Electronic Supplementary Information

Polyhedron-aggregated multi-facet Cu_2O homogeneous structures

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Experimental

Synthesis of polyhedron-aggregated multi-facet Cu_2O homogeneous structures enclosed by high-index {522} facets and low-index {111}, {100} and {110} facets

In a typical synthesis, 2.9946 g of $Cu(CH_3COO)_2$ was dissolved in deionized water (50 mL) using a beaker, and then 0.10 g of cubic Cu_2O powder was added into the solution under a constant stirring at 70 °C for 2 min. A dark precipitate was produced when a sodium hydroxide solution (3.6 g, 30 mL) was added dropwise to the above solution. After being stirred for 5 min, D-(+)-glucose powder (0.6 g) was added into the dark precursor with a constant stirring for another 3 min at 70 °C, and then was allowed to cool to room temperature naturally. The precipitates were centrifuged twice more in deionized water and anhydrous ethanol, respectively. And finally they were dried at 70 °C for 12 hours in a vacuum oven.

Synthesis of polyhedron-aggregated Cu_2O homogeneous structures composed of cubic cores and abridged truncated edge octahedral building blocks

In a typical synthesis, 2.9946 g of $Cu(CH_3COO)_2$ was dissolved in deionized water (50 mL) using a beaker, and then 0.10 g of cubic Cu_2O powder was added into the solution under a constant stirring at 70 °C for 2 min. A dark precipitate was produced when a sodium hydroxide solution (3.6 g, 15 mL) was added dropwise to the above solution. After being stirred for 5 min, D-(+)-glucose powder (0.6 g) was added into the dark precursor with a constant stirring for another 20 min at 70 °C, and then was allowed to cool to room temperature naturally. The precipitates were centrifuged twice more in deionized water and anhydrous ethanol, respectively. And finally they

were dried at 70 °C for 12 hours in a vacuum oven.

Characterization

The crystal phase of as-prepared products was characterized by an X-ray diffractometer Bruker-AXS D8 ADVANCE) using Cu Kα radiation (λ = 1.54 Å) in the range (20 ~ 80 °). The morphology of the products was investigated by field-emission scanning electron microscopy (FE-SEM) using JEOL (JSM-7000F) at an accelerating voltage of 20 KV.

Photocatalytic property

The catalytic activity experiments of the above two kinds of Cu_2O for the oxidation and decoloration of the methyl orange (MO) dyes were carried out at ambient temperature. The original solution was prepared by adding 50 mL MO solution (5 mg/L), and then 0.1 g Cu_2O powder was added into the solution to form the aqueous dispersion. Before illumination, the solution was magnetically stirred in the dark for 30 min to ensure establishing an adsorption–desorption equilibrium. Afterwards, the dispersion was irradiated by a 500 W xenon lamp equipped with a filter cutoff (λ≥420 nm) under magnetic stirring. At given time intervals, the dispersion was sampled and centrifuged to separate the catalyst. UV-vis absorption spectra were recorded at different intervals to monitor the reaction using a UV/vis/NIR spectrophotometer (Hitachi U-4100).

Table S1. Sample denotations and their corresponding detailed experimental conditions and surface area percentages: (A) NaOH = 1 M (Fig. 3a); (B) NaOH = 3 M (Fig. 1); (C) NaOH = 6 M (Fig. 2); (D) NaOH = 9 M (Fig. 3c).

sample	NaOH	{100}	{110}	{111}	{522}	{211}
A	1 M	27.4%	60.3%	12.3%	0.0%	0.0%
B	3 M	35.9%	42.7%	6.1%	15.3%	0.0%
C	6 M	12.7%	15.8%	71.5%	0.0%	0.0%
D	9 M	11.6%	13.0%	69.7%	0.0%	5.7%

