

Electronic Supplementary Information

Investigation of CO₂ reaction with Copper Oxide Nanoparticles for Room Temperature Gas Sensing

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Section S1. Instrumentation

Section S2. Material Characterization

Section S3. Thermodynamical Investigations

Section S4. Gas Sensing Response and Recovery Times

Section S1. Instrumentation

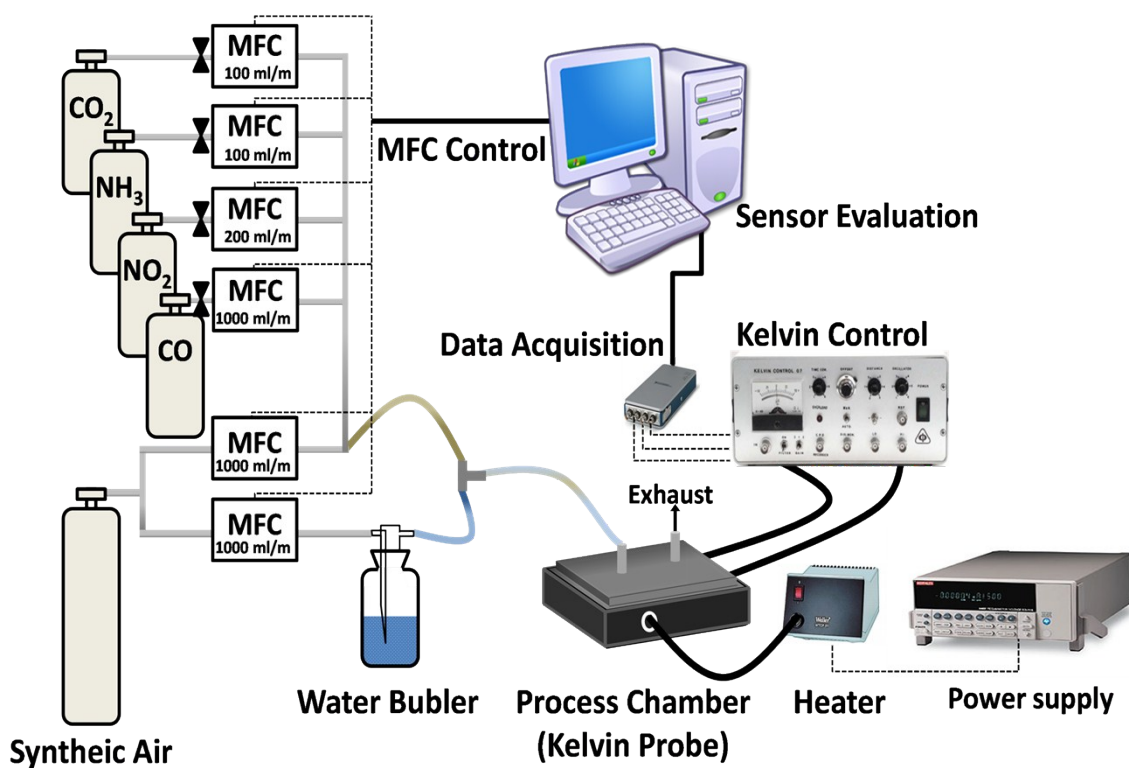


Figure S1. The schematic representation of developed Kelvin probe setup, which allow for the work function change measurement of gas sensitive materials under investigation.

