

Supplementary Information

Enlarging {110} Exposed Facets of Anatase TiO₂ by the Synergistic Action of Capping Agents

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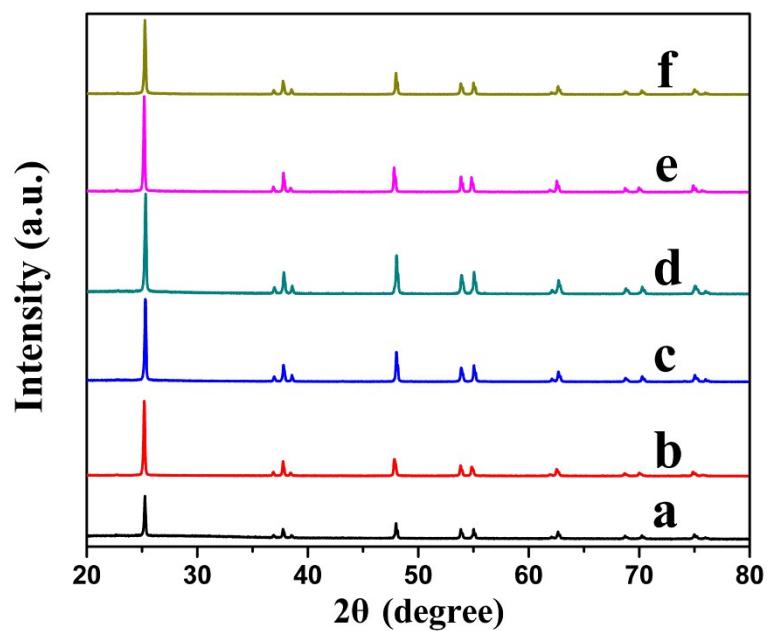


Fig. S1. XRD patterns of TiO_2 samples prepared in different concentrations of H_2O_2 solutions: (a) 0 M; (b) 0.6 M; (c) 0.9 M; (d) 1.5 M; (e) 2.4 M; (e) 3.0 M.

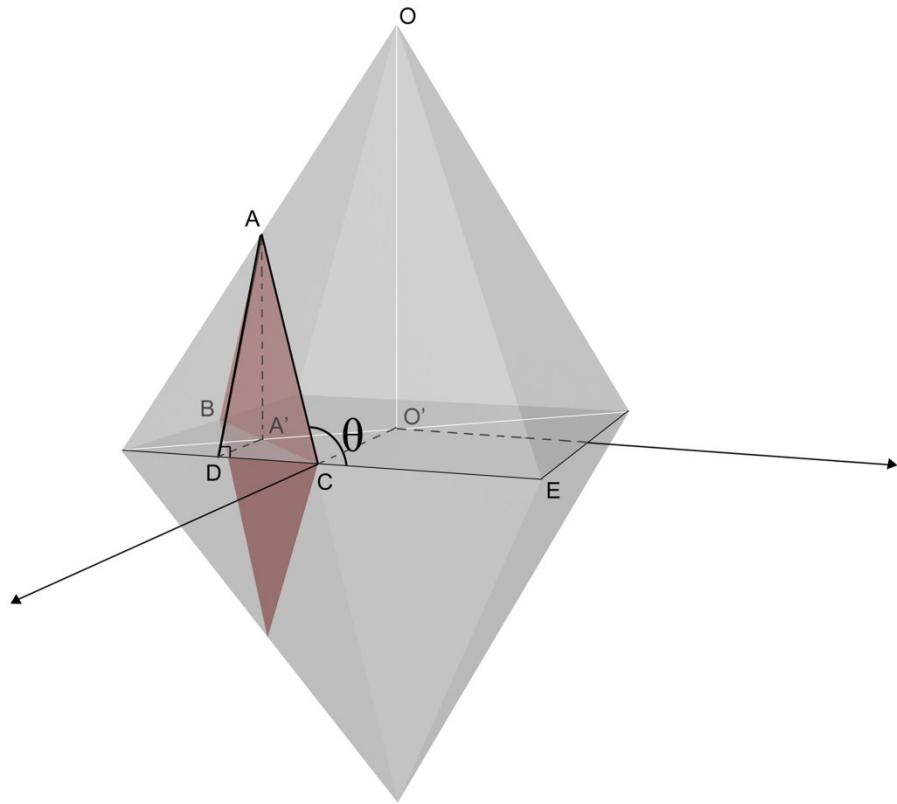


Fig. S2. Schematic diagram of the anatase TiO_2 single crystal.

