Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

High temperature activation of hematite nanorods for sunlight driven water oxidation reaction

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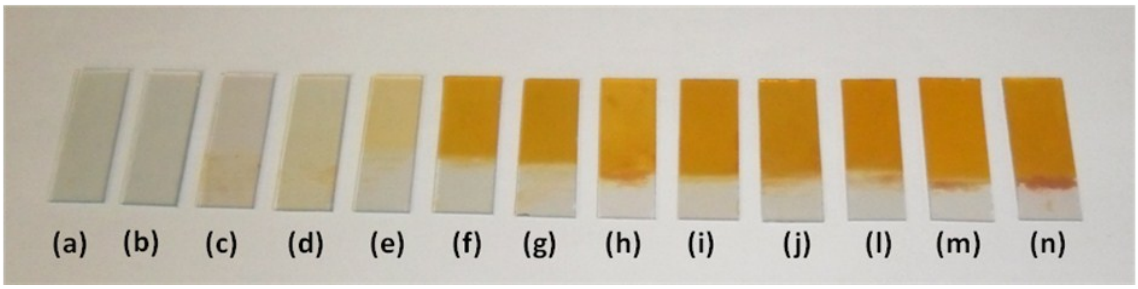

Fig. S1. Picture of as-synthesized films obtained at different time in iron oxyhydroxide phase (*β*-FeOOH) by purpose built material (*PBM*) method; (a) pure FTO substrate, (b) 0.25 h, (c) 0.5 h, (d) 0.75 h (e) 1 h, (f) 2 h (g) 3 h (h) 4 h (i) 5 h, (j) 6 h (l) 8 h (m) h 12 (n) 24 h.

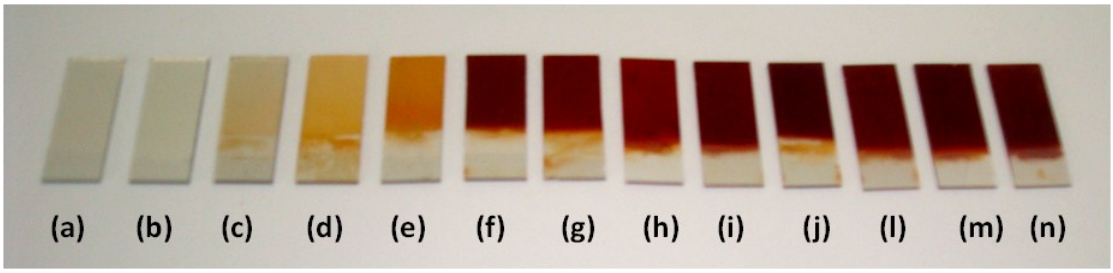

Fig. S2. Pictures of as-synthesized film at different time in hematite phase after annealing at 390 °C per 1h. (a) pure FTO substrate, (b) 0.25 h, (c) 0.5 h, (d) 0.75 h (e) 1 h, (f) 2 h (g) 3 h (h) 4 h (i) 5 h, (j) 6 h (l) 8 h (m) h 12 (n) 24 h.

