Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supporting Information

A dual-function photoelectrochemical solar cell which assimilates light-harvesting, charge-transport and photoelectrochromic nanomaterials in a tandem design

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Brunauer-Emmett-Teller (BET) surface area analysis and Barrett-Joyner-Halenda (BJH) pore size and volume analysis were performed under Nitrogen at 77.3 K, after degassing at 300 °C for 3 h. This analysis was performed on a Nova 2200e Quantachrome instrument.

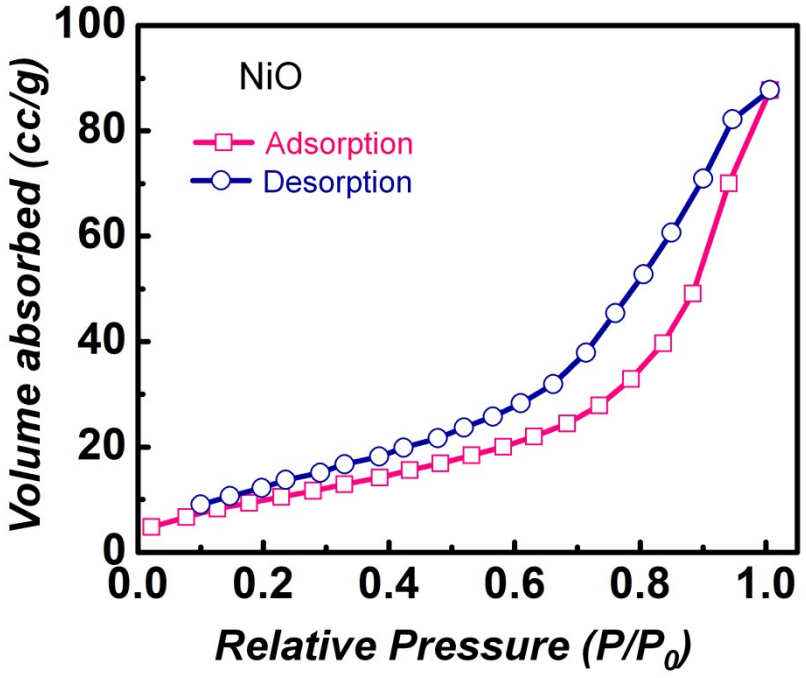

Figure S1 Nitrogen adsorption-desorption isotherm for NiO.

