Supporting Materials for:

Synthesis of anatase TiO$_2$ nanocrystals with \{101\}, \{001\} or \{010\} single facets of 90\% level exposure and liquid phase photocatalytic reduction and oxidation activity orders

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**Fig. S1** XRD patterns of PT-W and PT-E.

Fig. S1 shows the X-ray diffraction patterns (XRD) patterns of PT-W and PT-E. The peaks are indexed to that of K$_2$Ti$_{16}$O$_{33}$ with the monoclinic structure (JCPDS file No. 00-40-0403, $a = 1.559$ nm, $b = 0.3796$ nm and $c = 0.9108$ nm).
Fig. S2 FESEM images of PT-E (a) and PT-W (b).

Fig. S3 Calculation of facets percentage of 101 sample.

- \( a = 100 \text{ nm} \); \( b = 60 \text{ nm} \)
- \( c = 2\times\tan(22/\tan22-a/2) = 19.6 \text{ nm} \)
- \( S_{101} = 8[1/2(b+c)*(a/2)/\cos22] = 15013 \text{ nm}^2 \)
- \( S_{001} = 2c^2 = 768 \text{ nm}^2 \)
- Percentage of 101 = \( 15013/(15013+768) = 95\% \)
Fig. S4 Calculation of facets percentage of 001 sample.

\[a = 200 \text{ nm}; \ b = 10 \text{ nm}\]
\[c = a - 2 \times (b/2)/\tan79 = 198 \text{ nm}\]
\[S_{001} = 2c^2 = 78408 \text{ nm}^2\]
\[S_{201} = 8c \times (5/\cos11) = 8160 \text{ nm}^2\]
Percentage of 001 = \[\frac{78408}{78408 + 8160} = 91\%\]

Fig. S5 Calculation of facets percentage of 010 sample.

\[a = 500 \text{ nm}; \ b = 50 \text{ nm}; \ c = 450\]
\[d = b - (a-c)\tan22 = 30 \text{ nm}\]
\[S_{001} = 2d^2 = 1800 \text{ nm}^2\]
\[S_{101} = 8[1/2(b+c)\times((a-c)/2)]/\cos22] = 8000 \text{ nm}^2\]
\[S_{010} = 4bc = 90000 \text{ nm}^2\]
Percentage of 010 = \[\frac{90000}{90000 + 8000 + 1800} = 90\%\]

Fig. S6 K 2p XPS spectra of TiO$_2$-101, TiO$_2$-001 and TiO$_2$-010.
Fig. S7 Reaction of NBT with superoxide ion.

Fig. S8 UV-Vis absorption spectra of NBT in TiO$_2$ suspension.
Fig. S9 PL spectra of TAOH in TiO$_2$ suspension.

Fig. S10 Photocatalytic (a) reduction and (b) oxidation activity orders upon normalization by the surface area.
**Fig. S11.** Reaction constant $K$ and ratio $R$ between $K_1$ and $K_2$ of TAOH in TiO$_2$ suspension.

The results of fluorescence emission spectra of TiO$_2$ samples with different irradiation times are shown in Figure S9 and Figure S10. Obviously, the linear relationship between the fluorescence intensity and irradiation time during 60 min was observed for TiO$_2$-001, while the increment rate decreased after 30 min irradiation for TiO$_2$-101 and TiO$_2$-010. And the reaction constant $K$ can be divided into $K_1$ (0-30 min) and $K_2$ (30-60 min). The ratio $R$ between $K_1$ and $K_2$ can used to estimate the separate efficiency of photoexcited holes and electrons.$^{[12]}$ It can be seen that the $R_{001} = 1$, $R_{101} = 1.4$ and $R_{010} = 3.5$. This result demonstrated that the order of separate efficiency of photoexcited holes and electrons also is $\{001\} > \{101\} > \{010\}$. 

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**Fig. S12** Surface atomic structure of \{001\}, \{101\} and \{010\} facets.