Supporting Information:

Facet-Dependent Interfacial Charge Transfer in Fe(III)-Grafted TiO_2 Nanostructures Activated by Visible Light

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Chemicals and materials

$Ti(OC_4H_9)_4$, TiO_2 nanoparticles (Aeroxide P25), phenol, 2,3-bis(2-methoxy-4-nitro-5-sulfophehyl)-2H-tetrazolium-5-carboxanilide (XTT), p-hydrophenylacetic acid (POPHA) were purchased from Sigma-Aldrich (St.Louis, MO, USA). HPLC-grade methanol was obtained from Fisher Scientific (Pittsburgh, PA, USA). All other chemicals were of analytical reagent grade and used without further purification. All solutions were freshly prepared with deionized water obtained using a Milli-Q system from Millipore (Bedford, MA, USA).

Determination of the percentage of the predominant facet

According to the crystal model built by Wulff construction, the percentages of different crystal planes in the as-synthesized TiO_2 nanocrystals can be calculated by the geometrical parameters of different crystals through statistic based on the TEM results.

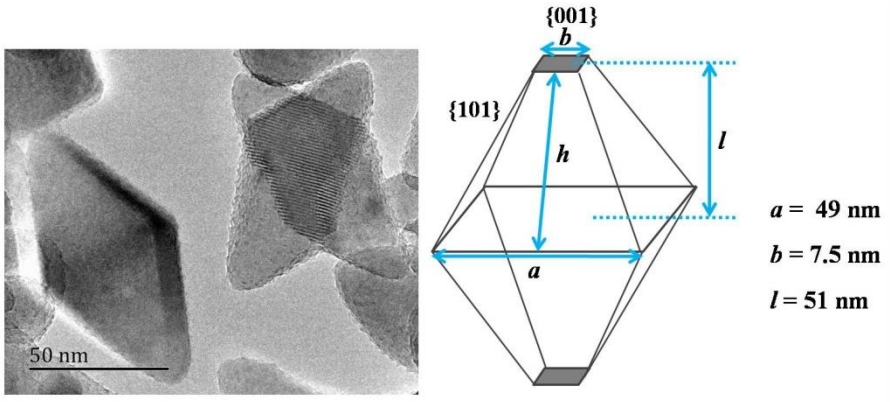

Figure S1. Typical TEM image of TiO_2 {101} crystals and its geometrical models.

The TiO_2 {101} crystals have an octahedron-like geometry. According to the geometrical models, the percentage of the dominant {101} facet can be calculated by

the following equation:

$$S_{101} = \frac{a+b}{2} h = \frac{(a+b)l}{2\sin\theta}$$

$$S_{001} = b^2$$

$$P_{101}(\%) = \frac{8S_{101}}{8S_{101} + 2S_{001}} \times 100\%$$

Where θ=68.3° represents the angle between the {101} and {001} facets. The percentage of the predominant {101} facet is calculated to be 99%.

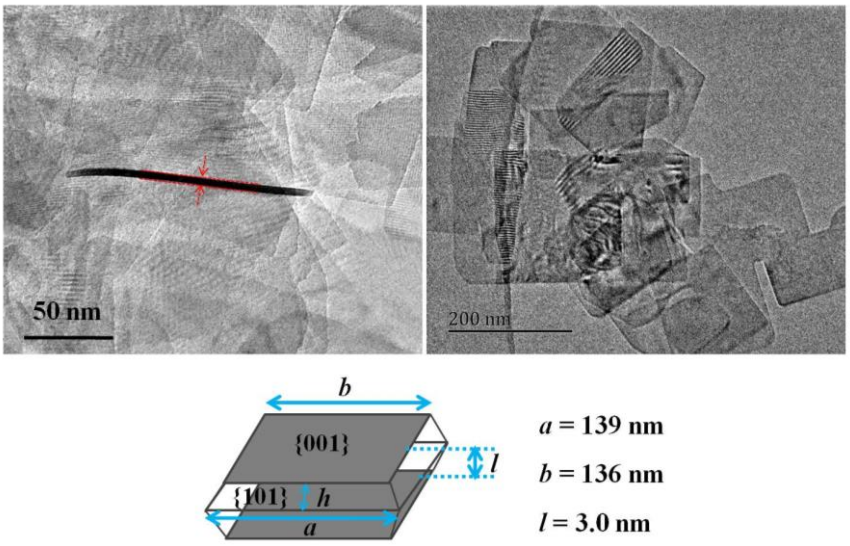

Figure S2. Typical TEM image of TiO_2 {001} crystals and its geometrical models.