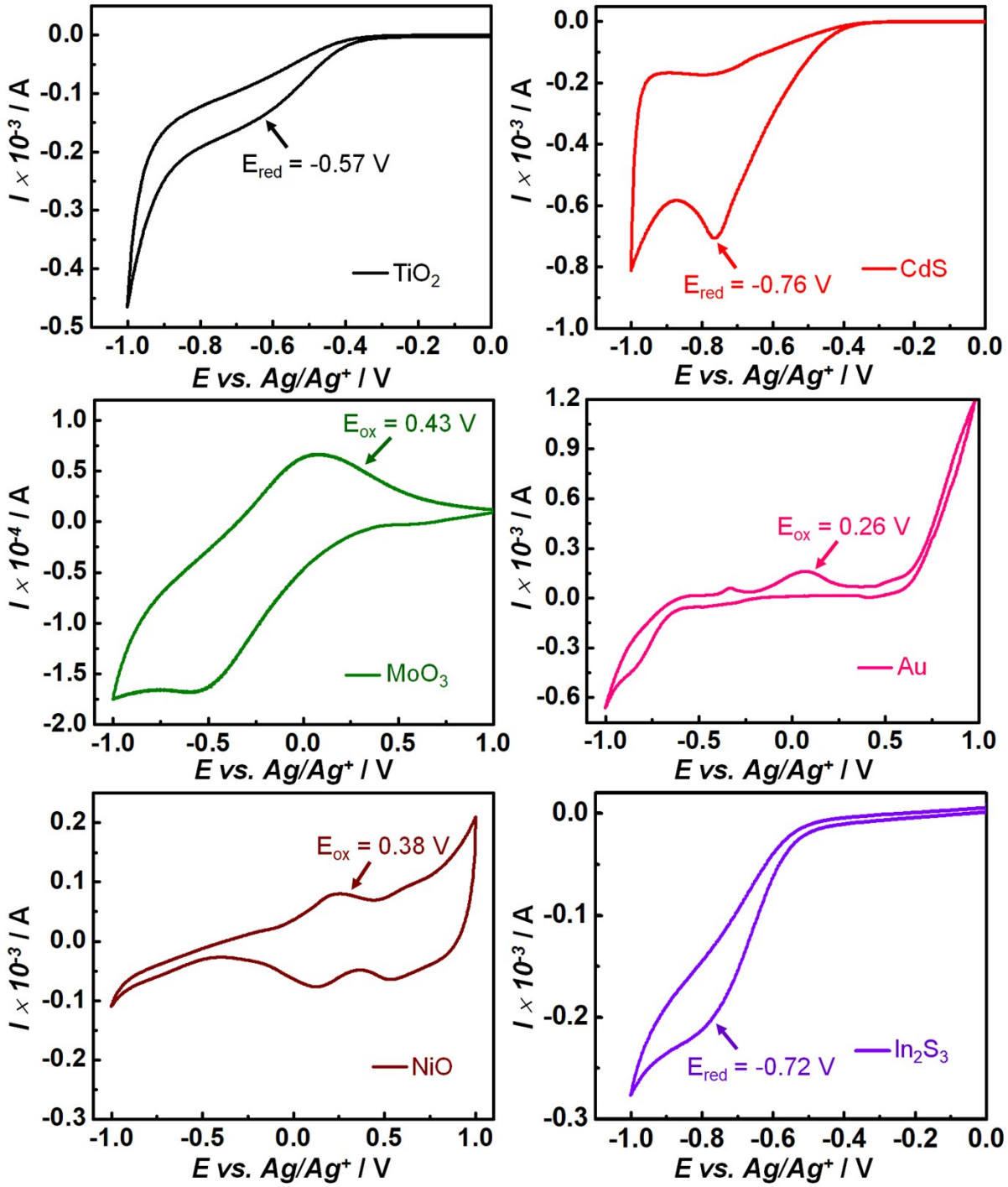

Figure S2 Cyclic voltammograms of TiO_2, CdS, MoO_3, Au, NiO and In_2S_3 films deposited over FTO substrates.All plots were recorded in a 0.1 M KCl solution as electrolyte, with a Pt rod as the counter electrode and Ag/AgCl/KCl as the reference electrode, at a scan rate of 20 mVs^{-1}.

The HOMO (VB), LUMO (CB) and band gap values of different materials used in PECD fabrication were acquired from cyclic voltammograms and absorbance spectra using the equations provided below.

E_{red} = –4.5 eV (≡ 0 V *versus* NHE) – (Red. Peak (V) vs. Ag/AgCl/KCl + 0.197 V) (1)

E_{ox} = –4.5 eV (≡ 0 V *versus* NHE) – (Ox. Peak (V) vs. Ag/AgCl/KCl + 0.197 V) (2)

Table S1 Energy level positions of the photoanode and photocathode components.

Material	Reduction peak / V vs. Ag/AgCl	Oxidation peak / V vs. Ag/AgCl	E_{red} (versus NHE) / eV ≡ LUMO	Band Gap / eV	E_{ox} (versus NHE) / eV ≡ HOMO
TiO_2	–0.571	---	–4.126	3.16	–7.286
CdS	–0.758	---	–3.939	2.29	–6.229
NiO	---	0.377	1.484	3.59	–5.074
In_2S_3	–0.723	---	–3.974	2.22	–6.194

Material	Peak / V vs. Ag/AgCl	E (versus NHE) / eV
Au	0.257	–4.954
MoO_3	0.434	–5.131

