Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary information

Beta-Fe_2O_3 nanoparticle-assembled film for photoelectrochemical water splitting

Ningsi Zhang [a], Yongsheng Guo[a], Xin Wang [a], Shiying Zhang [b], Zhaosheng Li [a,*],Zhigang Zou [a]

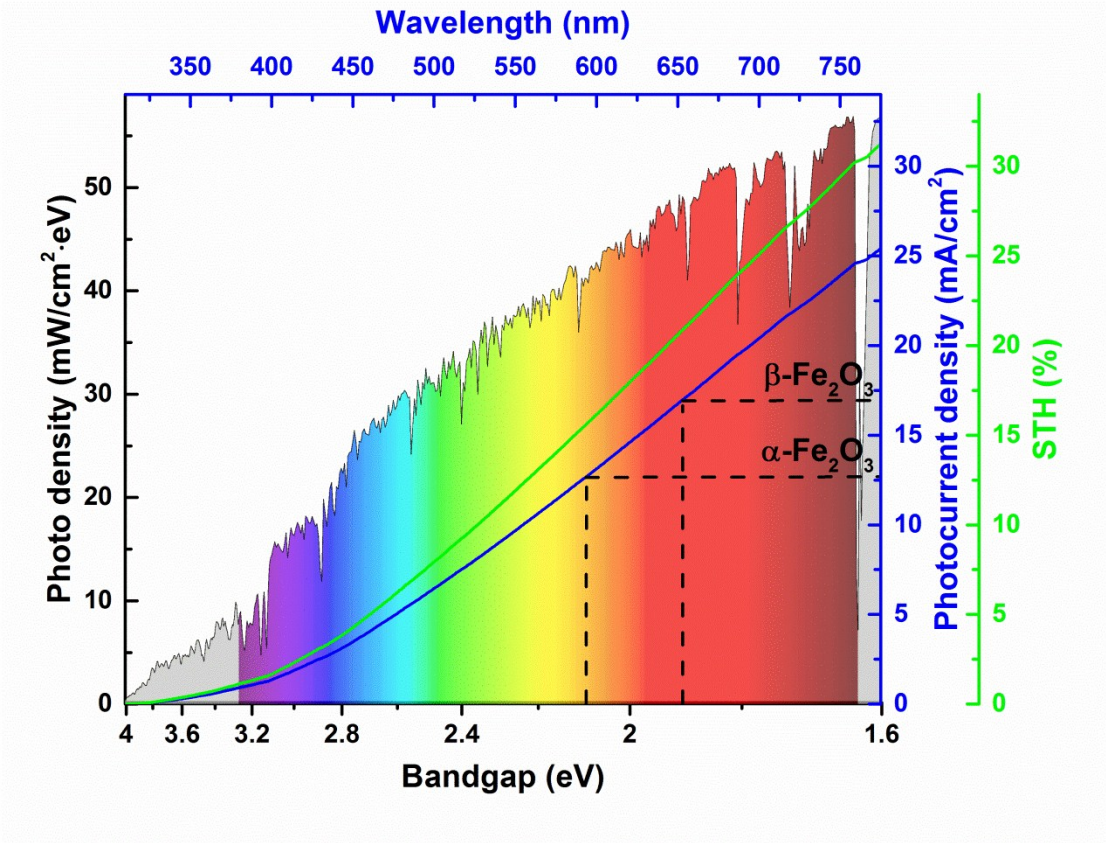

Figure S1. The theoretical value of saturated photocurrent and solar to hydrogen conversion efficiency (STH) calculate by integrating standard solar spectrum AM1.5G (NASA 2013).

