Electronic Supplementary Information (ESI)

Quantum dot material engineering boosting quantum dot sensitized solar cells efficiency over 13%

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Table S1. ZnSe thickness dependent ZCISe/ZnSe cell devices' photovoltaic performance parameters

ZnSe thickness		J_{sc} (mA·cm^{-2})	V_{oc} (V)	FF	PCE (%)
1 ML	average	26.69	0.770	0.668	13.71±0.11
	champion	26.70	0.780	0.664	13.84
2ML	average	26.04	0.773	0.664	13.36±0.11
	champion	26.19	0.773	0.665	13.46
3ML	average	25.68	0.771	0.663	13.14±0.10
	champion	25.75	0.775	0.663	13.23

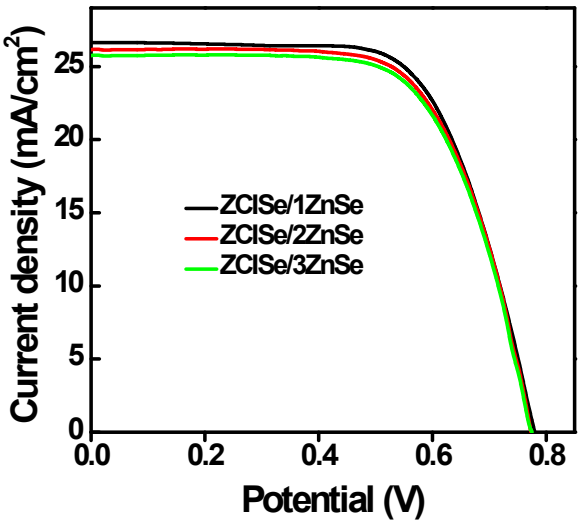


Fig. S1 $J-V$ curves for ZCISe/ZnSe QDs with different ZnSe shell thickness.

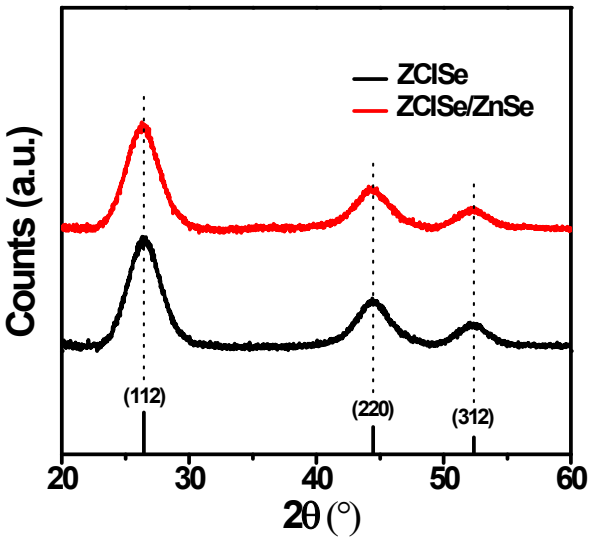


Fig. S2 XRD patterns of ZCISe, and derived ZCISe/ZnSe QDs. Line XRD pattern corresponds to bulk tetragonal chalcopyrite CISe.

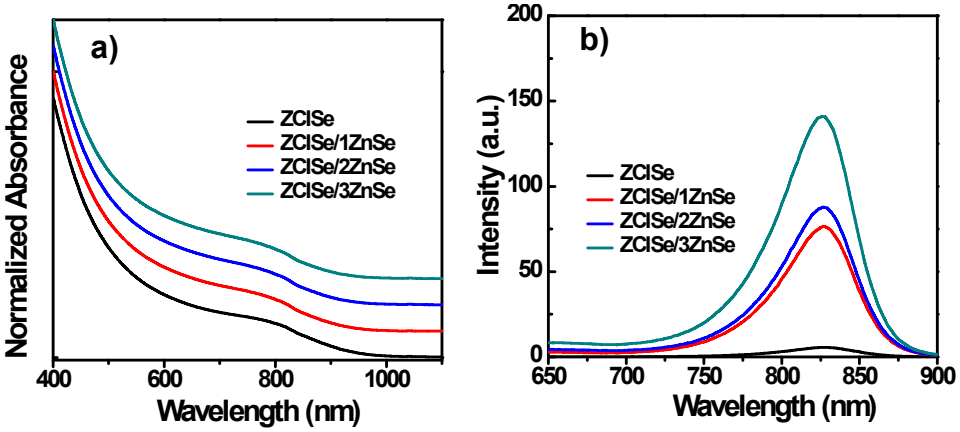


Fig. S3 ZnSe thickness dependent (a) UV−vis absorption, and (b) PL emission spectra.