Section S2. Material Characterization

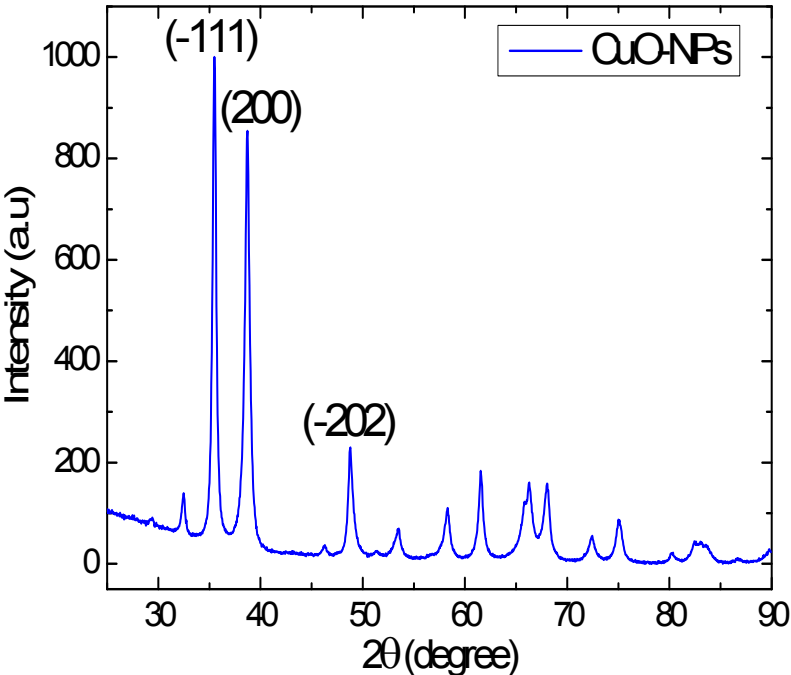


Figure S2. X-ray diffraction spectrum of copper oxide nano-powder.

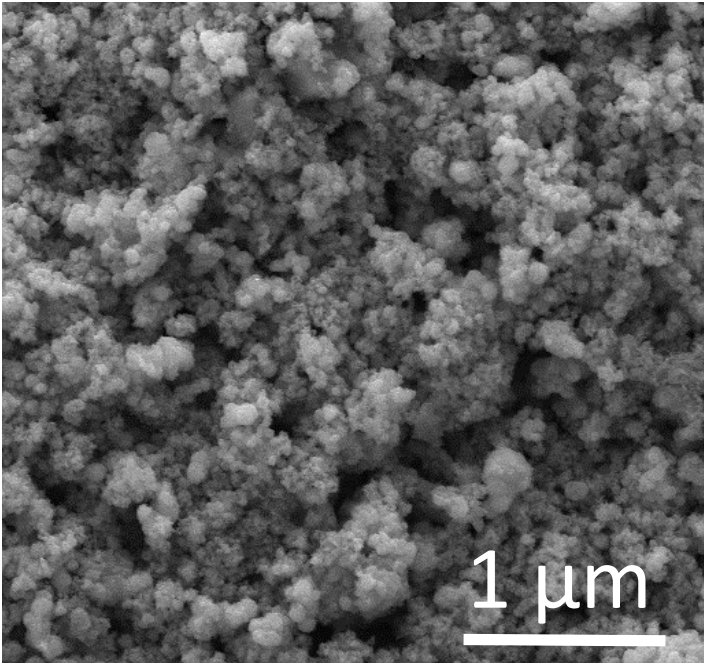


Figure S3. SEM-image of as deposited copper oxide nanoparticles layer

Section S3. Thermodynamical Investigations

The Gibbs free energy change $\Delta_R G$ for the reactions taking place at 298.15 K and partial pressures of participating gases differing from 1 bar can be calculated by the following equation ¹:

$$\Delta_R G = \Delta_R G^\circ + RT \ln Q \quad (\text{S1})$$

where $\Delta_R G^\circ$ is the free energy change at standard conditions, R is the ideal gas constant and its value is 8.314 J/mol.K, T is the temperature in kelvin, Q is the reaction quotient and for the kind of reaction shown in eq. (S2) with gaseous components as reactants and products, Q is given by eq. (S3):



$$Q = \frac{(P_C)^c (P_D)^d}{(P_A)^a (P_B)^b} \quad (\text{S3})$$

where p_A, p_B, p_C, p_D are the partial pressures of the corresponding gases in bar.

Correspondingly, $\Delta_R G^\circ$ for the reaction of malachite formation is given by:

$$\Delta_R G = \Delta_R G^\circ + RT \ln (P_{CO_2})^{-1} \quad (\text{S4})$$

At equilibrium, $\Delta_R G$ is zero, and the equilibrium partial pressure of CO_2 for the reaction of malachite formation can be calculated according to eq. S4 and S5:

$$\Delta_R G^\circ = -RT \ln K_{eq.} = -RT \ln (P_{CO_2})^{-1} \quad (\text{S4})$$

$$\log \frac{1}{p_{CO_2}} = -\frac{\Delta_R G^\circ}{2.303 RT} \quad (\text{S5})$$

where $K_{eq.}$ is the equilibrium constant.