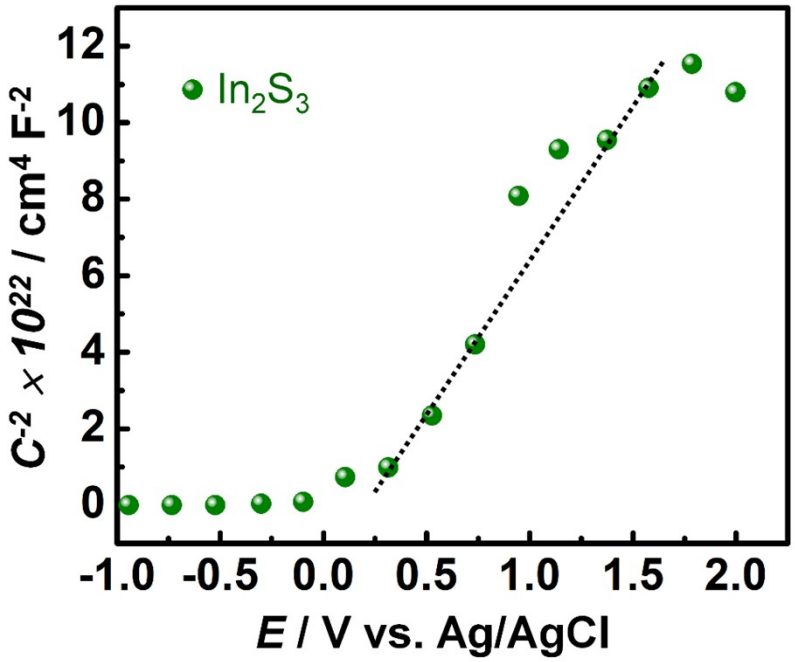

Figure S3 Mott−Schottky plot of the In_2S_3 film.

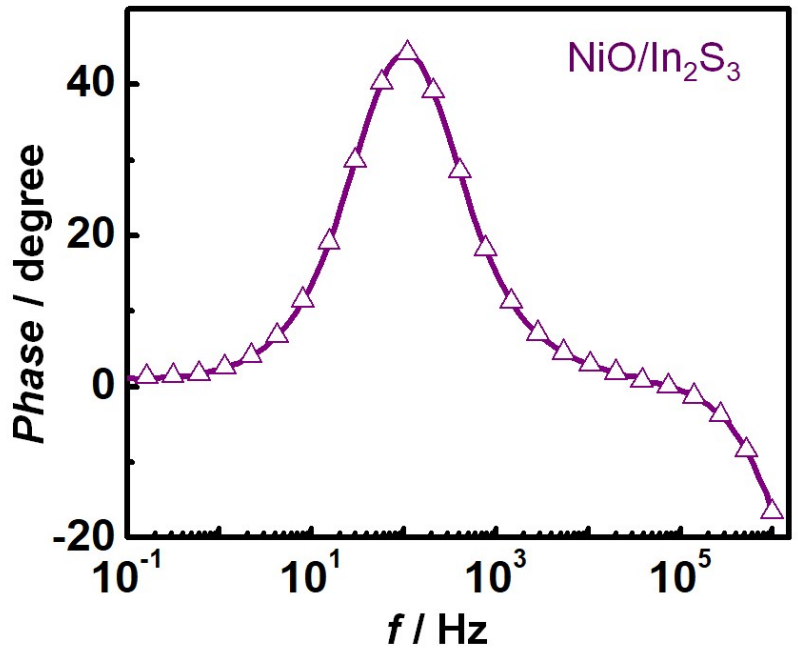

Figure S4 Bode plot of the NiO/In_2S_3-nS^{2-}/S_n^{2-} C-fabric half-cell, with NiO/In_2S_3 as the photoanode.

Table S2 Solar cell parameters of the 3-cells in a 1 M polysulfide gel electrolyte, exposed cell area: 0.12-0.15 cm^2, under 1 sun illumination (AM 1.5, 100 mW cm^{-2}).

Cells	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	Efficiency (η %)
TiO_2/CdS/Au/MoO_3 –In_2S_3/NiO/C-fabric				
Cell 1	0.785	17.99	56.54	7.987
Cell 2	0.787	17.67	52.60	7.314
Cell 3	0.783	17.32	51.63	7.002
Average	0.785	17.66	53.59	7.434

