

Supporting information

Coupling Ti-doping and Oxygen Vacancy in Hematite Nanostructures for Solar Water Oxidation with High Efficiency

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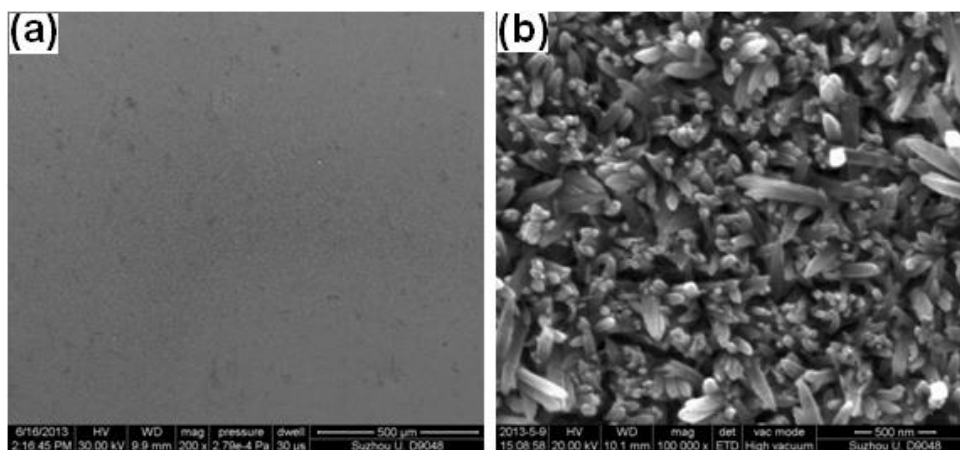
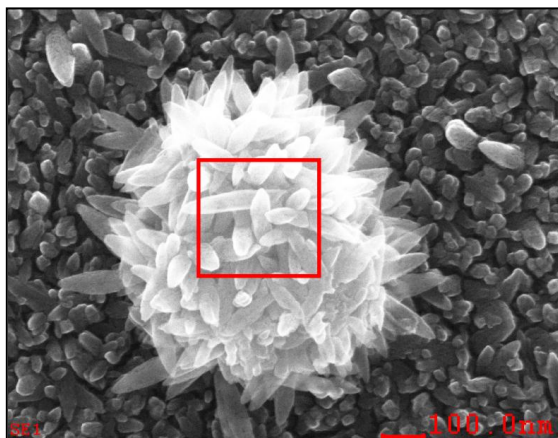


Figure S1: (a) and (b): SEM images of undoped hematite nanostructures sintered in a partial oxygen pressure of 2.1×10^{-2} Torr.



<i>Element</i>	<i>Wt%</i>	<i>At%</i>
<i>OK</i>	35.54	65.70
<i>TiK</i>	01.83	01.13
<i>FeK</i>	62.62	33.16
<i>Matrix</i>	Correction	ZAF

Figure S2: SEM image (left) and elemental analysis of the coral-like nanostructures (right).

