

## Supporting Information

# Effects of Defects on Photocatalytic Activity of Hydrogen-Treated Titanium Oxide Nanobelts

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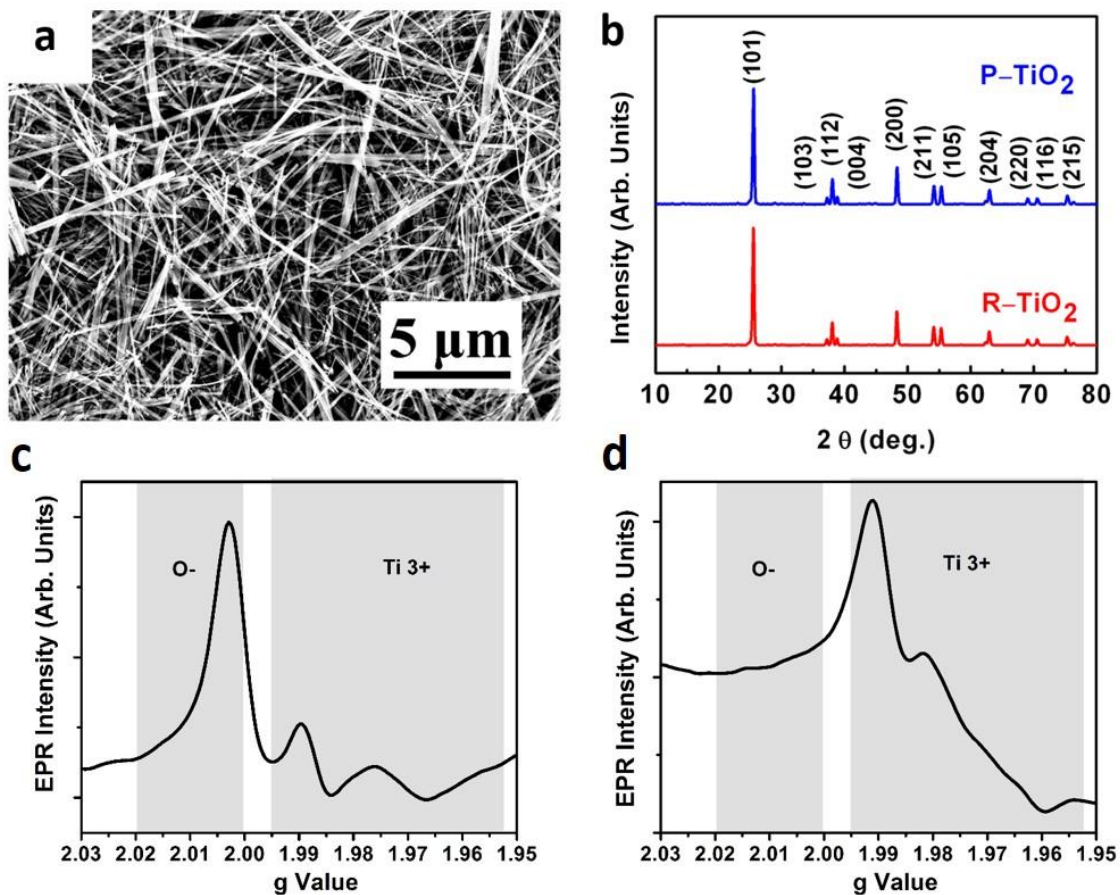
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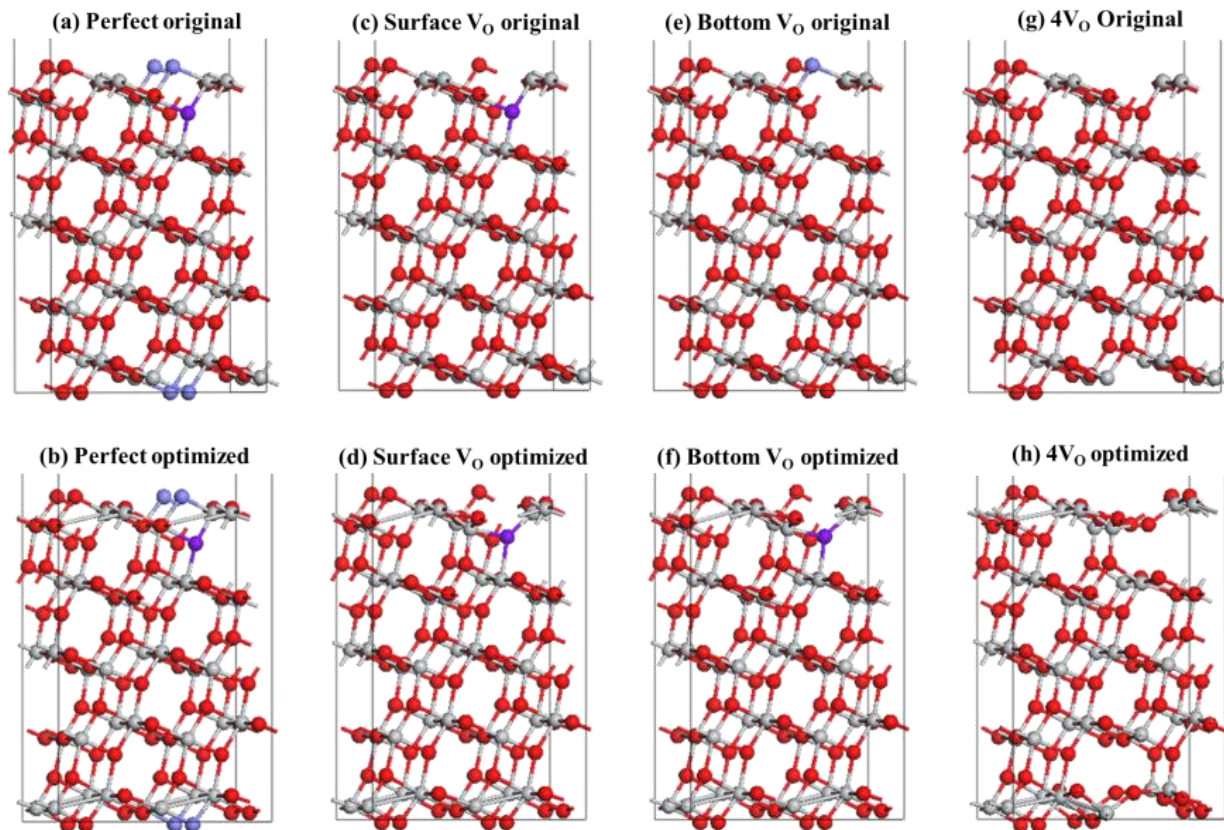
