Electronic Supplementary Information

Enhanced photocatalytic activity of anatase by rational modification of {001} facets with Fe(III) ions

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Experimental results

Figure S1. Photographs of (a) TiO_2-80%, (b) Fe-0.5-TiO_2, (c) and Fe-5-TiO_2.

Percentage of {001} facets was calculated as follows, which is refer to our previous study and other authoritative references. [1-3] According to the value of **Table S1** and following equations, S_{001}%=~80%

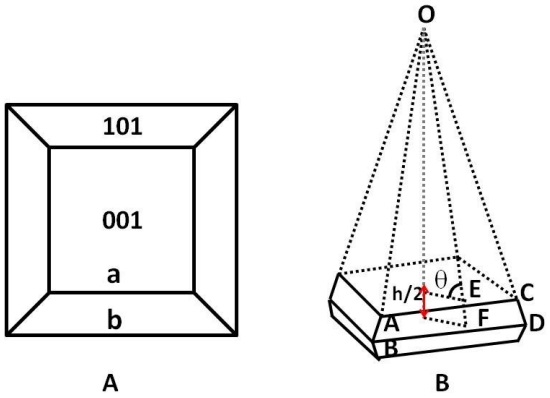

Figure S2. (A) The planform of anatase TiO_2 nanosheet. (B) Equilibrium model of anatase TiO_2 crystal.

Equations:

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

$$S_{101} = 8(S_{OBD} - S_{OAC})$$

$$= 8\left(\frac{1}{2}OF \cdot BD - \frac{1}{2}OE \cdot AC\right)$$

$$= 8\left(\frac{1}{2} \times \frac{\frac{1}{2}b}{\cos\theta} \times b - \frac{1}{2} \times \frac{\frac{1}{2}a}{\cos\theta}\right)$$

$$= \frac{2(b^2 - a^2)}{\cos\theta}$$

$$S_{001}\% = \frac{S_{001}}{S_{001} + S_{101}}$$

$$= \frac{2a^2}{2a^2 + \frac{2(b^2 - a^2)}{\cos\theta}}$$

$$= \frac{1}{1 + \frac{(\frac{b^2}{a^2} - 1)}{\cos\theta}}$$

$$= \frac{\cos\theta}{\cos\theta + (\frac{a}{b})^{-2} - 1}$$

Where $a = b - h/\tan\theta$. The values of b and h were determined as showed as TEM image, θ is the theoretical value for the angle between the {101} and {001} facets of

anatase, 68.3°. As indicated in the planform, two parameter *a* and *b* denote lengths of the side of square {001} 'truncation' facets and the side of bipyramid. The ratio of {001} facets to total surface area can be described by the value of S_{001}/S or a/b ($0 \leq a/b \leq 1$).

Table S1. Physical Properties of Different Samples

sample	phase	b (nm)[a]	h (nm)[a]	S_{001} %	BET (m^2/g)
TiO_2-80%	A	80-90	7-9	~80	89
TiO_2-60%	A	30-40	6-8	~60	87
Fe-0.5-TiO_2	A	80-90	7-9	~80	95
P25	A, R	25	-	-	90

[a] b and h: side length and thickness of TiO_2-60% nanosheets, respectively, are estimated by TEM image analysis (Figure S4).

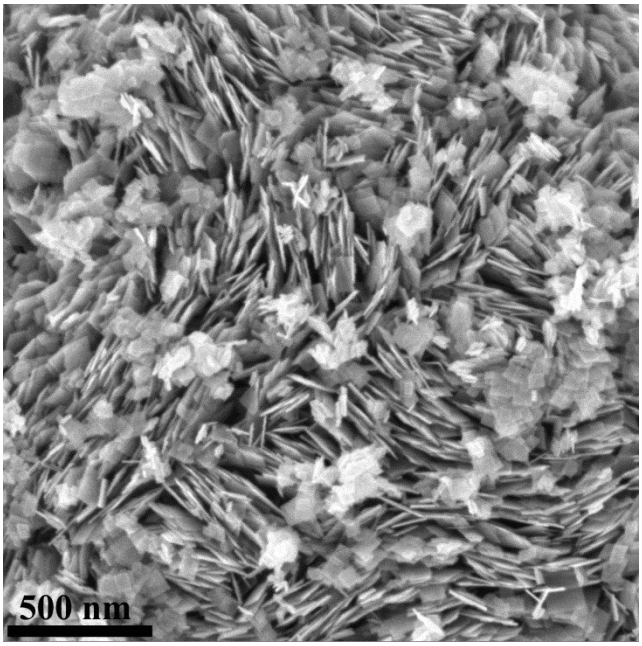

Figure S3. SEM image of Fe-0.5-TiO_2.

