Supporting Information

Photoelectrochemical H_2 evolution using TiO_2-coated $CaFe_2O_4$ without an external applied bias under visible light irradiation at 470 nm based on device modeling

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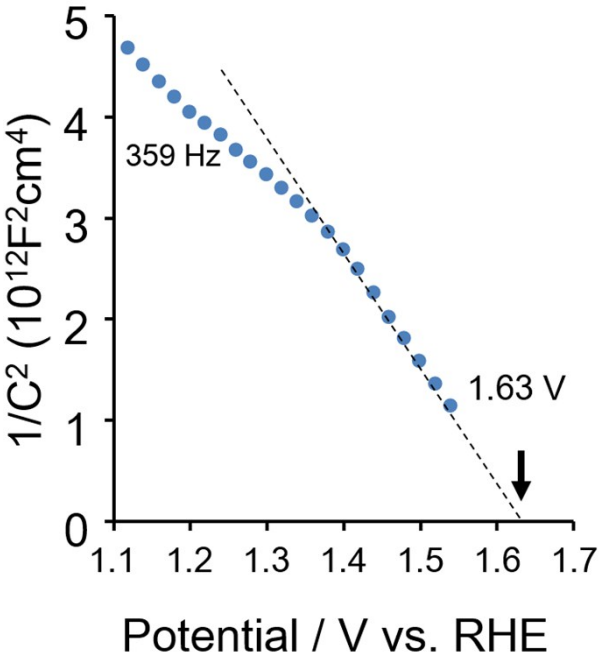

Figure S1 Mott-Schottky plot of a bare CFO electrode in 0.1 M NaOH solution.

