Supporting information

Sensing Performance and Mechanism of Shape-Tunable CuO Nanocrystals for Monohydric Alcohol Gases

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Table S1. The detailed list of experimental conditions

Sample	**$CuCl_2{\cdot}2H_2O$**	**PVP/g**	**T/°C**
Cu_2O-cube	0.0l mol, 100 mL	0	55
Cu_2O-Truncated Cube	0.0l mol, 100 mL	0.833	55
Cu_2O-cubooctahedron	0.0l mol, 100 mL	1.667	55
Cu_2O-Truncated octahedral-1	0.0l mol, 100 mL	2.778	55
Cu_2O-Truncated octahedral-2	0.0l mol, 100 mL	3.333	55
Cu_2O-octahedral	0.0l mol, 100 mL	3.988	55

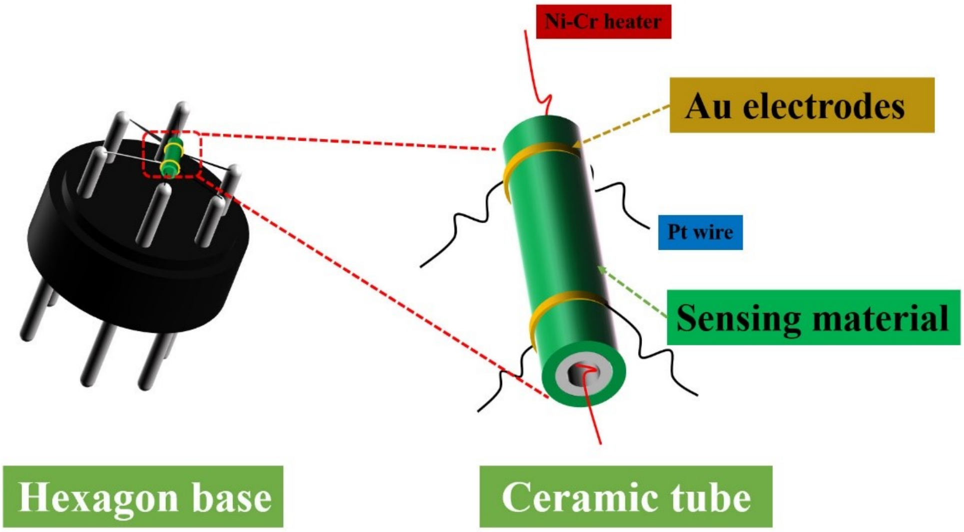

Fig. S1 The schematic diagram of the gas sensor device.