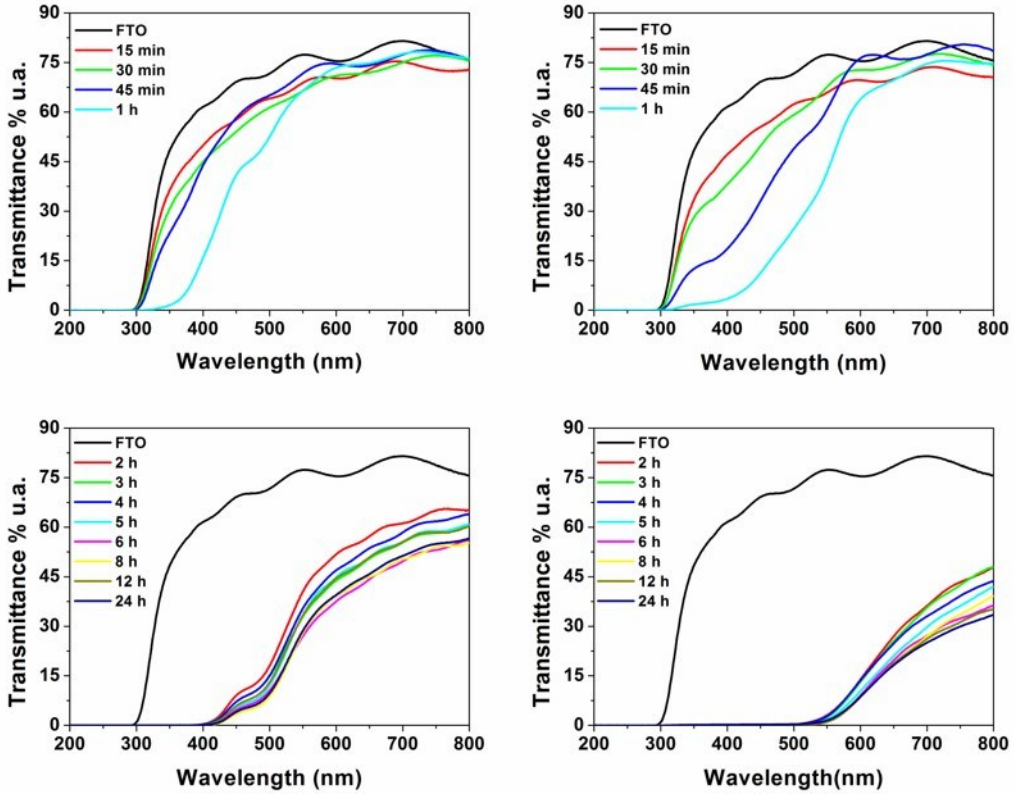

Figure S3: Transmittance (%) versus wavelength (nm) curves measured for the as-synthesized film before annealing treatment: (a) and (c) *β*-FeOOH films (yellow), and after annealing treatment at low 390 ^{o}C per 1h: (b) and (d) hematite films (red-brown).

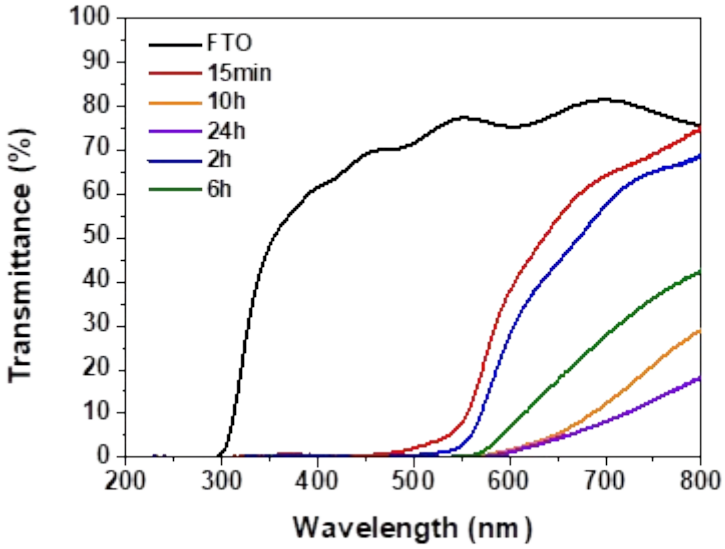

Figure S4: Transmittance (%) versus wavelength (nm) curves measured for the as-synthesized film annealed at 750 ^{o}C per 30 min.

