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## Supporting Information For

## Delicate Control of Crystallographic-Facet-Oriented $\mathrm{Cu}_{2} \mathrm{O}$ Nanocrystals and Its Correlated

## Adsorption Ability

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Fig. S1 The broad views of different shaped $\mathrm{Cu}_{2} \mathrm{O}$ polyhedrons synthesized at $55^{\circ} \mathrm{C}$ for 3 h . (a) $\mathrm{R}=0$, cubes, (b) $\mathrm{R}=5$, truncated cubes, (c) $\mathrm{R}=10$, cubooctahedrons, (d) $\mathrm{R}=15$, cubooctahedrons, (e) $\mathrm{R}=25$, truncated octahedrons, and (f) $R=30$, octahedrons.

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Table S1 The detailed list of the experimental conditions

| Sample | $\mathbf{C u C l}_{2} \bullet \mathbf{2 H} \mathbf{2} \mathbf{O} / \mathbf{g}$ | PVP/g | R | T/ ${ }^{\circ} \mathrm{C}$ |
| :---: | :---: | :---: | :---: | :---: |
| Fig.S1(a) | 0.171 | 0 | 0 | 55 |
| Fig.S1(b) | 0.171 | 0.556 | 5 | 55 |
| Fig.S1(c) | 0.171 | 1.111 | 10 | 55 |
| Fig.S1(d) | 0.171 | 1.667 | 15 | 55 |
| Fig.S1(e) | 0.171 | 2.778 | 25 | 55 |
| Fig.S1(f) | 0.171 | 3.333 | 30 | 55 |
| Fig.4(a) | 0.171 | 3.333 | 30 | 55 |
| Fig.4(b) | 0.171 | 3.333(Mw58 000) | 30 | 55 |
| Fig.4(c) | 0.171 | 3.333(Mw630000) | 30 | 55 |
| Fig.5(a) | 0.171 | 3.333 | 30 | 25 |
| Fig.5(b) | 0.171 | 3.333 | 30 | 40 |
| Fig.5(c) | 0.171 | 3.333 | 30 | 55 |
| Fig.5(d) | 0.171 | 3.333 | 30 | 75 |

The molar ratio of PVP to $\mathrm{CuCl}_{2} \cdot 2 \mathrm{H}_{2} \mathrm{O}$ was defined as R . The introduced PVP refer to Mw 30000 , if not specially noted. All reaction were carried out in $100 \mathrm{~mL} \mathrm{H}_{2} \mathrm{O}$, and the amount of added $\mathrm{NaOH}(2.0$ $\mathrm{M})$ and $\mathrm{Vc}(0.6 \mathrm{M})$ were 10.0 mL .


Fig. S2 XRD patterns of $\mathrm{Cu}_{2} \mathrm{O}$ crystals with different geometries, (a) cubes, (b) truncated cubes, (c) cubooctahedrons, (d, e) truncated octahedrons, (f) octahedrons. The lower part is the standard XRD data of bulk $\mathrm{Cu}_{2} \mathrm{O}$. Inset shows that the intensity ratio of $(111) /(200)$ increased as the shape of the products evolved from cubes through truncated cubes, cubooctahedrons, truncated octahedrons and finally to octahedrons.

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Fig. S3 The detailed structure analysis of the $\mathrm{Cu}_{2} \mathrm{O}$ nanocubes and nanooctahedrons. (a) The sketch of the cubic $\mathrm{Cu}_{2} \mathrm{O}$ nanocrystals; (a1-a3) The bright TEM images, and (a4-a6) the corresponding selected area electron diffraction (SAED) patterns with the electron beams parallel to [001], [110], and [111], respectively. (b1-b6) are the counterpart of the octahedral $\mathrm{Cu}_{2} \mathrm{O}$ nanocrystals.

As for a cubic particle in Figure a, the exposed surfaces are made of six $\{100\}$ facets, and the joints among the $\{100\}$ facets are the edge of [100]. If the electron beam was aligned to be perpendicular to $\{001\}$, a two-dimensional (2-D) square-shaped projection will be observed. Four facets in the $\{100\}$ family, which are parallel to [001] zone axis, are marked in Figure a1. With the zone axis as [110] and [111], 2-D rectangle (Figure a2) or hexagon (Figure a3) shaped projections will be resulted, respectively. The ideal projection drawing of a cube parallel to [110] zone axis is rectangle with length versus width ratio being about 1.414 . The rectangle in Figure a matches well with the above

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ratio. The blue dashed lines in Figure a 2 present $\{100\}$ facets, while the red dashed ones present the edge of [100]. From Figure a3, the simulated projection of the cube parallel to [111] zone axis is a hexagon made of six (100) edge. The brighter edge areas comparing to the center of the hexagon derives from the thickness contrast viewed down the vertices of the cube.

For an octahedral particle as depicted in Figure b, viewed from [001] zone axis, the projection is square (Figure b1), which is different from those in Figure a1. The four edges of the square correspond to the edge of $(110)$ instead of the projects of $\{100\}$ facets. The different SAED pattern in Figure b4 from that in Figure a4 supplied further proof. Viewed along [110] zone axis, the projection drawing of the octahedron is a parallelogram made of the projections of four $\{111\}$ facets (Figure b2). Figure b3 shows the projection drawing along [111] of the octahedron, which is a hexagon but different from that in Figure a3 as illustrated by the corresponding inserted 3D models.


Fig. S4 FESEM images of $\mathrm{Cu}_{2} \mathrm{O}(\mathrm{a}-\mathrm{c})$ nanocubes, and (d-f) nanocubooctahedrons produced under 25, 40 , and $55^{\circ} \mathrm{C}$, respectively.

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Figure S5. The FTIR spectra of pure PVP (Mw30 000), $\mathrm{Cu}_{2} \mathrm{O}$ octahedrons and $\mathrm{Cu}_{2} \mathrm{O}$ cubes, respectively.

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