The TiO_2 {001} crystals have a plate-like morphology. According to the previous report, the percentage of the dominant {001} facet is given according to the equation shown below:

$$S_{101} = \frac{a+b}{2} h = \frac{(a+b)l}{2\sin\theta}$$

$$S_{001} = b^2$$

$$P_{001}(\%) = \frac{2S_{001}}{8S_{101} + 2S_{001}} \times 100\%$$

Where θ =68.3° is the angle between the {101} and {001} facets. The percentage of the predominant {001} facet is calculated to be 91%.

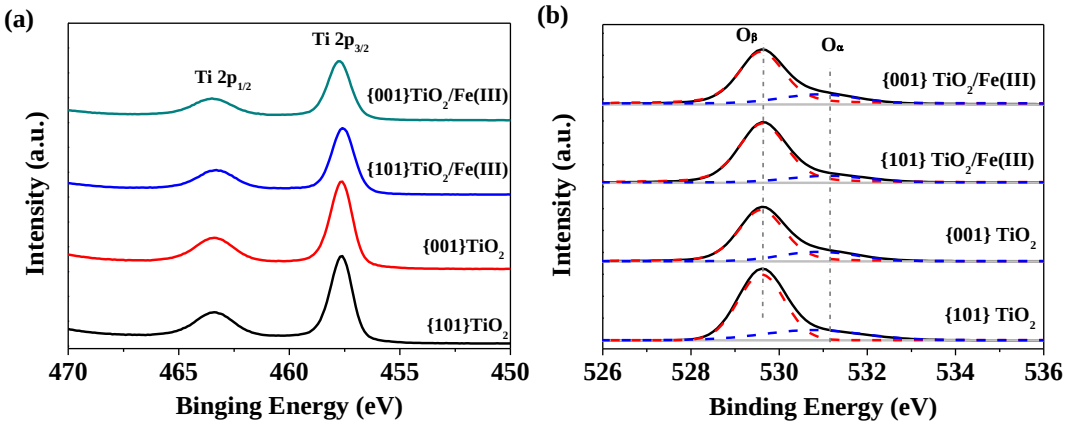

Figure S3. (a) Ti 2p core-level spectra and (b) O 1s spectra of bare TiO_2 and TiO_2/Fe(III) samples.

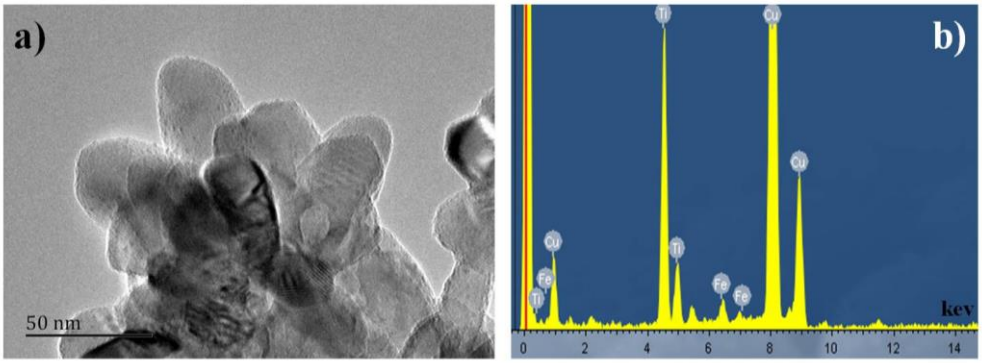

Figure S4. (a) TEM and (b) EDS images of TiO_2(Rutile)/Fe(III) hybrid. The loading amount of Fe(III) in TiO_2(Rutile)/Fe(III) hybrids was about 0.36 wt%, which was measured by ICP-OES.

