Supporting information for

Combinatorial chemical bath deposition of CdS contacts for chalcogenide photovoltaics

Krishnaiah Mokurala [a, b,*], Lauryn L. Baranowski[a,c], Francisco W. de Souza Lucas[a,d], Sebastian Siol [a], Maikel F. A. M van Hest[a] , Sudhanshu Mallick [b] , Parag Bhargava [b], Andriy Zakutayev[a,*]

[a] National Renewable Energy Laboratory, Golden, Colorado 80401, USA

[b] Indian Institute of Technology Bombay, Mumbai 400076, India

[b] Colorado School of Mines, Golden, Colorado, 80401, USA

[d] Federal University of Sao Carlos, São Carlos-SP, 13565-905, Brazil

* Corresponding authors: krishrama33@gmail.com, andriy.zakutayev@nrel.gov

Methods:

CdS chemical bath deposition process

The chemical bath consisted of 100 mL of deionized water, 10 mL of 0.015 M cadmium sulfate ($CdSO_4.2.7H_2O$, Sigma-Aldrich, ACS regent > 99.0%), 12.5 mL of concentrated ammonium hydroxide (28 – 30% NH_4OH, Fisherconc.) and 5 mL of 1.5 M thiourea (CH_4N_2S, Sigma-Aldrich, ACS regent > 99.0%). First, the temperature of a water circulator unit was set at 65° C, and it was connected to a clean double-walled reaction beaker to maintain constant temperature during the deposition. Second, the double-walled reaction beaker was placed on a magnetic stirrer, and the magnetic stirring rod was placed at the bottom of the beaker. The aforementioned chemical solutions were added to the reaction beaker in a sequential manner, and were constantly stirred by the magnetic rod. The substrate was inserted into the reaction beaker with help of dip coater for film deposition.

Photovoltaic device characterization

The automated spatially-resolved J-V mapping under the solar simulator was performed with the stationary back contact probe in the corner of the library, placed on the x-y stage under the front contact probe enabled with the z-axis motion. The solar simulator lamp intensity was calibrated using a standard reference Si solar cell. The area of the device (0.25 cm^2) was used to calculate the current density.

Tables:

Table S1 Thickness of the CdS films measured by XRF and Dectak8

Dipping time (min)	Thickness (nm) XRF	Thickness (nm) Dectak8
5	-	-
10	48	52
15	74	76
15 (STD - CBD)	70	72
20	98	101

Table S2 Average photovoltaic parameters of CZTSe solar cells

Deposition time (min)	J_{sc} (mA/cm^2)	V_{oc} (mV)	FF (%)	η (%)
5	23.3	291	38.2	2.7
10	25.9	308	40.4	3.3
15	28.5	333	44.3	4.3
15 (Std – CBD)	29.7	340	45.4	4.8
20	27.2	319	42.8	3.8

Table S3 Average photovoltaic parameters of CIGSe solar cells

Deposition time (min)	J_{sc} (mA/cm^2)	V_{oc} (mV)	FF (%)	η (%)
5	28.5	604	62.3	10.7
10	29.4	616	63.35	11.3
15	31.8	628	64.7	12.9
15 (Std – CBD)	32.7	634	65.8	13.8
20	30.0	629	63.1	12.2

Figures:

