

Uniform Anatase Single-Crystal Cubes with Highly Thermal Stability and Fully Enclosed by Active {010} and {001} Facets

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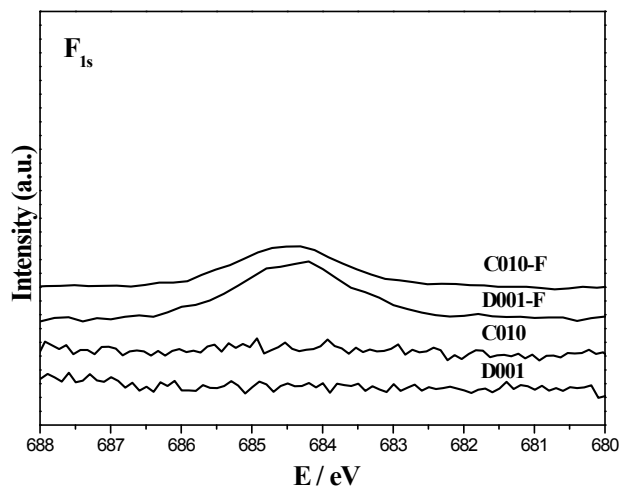


Figure S1. F_{1s} XPS spectra of samples before and after calcination.

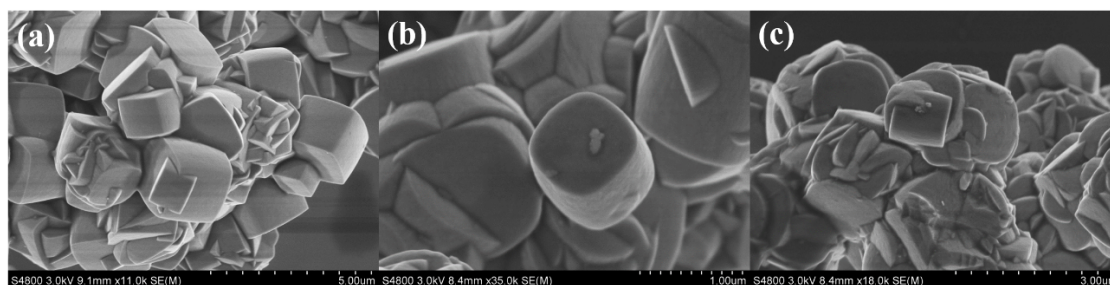


Figure S2. FE-SEM images of anatase TiO₂ crystals obtained in the absence of surfactant (a), in the presence of SDS (b), and CTAB (c), respectively.

