Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Open-top TiO_2 Nanotube Arrays with Enhanced Photovoltaic and Photochemical Performances *via* a Micromechanical Cleavage Approach

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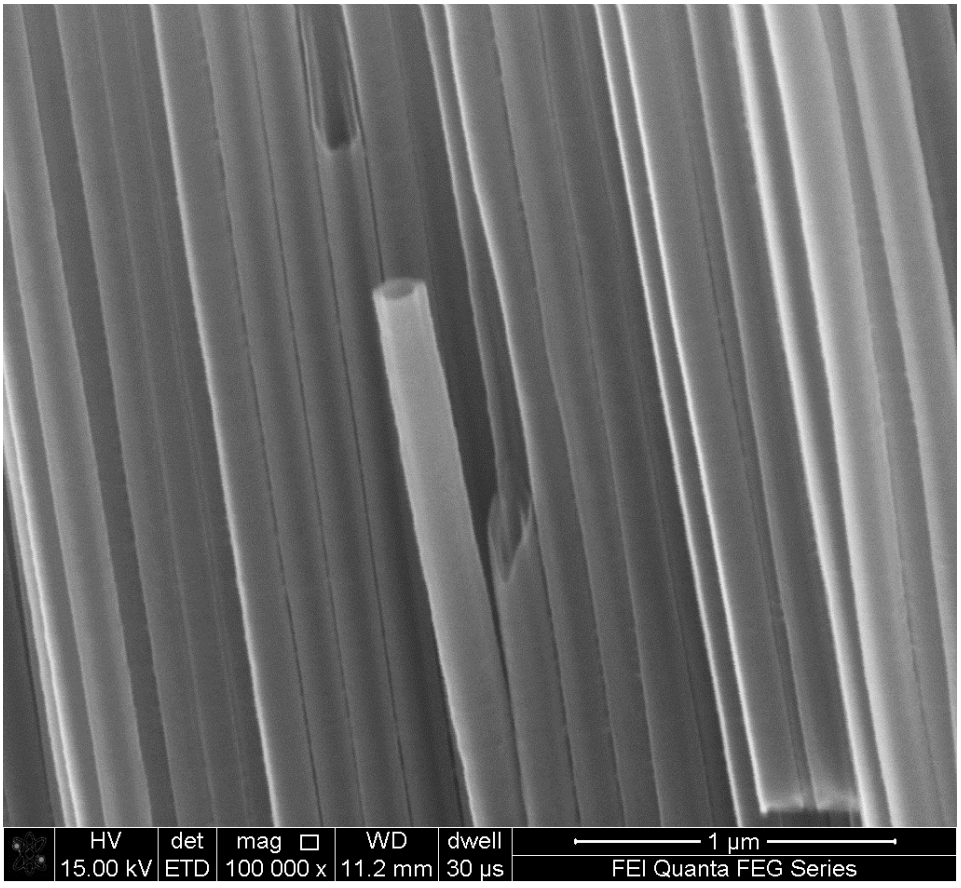

Figure S1. SEM image of the side view of anodic TiO_2 NTs, showing the TiO_2 NTs are uniform and well aligned with smooth wall.

