SUPPORTING INFORMATION

High Efficiency Quantum Dot-Sensitized Solar Cells based on Direct Adsorption of Quantum Dots on Photoanodes

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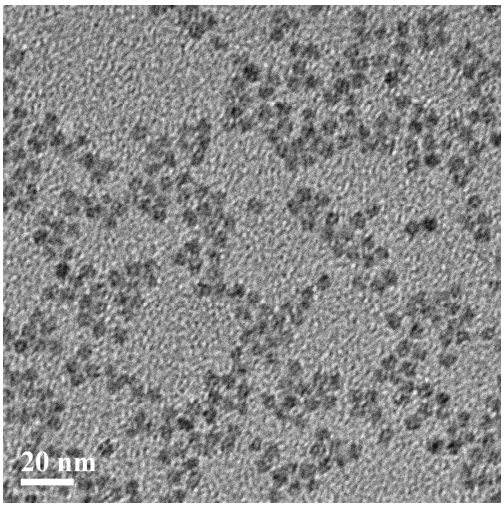

Figure S1. TEM image of as-prepared CdSe QDs.

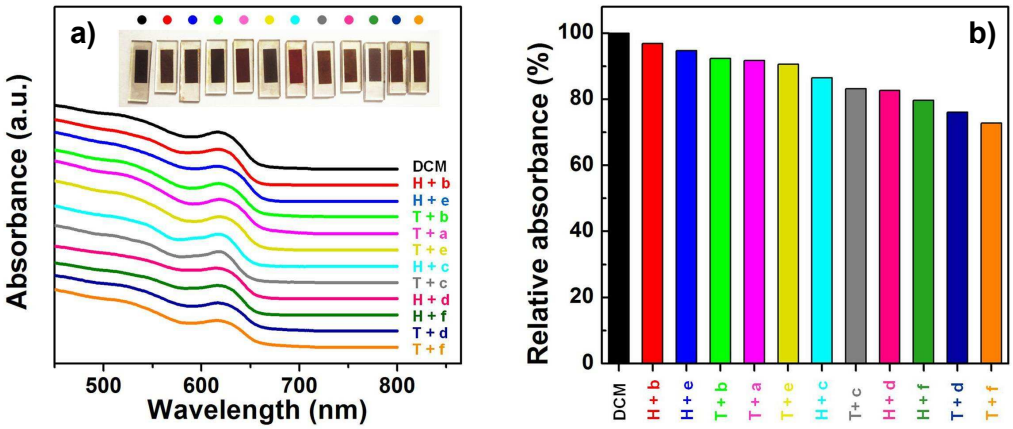

Figure S2. (a)Absorption spectra of CdSe sensitized TiO_2 films sensitized *via* DA mode based on a series of mixed solvent. The results deducted the absorbance of blank TiO_2 film. For the abbreviations, DCM = dichloromethane, H = hexane, T = toluene, a = methanol, b = ethanol, c = isopropanol, d = butanol, e = acetone, and f = butylamine. The QD suspensions based on mixed solvents were prepared by dropwise adding corresponding polar solvent into original nonpolar QD suspensions just before flocculation appeared. Inset: photographs of corresponding films. (b)Relative absorbance of corresponding films at 618 nm. The absorbance based on DCM was set as 100%.

Table S1. Details of Photovoltaic Performance of Solar Cells *via* DA Mode Based on a Series of Purification Cycles.

PC number	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
	0.603	13.52	0.667	5.44
	0.601	13.74	0.655	5.41
1	0.600	13.84	0.660	5.48
	0.594	13.77	0.659	5.39
	0.608	13.68	0.656	5.46
Average	0.601 ± 0.007	13.71 ± 0.19	0.659 ± 0.008	5.44 ± 0.05
	0.615	14.32	0.667	5.87
	0.608	14.45	0.661	5.81
2	0.611	14.66	0.661	5.92
	0.607	14.54	0.656	5.79
	0.616	14.62	0.660	5.94
Average	0.611 ± 0.005	14.52 ± 0.20	0.661 ± 0.006	5.87 ± 0.08
	0.615	14.97	0.656	6.04
3				
	0.622	15.18	0.655	6.19

