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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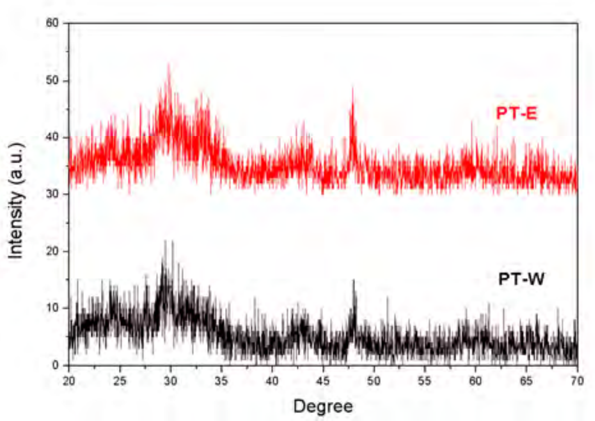

Fig. S1 XRD patterns of PT-W and PT-E.

Fig. S1 shows the X-ray diffraction patterns (XRD) patterns of PT-W and PT-E. The peaks are indexed to that of $K_2Ti_{16}O_{13}$ with the monoclinic structure (JCPDS file No. 00-40-0403, a = 1.559 nm, b = 0.3796 nm and c = 0.9108 nm).

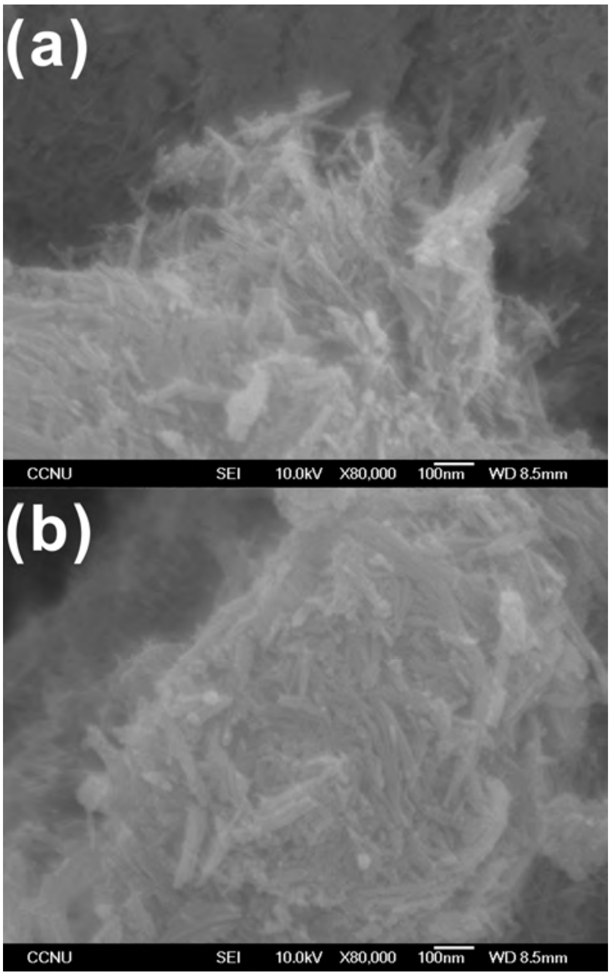

Fig. S2 FESEM images of PT-E (a) and PT-W (b).

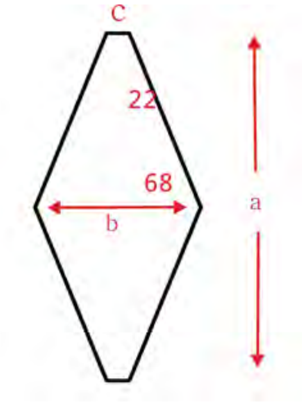

Fig. S3 Calculation of facets percentage of 101 sample.

a = 100 nm; b = 60 nm

c = 2*tan22(25/tan22-a/2) = 19.6 nm

S101 = 8[1/2(b+c)*(a/2)/cos22] = 15013 nm^2

S001 = $2c^2$ = 768 nm^2

Percentage of 101 = 15013/(15013+768) = 95%

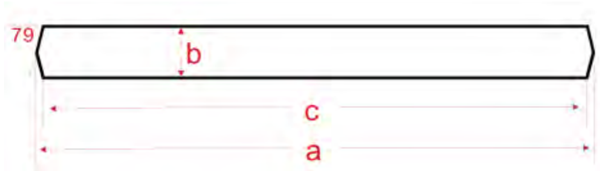

Fig. S4 Calculation of facets percentage of 001 sample.