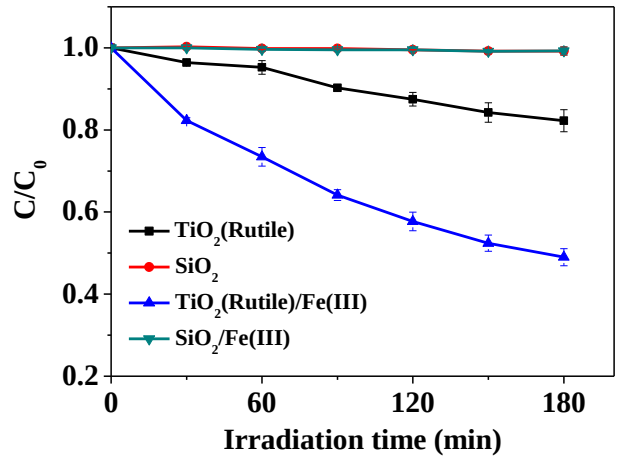

Figure S5. Photocatalytic degradation phenol curves in TiO_2(Rutile)/Fe(III) and SiO_2/Fe(III) suspensions under visible light irradiation ($\lambda > 400$ nm).

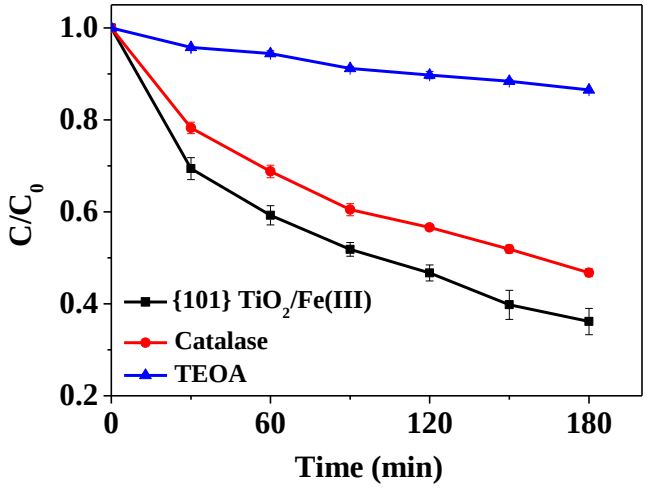

Figure S6. Phenol degradation curves in {101} TiO_2/Fe(III) suspensions with the addition of different scavengers (TEOA for hole, catalase for H_2O_2).

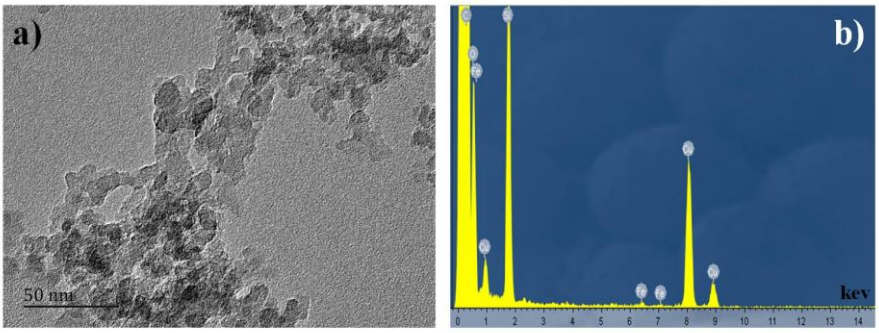

Figure S7. (a) TEM and (b) EDS images of SiO_2/Fe(III) hybrids. The loading amount of Fe(III) in SiO_2/Fe(III) hybrids was about 0.39 wt%, which was measured by ICP-OES.