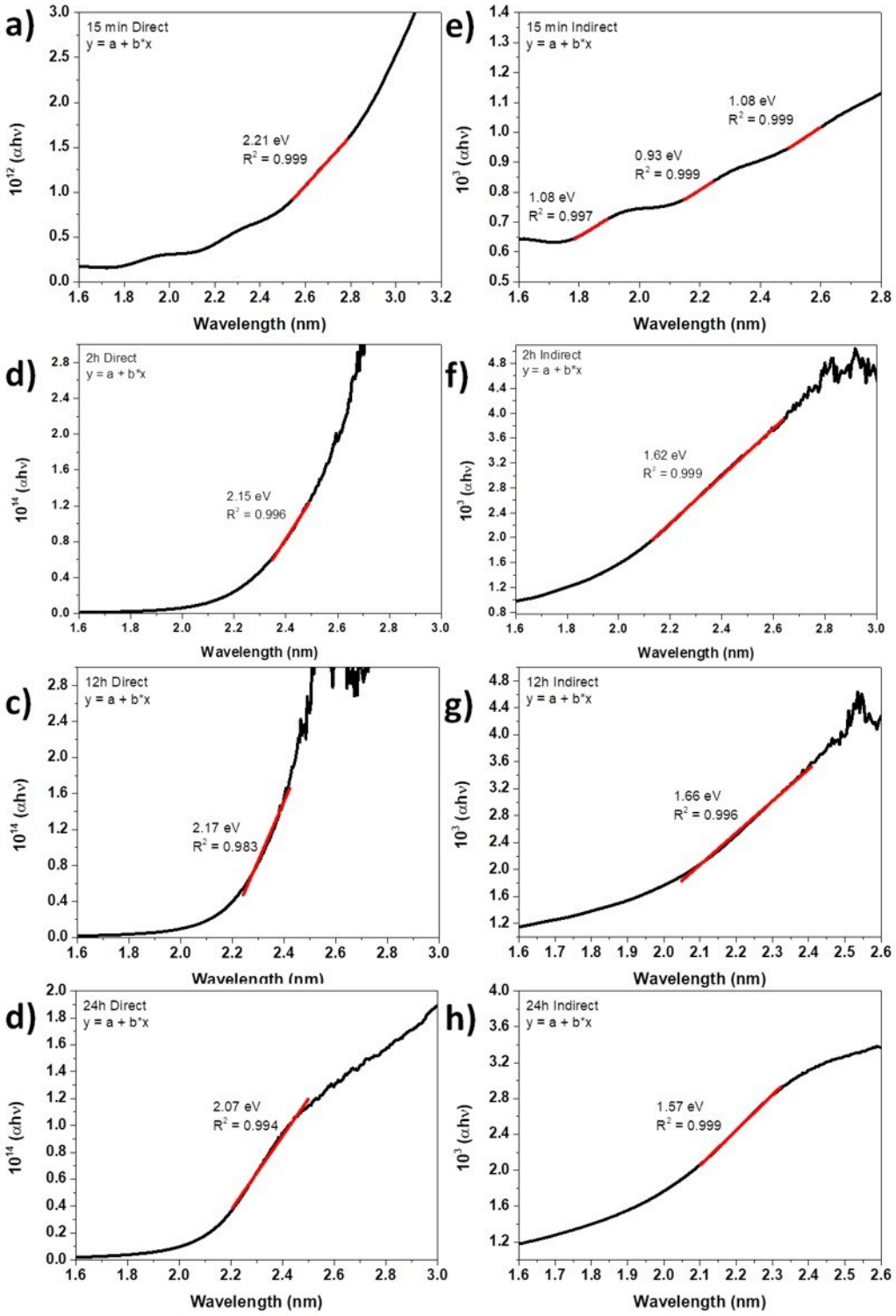

Fig. S5 Plot of absorption data according to reference (38) in the manuscript: (Left side) direct band gap. (right side) indirect optical band gap for hematite films annealed at 390 ^{o}C per 1 hour.