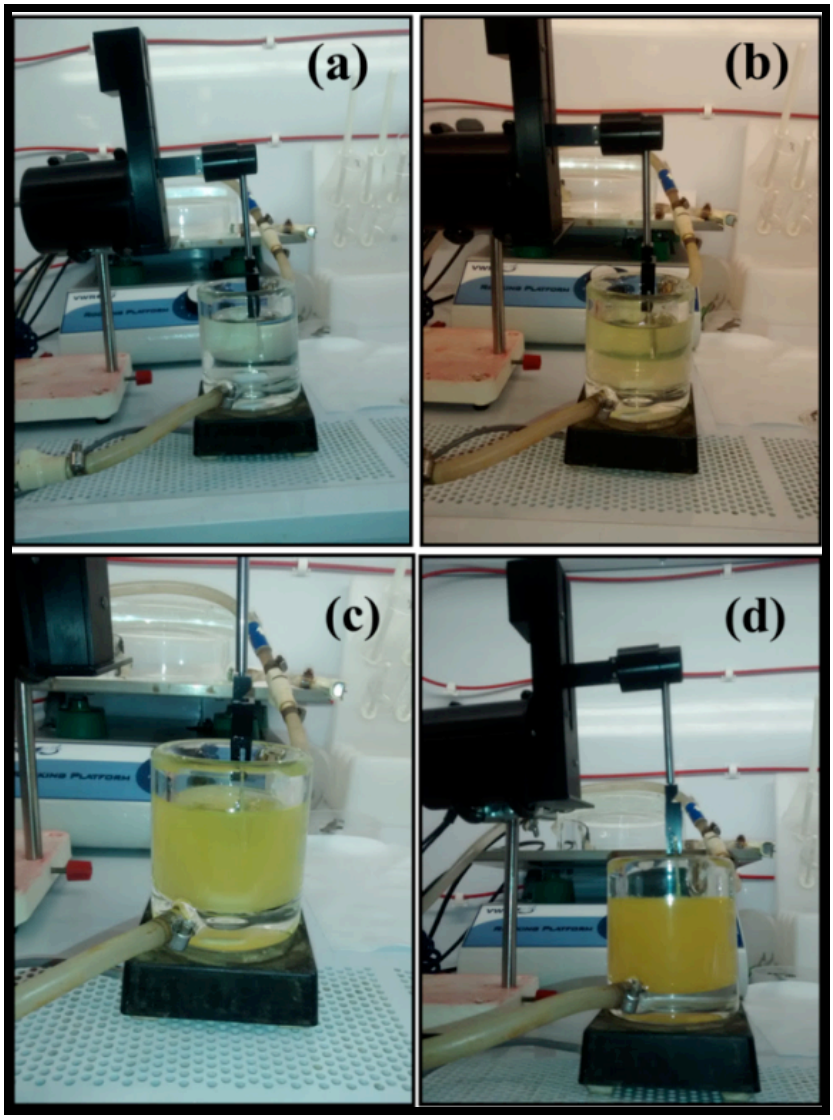

Fig. S1 Photographs of dip coating process (a) after 5 min, (b) 10 min, (c) 15 min, and (d) 20 min

