Supporting Information

Heating-induced Transformation of Anatase TiO_2 Nanorods to Rock Salt TiO Nanoparticles: Implications for Photocatalytic and Gas Sensing Applications

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Supporting Figures

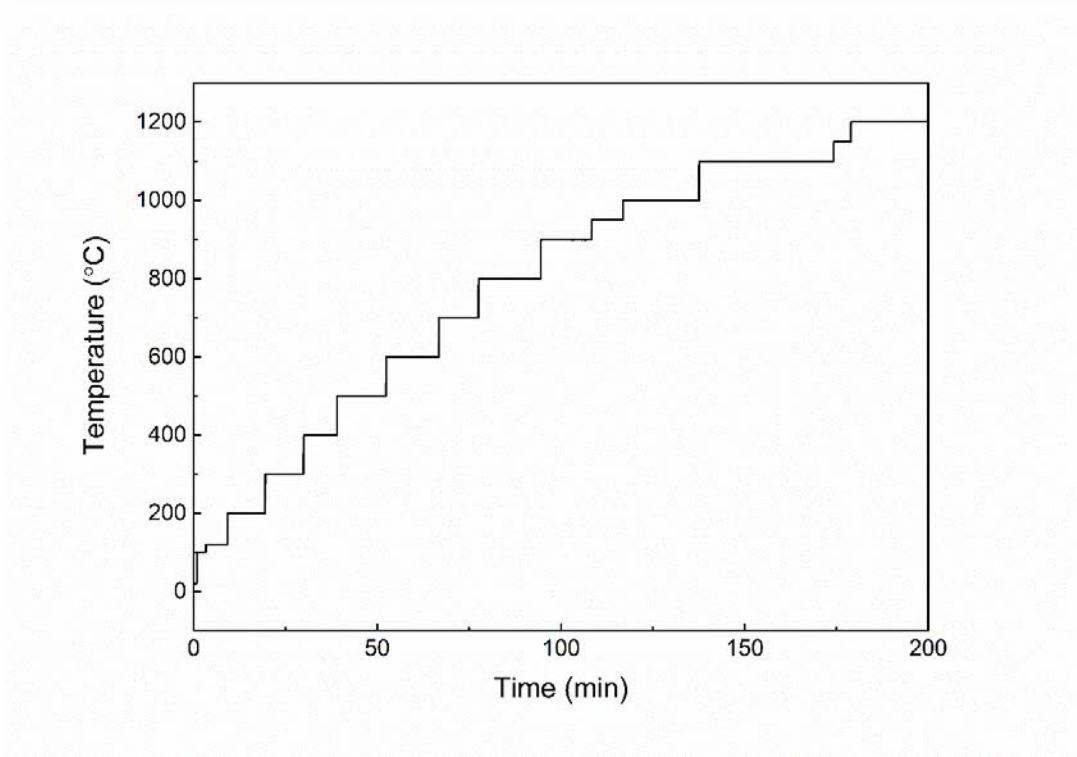

Figure S 1 Typical heating temperature profile of the experiments (the heating profile of one actual experiment is shown). The experiments were conducted several times, some steps may take longer time for more inspections, which does not affect the final result.

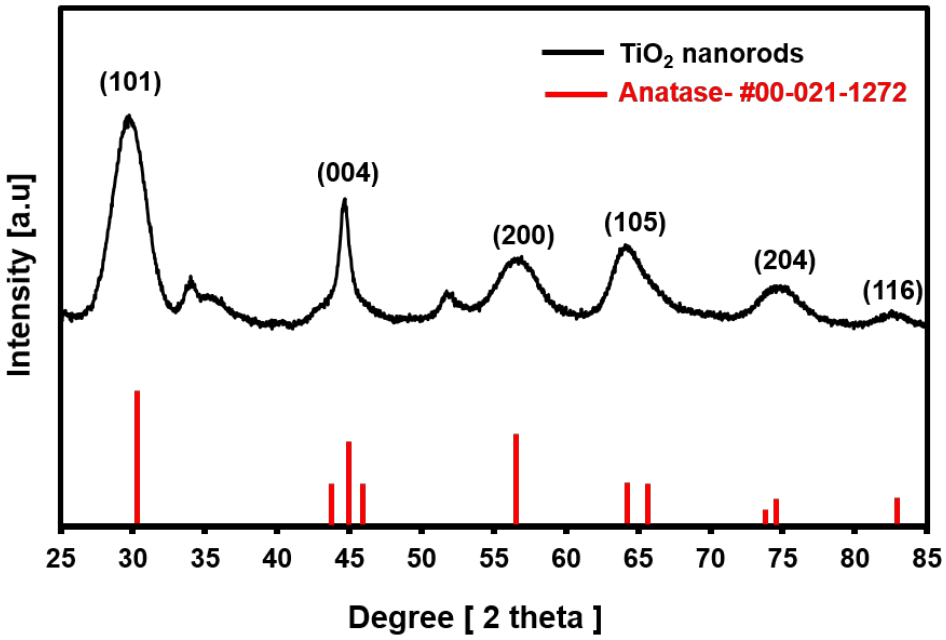

Figure S 2 X-ray diffraction spectrum of the as-synthesized TiO_2 NRs, confirming the anatase crystallographic phase.

