

Supporting Information

Electrochemically self-doped hierarchical TiO₂ nanotube arrays for enhanced visible- light photoelectrochemical performance: an experimental and computational study

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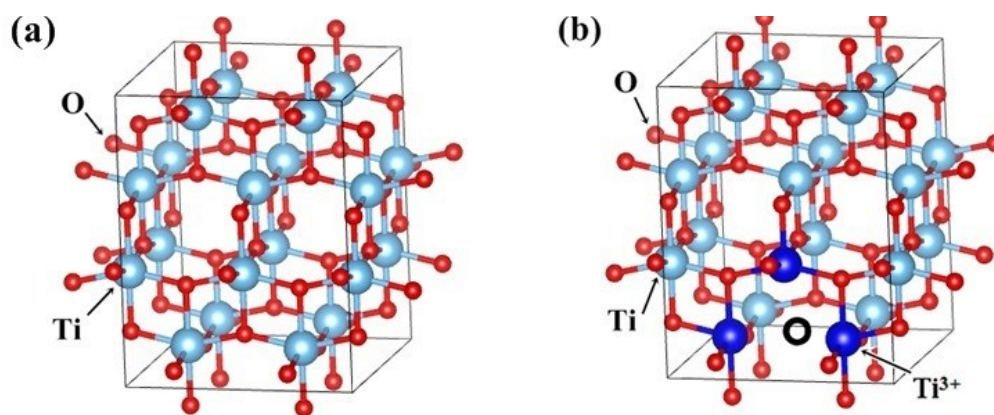


Fig. S1. (a) The schematic plots of the $2 \times 2 \times 1$ supercell of TiO_2 and (b) the $2 \times 2 \times 1$ supercell of the self-doped TiO_2 with an oxygen vacancy. The black circle shows the position of the oxygen vacancy.

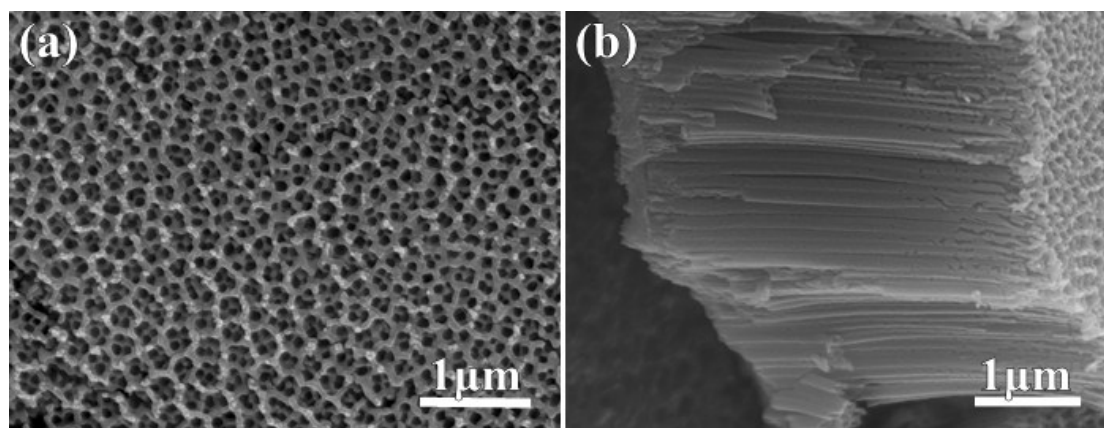


Fig. S2. SEM images of (a) the large-scale top view and (b) the cross-sectional view of the pristine TNTAs showing the top-ring/bottom-tube structure.

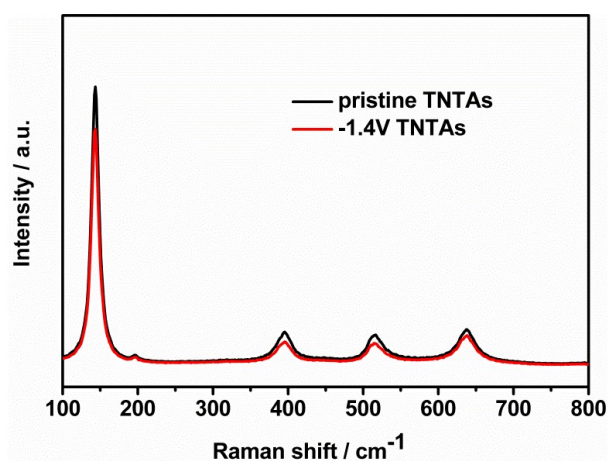


Fig. S3. Raman spectra of the pristine and -1.4 V TNTAs.

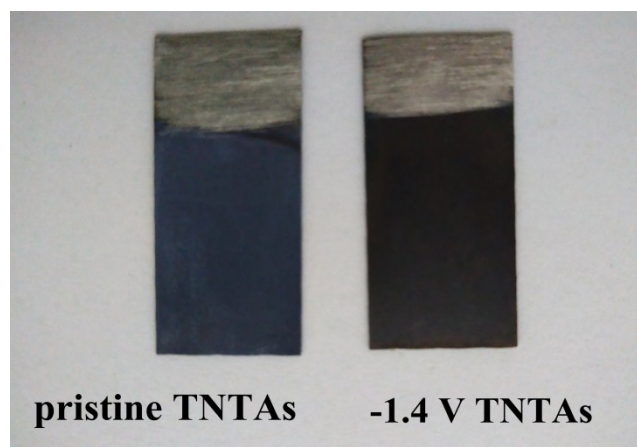


Fig. S4. Optical images of the pristine and -1.4 V TNTAs.