

## Supporting Information (SI)

### **Engineering defects and photocatalytic activity of TiO<sub>2</sub> nanoparticles by thermal treatments in NH<sub>3</sub> and subsequent surface chemical etchings**

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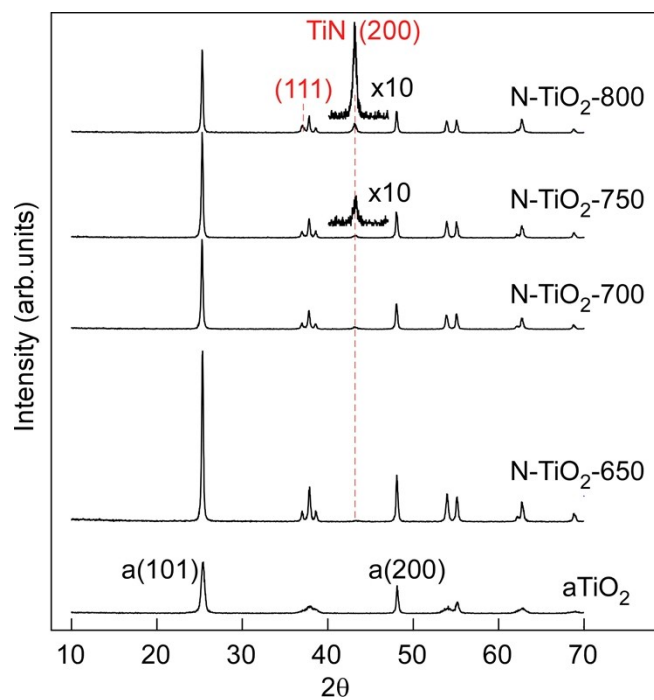
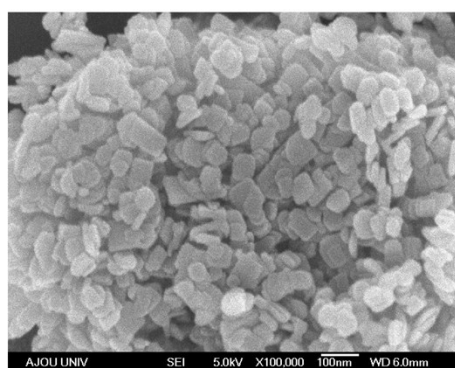
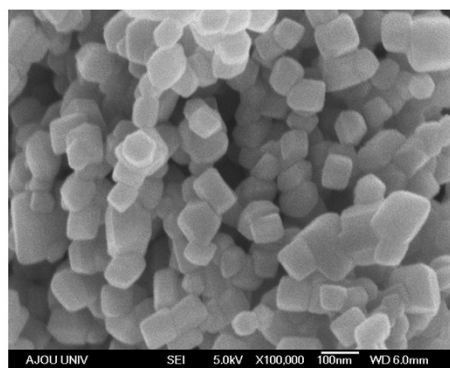


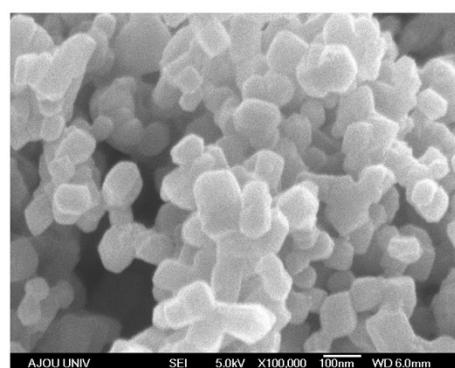
Figure S1. XRD patterns of as-synthesized aTiO<sub>2</sub> and N-doped aTiO<sub>2</sub> prepared at temperatures of 650 – 800 °C. Anatase phase remains as a major phase up to 800 °C. Only a trace of a crystalline peak of TiN is observed above 700 °C, and the peak remains small up to 800 °C.