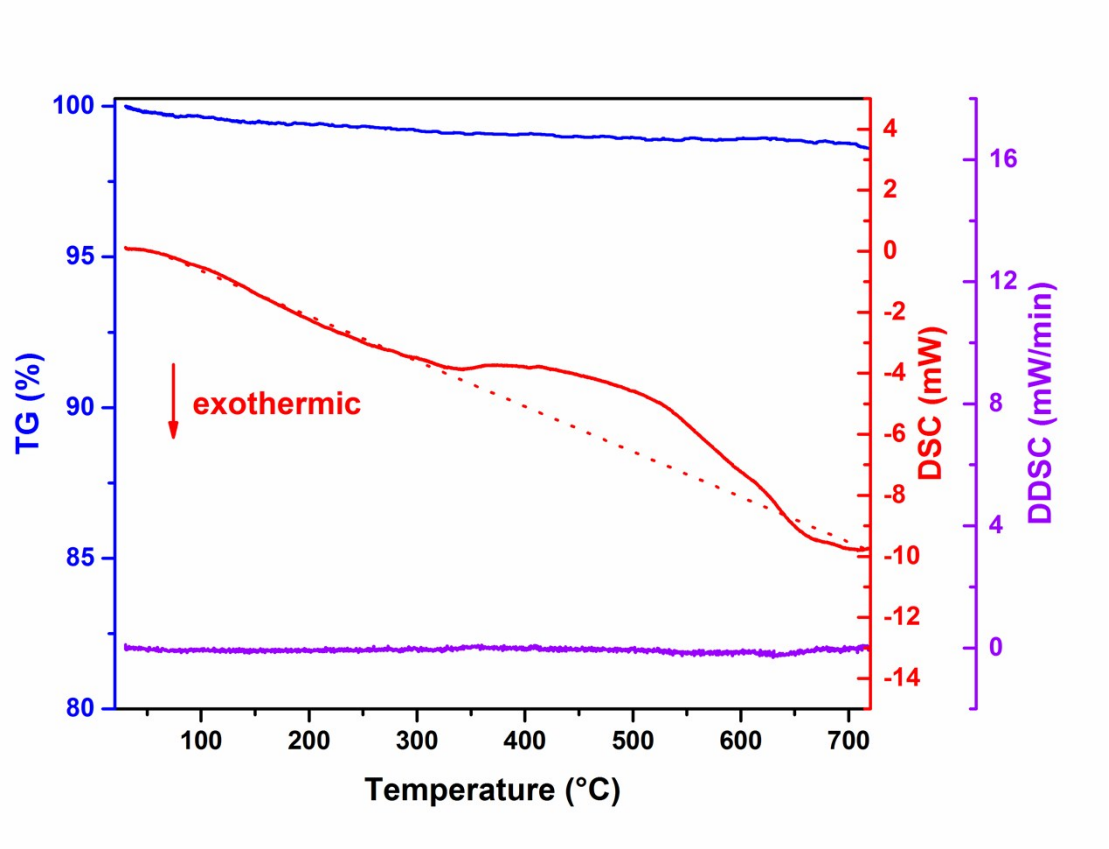

Figure S2. Differential thermal analysis of beta iron oxide nanopowder.

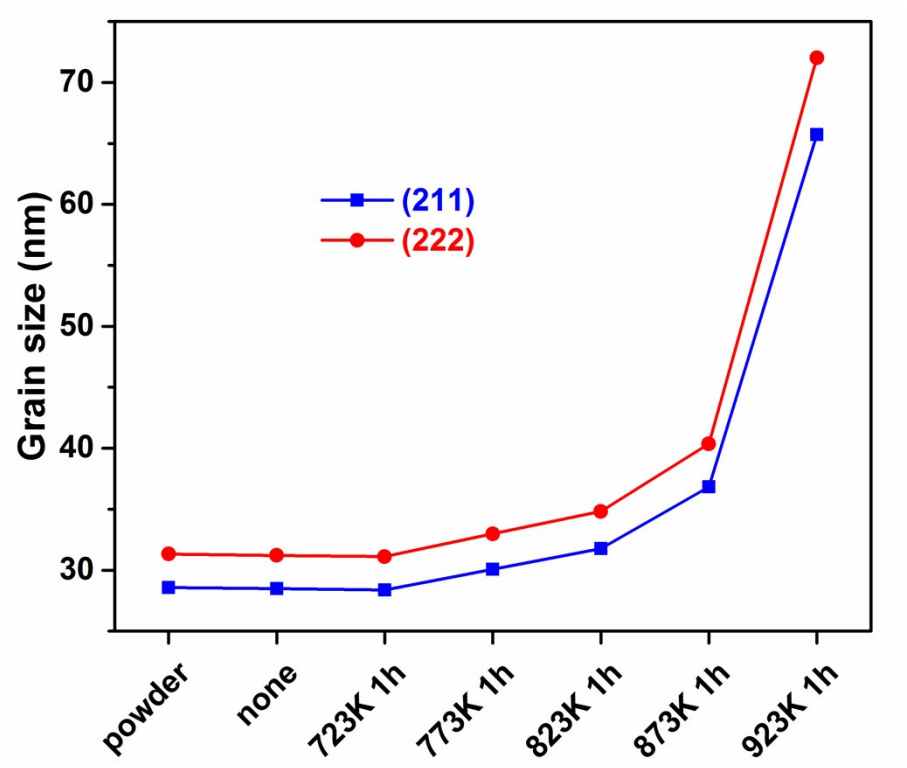

Figure S3. The grain size of β-Fe_2O_3 nanopowder and photoanode annealed at different temperature. Debye-Scherrer formula: $D = K\gamma/Bcos\theta$ was used to calculate the average grain size of two grain orientations (211) and (222).