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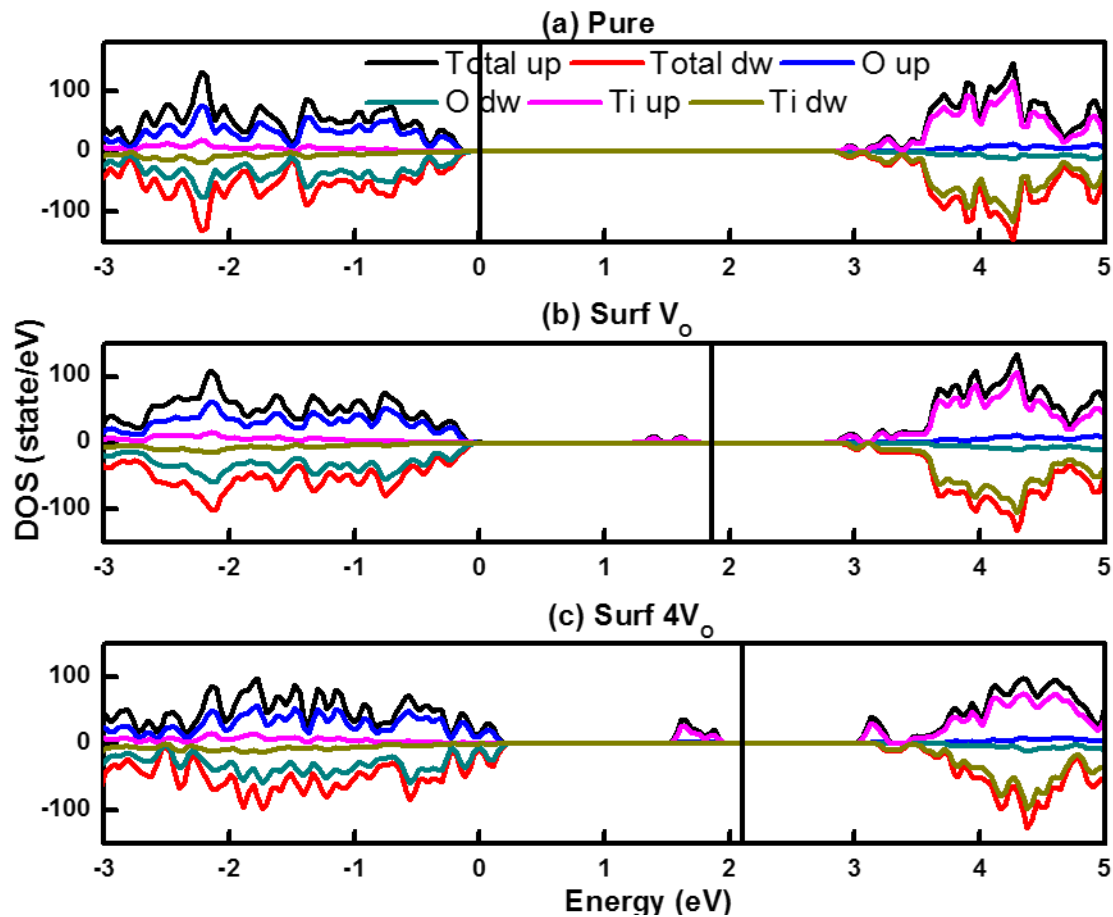
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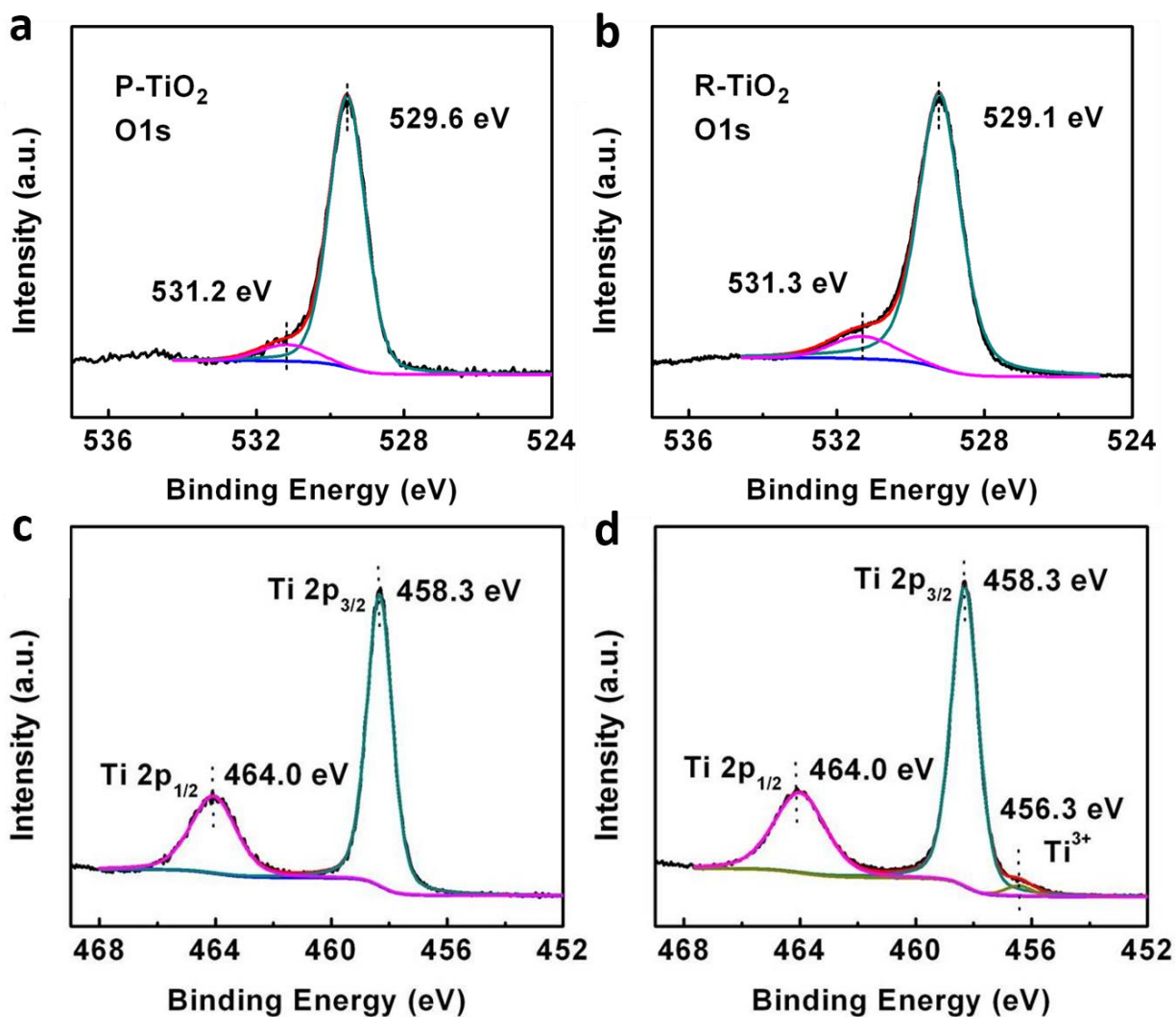
**Figure S1.** Characterization of TiO<sub>2</sub> nanobelts. (a) SEM image of hydrogen-treated TiO<sub>2</sub> nanobelts. (b) XRD patterns for the pristine and reduced TiO<sub>2</sub>. EPR spectrum for (c) pristine and (d) hydrogen-treated TiO<sub>2</sub> including the g-value range from Reference 46 and 47 showing the location of the O<sup>-</sup> surface oxygen vacancy and bulk Ti<sup>3+</sup> sites.