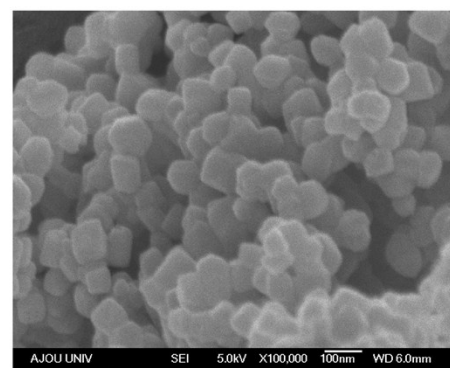
(a) N-TiO<sub>2</sub>-300



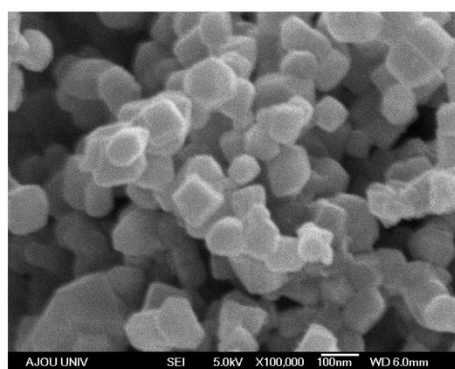
(b) N-TiO<sub>2</sub>-650



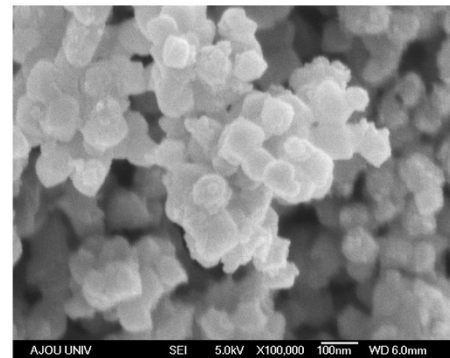
(c) N-TiO<sub>2</sub>-750



(d) After HF 5 min



(e) N-TiO<sub>2</sub>-800



(f) After HF 50 min

Figure S2. SEM images of N-doped TiO<sub>2</sub> prepared at temperatures of (a) 300, (b) 650, (c) 750 and (e) 800 °C. Also, shown are the SEM images after the RT HF treatment of N-TiO<sub>2</sub>-700 for 5 min (d) and of N-TiO<sub>2</sub>-800 for 50 min (f). The SEM images after the HF treatment up to 50 min show little difference in morphology from those of as-prepared N-TiO<sub>2</sub> nanocrystals.

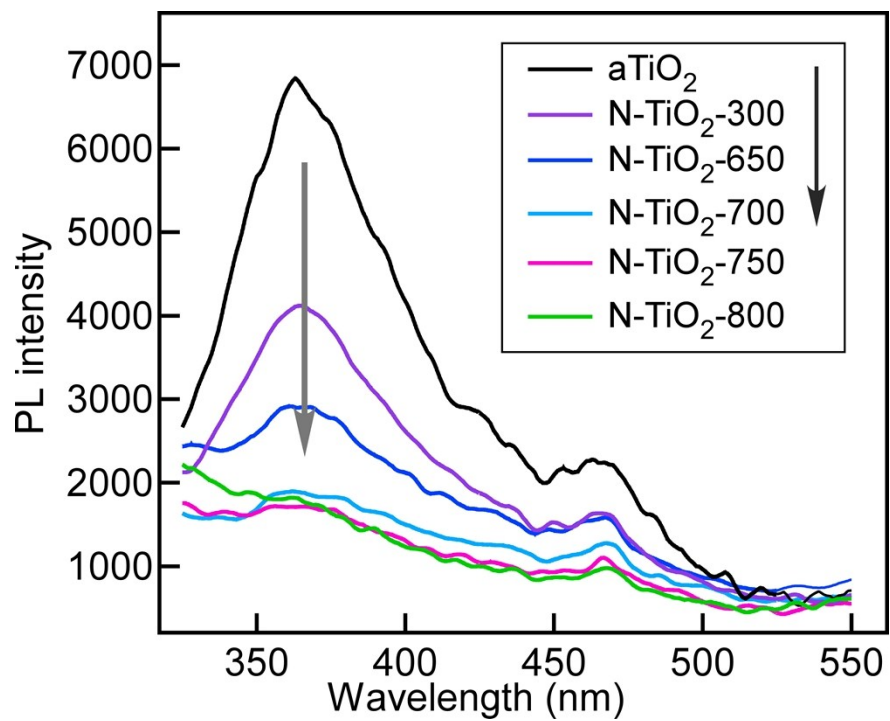


Figure S3. Photoluminescence spectra of aTiO<sub>2</sub> and N-TiO<sub>2</sub> nanocrystals prepared at 300 – 800 °C taken with excitation at 300 nm.