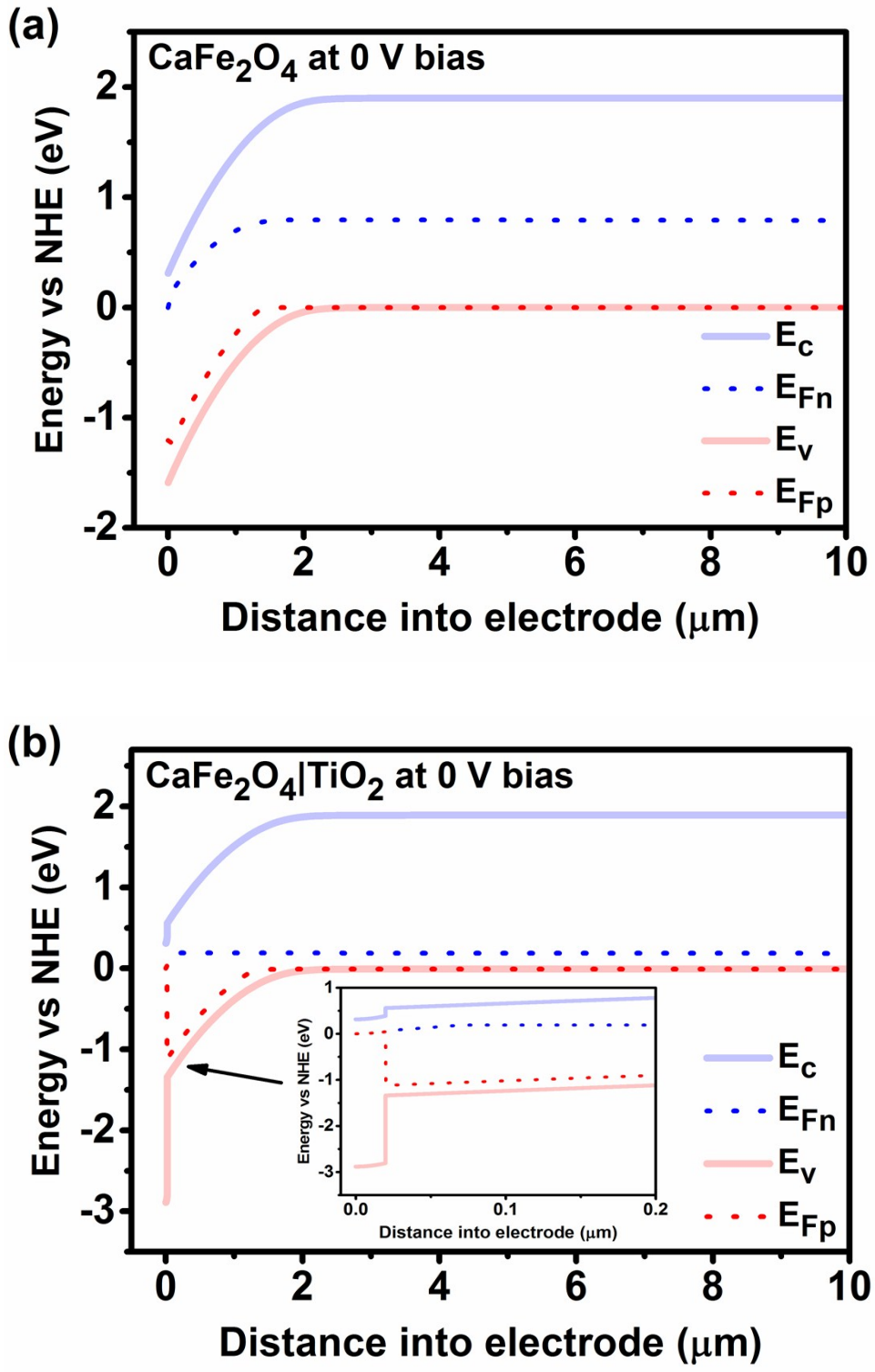

Figure S2. Band structures of $CaFe_2O_4$ and TiO_2-coated $CaFe_2O_4$ electrodes at 0 V vs NHE under 470 nm excitation.

