Supporting Information

## Facile synthesis of uniform $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> crystals and the facet-dependent

## catalytic performance in photo-Fenton reaction

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## **Characterization:**

The morphology of the catalyst samples were determined by scanning electron microscope (SEM) and high resolution transmission electron microscope (HRTEM) on JEOL 6700F and JEOL 3010, respectively. X-ray diffraction patterns of the catalysts were obtained on a Rigaku D/MAX 2500 diffractometer with Cu radiation (Cu K $\alpha$ =0.15406 nm). BET surface area was measured via nitrogen sorption at 77 K on a surface area analyzer (QuadraSorb SI); the samples were degassed at 150 °C for ten hours before nitrogen adsorption

## Dye adsorption measurement:

10 mg  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> catalysts, 50 ml aqueous solution containing Rhodamine B (2×10<sup>-5</sup> mol/L) and 0.2 ml H<sub>2</sub>O<sub>2</sub> (30 *wt*.%) was mixed in the Pyrex reactor. After 40 min of stirring in the dark, the solution was centrifuged and measured by a UV-Vis spectrometer. The dye adsorption on the catalyst was calculated from the following equation.

$$b = \frac{A_0 - A_s}{A_0} \times C_0 \times V \div m_{cata}.$$

*b*: adsorption of RhB on the catalyst;  $A_0$ : the absorbance of the raw dye solution;  $A_s$ : the absorbance of filtrate after adsorption;  $C_0$ : the concentration of the raw dye solution; *V*: the volume of the solution;  $m_{cata}$ : the mass of the catalyst.



*Figure S1.* Atomic arrangement of  $\{10-10\}$ ,  $\{0001\}$  and  $\{10-12\}$  crystal facet. Red ball, oxygen atoms; yellow ball, surface exposed iron atoms; blue ball, bulk iron atoms. Fe<sub>3c</sub>, Fe<sub>4c</sub> and Fe<sub>5c</sub> represents 3, 4 and 5-fold coordinated Fe atoms, respectively.



*Figure S2.* Atomic arrangement of  $\{10-10\}$ ,  $\{0001\}$  and  $\{10-12\}$  crystal facet. Red ball, oxygen atoms; yellow ball in the white line boundary, surface exposed iron atoms; blue ball, iron atoms. Surface Fe density on  $\{0001\}$  facet is  $4.55/\text{nm}^2$  ( $1/0.22 \text{ nm}^2$ );  $\{10-10\}$ :  $5.79/\text{nm}^2$  ( $4/0.69 \text{ nm}^2$ );  $\{10-12\}$  facet:  $9.76/\text{nm}^2$  ( $4/0.41 \text{ nm}^2$ ).