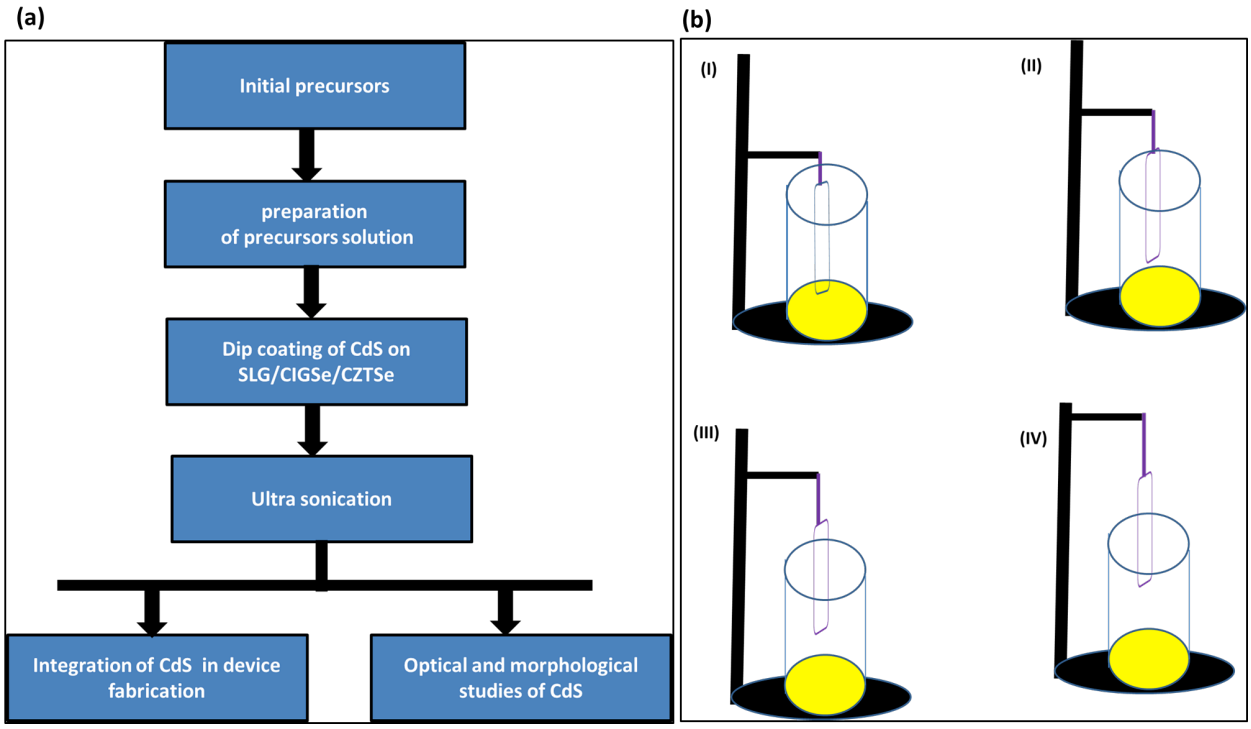

Fig. S2 Flow chat for dip coating technique: (a) processing steps involved in CdS film deposition and (b) steps involved in dip coating process