a = 200 nm; b = 10 nm

c = a-2* (b/2)/tan79 = 198 nm

S001 = $2c^2$ = 78408 nm^2

S201 = 8*c*(5/cos11) = 8160 nm^2

Percentage of 001 = 78408/(78408+8160) = 91%

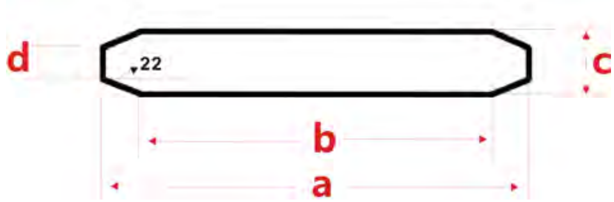

Fig. S5 Calculation of facets percentage of 010 sample.

a = 500 nm; b = 50 nm; c= 450

d = b – (a-c)tan22 = 30 nm

S001 = $2d^2$ = 1800 nm^2

S101 = 8[1/2(b+c)*((a-c)/2)]/cos22] = 8000 nm^2

S010 = 4bc = 90000 nm^2

Percentage of 010 = 90000/(90000 + 8000 + 1800) = 90%

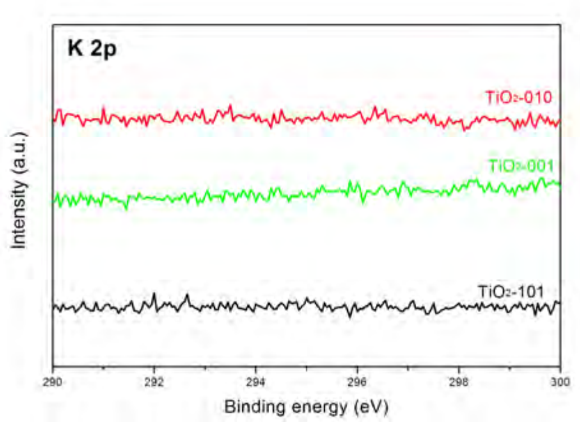

Fig. S6 K 2p XPS spectra of TiO_2-101, TiO_2-001 and TiO_2-010.

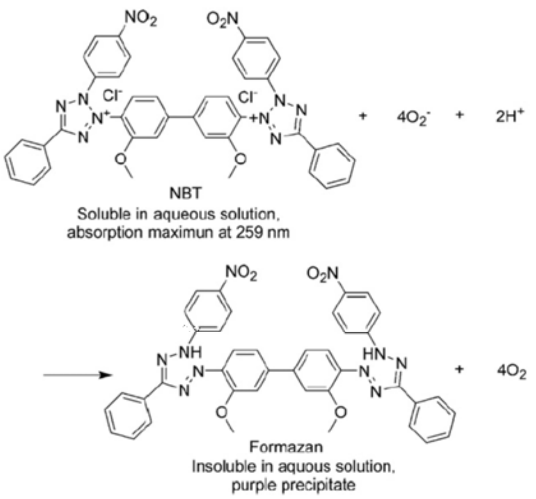

Fig. S7 Reaction of NBT with superoxide ion.