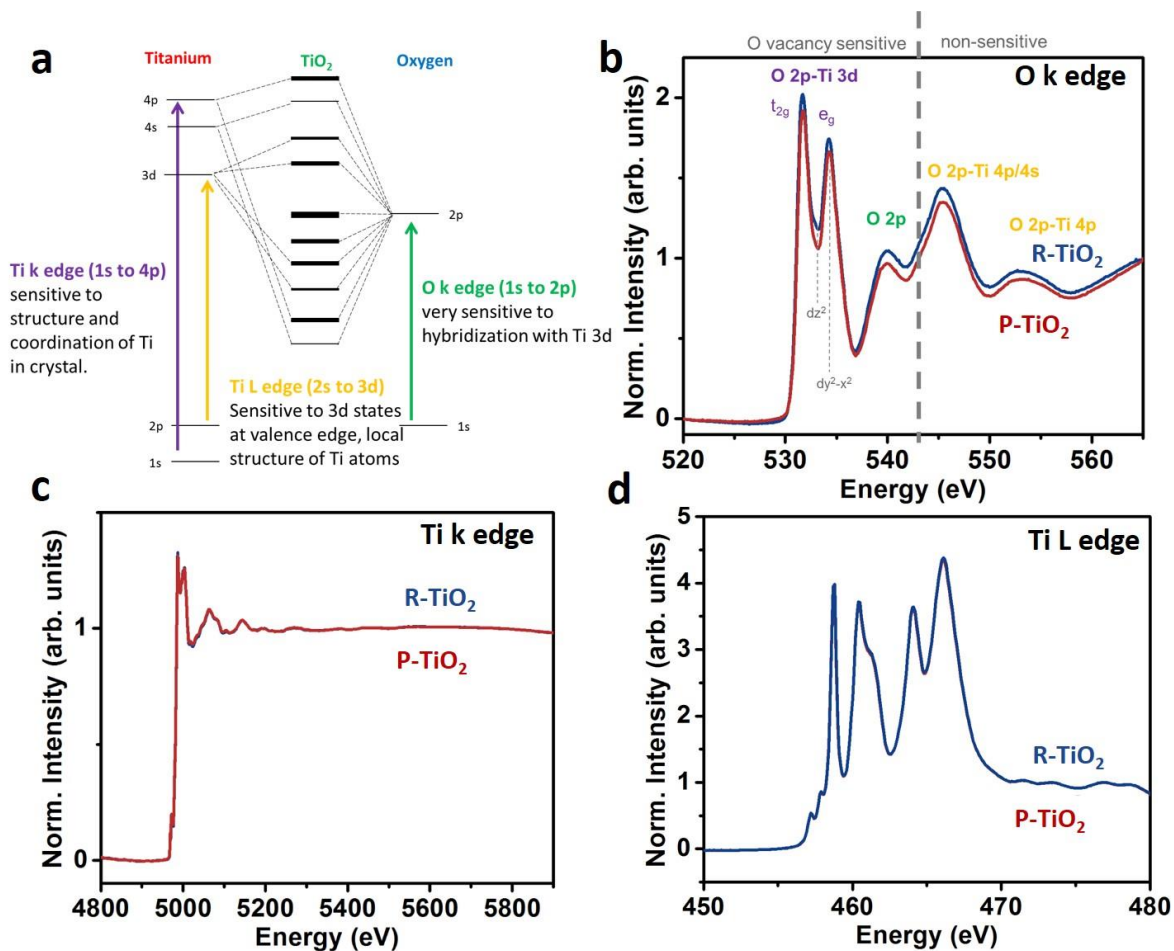
**Figure S2.** Inclusion of oxygen vacancies in DFT calculation. (a) Position of vacancies in  $\text{TiO}_2$  nanobelt, (b) optimized  $\text{TiO}_2$  nanobelt, (c) original, and (d) optimized  $\text{TiO}_2$  nanobelt with an oxygen vacancy on the surface, (e) original and optimized  $\text{TiO}_2$  nanobelt with an oxygen vacancy on the bottom of the surface layer, (g) original, and (h) optimized  $\text{TiO}_2$  nanobelt with four surface vacancies.