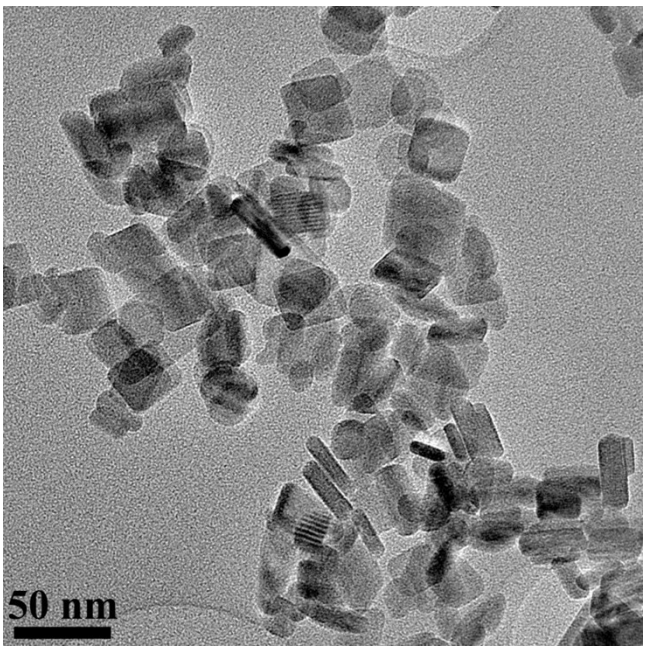

Figure S4. TEM image of TiO_2-60%.

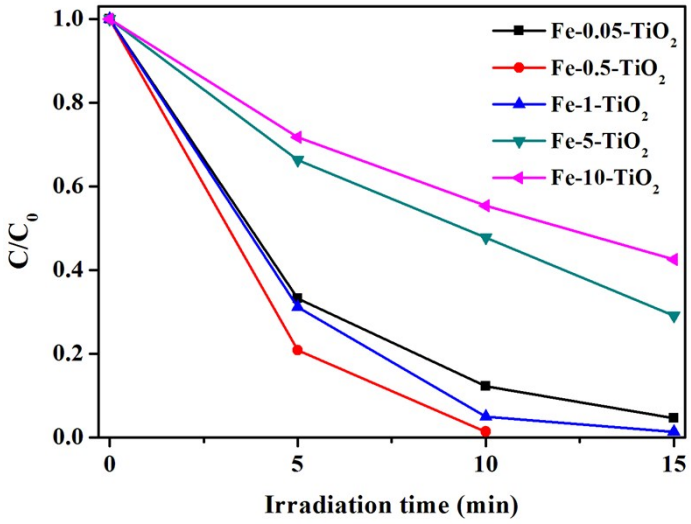

Figure S5. Photocatalytic degradation of MO under UV-light irradiation (200-400 nm, 310 mW/cm^2) over Fe-X-TiO_2 (X = Fe/TiO_2 wt%).

In order to comparison the photocatalytic activity between the Fe-0.5-TiO_2 and noble metal-modified anatase TiO_2, TiO_2-$Pt_{0.5}$ was prepared according to our previous study. [4] And the photocatalytic activity was estimated by degradation of MO under simulate solar-light illumination. The result was shown in **Figure S6**. It can be seen that, TiO_2-$Pt_{0.5}$ shows high photocatalytic efficiency than that of Fe-0.5-TiO_2. The MO was completely degraded within 20 min with the degradation rate of 100%.

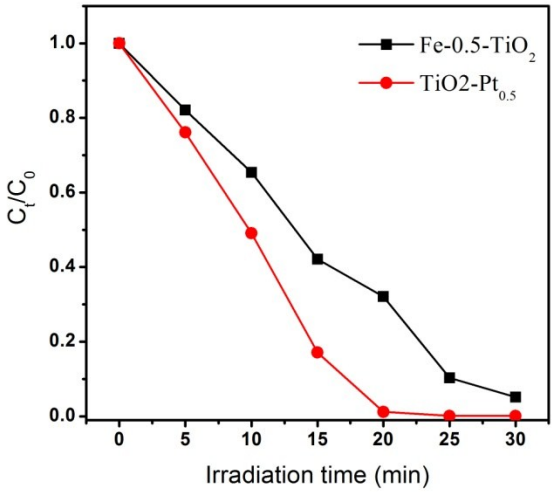

Figure S6. The photocatalytic activity of Fe-0.5-TiO_2 and TiO_2-$Pt_{0.5}$

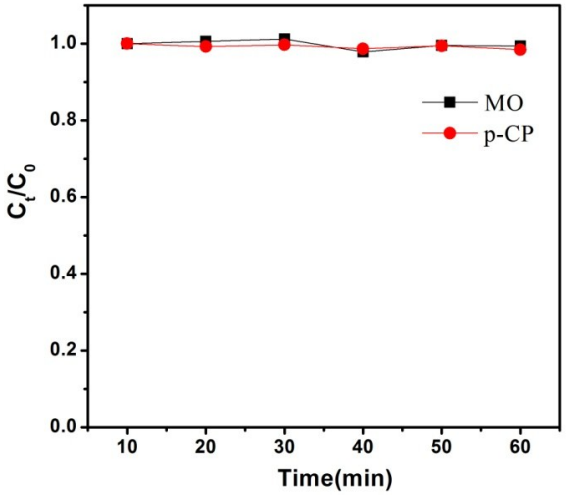

Figure S7. Adsorption capability of Fe-0.5-TiO_2 towards MO and p-CP within 1h in dark.