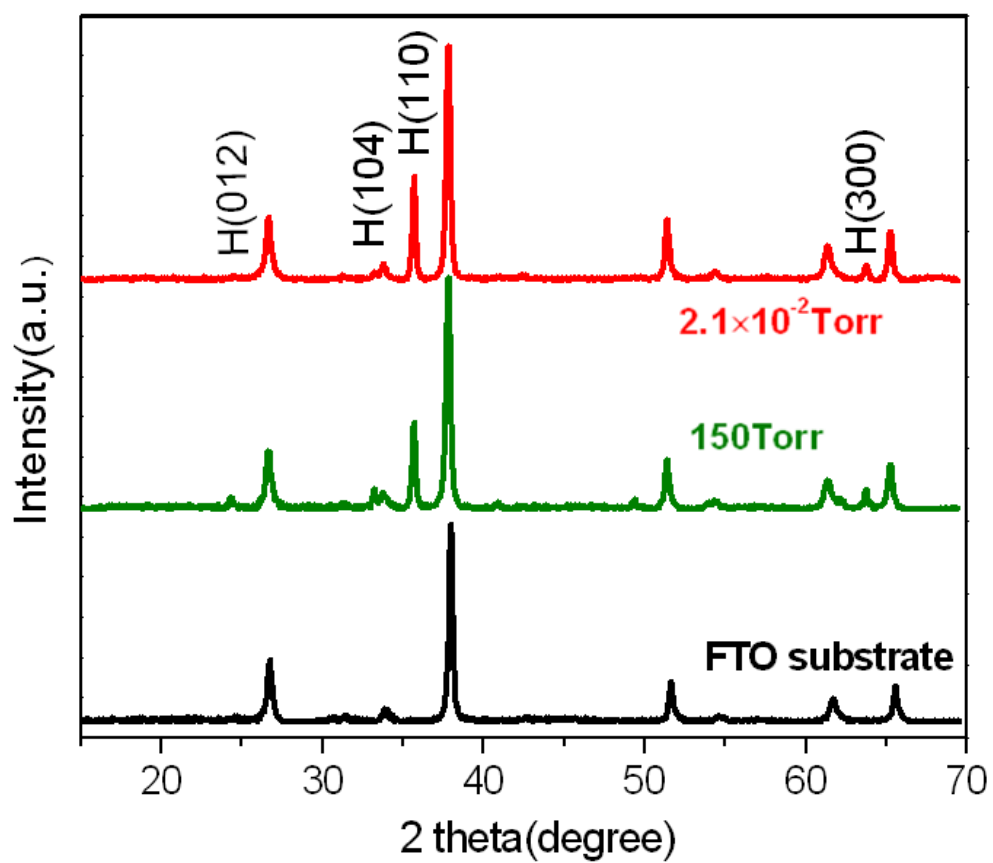


Figure S3: XRD spectra of undoped hematite nanostructures sintered in various partial oxygen pressures.

