between the two in the region 900-1,100 cm⁻¹.

Fig. S9 (a) SEM image of MWCNTs coated with Ag NPs. Inset is an SEM image showing the hybrid structure bridging two gold electrodes. (b) I-V characteristics of MWCNTs and MWCNTs/Ag. (c) and (d) are sensing responses of bare MWCNTs and MWCNTs/Ag structures to 100 ppm NO_2 and 1% NH_3 at room temperature, respectively.



Fig. S10 SEM image of MWCNTs with full surface coverage of SnO₂ NPs



Fig. S11 *I-V* curve evolution of the control sample, which was obtained by first coating MWCNTs with SnO_2 NPs at a high coverage followed by additional coating of Ag NPs.