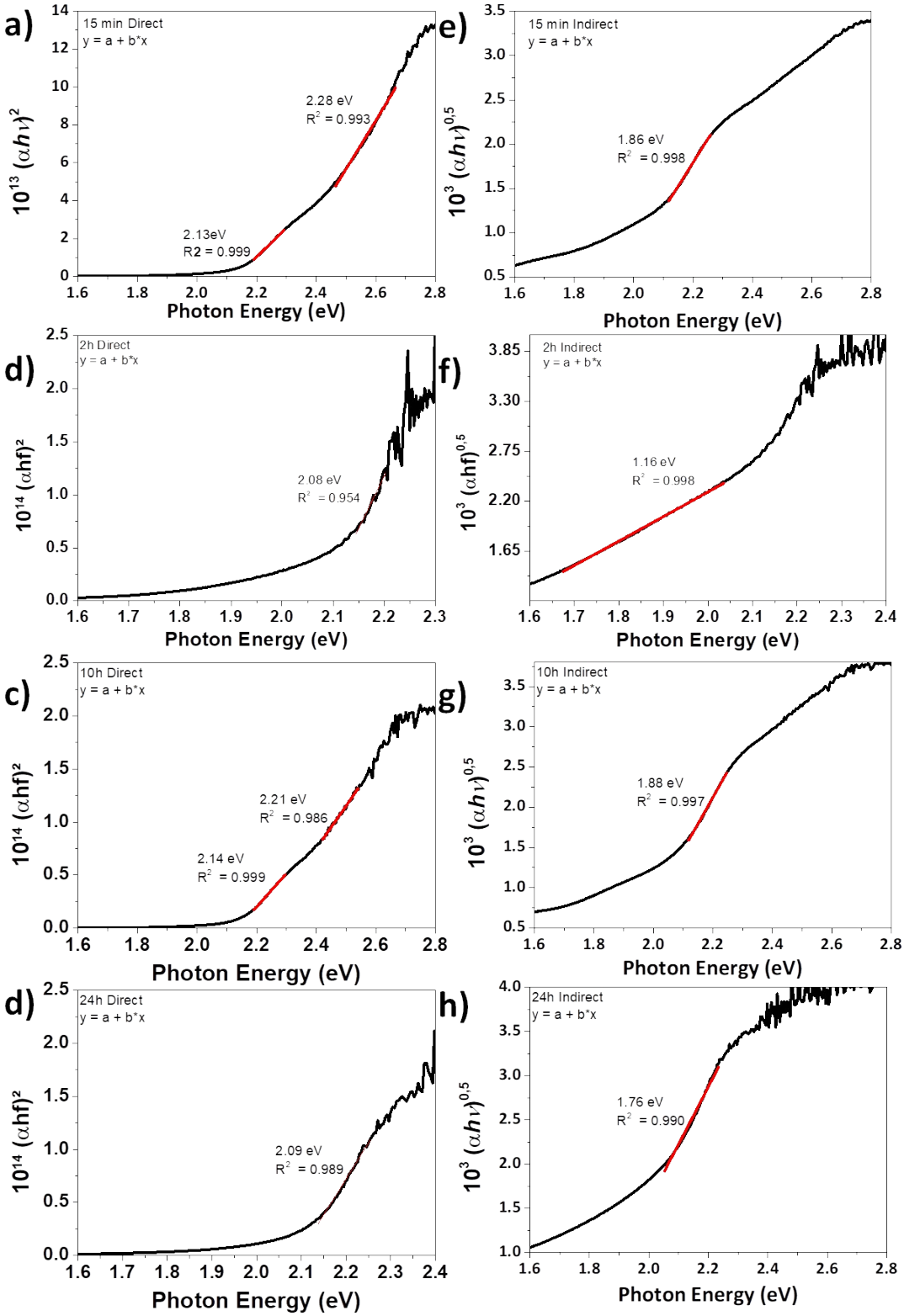

Fig. S6 Plot of absorption data according to the reference (38) in the manuscript: (Left side) direct band gap. (right side) indirect optical band gap for hematite films annealed

at 750 ^{o}C per 1 hour.

Table S1. Lattice parameters and the preferential crystal orientation plane (P.O.) for the hematite films synthesized at different time and annealed at 390 °C per 1h.

Samples	a (Å)	c (Å)	V (Å^3)	P.O.
JCPDS	*5.04*	*13.7*	*302*	
0.25 h	5.09 (±0.06)	13.1 (±0.2)	295 (±8)	104
0.5 h	5.11 (±0.05)	13.1 (±0.2)	296 (±7)	116
0.75 h	5.11 (±0.05)	13.1 (±0.2)	296 (±7)	116
1 h	5.04 (±0.07)	13.3 (±0.3)	292 (±9)	104
2 h	5.06 (±0.03)	13.2 (±0.2)	293 (±5)	300
3 h	5.07 (±0.03)	13.2 (±0.2)	294 (±6)	300
4 h	5.07 (±0.03)	13.2 (±0.2)	293 (±6)	300
5 h	5.06 (±0.03)	13.2 (±0.2)	293 (±6)	104
6 h	5.06 (±0.04)	13.2 (±0.2)	292 (±6)	104
8 h	5.06 (±0.04)	13.2 (±0.2)	293 (±6)	300
24 h	5.03 (±0.07)	13.2 (±0.3)	290 (±9)	116

Table S2. Lattice parameters and the preferential crystal orientation plane (P.O.) of hematite films annealed at 750 °C per 0.5h.

Samples	**Lattice parameter**			
	a (Å)	c (Å)	V ($Å^3$)	P.O.
JCPDS	5.04	13.7	302	
0.25 h	4.98 (±0.03)	13.2 (±0.2)	295 (±4)	110
2 h	4.98 (±0.02)	13.2 (±0.2)	285 (±4)	110
6 h	4.98 (±0.02)	13.2 (±0.2)	285 (±4)	110
10 h	4.98 (±0.03)	13.2 (±0.2)	284 (±4)	110
24 h	4.97 (±0.03)	13.1 (±0.2)	281 (±4)	110

Table S3. Direct and indirect optical band gap calculated from the electronic transition spectra for hematite films annealed at 390 °C per 1h.

Synthesis time	Direct optical band gap (eV)	Indirect optical band gap (eV)
24 h	2.07	1.57
12 h	2.17	1.66
8 h	2.16	1.63
6 h	2.16	1.62
5 h	2.15	1.64
4 h	2.19	1.62
3 h	2.14	1.59
2 h	2.15	1.62
1 h	2.60	1.62
45 min	2.68	1.63
30 min	2.88	1.25
15 min	2.21	1.08 and 0.93

Table S4. Direct and indirect optical band gap calculated from the electronic transition spectra for hematite films annealed at 750 °C per 0.5h.