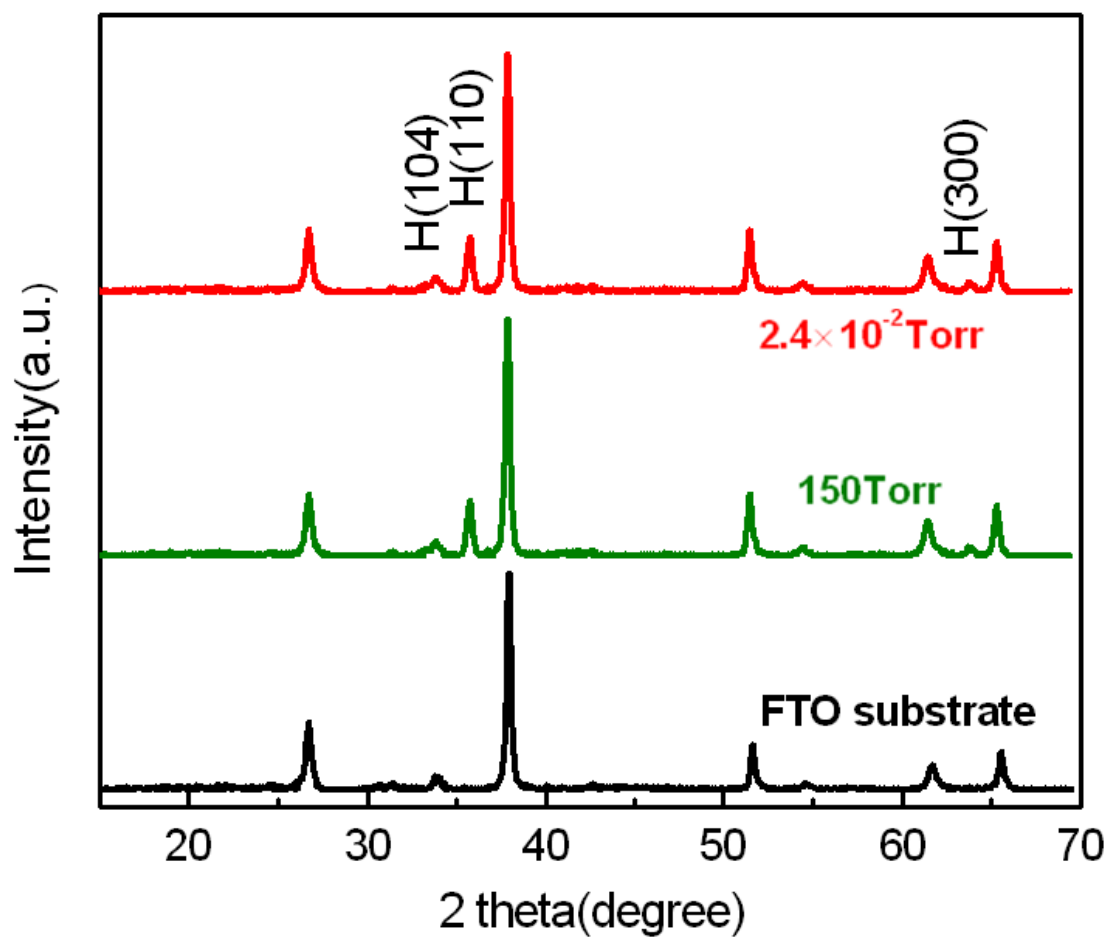


Figure S4: XRD spectra of Ti-doped hematite nanostructures sintered in various partial oxygen pressures.