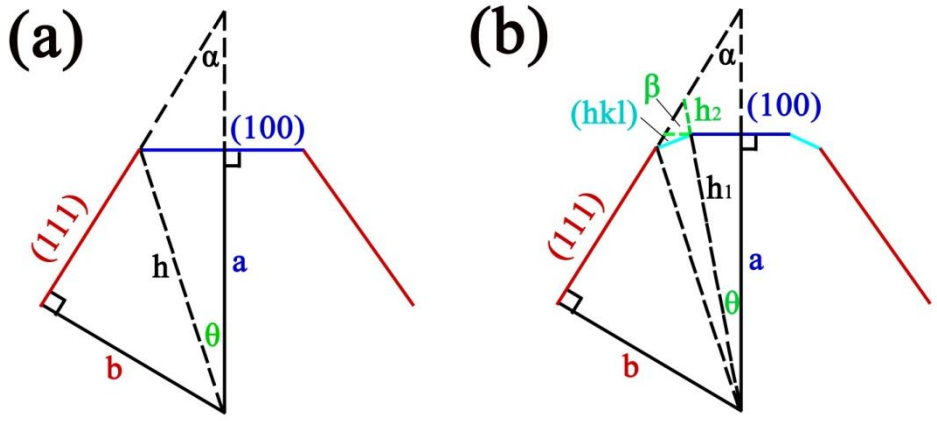


Fig. S1 The relation between R value and morphology of crystal with different index planes. (a) Low-index {111} and {100} planes; (b) Both low-index {111} and {100} planes and high-index {hkl} planes.

Detailed calculations of R value and morphology of crystal with different index planes:

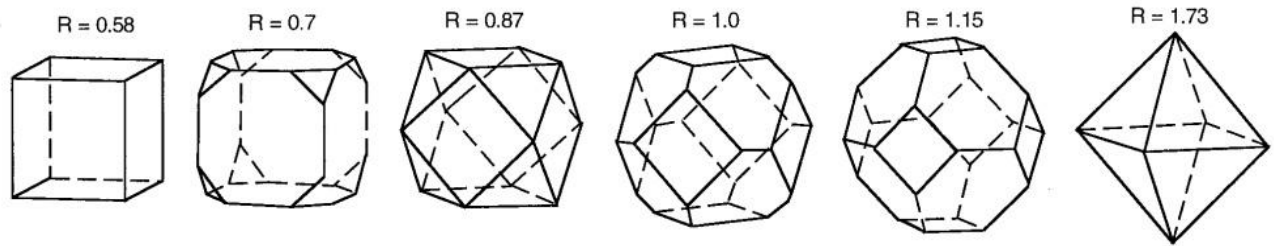
(1) As shown in Fig. S1a, the polyhedral architecture is made up of only low-index {100} and {111} facets. The red and blue lines represent the projection of {100} and {111} facets perpendicular to the [110] zone axis, respectively. The theoretical values of angle α = (180°—109.5°) ÷ 2 = 35.25° between {111} vs {111} facets. Where θ is the variable, and R is the function.

∵

$$R = \frac{v_{\{100\}}}{v_{\{111\}}} = \frac{a}{b} = \frac{h\cos\theta}{h\sin(\theta+\alpha)} = \frac{\cos\theta}{\sin\theta\cos\alpha+\cos\theta\sin\alpha} = \frac{\cos\theta}{\sin\theta\cos 35.25^\circ+\cos\theta\sin 35.25^\circ}$$

∴ When θ=0°, R= 1.73, while θ=90°, R= 0.58. It is in good agreement with the previous report by Wang ZL.

Hence, the relation between R values and shapes can be described as the following figure.



Reference: Wang ZL. Journal of Physical Chemistry B, 2000, 104 (6): 1153-1175.

(2) When the polyhedral architecture is made up of {100}, {111} and high-index {hkl} planes, the projection of {100}, {111} and {hkl} facets perpendicular to the [110] zone axis was shown in Fig. S1b. The red, blue and cyan,

lines represent the {111}, {100} and {hkl} planes, respectively. The *R* value can be calculated based on Fig. S1b, where α = 35.25°, and β = 54.7° is the acute angle between {111} vs {100}. Where θ is the variable, *R* is the function. Similarly, *R* value can be described by the following equation.

$\because$

$$a = h_1 \cos\theta$$

$$b = h_1[\frac{\sin(\theta+\alpha) - \cos\theta \cdot \tan\alpha \cdot \sin\beta - \sin\theta \cdot \sin\beta}{1 - \cos\alpha \cdot \sin\beta}]$$

$$R = \frac{v_{\{100\}}}{v_{\{111\}}} = \frac{a}{b} = \frac{(1 - \cos\alpha \cdot \sin\beta)\cos\theta}{\sin(\theta+\alpha) - \cos\theta \cdot \tan\alpha \cdot \sin\beta - \sin\theta \cdot \sin\beta}$$

$\therefore$ $$R = \frac{(1 - \cos 35.25° \cdot \sin 54.7°)\cos\theta}{\sin(\theta+35.25°) - \cos\theta \cdot \tan 35.25° \cdot \sin 54.7° - \sin\theta \cdot \sin 54.7°}$$

Based on the above discussion, it can be seen that the controllable high-index planes can be formed via changing the *R* values under appropriate reaction conditions.