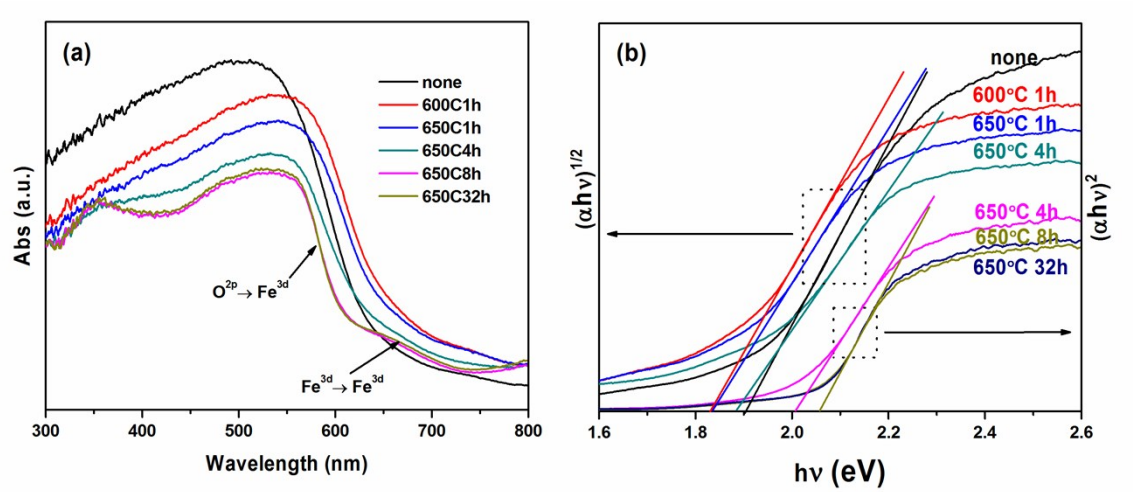

Figure S4. UV-vis diffuse reflection spectra and band gap obtained by Tauc plot of beta-Fe_2O_3 photoanode annealed at different temperature. The sample annealed at 650°C for 1hour contains a small amount of α-Fe_2O_3, exhibit the properties of direct band gap semiconductor. The sample annealed at 650°C for 32hours pure α-Fe_2O_3, exhibit the properties of indirect band gap semiconductor.

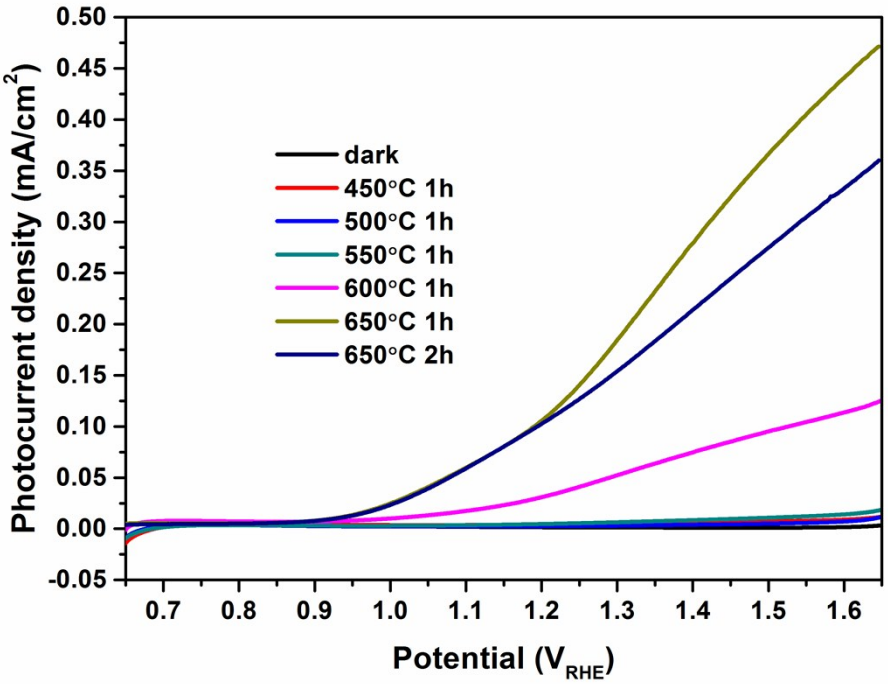

Figure S5. Photocurrent density of photoanode after heat treatment with different annealing temperature. Light source is solar AAA(Newport) and use 1mol/L NaOH as electrolyte.