Synthesis time	Direct optical band gap (eV)	Indirect optical band gap (eV)
24 h	2.09	1.76
10 h	2.21	1.88
6 h	2.01	1.7
2 h	2.08	1.16
15 min	2.28 and 2.13	1.86

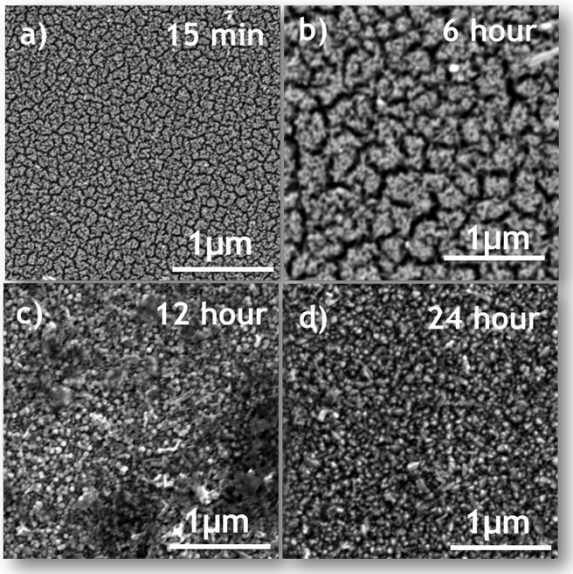

Fig. S7. Top-view scanning electron microscopy (SEM) images of the as-synthesized films at (a) 15 min, (b) 6 h, (c) 12 h (d) 24 h and annealed at 750 °C for 0.5 hour.

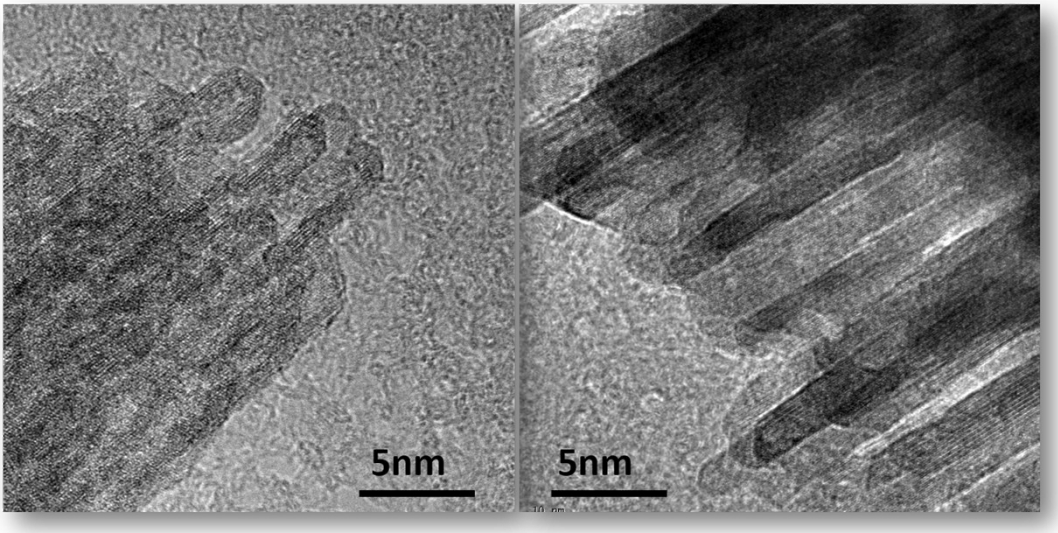

Fig. S8. Transmission electron microscopy (TEM) images of the hematite films obtained at 6 hours and annealed at (a) 390 for 1.0 hour and (b) 750 °C for 0.5 hour.

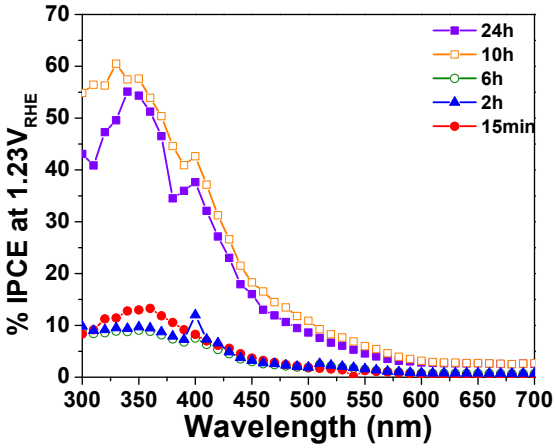

Fig. S9. IPCE curve at 1.23 V_{RHE} for the hematite electrodes synthesized during 0.25, 2, 6, 10 and 24 hours with additional thermal treatment at 750 °C per 0.5h.