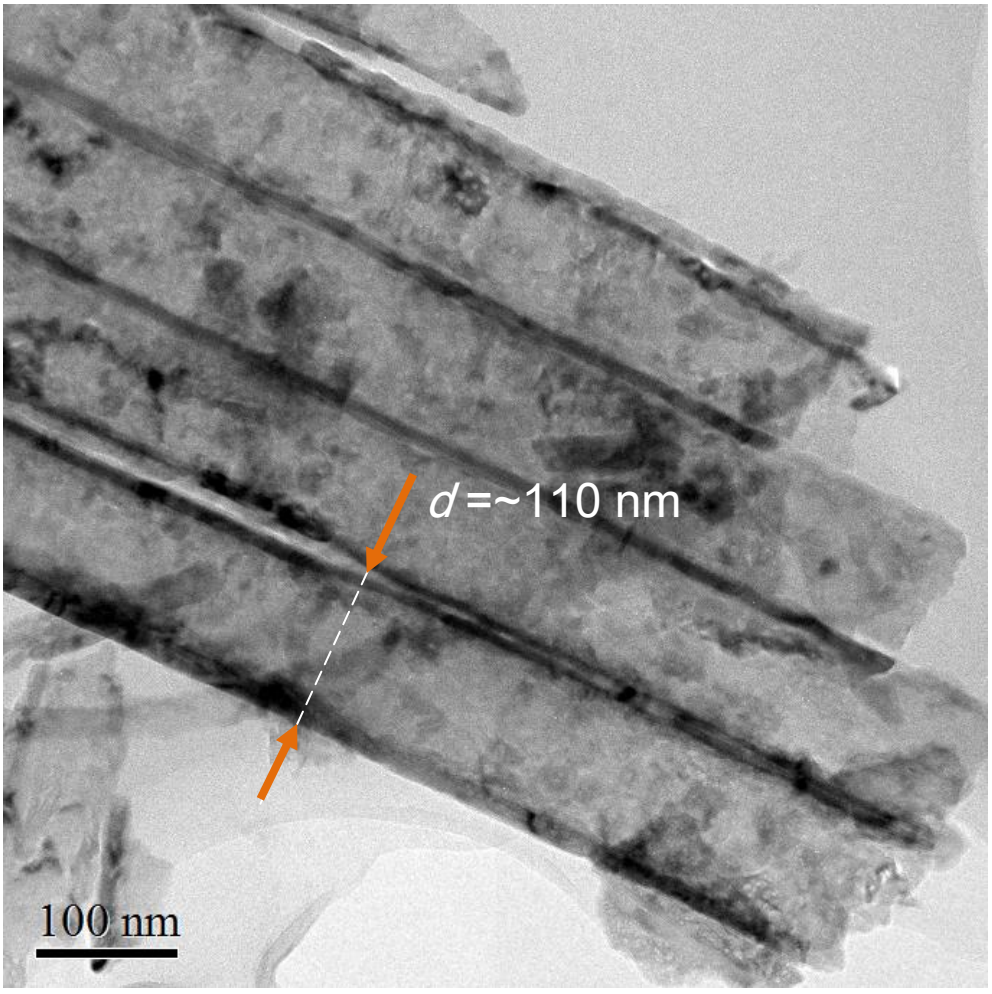

Figure S2. TEM image of the anodic TiO_2 NTs, showing highly ordered and uniform the TiO_2 NTs with diameter of ~110 nm.

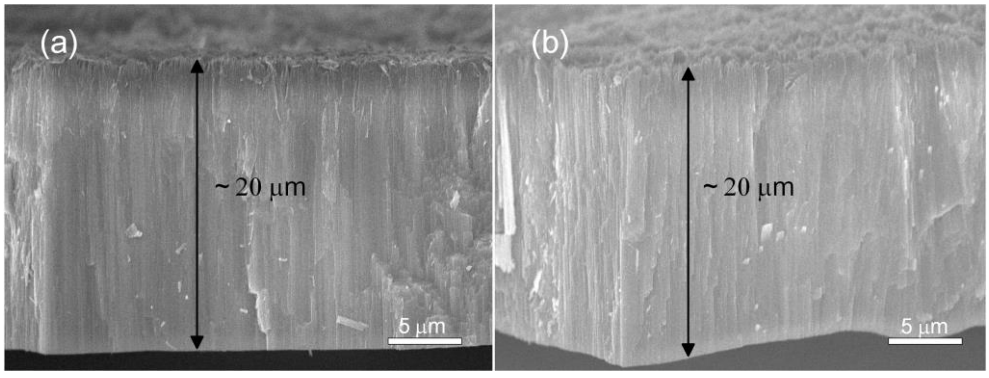

Figure S3. SEM images of the side view of anodic TiO_2 NT arrays (a) before and (b) after peeling off the nanograss layer, showing negligible change in thickness.