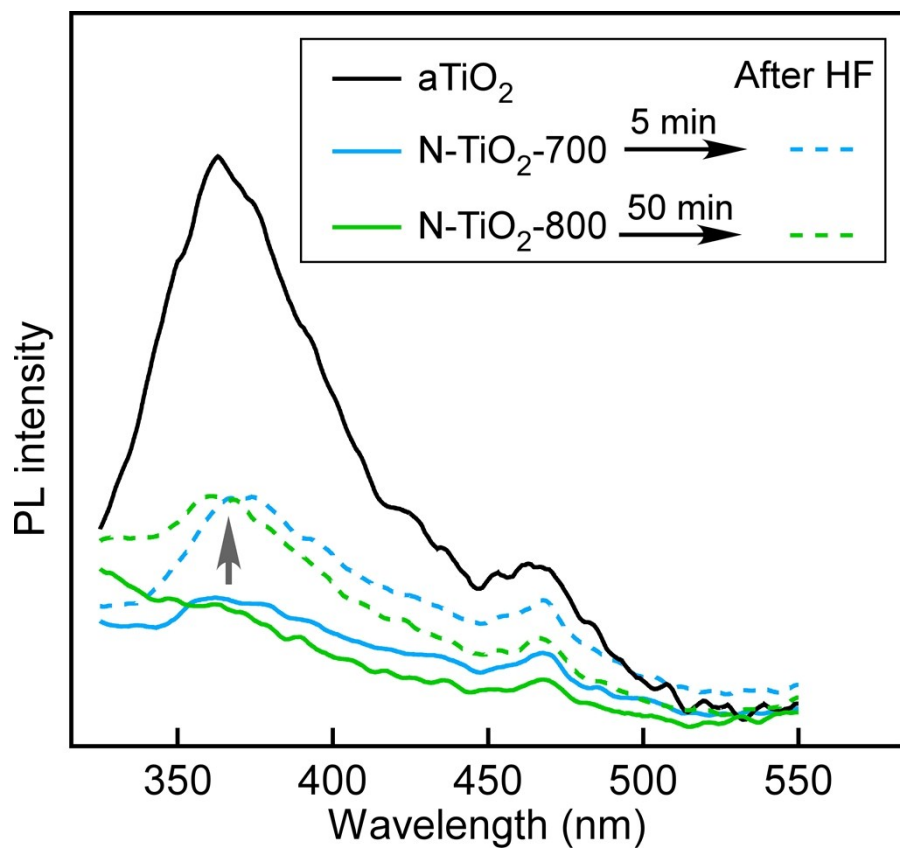


Figure S4. Photoluminescence spectra of  $\text{N-TiO}_2$  nanocrystals prepared at 700 – 800 °C in comparison with those after the HF treatments taken with excitation at 300 nm.

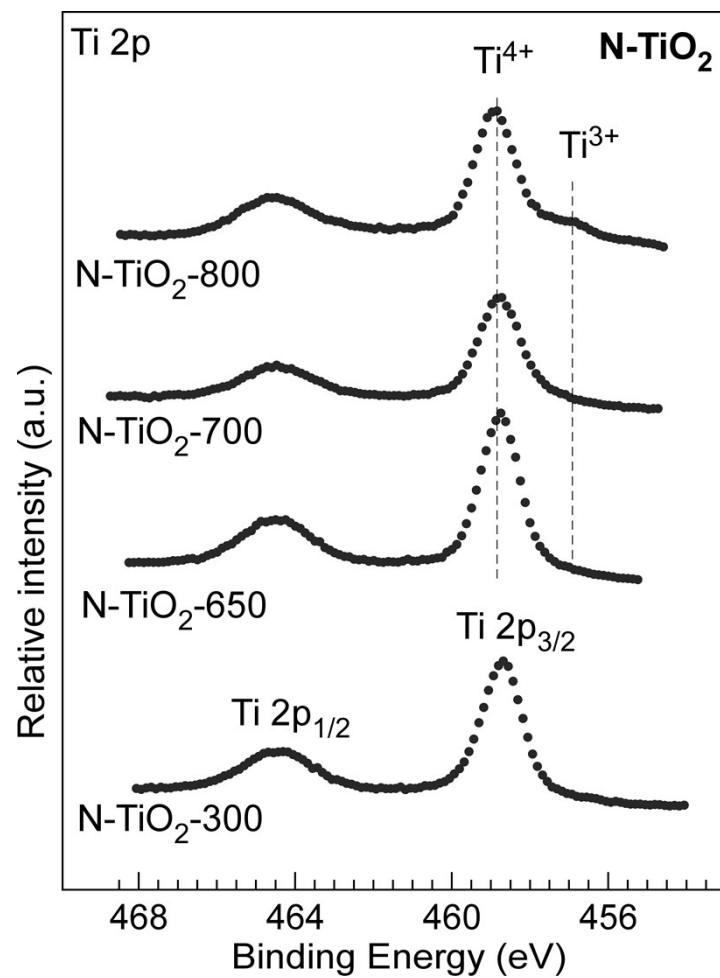


Figure S5. Ti 2p core level of N-TiO<sub>2</sub> prepared at 300, 600, 700 and 800 °C.

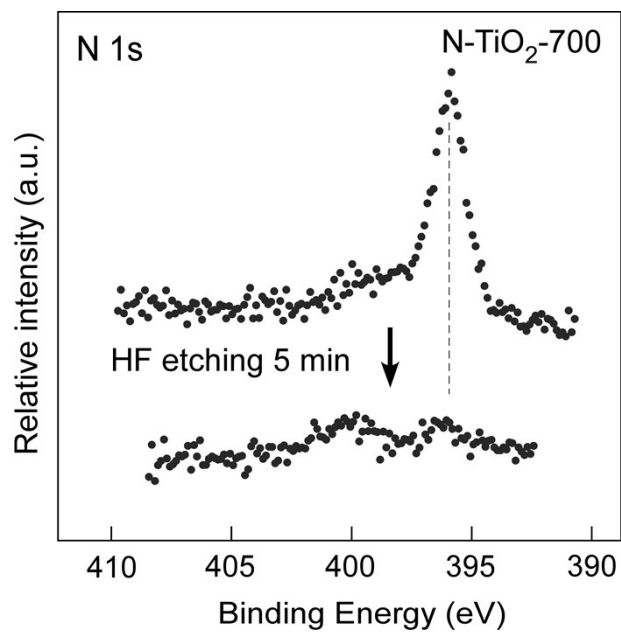


Figure S6. N 1s core level spectra of N-TiO<sub>2</sub>-700 before and after the HF etching for 5 min.