Table S2. Photovoltaic parameters of ZCISe and ZCISe/ZnSe core/shell based QDSCs under the illumination of one full sun intensity (100 mW/cm^2).

QDs	J_{sc} (mA/cm^2)	V_{oc} (V)	FF	PCE (%)
ZCISe NMC/Ti	26.25	0.752	0.635	12.54
	26.10	0.748	0.633	12.35
	26.45	0.746	0.632	12.57
	26.09	0.754	0.635	12.49
	26.30	0.744	0.645	12.65
Average	26.22±0.17	0.750±0.004	0.634±0.002	12.49±0.10
ZCISe/ZnSe NMC/Ti	27.00	0.769	0.664	13.79
	26.54	0.761	0.674	13.62
	26.70	0.780	0.664	13.84
	26.68	0.765	0.676	13.69
	26.55	0.776	0.660	13.59
Average	26.69±0.19	0.770±0.008	0.668±0.007	13.71±0.11

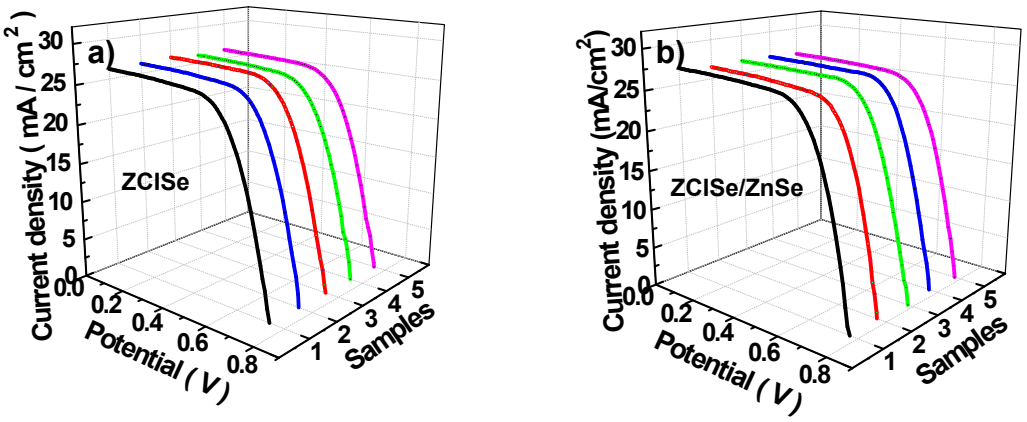
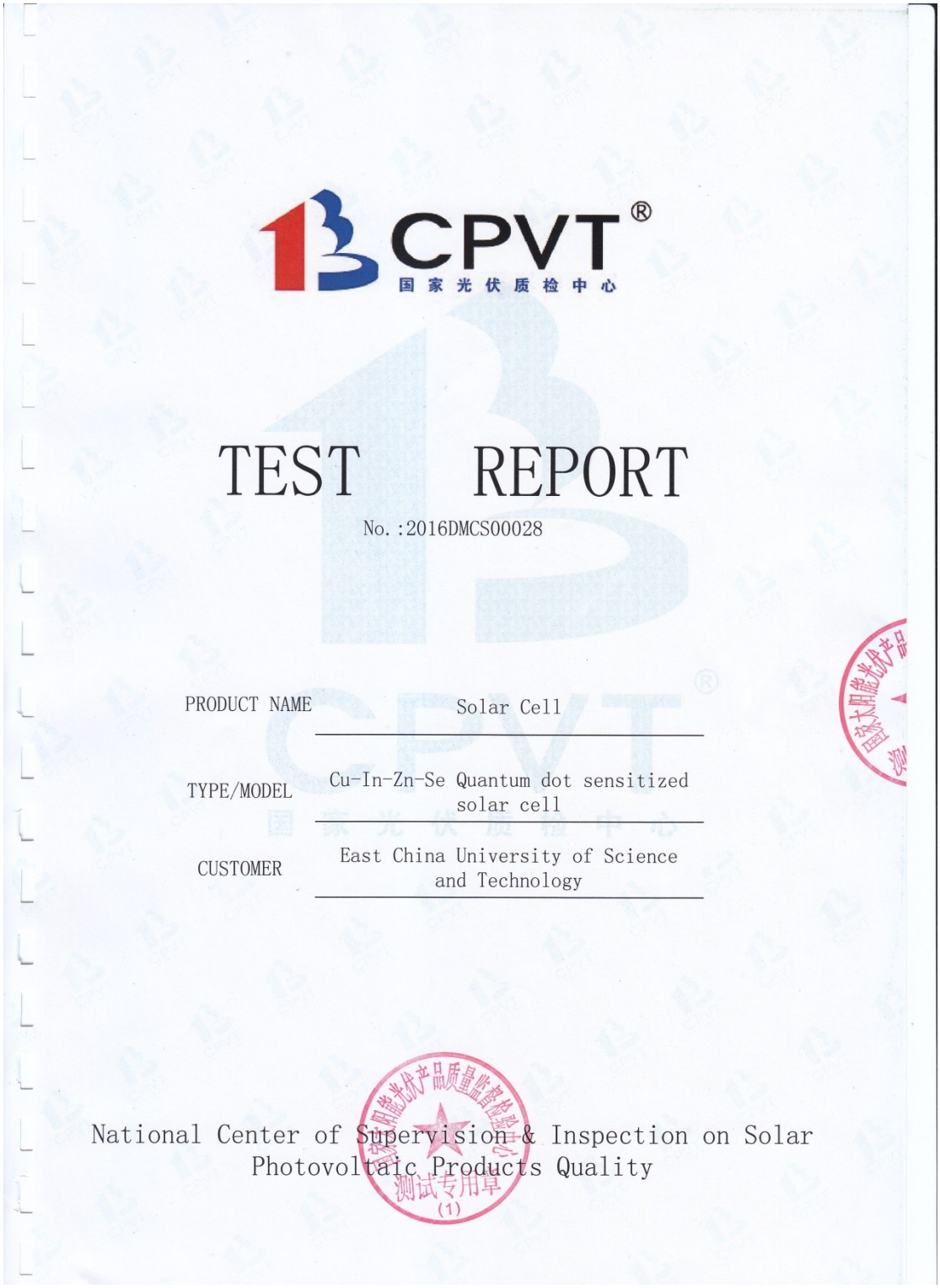