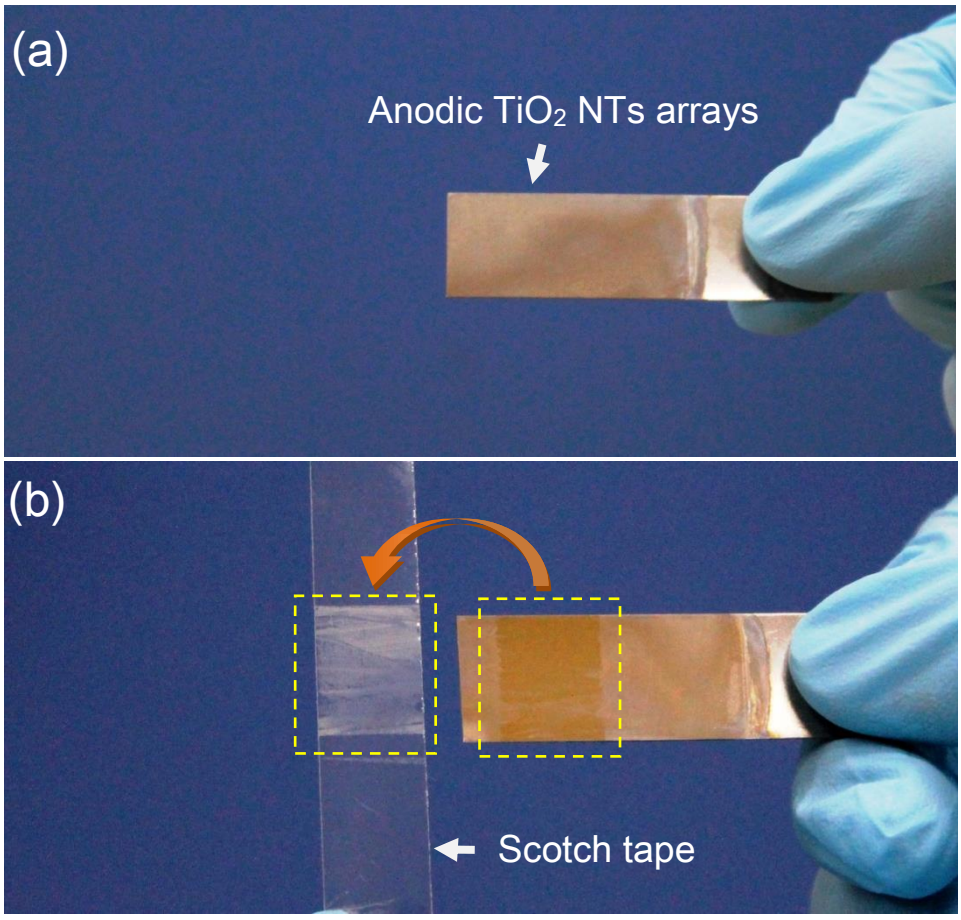

Figure S4. Photograph of (a) the as-prepared anodic TiO_2 NT arrays on metal Ti substrate and (b) the peeling off process to remove the nanograss top layer by using scotch tape technique.