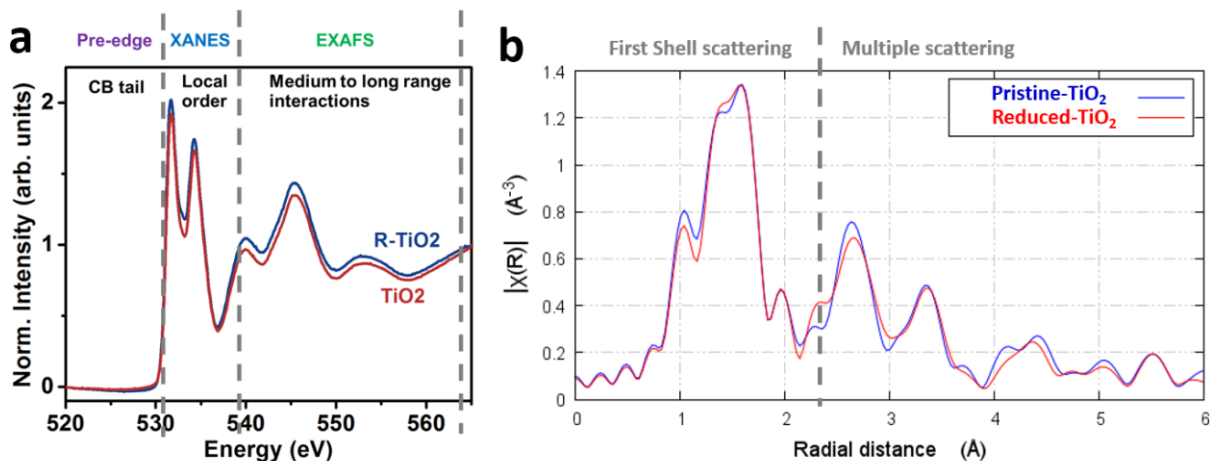
**Figure S3.** Total and partial density of states from GGA+U calculation. (a) pristine TiO<sub>2</sub> nanobelt, (b) TiO<sub>2</sub> nanobelt with one oxygen vacancy on the surface or the bottom of the surface layer, and (c) TiO<sub>2</sub> nanobelt with four surface vacancies. The solid line indicates the Fermi level. Unlike in Figure 1 of the main manuscript, the DOS here have not been aligned using the energy of the semicore levels, hence the apparent shift of the VB and CB.