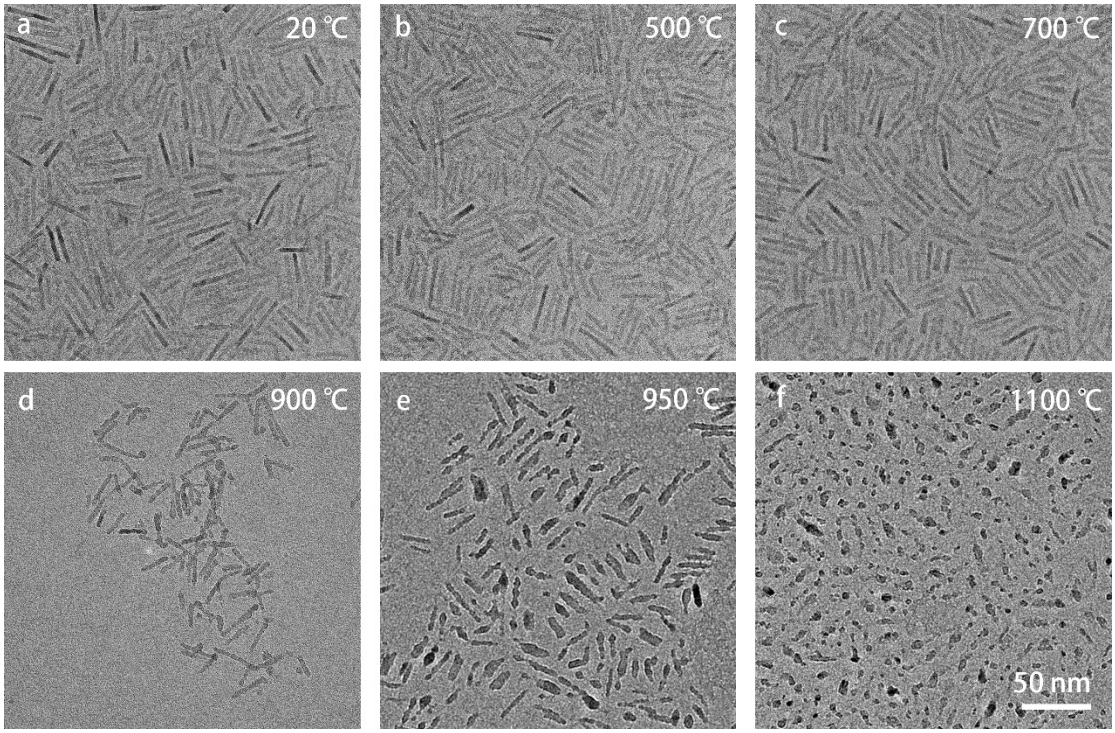

Figure S 3 Bright-field TEM images of TiO_x nanocrystals during heating. Some of the nanorods appear darker due to diffraction contrast. Upon heating to 500 °C, the edges became rounded. At 700 °C, the surfaces of the nanorods deformed more and are no longer sharp. At 900 °C, some nanorods broke up into multiple segments, and sometimes neighboring rods had coalesced. Upon heating to 1000 °C, most nanorods had transformed into smaller nanoparticles.

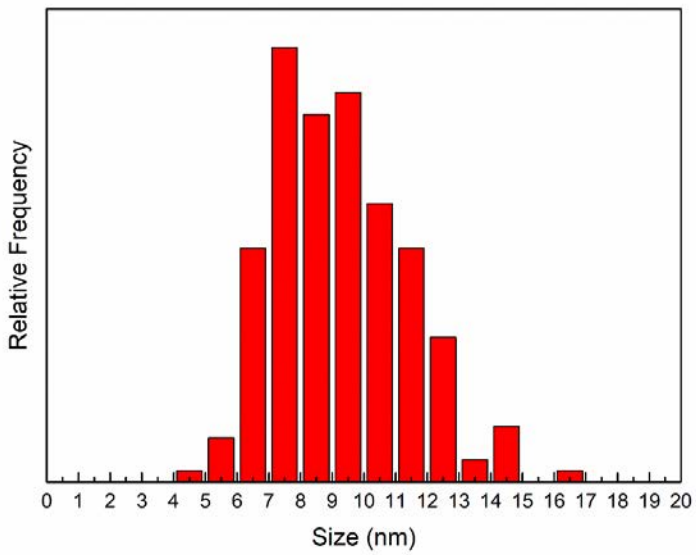

Figure S 4 Size distribution plot of TiO nanoparticles obtained after heating to 1200 °C, measured after cooling down to room temperature. The sizes of 200 particles are included for the statistics.