	0.626	15.00	0.646	6.07
	0.618	15.19	0.658	6.18
	0.614	15.28	0.653	6.13
Average	0.619 ± 0.007	15.12 ± 0.16	0.654 ± 0.008	6.12 ± 0.08
	0.613	15.07	0.648	5.99
	0.626	14.95	0.643	6.02
4	0.617	14.88	0.656	6.02
	0.614	14.72	0.654	5.91
	0.618	14.71	0.649	5.90
Average	0.618 ± 0.008	14.87 ± 0.20	0.650 ± 0.007	5.97 ± 0.07
	0.610	14.26	0.656	5.71
	0.603	14.43	0.663	5.77
5	0.606	14.33	0.659	5.72
	0.607	14.55	0.646	5.70
	0.599	14.43	0.658	5.69
Average	0.605 ± 0.006	14.40 ± 0.15	0.656 ± 0.010	5.72 ± 0.05

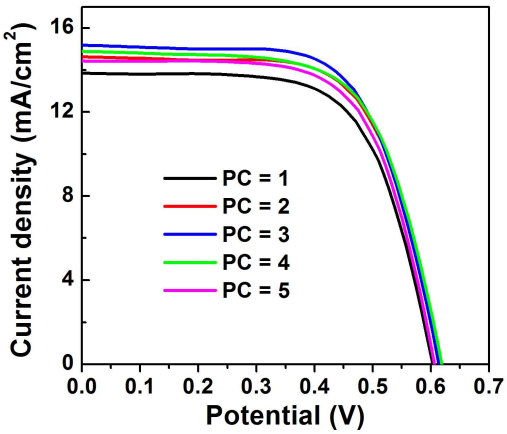

Figure S3. *J-V* curves of champion CdSe QDSCs *via* DA mode based on a series of purification cycles.

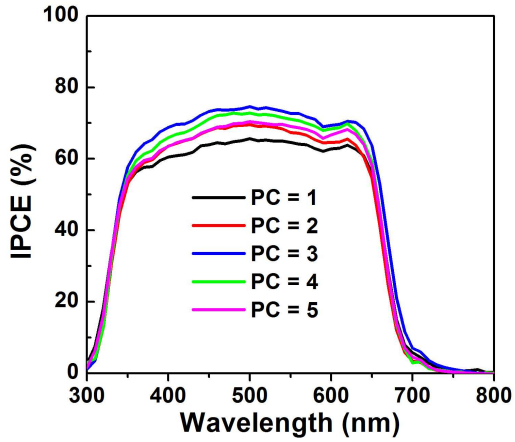

Figure S4. Comparison of IPCE of QDSCs *via* DA mode based on a series of purification cycles.

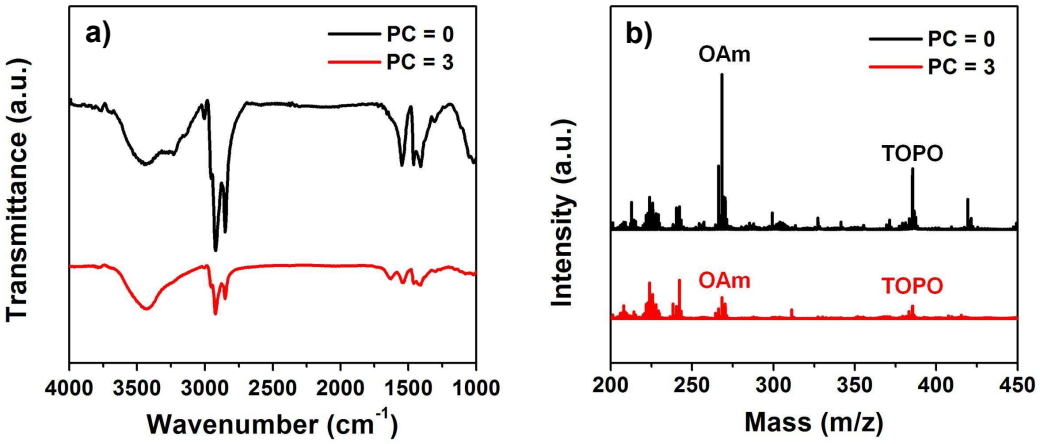

Figure S5. (a) FTIR and (b) mass spectra of CdSe QDs based on a series of purification cycles. In mass spectra, all peaks were calibrated to Cd−114 peak.

