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Surface passivation of hematite photoanodes using iron phosphate

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Table. S1. Different percentages of elements obtained from EDS analysis for crystalline and amorphous iron phosphate

Element	Weight%	Atomic%
Crystalline		
O	23.04	67.42
P	0.42	0.63
Fe	3.95	3.31
Sn	72.59	28.63
Sum	100.00	100.00
Amorphous		
O	23.71	67.68
P	0.67	0.99

Fe	5.16	4.22
Sn	70.47	27.12
Sum	100.00	100.00

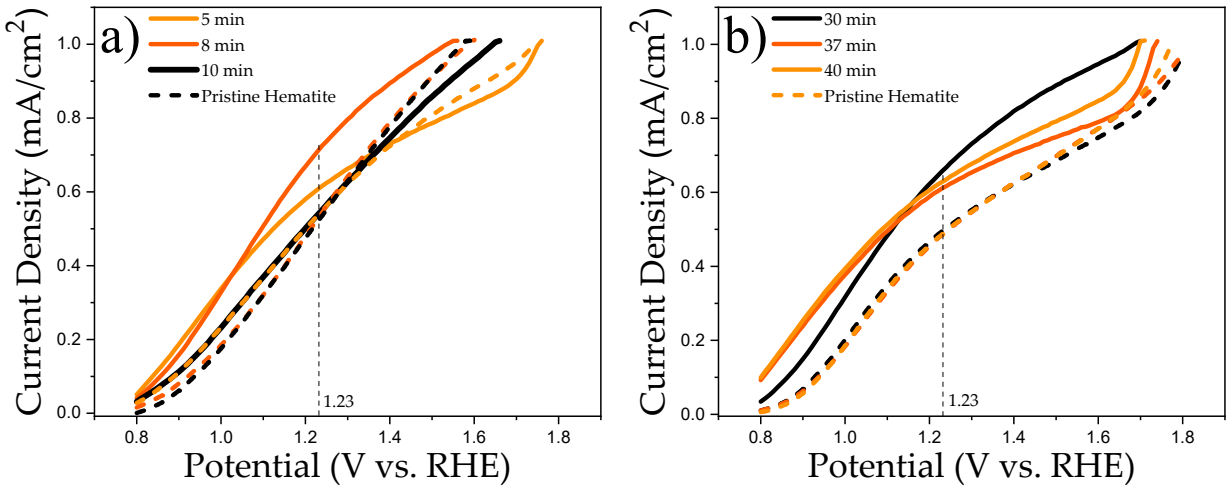

Figure. S1. J-V curves of the samples with different deposition time for $FePO_4.2H_2O$ in **a)** crystalline and **b)** amorphous states at 1.23 V vs. RHE under 1.5 G AM light.

Table. S2. Photocurrent density for thin films of (α-Fe_2O_3) and modified with crystalline and amorphous iron phosphate, with different thicknesses at 1.23 V vs. RHE.

Sample	**Current density ($mA.cm^{-2}$) of (α-Fe_2O_3)**	**Current density ($mA.cm^{-2}$) of (α-Fe_2O_3/Fe-Pi)**	**V_{on} (V vs. RHE) before and after the modification**

Crystalline			
5 min	0.53	0.60	0.80 ⟶ 0.75
8 min	0.52	0.71	0.81 ⟶ 0.76
10 min	0.53	0.55	0.83 ⟶ 0.77
Amorphous			
30 min	0.49	0.65	0.83 ⟶ 0.74
37 min	0.48	0.61	0.83 ⟶ 0.72
40 min	0.48	0.62	0.83 ⟶ 0.72

The separation and catalytic efficiencies of the photo electrode were evaluated uisng the method reported by Dotan et al. [1]. The photocurrent relates to the separation and catalytic efficiencies according to the following equation [1]:

$$J_{H_2O} = J_{abs} \times \eta_{separation} \times \eta_{catalytic} \quad (1)$$

where J_{abs} is the photon absorption rate, which is presented as a current. It is determined by multiplying the AM1.5G spectrum by the absorption spectrum followed by integration over wavelength. $\eta_{separation}$ is the charge separation efficiency. $\eta_{catalytic}$ is also the catalytic efficiency for water oxidation. By adding Na_2SO_3 to the electrolyte, it acts as a very effective hole scavenger and the corresponding photocurrent is denoted as $J_{Na_2SO_3}$as following:

$$J_{Na_2SO_3} = J_{abs} \times \eta_{separation} \quad (2)$$

Based on the above two equations, $\eta_{separation}$ and $\eta_{catalytic}$ are obtained according to the following equations:

$$\eta_{catalytic} = \frac{J_{H_2O}}{J_{Na_2SO_3}} \tag{3}$$

$$\eta_{separation} = \frac{J_{Na_2SO_3}}{J_{abs}} \tag{4}$$

1. H. Dotan, K. Sivula, M. Gr_tzel, A. Rothschild, S. C. Warren, Energy Environ. Sci. 2011, 4, 958 –964.