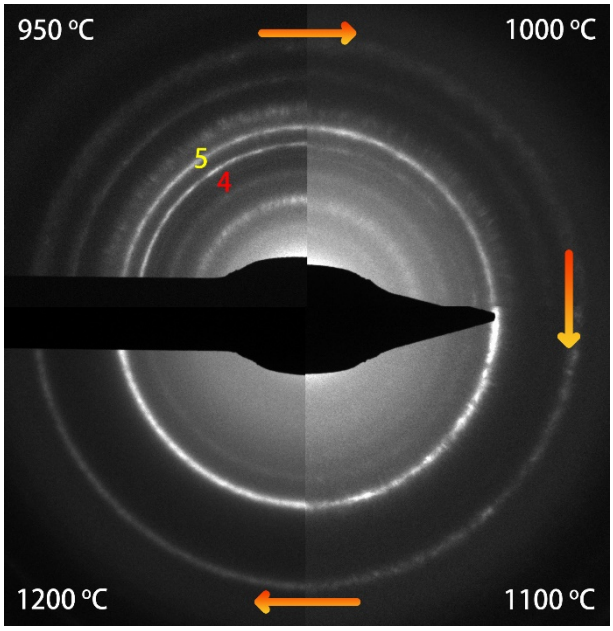

Figure S 5. Comparison of selected area diffraction patterns (SADPs) of TiO_x at temperatures of 950 °C (top-left), 1000 °C (top-right), 1100 °C (bottom-right), and 1200 °C (bottom-left). The rings corresponding the anatase phase (ring #4 and other inner rings) disappeared gradually, and finally only rings belonging to cubic TiO remain. Ring #5 corresponding to (200) of TiO appeared at 950 °C, and remained until 1200 °C.

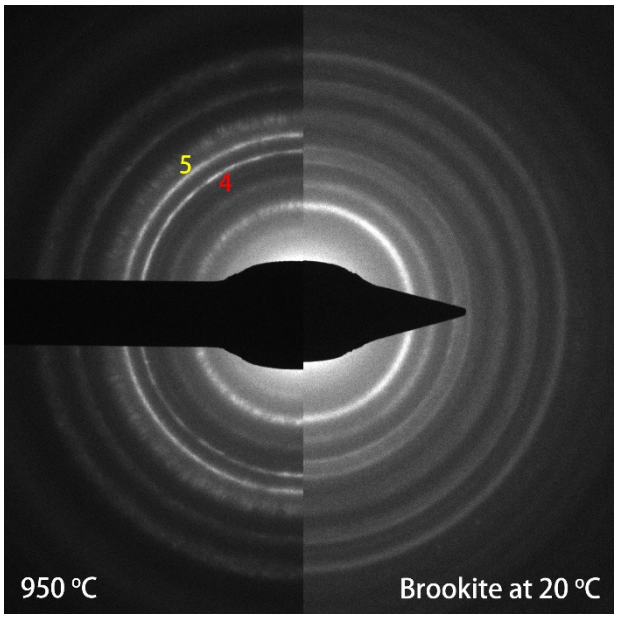

Figure S 6. Electron diffraction pattern (DP) of the sample annealed at 950 °C (left) and DP of pure brookite nanorods at room temperature (right). Most of the rings in both DPs are the same, except for ring No. 4 and 5 at 950 °C. Ring No. 4 corresponds to the anatase (004) reflection and ring No. 5 corresponds to the TiO (200) reflection.