Calculated θ angle

$$\theta = 180^\circ - \arccos \frac{DC}{AC}$$

Here we set $O'C = 2a$, $O'G = 2b$, $OO' = 2c$, $a = b = 3.785$, $c = 9.514$, A is the midpoint of line OE .

$$AC^2 = AA'^2 + A'C^2 = \left(\frac{OO'}{2}\right)^2 + (A'D^2 + DC^2) = c^2 + (a^2 + b^2) = 119.168,$$

$$AC = 10.916,$$

$$DC = b = 3.785$$

$$\theta = 180^\circ - \arccos \frac{DC}{AC} = 180^\circ - \arccos \frac{3.785}{10.916} = 110^\circ.$$

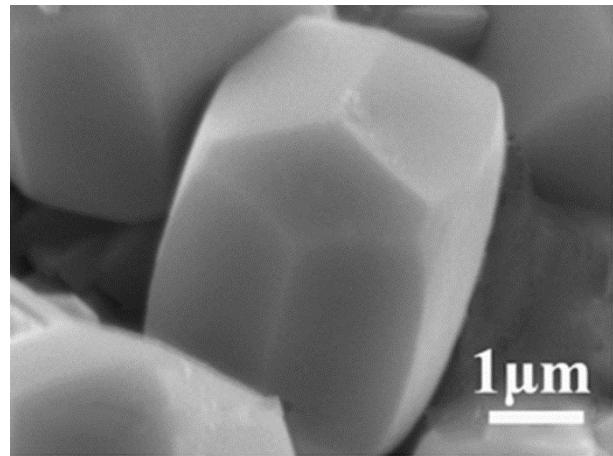


Fig. S3. SEM image of TiO₂ prepared by using TiCl₄ as Ti source in presence of H₂O₂ (2.4 M) and HF (0.1 M).

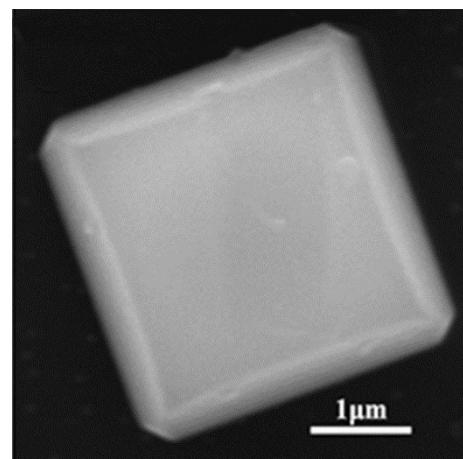


Fig. S4. SEM images of anatase TiO₂ single crystals prepared using Ti (OC₃H_{7-i})₄ as titanium source in the presence of H₂O₂ (2.4 M) and HF (0.1 M).

Table S1. The dependence of exposed facets on titanium source, H_2O_2 , HCl , and HF

Composition of reaction solution					Exposed facets
	Titanium source	H_2O_2	HF	HCl	
A ^a	TiCl_3	Yes	No	No	Irregular particles
B ^a	TiCl_3	Yes	No	Yes	{101} and {001}
C ^a	TiCl_3	No	Yes	No	{101}, {001}, and minor {110}
D ^a	TiCl_3	Yes	Yes	No	{101}, {001}, and bigger {110}
E ^a	$\text{Ti}(\text{OC}_3\text{H}_7\text{-i})_4$	Yes	Yes	No	{101}, {001}, and minor {110}
F ^b	TiF_4	No	Yes	No	{101} and {001}
G ^c	Ti powder	Yes	Yes	No	{101}, {001}, and minor {110}
H ^d	TiCl_3	No	Yes	No	{101}, {001}, and minor {110}
I ^e	TiCl_3	Yes	No	No	{101} and {001}

^a This work.

^b *Nature*, *Nature* 2008, 453, 638.

^c *Chem. Commun.*, 2010, 46, 1664.

^d *J. Phys. Chem. Lett.* 2013, 4, 3910.

^e *Ind. Eng. Chem. Res.* 2013, 52, 6704.

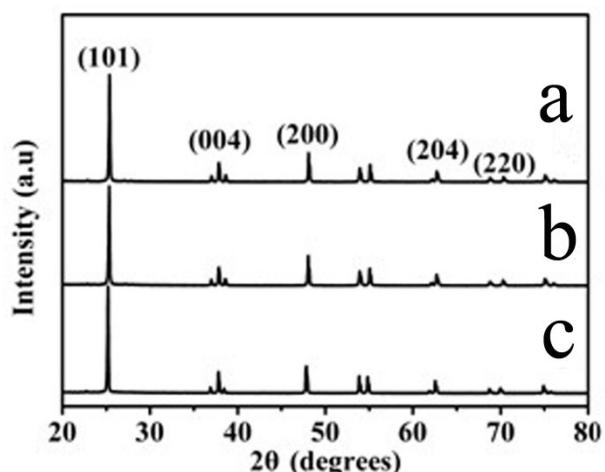


Fig. S5. XRD patterns of the {110} facet exposed TiO_2 single crystals calcined at different conditions: (a) Without calcination treatment; (b) Calcination at 600 °C for 2 h; (c) Calcination at 800 °C for 2 h.