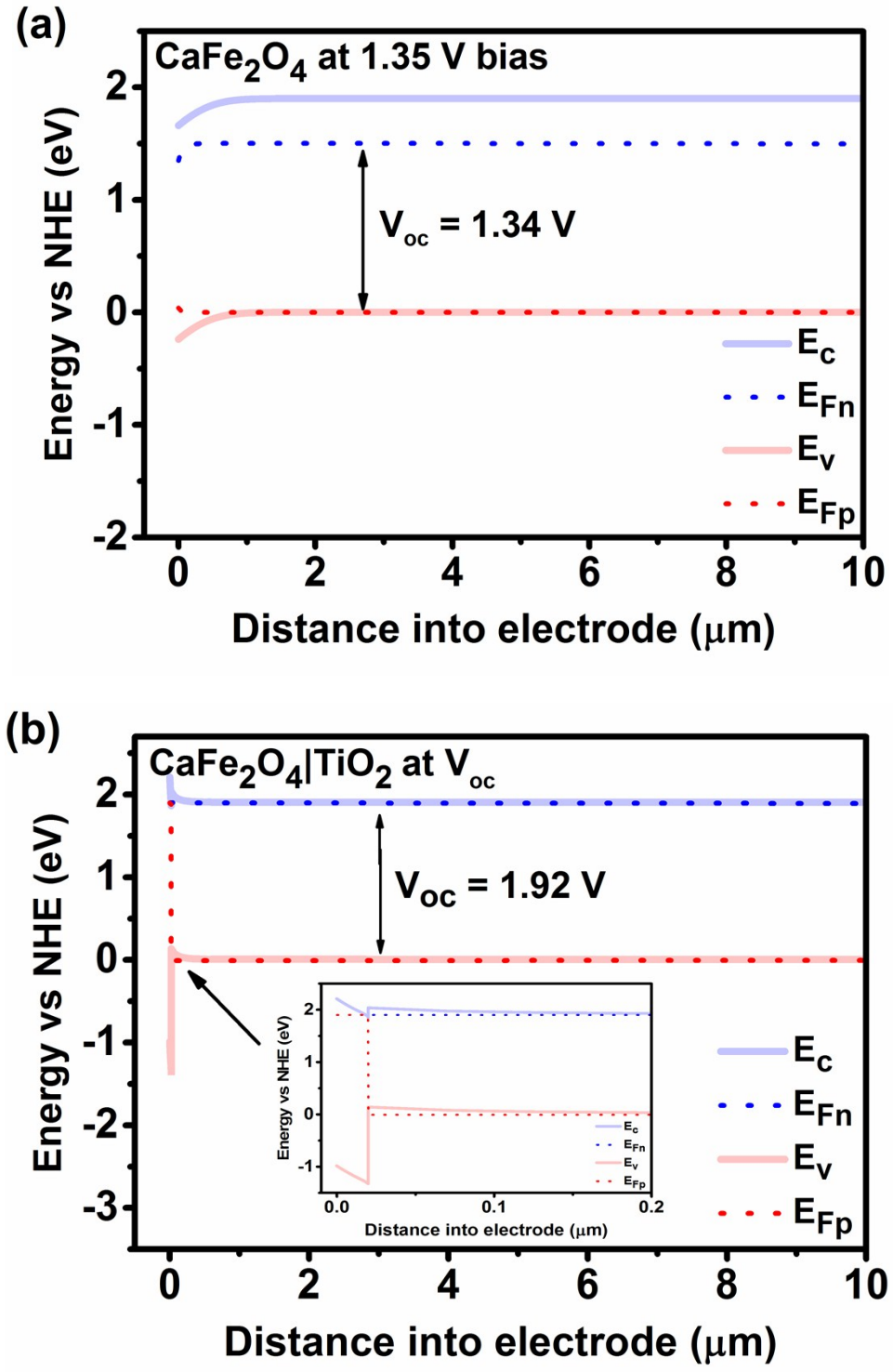

Figure S3. Band structures of $CaFe_2O_4$ and TiO_2-coated $CaFe_2O_4$ electrodes at the onset potential under 470 nm excitation.

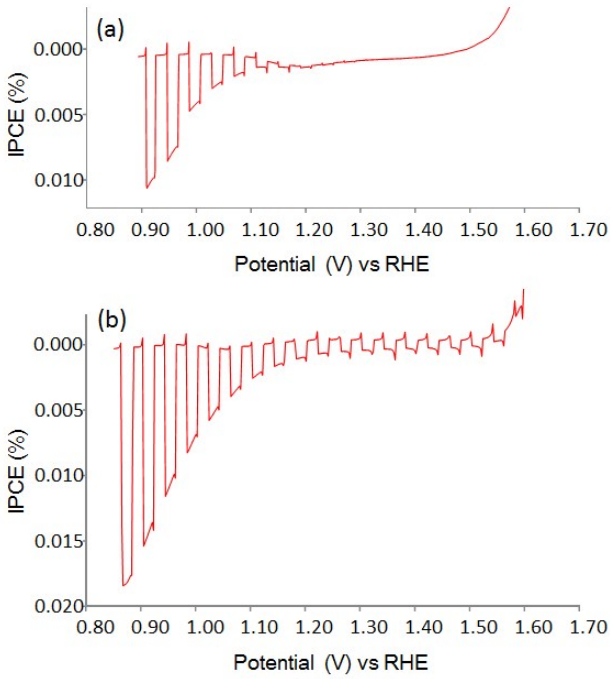

Figure S4. IPCE-potential curves of (a) CFO and (b) TiO_2-coated CFO electrodes in 0.1 M NaOH solution under chopped 470 nm light illumination.