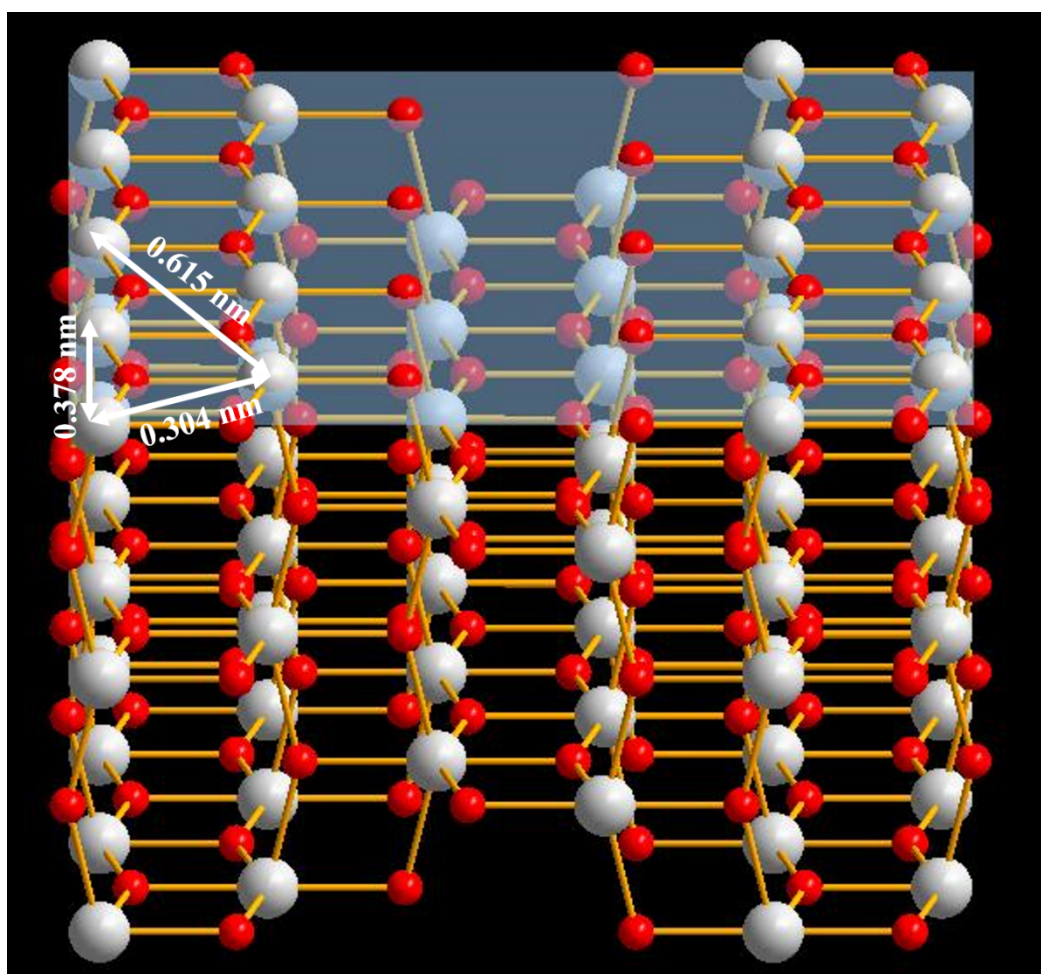


Figure S3. Distances between Ti atoms on the {010} surfaces of anatase.