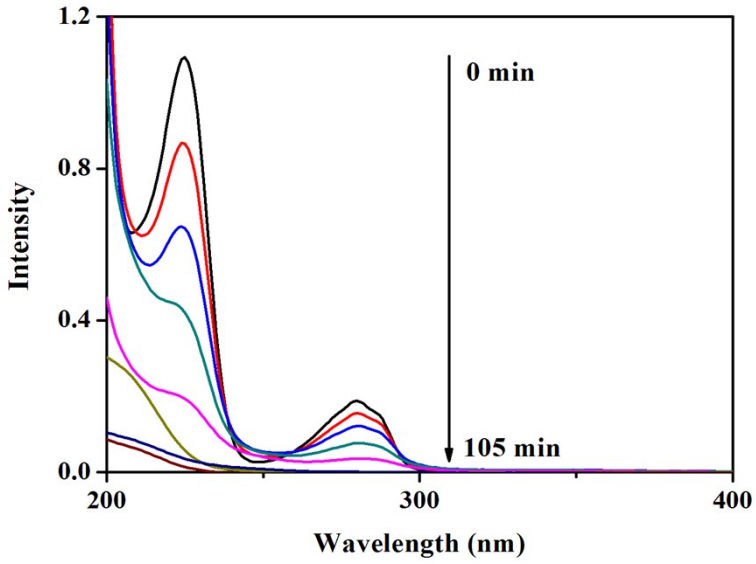

Figure S8. (a) UV−vis spectra variation of the p-CP solution under simulated solar-light irradiation (200 mW/cm^2) over Fe-0.5-TiO_2.

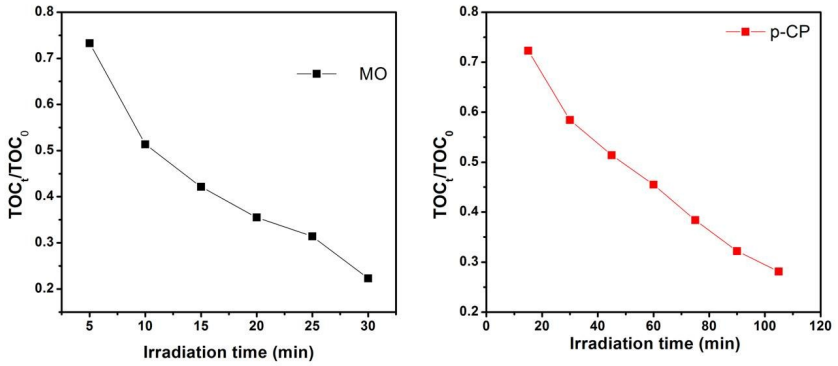

Figure S9 The content of TOC in each system.

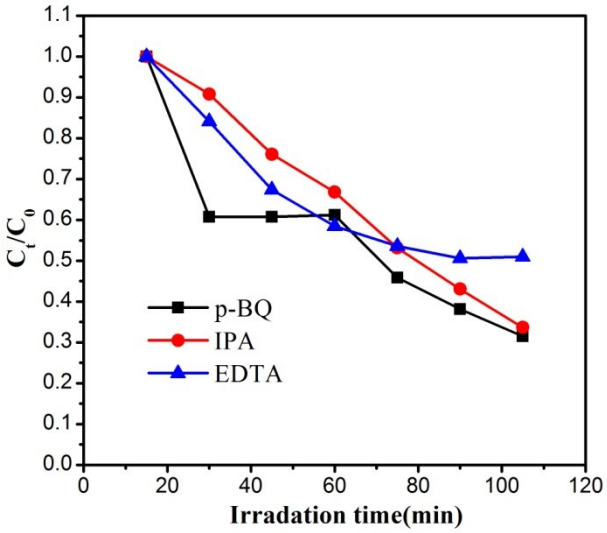

Figure S10. Photocatalytic activity of Fe-0.5-TiO_2 towards MO degradation in the presence of different scavengers.

References:

1. L. Sun, Z. Zhao, Y. Zhou and L. Liu, *Nanoscale*, 2012, **4**, 613-620.
2. H. G. Yang, C. H. Sun, S. Z. Qiao, J. Zou, G. Liu, S. C. Smith, H. M. Cheng and G. Q. Lu, *Nature*, 2008, **453**, 638-641.
3. Q. Xiang, J. Yu and M. Jaroniec, *Chemical Communications*, 2011, **47**, 4532-4534.
4. N. Guo, Y. Zeng, H. Li, X. Xu and H. Yu, *Materials Letters*, 2018, **221**, 183-186.