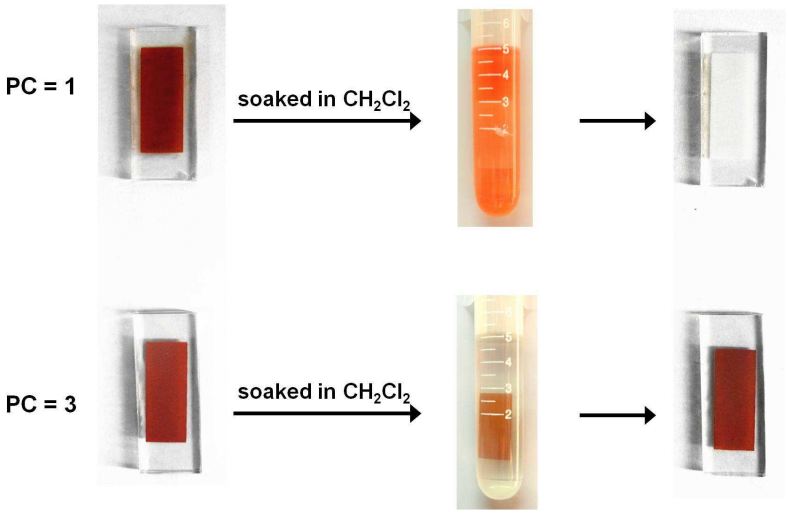

Figure S6. Photographs of CdSe sensitized TiO_2 photoanodes before and after soaking in 5 mL of fresh CH_2Cl_2. The original suspension had undergone 1 and 3 purification cycles.

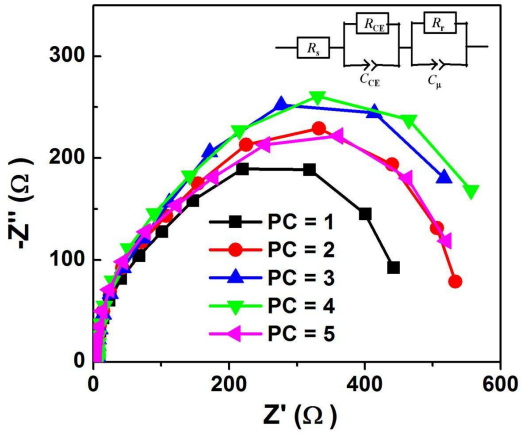

Figure S7. Nyquist plots of QDSCs *via* DA mode based on a series of purification steps at the forward bias of −0.60 V. Inset: the equivalent circuit used to fit EIS.

Table S2. Details of Photovoltaic Performance of Solar Cells *via* DA Mode at Sensitization Time of 2, 3, 5 and 24 h.

Sensitization time	V_{oc} **(V)**	J_{sc} **(mA/cm^2)**	**FF**	**PCE (%)**
	0.607	14.75	0.664	5.94
	0.610	14.43	0.657	5.78
2 h	0.609	14.62	0.649	5.78
	0.617	14.56	0.658	5.91
	0.614	14.71	0.662	5.98
Average	0.611 ± 0.006	13.32 ± 0.12	0.658 ± 0.009	5.88 ± 0.10
	0.615	14.97	0.656	6.04
	0.622	15.18	0.655	6.19
3 h	0.626	15.00	0.646	6.07
	0.618	15.19	0.658	6.18
	0.614	15.28	0.653	6.13
Average	0.619 ± 0.007	15.12 ± 0.16	0.654 ± 0.008	6.12 ± 0.08
5 h	0.619	14.97	0.656	6.08

	0.627	14.83	0.645	6.00
	0.618	14.71	0.652	5.93
	0.612	14.95	0.662	6.06
	0.620	15.06	0.647	6.04
Average	0.619 ± 0.007	14.90 ± 0.19	0.652 ± 0.010	6.02 ± 0.09
	0.594	13.63	0.620	5.02
	0.581	13.39	0.641	4.99
24 h	0.579	13.79	0.651	5.20
	0.578	13.45	0.652	5.07
	0.574	13.73	0.627	4.94
Average	0.581 ± 0.013	13.60 ± 0.21	0.638 ± 0.018	5.04 ± 0.16

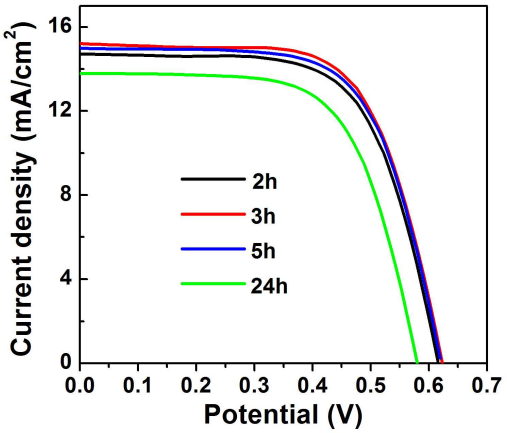

Figure S8. *J-V* curves of champion CdSe QDSCs *via* DA mode at sensitization time of 2, 3, 5 and 24 h.