Fig. S4 *J*−*V* curves of ZCISe and ZCISe/ZnSe core/shell QDs-based cells under the illumination of one full sun intensity (100 mW/cm^2).

Certified photovoltaic performance of ZCISe/ZnSe QDSC by CPVT (National Centre of Supervision and Inspection on Solar Photovoltaic Products Quality, China)



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TEST REPORT

No.:2016DMCS00028

PRODUCT NAME	Solar Cell
TYPE/MODEL	Cu-In-Zn-Se Quantum dot sensitized solar cell
CUSTOMER	East China University of Science and Technology

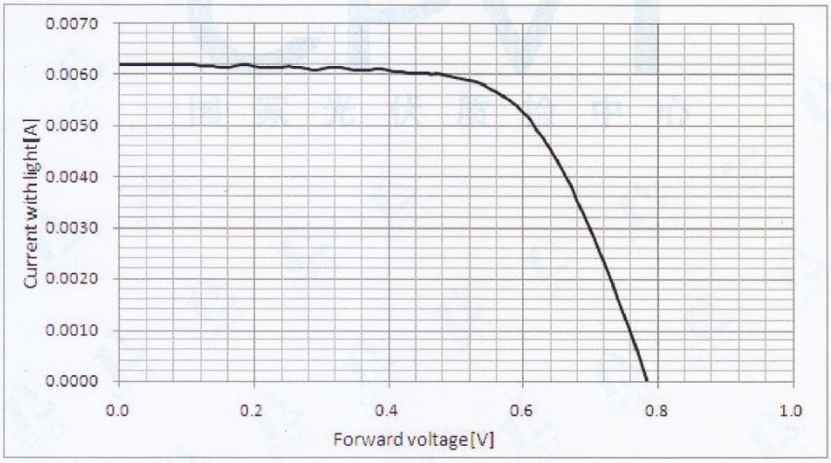
National Center of Supervision & Inspection on Solar Photovoltaic Products Quality