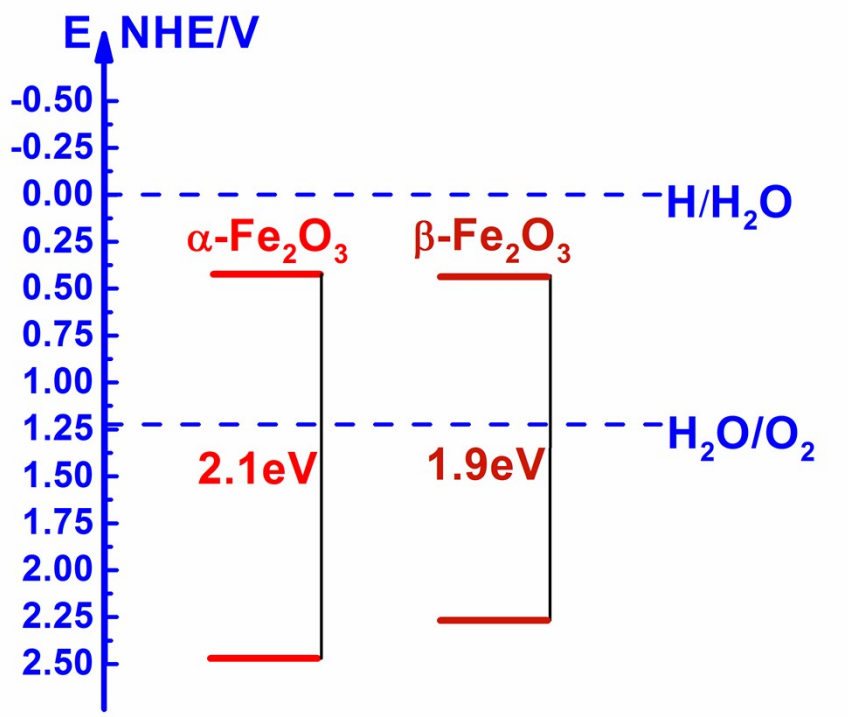

Figure S6. The schematic diagram of energy band. Band edges of α-Fe_2O_3 and β-Fe_2O_3 are obtained by GGA+U method via VASP package. fermi level and band edges are revised with the 1s orbit core states of the off-defect oxygen ions.

