Fabrication and enhanced visible-light photocatalytic activity of carbon self-doped TiO$_2$ 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$^{1,2}$

$S_{001} = 2a^2$

$S_{101} = 8(\frac{1}{2}EG \times b - \frac{1}{2}EF \times a)$
\[ S_{001} \% = \frac{S_{001}}{S_{001} + S_{101}} \]

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

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

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

Here \( \theta \) 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 \( \leq a/b \leq 1 \)). \( a/b \) is the degree of truncation.


**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.