Test Results

No:2016DMCS00028

Clause	Test item(s)	Unit	Technical requirements	Results	Verdict Pass/Fail
1	Current-voltage characteristic measurement (1#)	---	At STC (module temperature: 25 ℃, irradiance: 1000W/m², standard solar spectral irradiance distribution corresponds to IEC60904-3), measure the current-voltage characteristics of the cell with the variation of load	------	---
1.1	Open-circuit voltage, Voc	V	------	0.7824	---
1.2	Short-circuit current, Isc	mA	------	6.190	---
1.3	Maximun-power, Pmax	mW	------	3.184	---
1.4	Maximun-power voltage, Vmp	V	------	0.5800	---
1.5	Maximun-power current, Imp	mA	------	5.490	---
1.6	Fill factor, F.F. (%)	---	------	65.74	---
1.7	Calculate conversion efficiency	---	------	---	---
1.7.1	Conversion efficiency, η (%)	---	$\eta = \frac{Pmax}{1000W/m^2 \times S} \times 100\%$	13.49	---
1.7.2	Area, S	cm^2	S is determined by sample surface outer range	0.23602	---

1# - Current-voltage characteristic at STC



Remark: ------

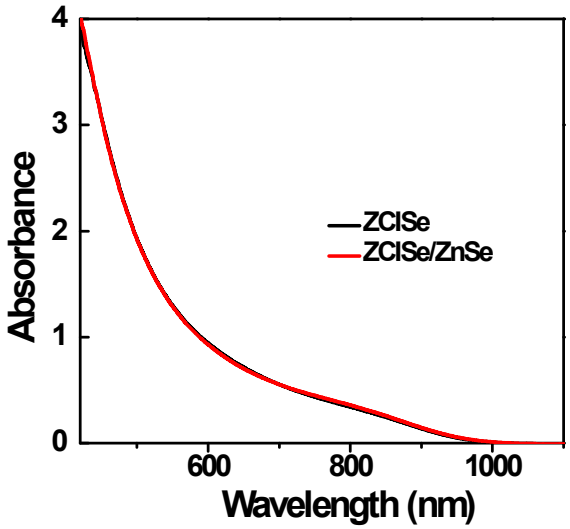


Fig. S5 ZCISe and ZCISe/ZnSe sensitized TiO2 mesoporous film electrodes. It is noted that the measured film is consisted of 5.0 μm transparent P25 layer.

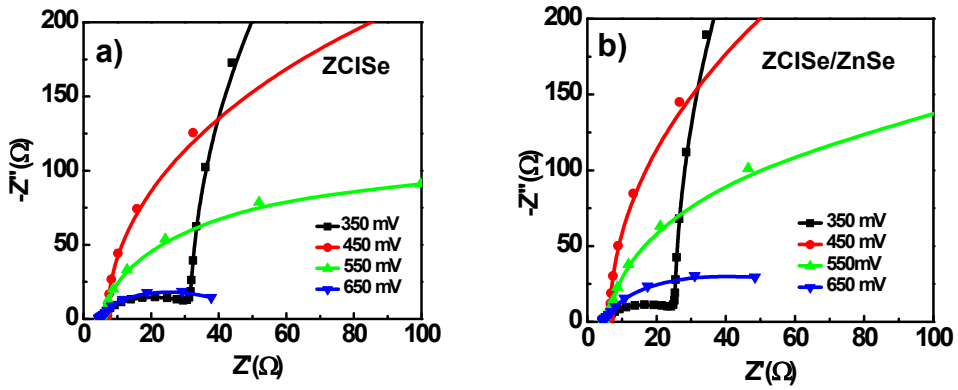


Fig. S6 Nyquist curves at different forward bias for (a) ZCISe, and (b) ZCISe/ZnSe based QDSCs.

Table S3. Extracted EIS parameter values for ZCISe and ZCISe/ZnSe based cells at bias voltage of −0.65 V.

Cells	R_s ($\Omega \cdot cm^2$)	R_{CE} ($\Omega \cdot cm^2$)	C_μ ($mF \cdot cm^{-2}$)	R_{rec} ($\Omega \cdot cm^2$)	τ_n (ms)
ZCISe	4.66	1.80	19.30	37.91	731.6
ZCISe/ZnSe	4.55	2.36	18.06	62.30	1125.0