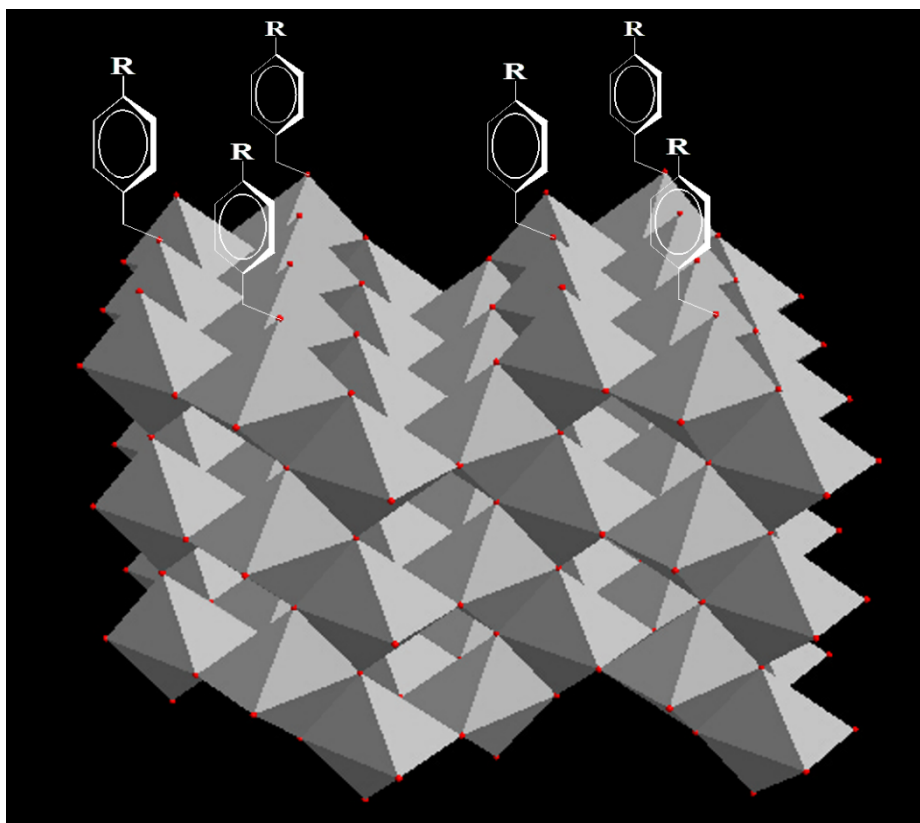


Figure S4. Schematic representation of the SDBS adsorbed on {010} facets of anatase TiO₂ through π - π stacking between aromatic rings.

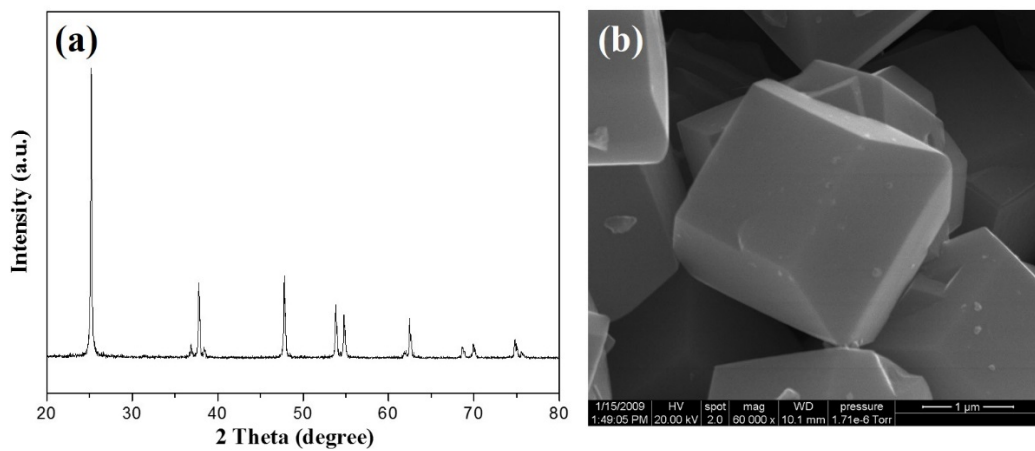


Figure S5. (a) XRD pattern and (b) FESEM images of samples D001-F prepared by a method previously published by our group.^[1]

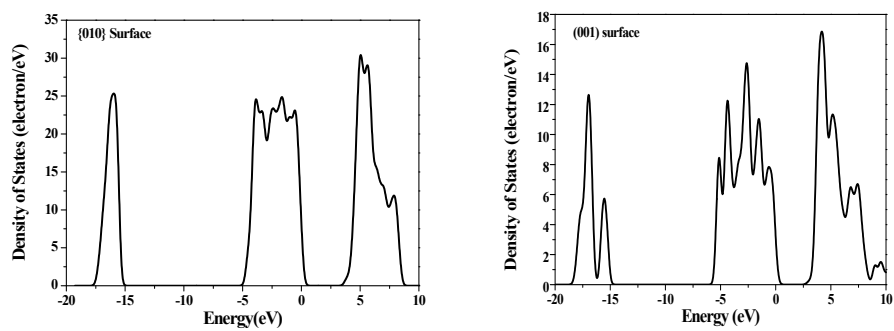


Figure S6. Partial density of states (PDOS) of {010} and {001} surface of anatase TiO₂.