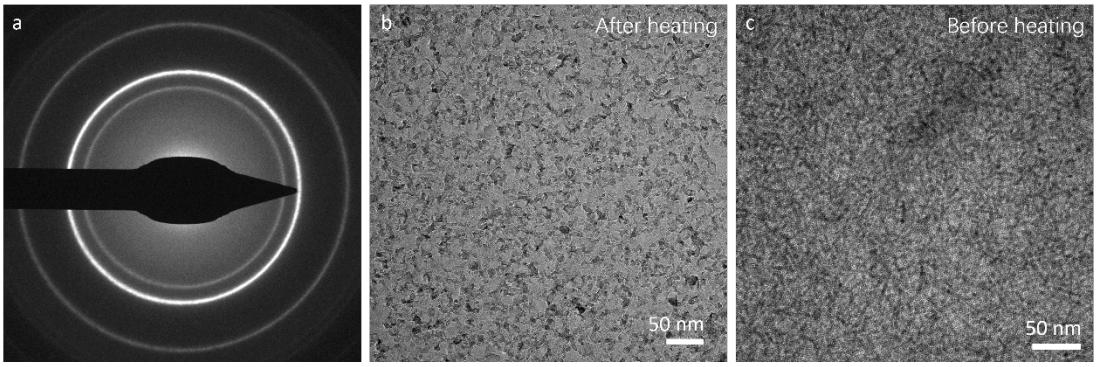

Figure S 7. Result of in-situ heating of very high concentration NRs to 1200 °C. (a)DP. (b) TEM image taken after heating. (c) TEM image taken at room temperature before heating. The diffraction pattern shows rock-salt TiO structure. The NRs sublimated during heating.

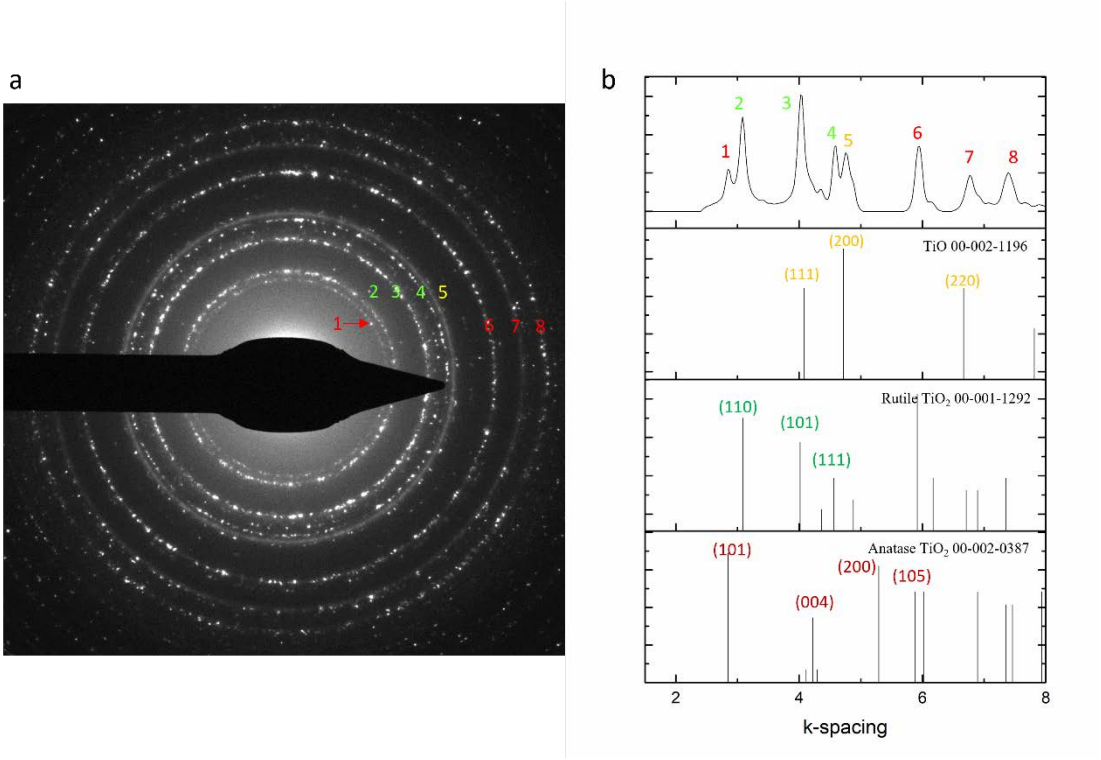

Figure S 8. Diffraction pattern (DP) of the sample after heating in a vacuum chamber to 1200 °C with the same heating rate as used in the electron microscope. The DP shows a mixture of anatase, rutile and cubic TiO phases. (a) The diffraction pattern; (b) integrated DP compared with the XRD spectra of anatase, rutile, and cubic TiO. The peaks in the DP are marked with different colors and correspond to lattice reflections of different phases. Ring #1 correspond to the anatase structure. Rings # 2-4 correspond to the rutile structure. Ring #5 corresponds to cubic TiO. Rings #6-8 are close to both the anatase and rutile structures.