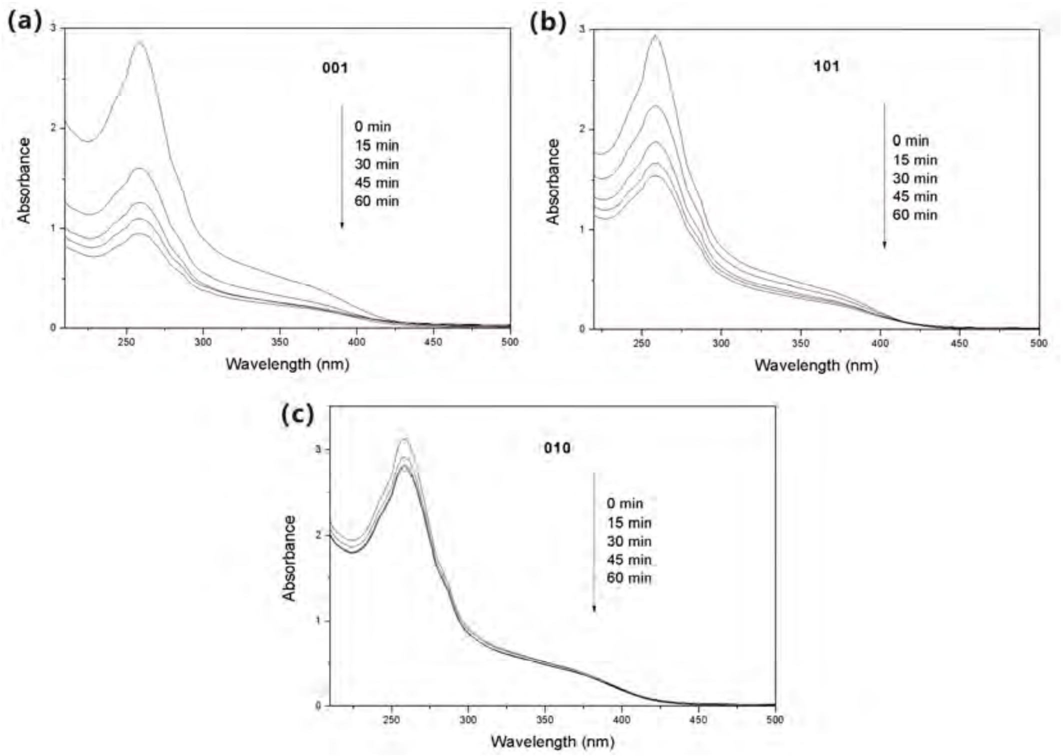

Fig. S8 UV-Vis absorption spectra of NBT in TiO_2 suspension.

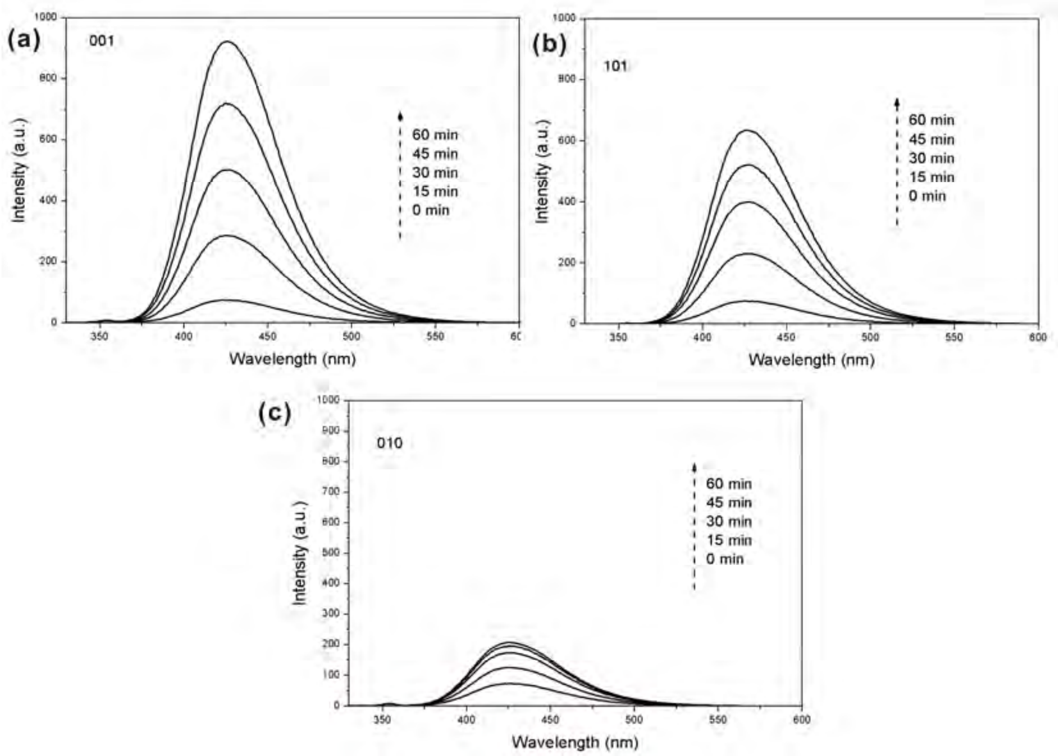

Fig. S9 PL spectra of TAOH in TiO_2 suspension.