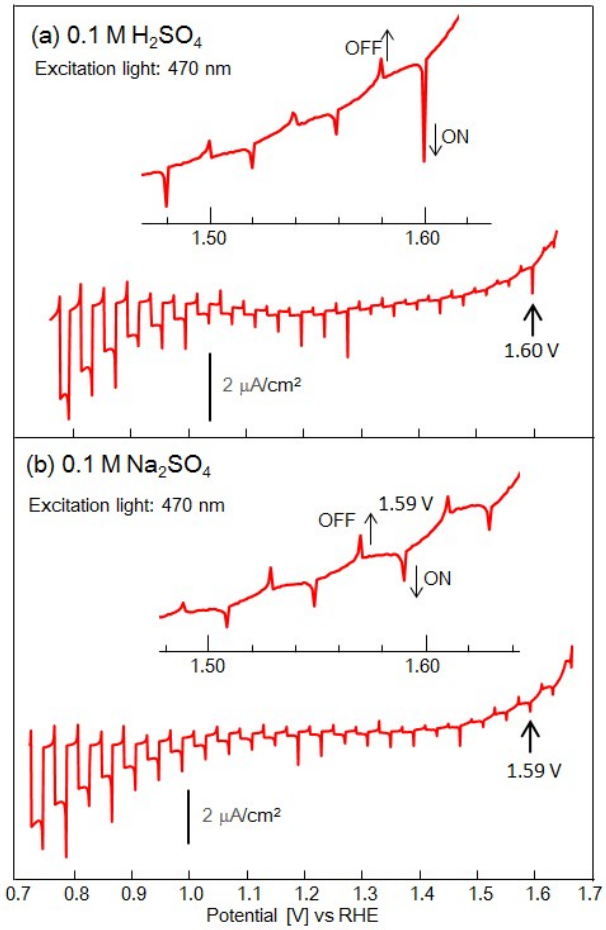

Figure S5. Current-potential curve of TiO_2-coated CFO electrode under chopped light illumination of 470 nm in (a) 0.1 M H_2SO_4 and (b) 0.1 M Na_2SO_4.

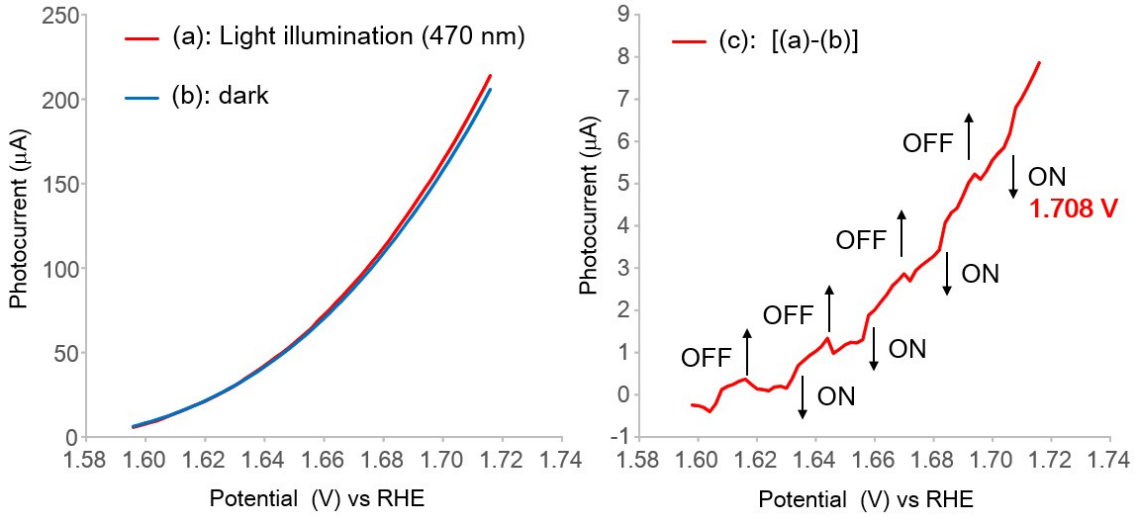

Figure S6 Current-potential curves of TiO_2-coated CFO electrodes in 0.1 M NaOH solution under chopped light illumination (470 nm); (a) light illumination, (b) dark condition and (c) difference spectrum [(a)-(b)].

Table S1. Electronic parameters used as inputs for $CaFe_2O_4$ and $CaFe_2O_4|TiO_2$ photoelectrodes.

Electronic Parameter	Units	$CaFe_2O_4$ (50 μm)	TiO_2 (20nm)
Permittivity		287	50
Band Gap (E_g)	eV	1.9	3.2
Electron Affinity	eV	4.12	4.3
Conduction Band Density of States (N_c)	cm^{-3}	10^{16}	10^{19}
Valence Band Density of States (N_v)	cm^{-3}	10^{16}	10^{19}
Electron Mobility (μ_n)	$cm^2\ V^{-1}\ s^{-1}$	0.01	0.001
Hole Mobility (μ_p)	$cm^2\ V^{-1}\ s^{-1}$	0.05	0.0001
Donor Dopant Density (N_d)	cm^{-3}	0	10^{18}
Acceptor Dopant Density (N_a)	cm^{-3}	10^{16}	0

Table S1-2. Defect parameters used as inputs for TiO_2 layer.

Defect Parameter	Units	Value
Type		Donor-like[1]
Density	cm^{-3}	10^{18}
Energy Level	eV	1.6
Capture Cross Section for Electrons	cm^2	5e-12
Capture Cross Section for Holes	cm^2	5e-12

[1]Discrete energetic distribution