**Figure S4.** XPS spectra for O *1s* of (a) pristine TiO<sub>2</sub> and (b) reduced TiO<sub>2</sub>. XPS spectra for the Ti *2p* of (c) pristine TiO<sub>2</sub> and (d) reduced TiO<sub>2</sub>. Based on the XPS analysis, the Ti<sup>3+</sup> content was estimated at 3.4 %, and accordingly the oxygen vacancy content was 0.85 %.

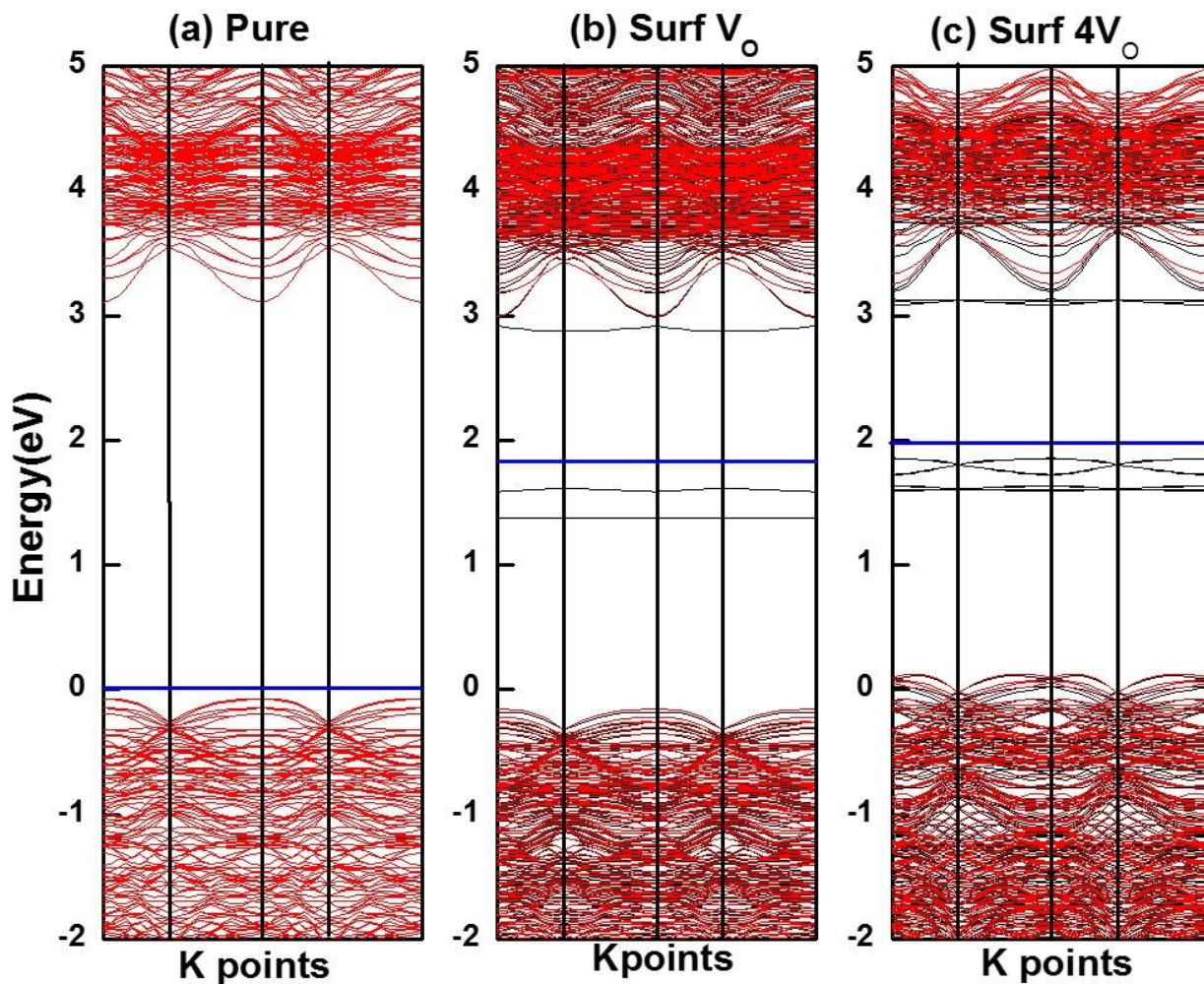


**Figure S5.** XANES spectra of pristine and reduced TiO<sub>2</sub>. (a) Explanation of the different XANES transitions and what they are sensitive to, adapted from Ref 41-46. (b) O K edge with transitions from Reference 41, (c) Ti K edge, and (d) Ti L edge.