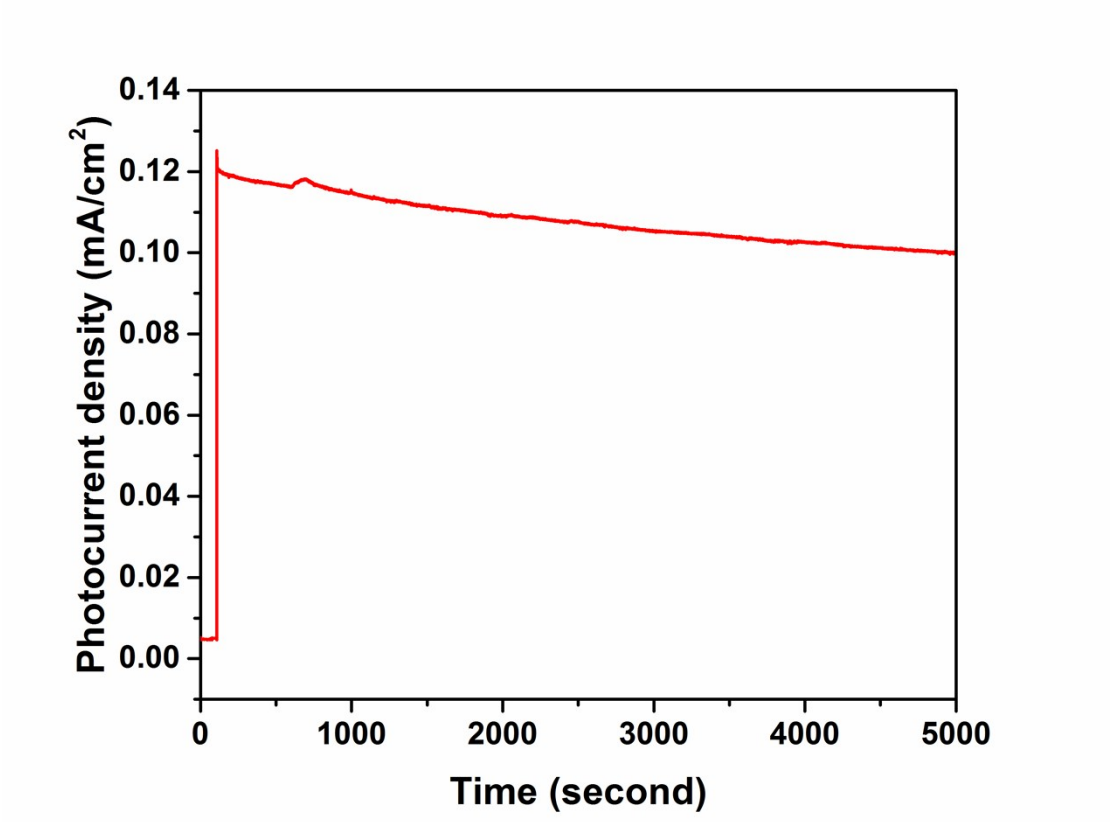

Figure S7. The I-t curve of β-Fe_2O_3 photoanode annealed at 600°C for 1h. Light source is solar AAA(Newport) and use 1mol/L NaOH as electrolyte.

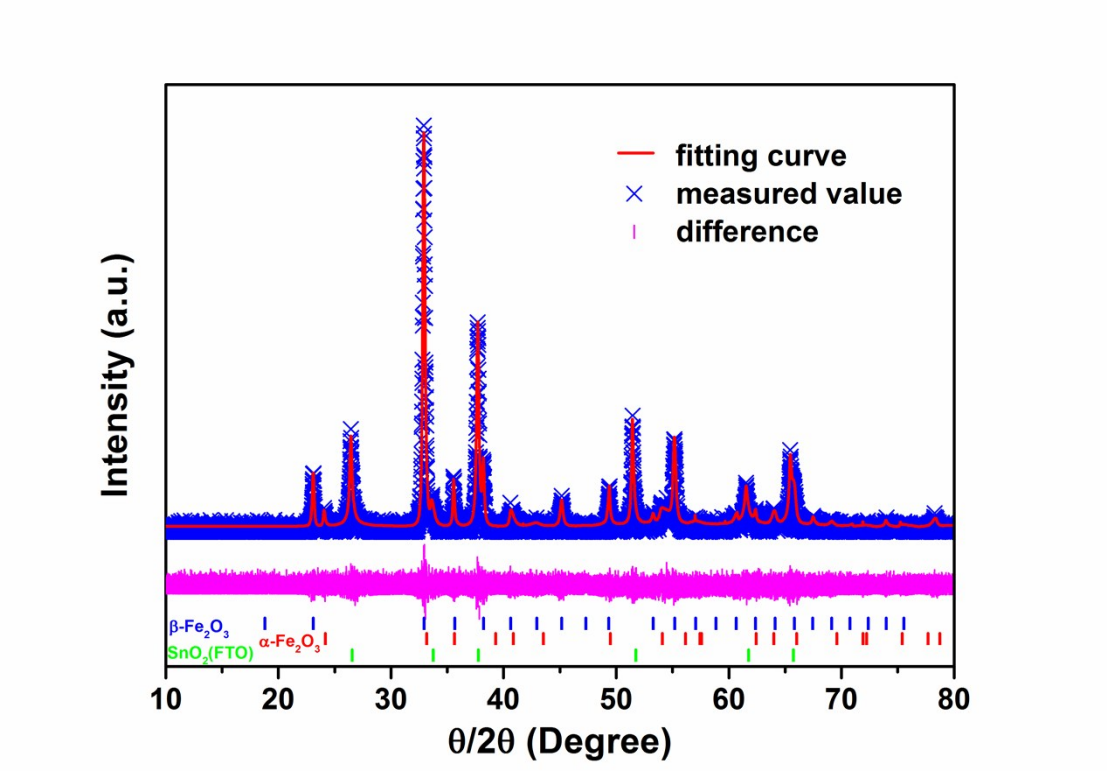

Figure S8. The rietveld refinement of XRD pattern of β-Fe_2O_3 annealed at 650°C for 1h. The content of alpha- Fe_2O_3 is 10.2%(α:β≈1:9)and the error factor R=7.84%.