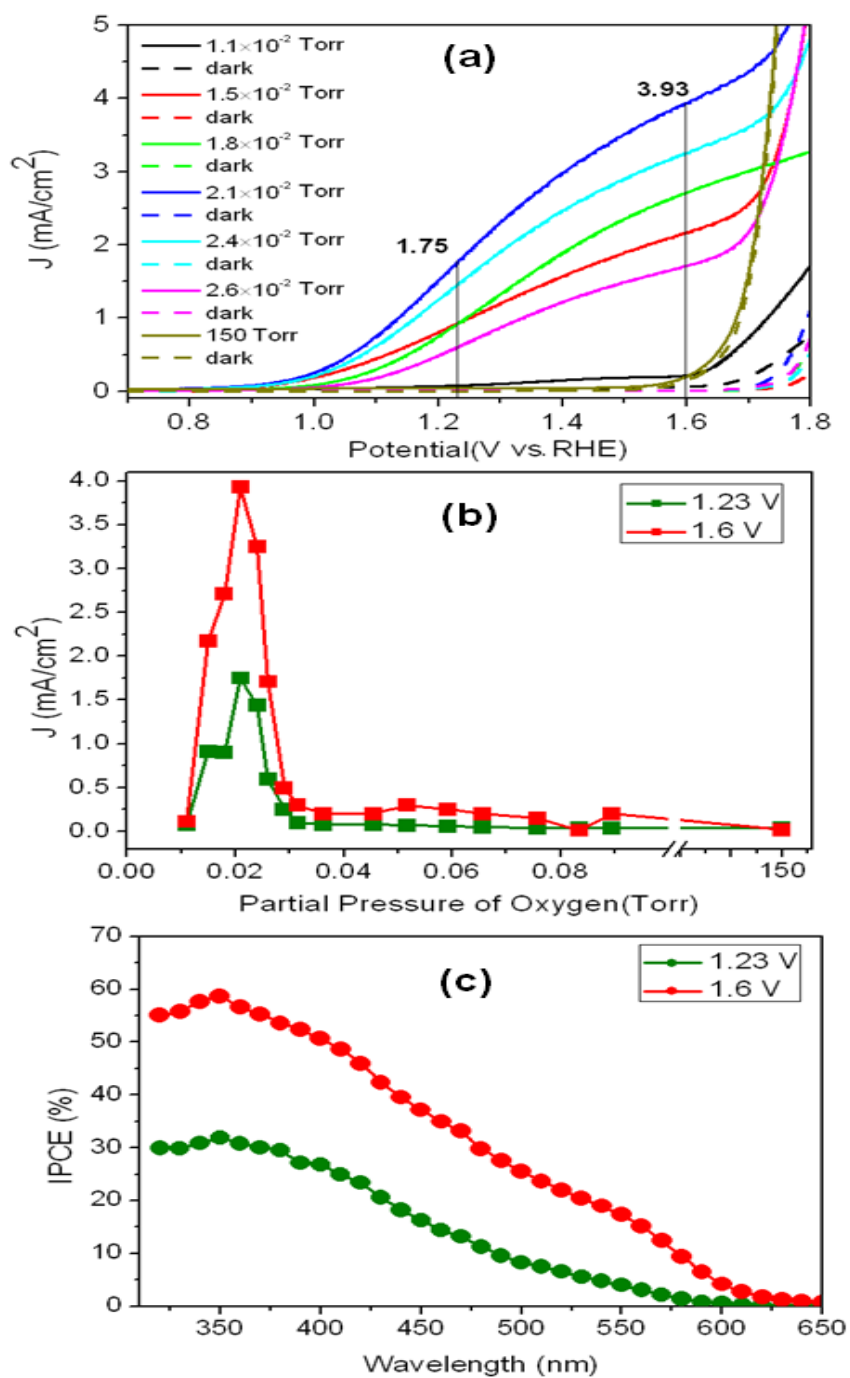


Figure S5: (a) J - V scans for undoped hematite sintered in various partial oxygen pressures at 550 °C. (b) Photocurrent density of undoped hematite at 1.23 and 1.6 V vs. RHE as a function of partial oxygen pressure. (c) IPCE spectra for undoped hematite sintered in a partial oxygen pressure of 2.1×10^{-2} Torr at 1.23 (green) and 1.6 (red) V vs. RHE.

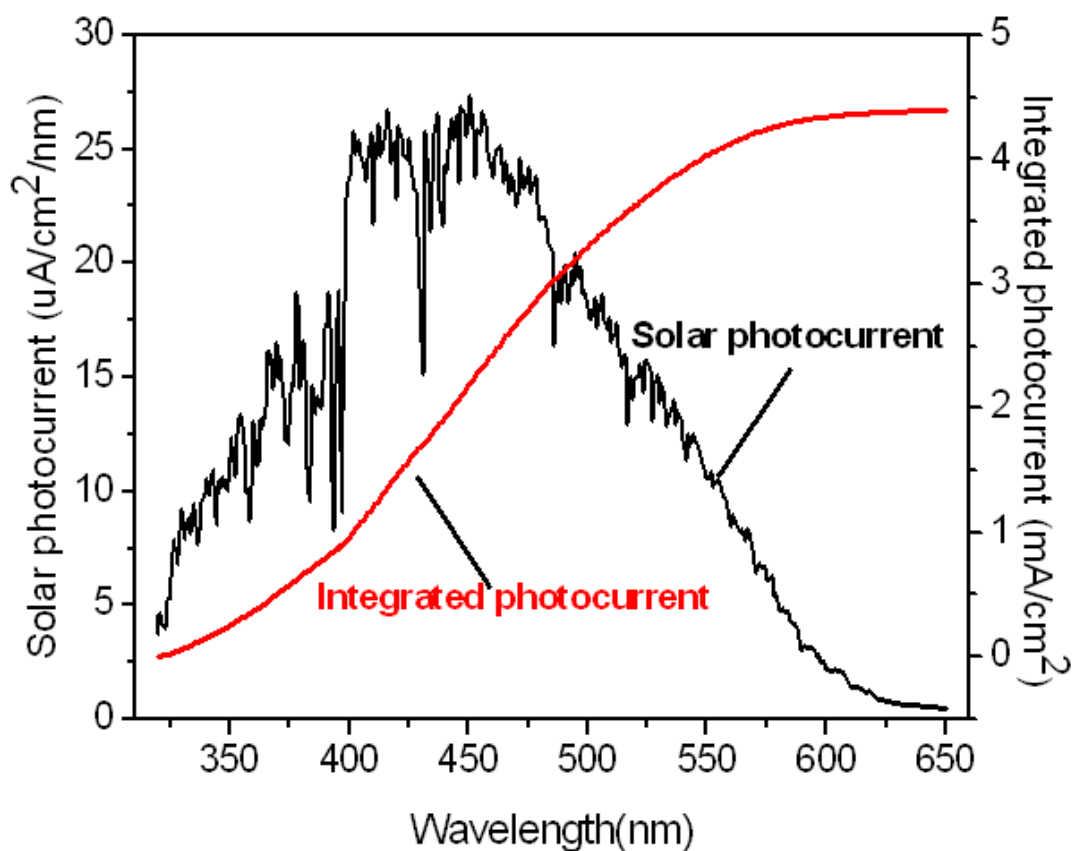


Figure S6: The integrated photocurrent based on the IPCE data (320 nm to 650nm) at 1.6 V vs. RHE. The photocurrent density was calculated by integrating the IPCE spectra with a standard AM 1.5G solar spectrum (ASTMG-173-03), using the following equation:

$$I = \int_{350}^{650} \frac{1}{1240} \lambda IPCE(\lambda) E(\lambda) d\lambda$$

where $E(\lambda)$ is the solar spectral irradiance at a specific wavelength (λ) and $IPCE(\lambda)$ is the obtained IPCE profile as a function of wavelengths (λ) at 1.6 V vs. RHE. The integrated photocurrent at 1.23 V vs. RHE was calculated by a similar way. The calculated photocurrents are 2.04 mA cm⁻² and 4.41 mA cm⁻² at 1.23 and 1.6 V vs. RHE, respectively.

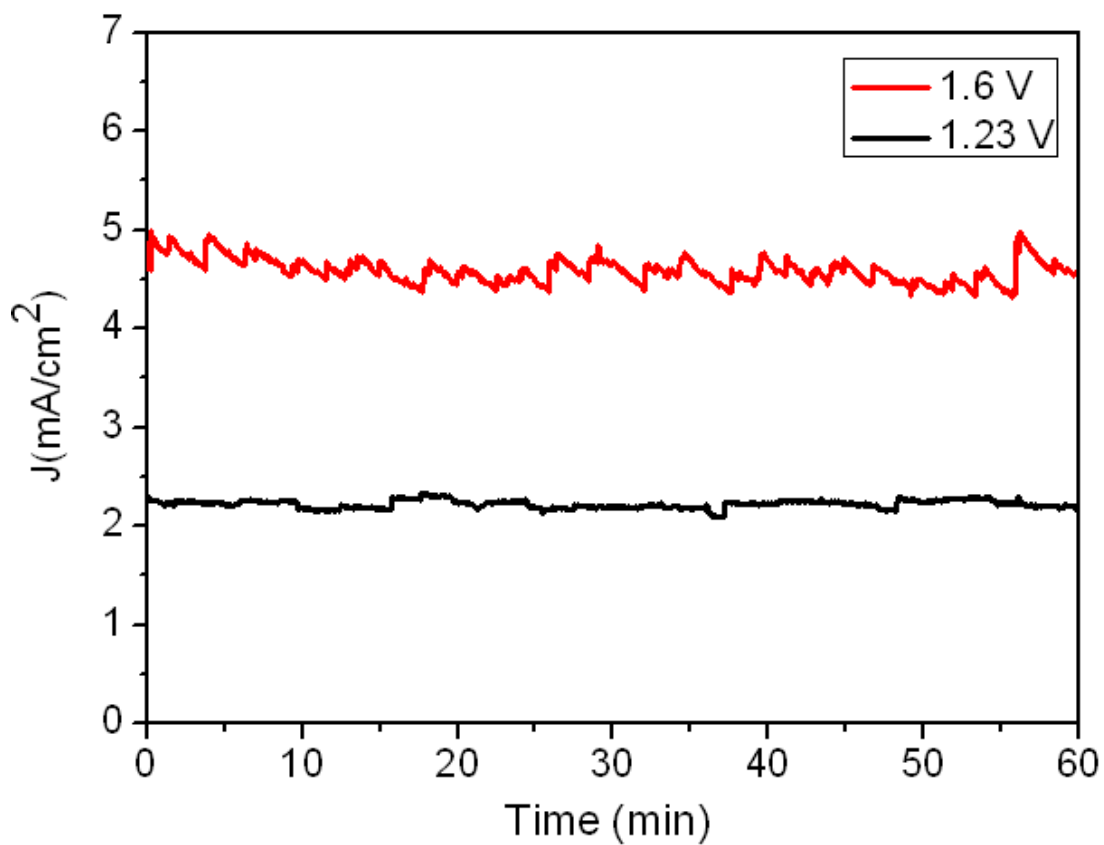


Figure S7: Photochemical stability curves for the Ti-doped sample (2.4×10^{-2} Torr) collected at 1.23 V and 1.6 V vs. RHE.