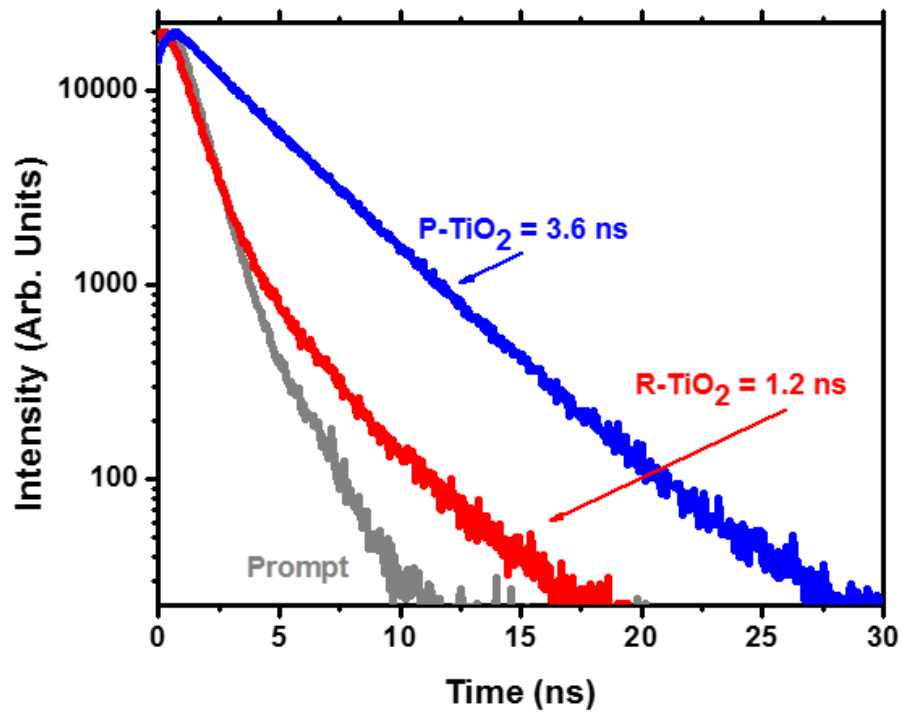
**Figure S6.** EXAFS for pristine and reduced  $\text{TiO}_2$ . **(a)** Different regions of the x-ray absorption spectrum and what they are sensitive to. **(b)** EXAFS data showing that to the first shell scattering, and even to multiple scattering, there is little disorder caused by reducing the  $\text{TiO}_2$ . EXAFS calculated using the ATHENA package: "ATHENA, ARTEMIS, HEPHAESTUS: data analysis for X-ray absorption spectroscopy using IFEFFIT", B. Ravel and M. Newville, *J. Synchrotron Rad.* 12, pp 537--541 (2005).