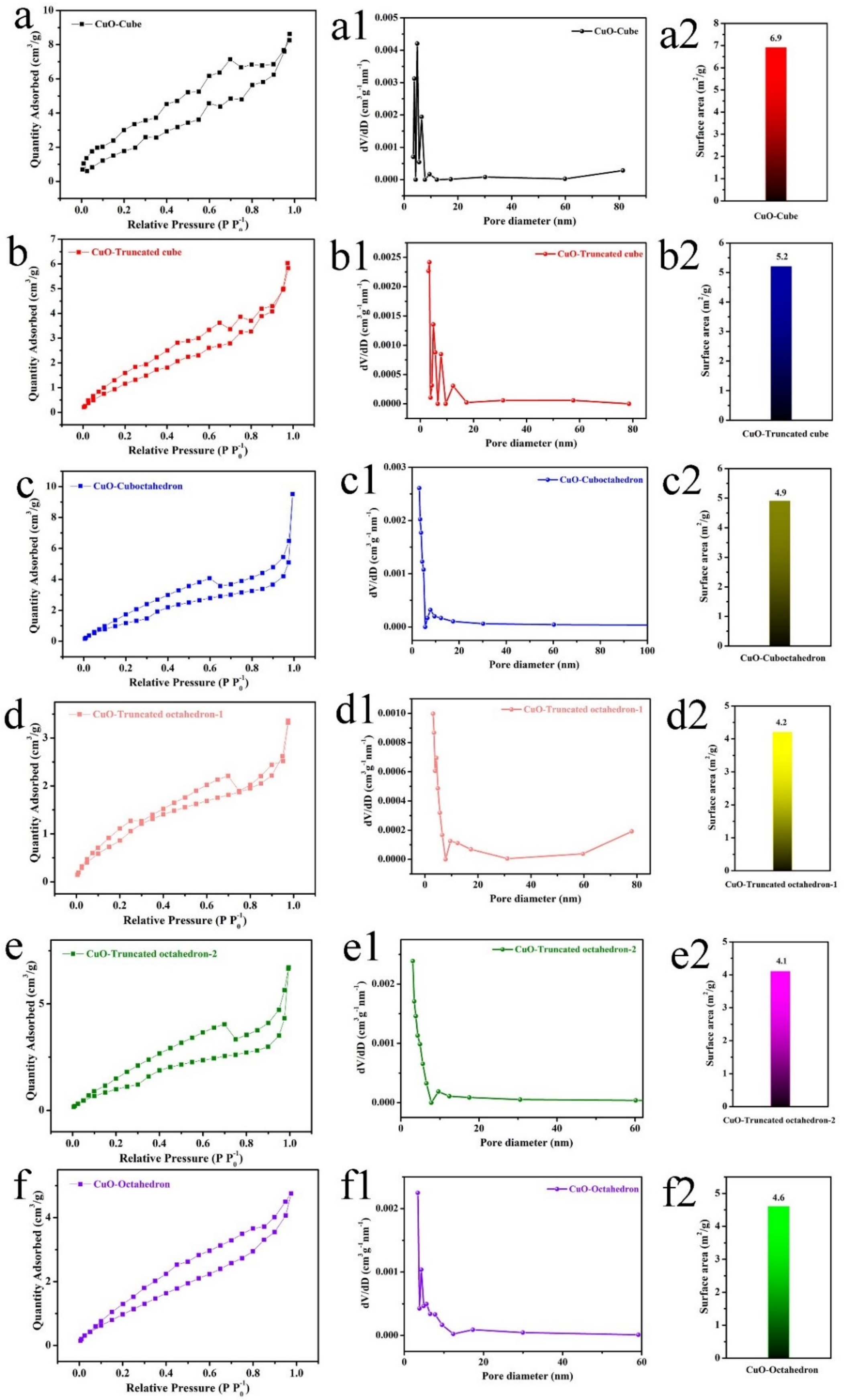

Fig. S2 N_2 adsorption–desorption isotherms, BET surface area and pore size distribution curve value of the six CuO sensors (a-a2: CuO-cube; b-b2: CuO-truncated cube; c-c2: CuO-cubooctahedron; d-d2: CuO-truncated octahedron-1; e-e2: CuO-truncated octahedron-2; f-f2: CuO-octahedron).

The detail about the DFT analyses:

The $C_nH_{2n+2}O$ adsorbed on CuO were modeled using repeated slab geometry with four-layer CuO (110) surface. The VASP was used to perform DFT calculations within the local atomic orbital (LCAO) approach. For the exchange-correlation function, generalized gradient approximation (GGA) proposed by Perdew-Burke-Ernzerhof (PBE) was used. Soft pseudopotentials were used for Cu, O, C and H to describe the interaction between valence electrons and ionic cores. In the models, vacuum spacing of 30 Å in c direction was used between the structures to avoid strong bond interaction between them. The cut-off energy was set to 400 eV for all the calculations. The K-grid was set to 5×5×1 to reduce the system energy and forces up to 10-5eV and 0.02eV/Å, respectively. The lowest two layers of CuO were fixed during the optimization, to represent the authentic surface.

(1) Molecular dissociation:

$C_nH_{2n+2}O \rightarrow C_nH_{2n+1}O + 1/2H_2$

$E_{dissociation}= E_{1/2H2}+ E_{CnH2n+1O} - E_{CnH2n+2O}$

(2) Surface adsorption:

$C_nH_{2n+2}O + * \rightarrow C_nH_{2n+2}O*$ (The process of molecules adsorbing on a surface)

$E_{adsorption}=E_{CnH2n+2O*}-E*-E_{CnH2n+2O}$

(3) Surface dissociation adsorption:

$C_nH_{2n+2}O*+* \rightarrow C_nH_{2n+1}O*+H*$（The molecules adsorbed on the surface dissociate into hydrogen atoms, and hydrogen atoms are also adsorbed on the surface）

$E_{adis}= E_{H*}+E_{CnH2n+1O*}-E*-E_{CnH2n+2O*}$

We calculated the above three processes of six different alcohol molecules from C1 to C6 on three different copper oxide crystal planes, and calculated the energy (internal energy) changes of the three processes. Thermodynamically speaking, the process of energy reduction, that is, the negative energy change, spontaneously occurs in an isolated system. The more energy reduction, the more favorable the progress of one process. Therefore, by comparing the energy changes, the strength of the interaction between different CuO crystal planes and different alcohol molecules can be inferred. Comparing with experimental data can explain why the detection signal for a certain alcohol molecule is stronger.