Section S4. Gas Sensing Response and Recovery Times

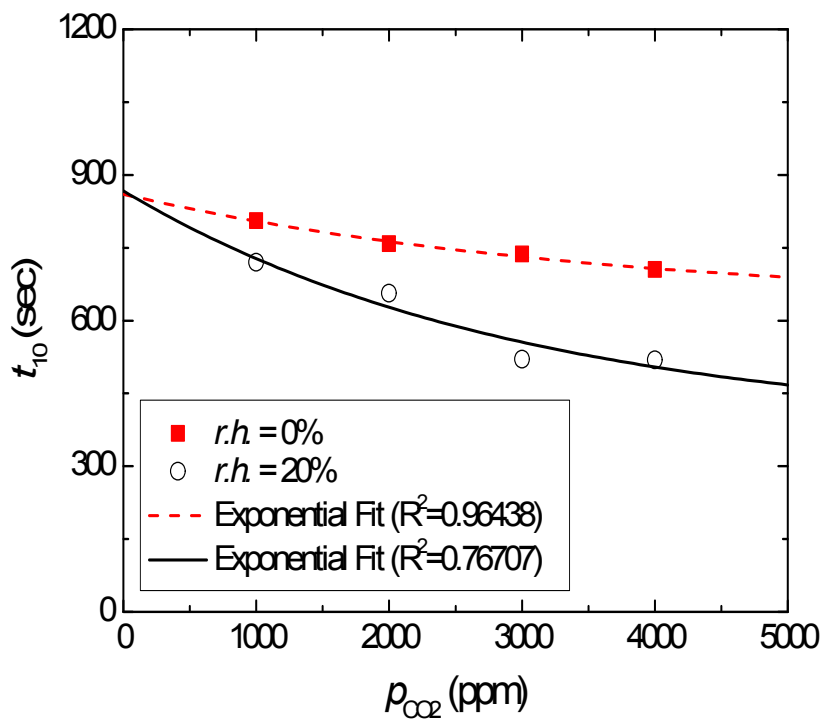
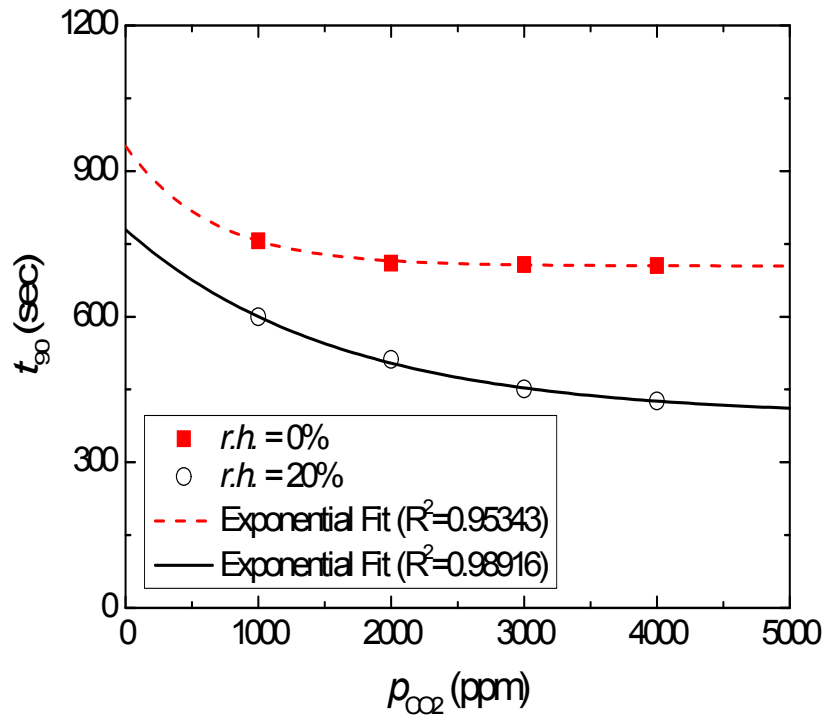


Figure S4. Dependence of response (t_{90}) and recovery (t_{10}) times on CO₂ concentration for dry ($r.h.$ = 0%) and humid ($r.h.$ = 20%) conditions at room temperature.