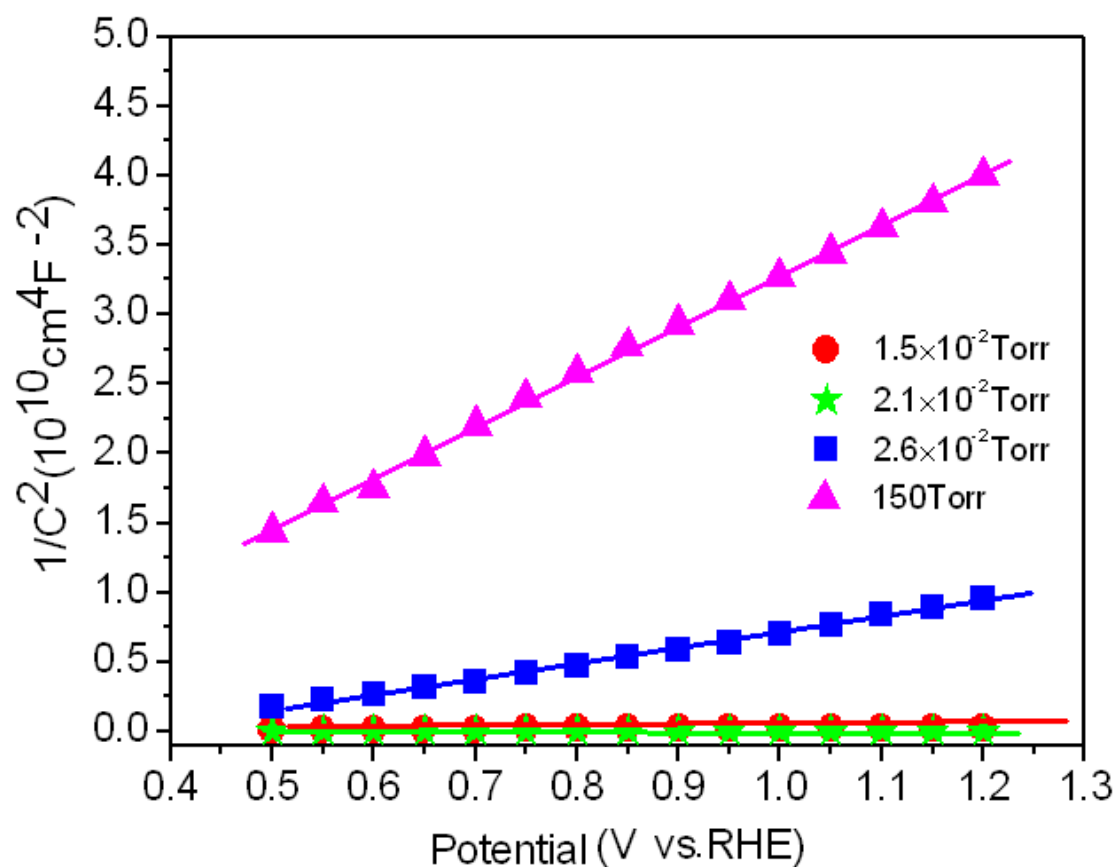


Figure S8: Mott-Schottky plots of undoped hematite samples sintered in various partial oxygen pressures at 550 °C. Results show that the best donor density of undoped hematite sample is $3.73 \times 10^{20} \text{ cm}^{-3}$ at 2.1×10^{-2} Torr, while the donor densities of other samples are $6.19 \times 10^{19} \text{ cm}^{-3}$ at 1.5×10^{-2} Torr, $1.5 \times 10^{18} \text{ cm}^{-3}$ at 2.6×10^{-2} Torr and $4.8 \times 10^{17} \text{ cm}^{-3}$ at 150 Torr.