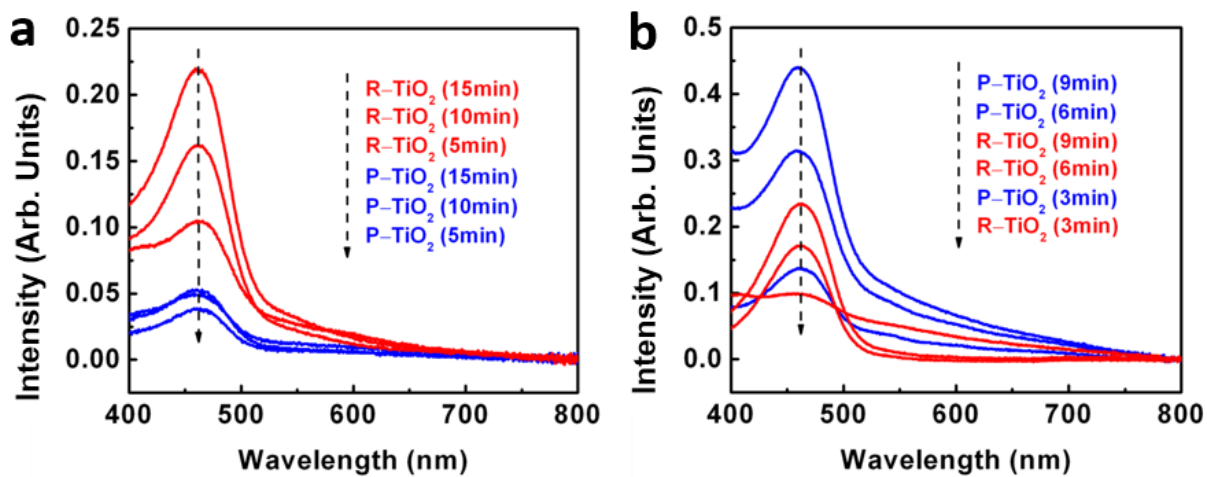


**Figure S7.** Energy band structures from GGA+U calculation. (a) pristine  $\text{TiO}_2$  nanobelt, (b)  $\text{TiO}_2$  nanobelt with one oxygen vacancy on the surface or the bottom of the surface layer, and (c)  $\text{TiO}_2$  nanobelt with four surface vacancies. The blue lines denoted Fermi energy levels. Unlike in Figure 1 of the main manuscript, the DOS here have not been aligned using the energy of the semicore levels, hence the apparent shift of the VB and CB.

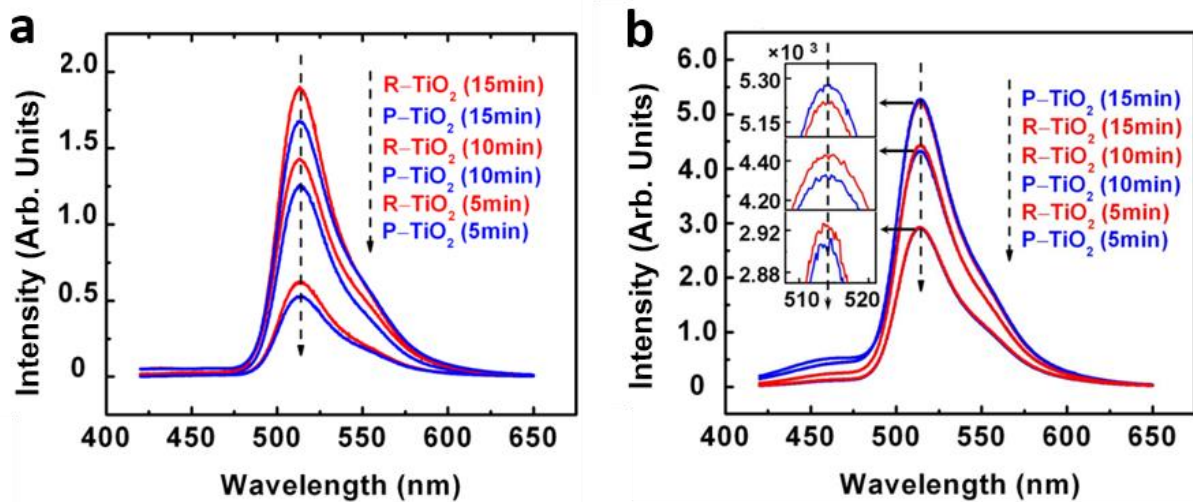




**Figure S8.** Time-resolved fluorescence for pristine and reduced TiO<sub>2</sub> under excitation at 325 nm. The lifetime is fit by convolution with the instrument response function shown in grey.



**Figure S9.** Absorption spectra of NBD-Cl solutions with TiO<sub>2</sub> nanobelts after radiation for different times in (a) visible-light and in (b) UV light for monitoring superoxide radicals ( $O_2^{\bullet-}$ ).



**Figure S10.** Emission spectra of HPF solution with TiO<sub>2</sub> nanobelts after radiation for different times in (a) visible-light, and in (b) UV light for monitoring hydroxyl radicals ( $\bullet$ OH).