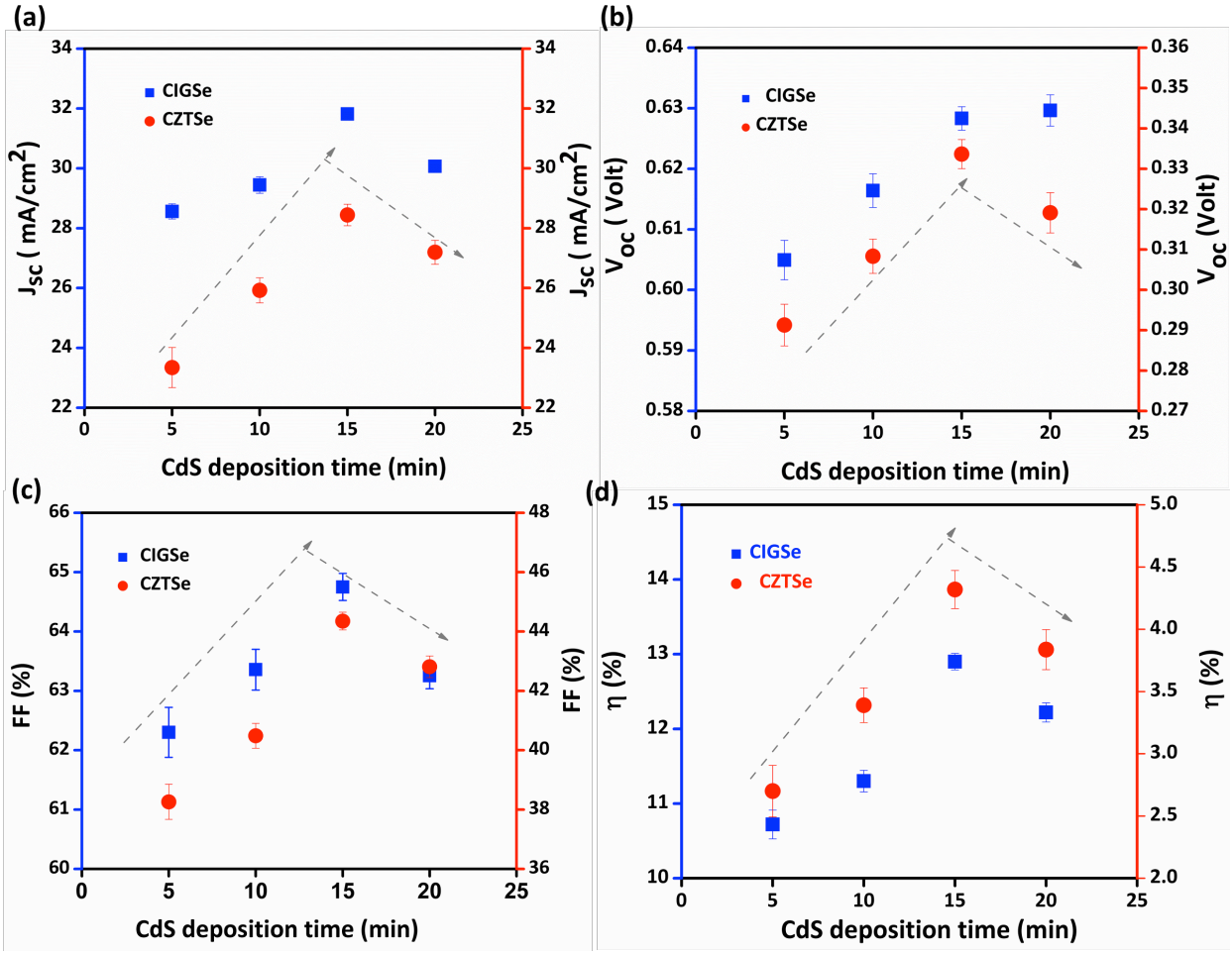

Fig. S3 Photovoltaic parameters of CZTSe and CIGSe solar cells as a function of CdS thickness prepared by combinatorial dip-coating CBD, including (a) short current density, (b) open circuit voltage, (c) fill factor, and (d) efficiency

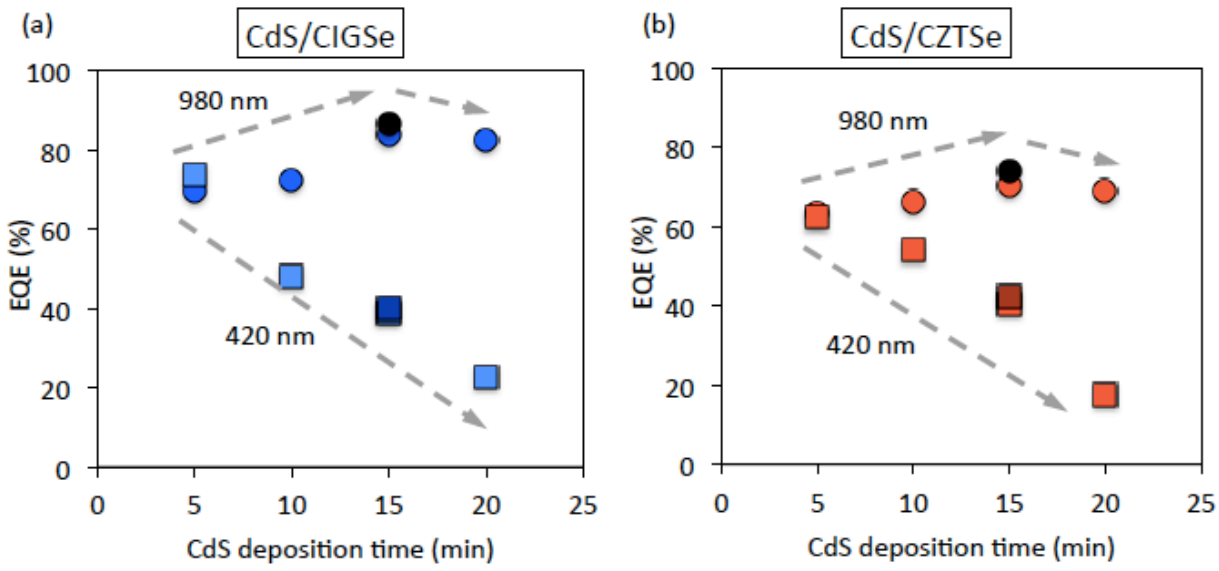

Fig. S4 External quantum efficiency of (a) CIGS and (b) CZTSe solar cells at short (420 nm) and long (980 nm) wavelengths, as a function of combinatorial CdS contact layer thickness. The dark-blue and dark-red squares, and black circles are for conventional CBD CdS.