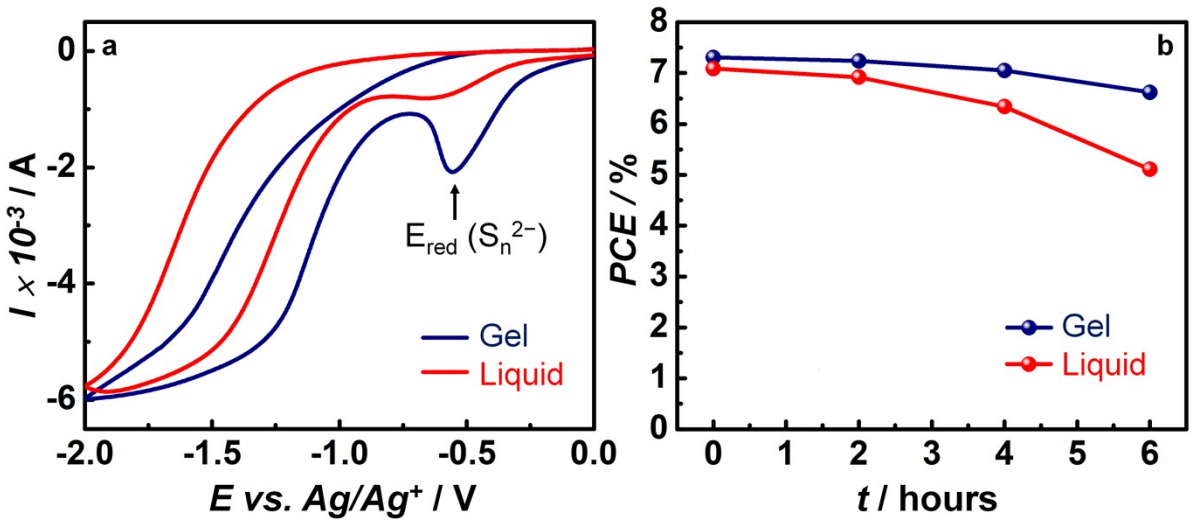

Figure S5 (a) Cyclic voltammograms of aqueous 1 M Na_2S/1 M S/SiO_2 gel and the same liquid electrolyte without SiO_2, recorded between two Pt electrodes at a scan rate of 20 mV s^{-1}. (b) Variation of PCE as a function of exposure time to 1 sun (100 mW cm^{-2}) for tandem cells with liquid and gel electrolytes.

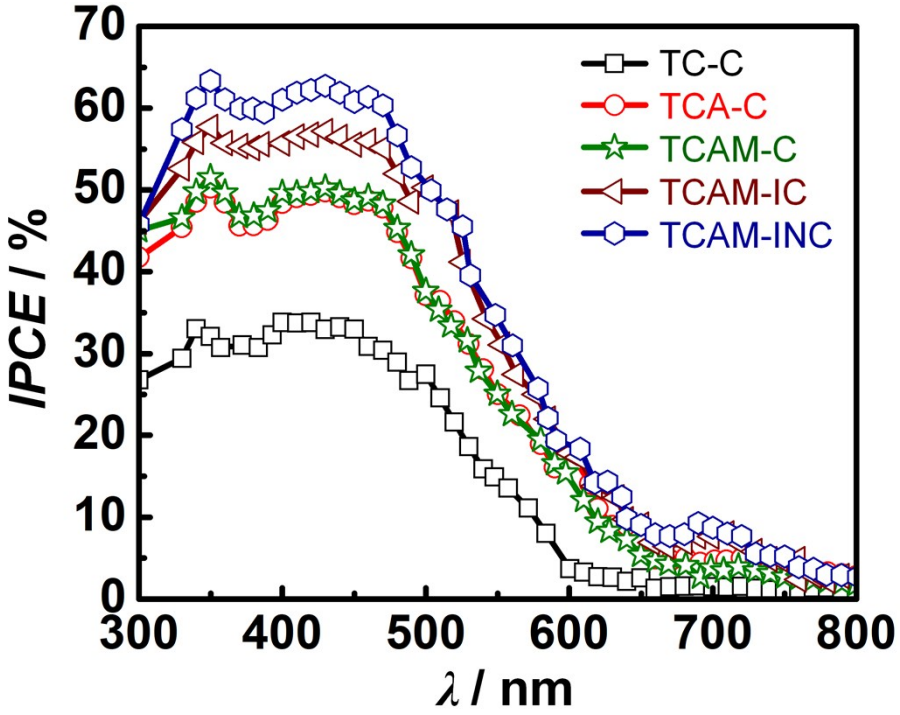

Figure S6 IPCE*versus* wavelength curves for TiO_2/CdS (TC), TiO_2/CdS/Au (TCA) and TiO_2/CdS/Au/MoO_3 (TCAM) photoanode-based cells each with three different counter electrodes: C-fabric (C), In_2S_3/C-fabric (IC), and In_2S_3/NiO/C-fabric (INC) (polysulfide gel electrolyte, under 1 sunillumination, AM 1.5).