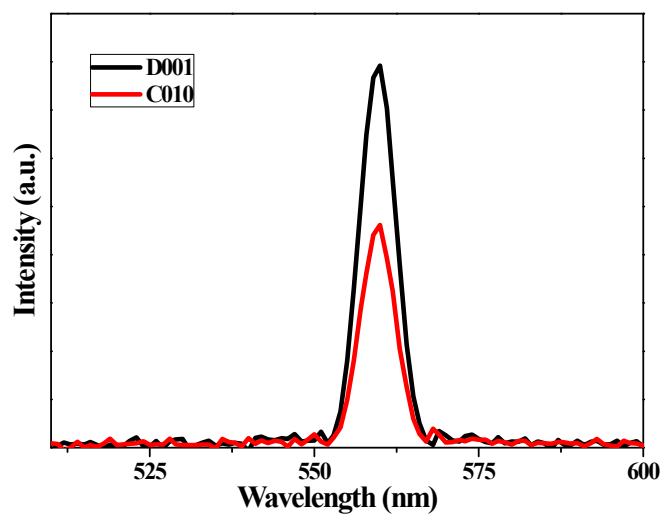


Figure S7. The photoluminescence spectroscopy spectra of the sample C010 and D001

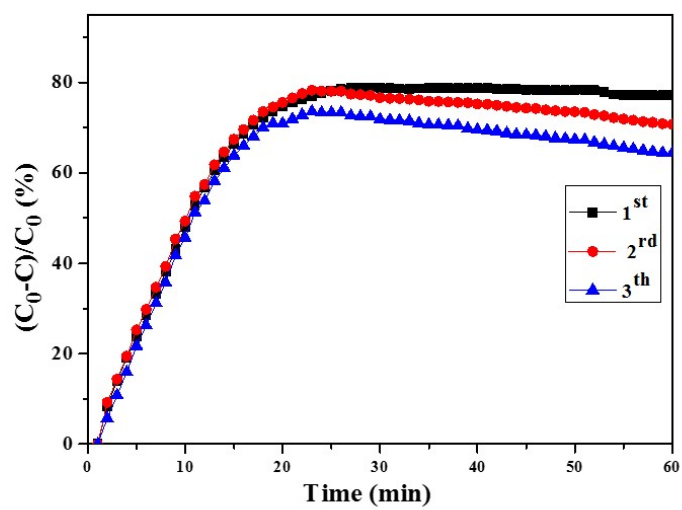


Figure S8. The recyclability of the photocatalytic oxidation of NO over C010

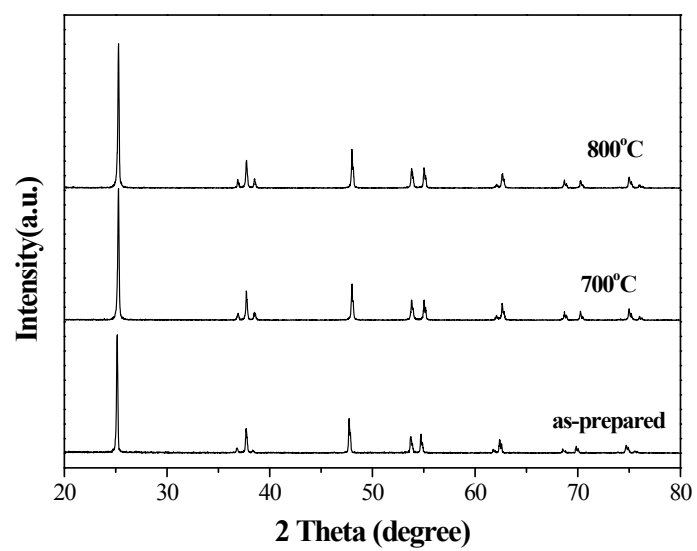


Figure S9. Wide-angle XRD patterns of the TiO₂ single-crystal cubes calcined at different temperatures under air atmosphere for 1h.

References:

- 1 D. Zhang, G. Li, H. Wang, K. M. Chan and J. C. Yu, *Crys. Growth Des.* 2010, 10, 1130-1137.