Fabrication and enhanced visible-light photocatalytic activity of carbon self-doped TiO₂ sheets with exposed {001} facets

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Figure S1. A) Slab model of anatase TiO_2 single crystal. B) Equilibrium model of anatase TiO_2 single crystal.

Calculation of percentage of $\{001\}$ facets^{1,2}

 $S_{001} = 2a^2$

 $S_{101} = 8(\frac{1}{2}EG \times b - \frac{1}{2}EF \times a)$

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

$$= \frac{2a^{2}}{2a^{2} + 8(\frac{1}{2}EG \times b - \frac{1}{2}EF \times a)} = \frac{a^{2}}{a^{2} + 4(\frac{1}{2} \times \frac{\frac{1}{2}b}{\cos\theta} \times b - \frac{1}{2}\frac{\frac{1}{2}a}{\cos\theta} \times a)} =$$

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

$$= \frac{\cos 68.3^{\circ}}{\cos 68.3^{\circ} + (\frac{490nm}{552nm})^{-2} - 1} = 57.8\%$$

Here θ is the theoretical value for the angle between the [001] and [101] facets of anatase. As indicated in the slab model, two independent parameters *b* and *a* denote lengths of the side of the bipyramid and the side of the square {001} 'truncation' facets, respectively. The values of *b* and *a* are equal to 552 and 490 nm, respectively; these values were measured directly from Fig. 2b. The ratio of highly reactive {001} facets to the total surface area can be described by the value of S_{001}/S or a/b (where $0 \le a/b \le 1$). a/b is the degree of truncation).

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 D. Q. Zhang, G. S. Li, X. F. Yang, J. C. Yu, *Chem. Commun.*, 2009, 4381.



Figure S2. XPS survey spectra of the CTS (a), CTNP (b), TNS (c) and TiC (d) samples. Inset shows the high-resolution XPS spectrum of F1s in CTS.