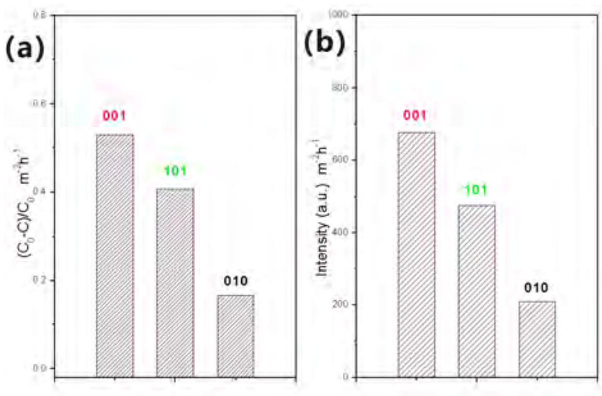

Fig. S10 Photocatalytic (a) reduction and (b) oxidation activity orders upon normalization by the surface area.

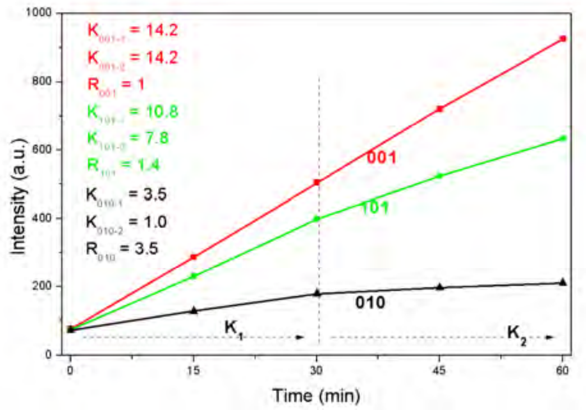

Fig. S11. Reaction constant K and ratio R between K_1 and K_2 of TAOH in TiO_2 suspension.

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}.

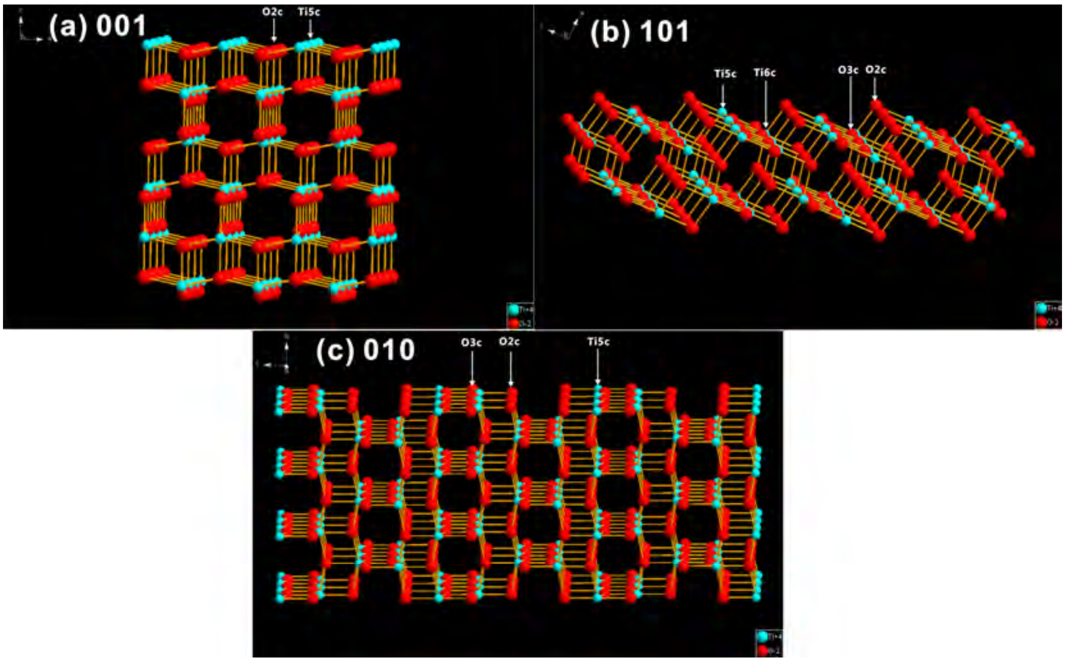

Fig. S12 Surface atomic structure of {001}, {101} and {010} facets.