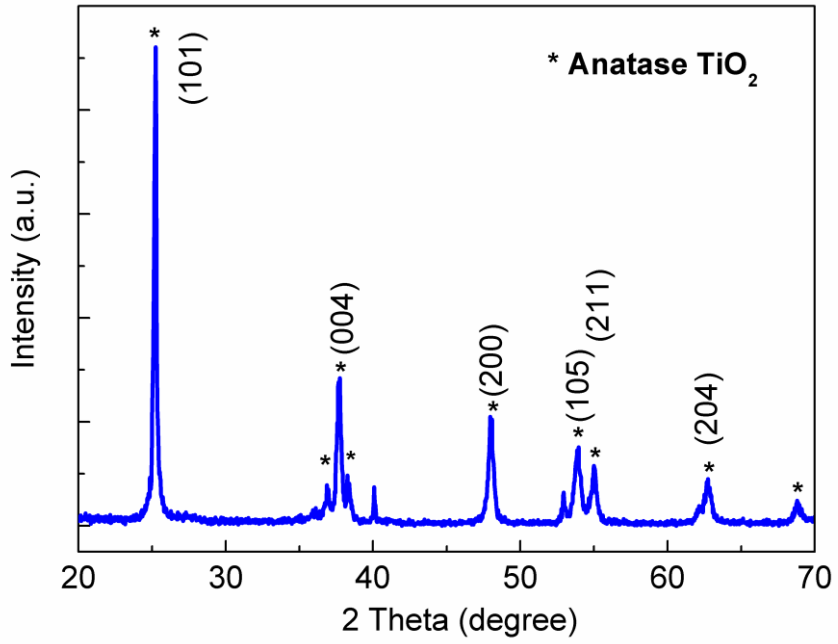

Figure S5. XRD patterns of the anodic TiO_2 NT arrays after sintered at 450 ^oC for 2 h, indicating the anodic TiO_2 NT arrays was crystallized to pure anatase phase.

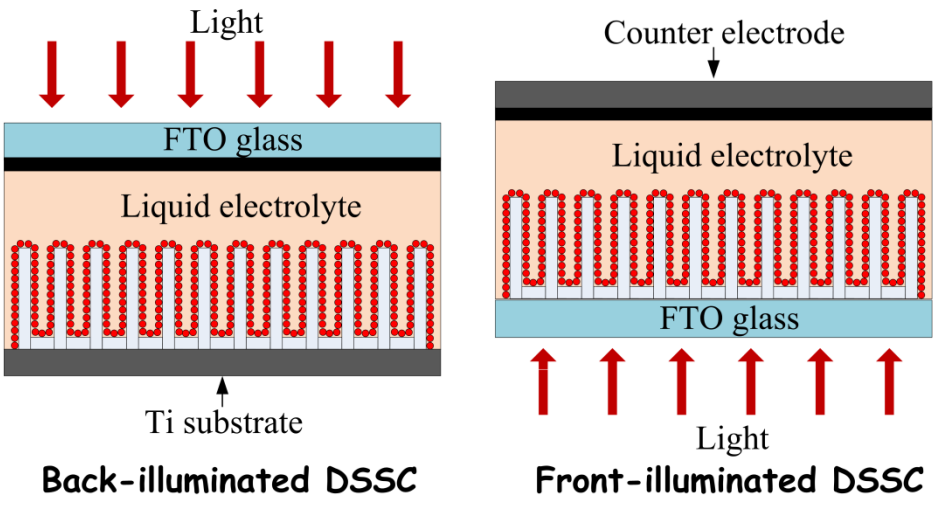

Figure S6. Illustration of the structure of a back-illuminated DSSC and a front-illuminated DSSC.

More Experimental Details:

Photocatalytic testing: The photocatalytic activities of the TiO_2 NT arrays with and without nanograss top-layer were evaluated on the basis of the degradation of methyl orange (MO, 20 mM L^{-1}) as model organic pollutants in aqueous solutions (40 mL total volume). The TiO_2 NT films (3.0 × 1.5 cm^2 surface area, total mass ~ 0.04 g) were immersed in the solution and irradiated with six 4-W UV bulbs (Eiko, Black Light Blue, Shawnee, KS; 18 W/m^2 measured illumination intensity). Before testing, the samples were soaked for 30 min in dark with magnetic stirring to reach adsorption/desorption equilibrium. The photo-degradation testing lasted for 120 min and were carried out in an open quartz photoreaction vessel with rapid stirring under room temperature. The concentration of the residual MO was measured by a Uv-vis spectrometer at 463 nm.

In order to simulate the molecular transportation (e.g. MO molecule) inside the TiO_2 NTs, we also solve the molecular diffusion equation by Finite-difference Methods for nanograss-capped TiO_2 NTs and top opened TiO_2 NTs.