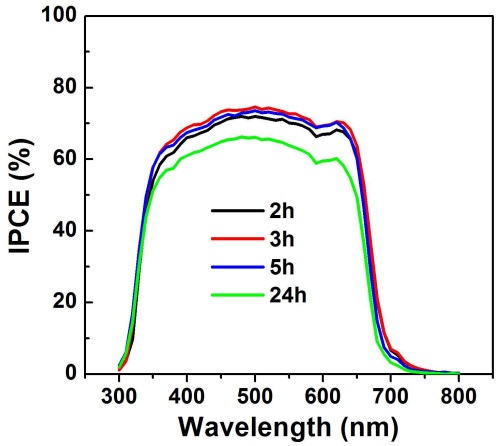

Figure S9. Comparison of IPCE of QDSCs *via* DA mode based on a series of sensitization time.

Table S3. Details of Photovoltaic Performance of Solar Cells *via* CLIS Mode at Sensitization Time of 2 and 24 h.

Sensitization time	V_{oc} **(V)**	J_{sc} **(mA/cm^2)**	**FF**	**PCE (%)**
	0.621	16.07	0.656	6.55
	0.621	15.99	0.656	6.51
2 h	0.621	15.79	0.658	6.45
	0.614	15.83	0.660	6.41
	0.616	15.95	0.648	6.37
Average	0.619 ± 0.005	15.93 ± 0.14	0.657 ± 0.008	6.46 ± 0.09
	0.619	15.92	0.649	6.40
	0.617	15.99	0.656	6.47
24 h	0.610	16.02	0.655	6.40
	0.618	15.81	0.646	6.31
	0.619	16.05	0.643	6.39
Average	0.617 ± 0.007	15.96 ± 0.15	0.650 ± 0.007	6.39 ± 0.08

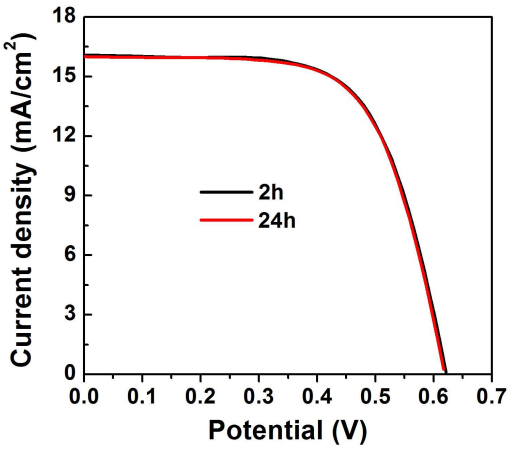

Figure S10. *J-V* curves of champion CdSe QDSCs *via* CLIS mode at sensitization time of 2 and 24 h.

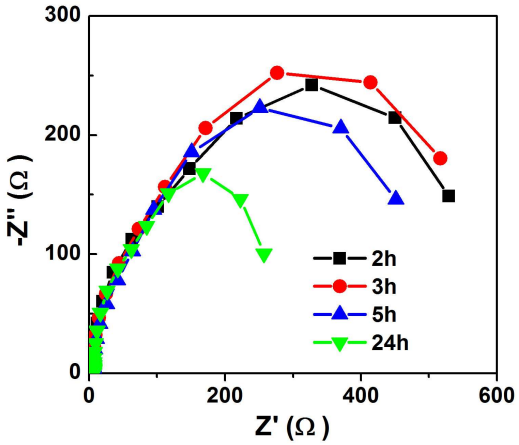

Figure S11. Nyquist plots of QDSCs *via* DA mode based on a series of sensitization times at the forward bias of −0.60 V.

Table S4. Details of Photovoltaic Performance of Solar Cells *via* DA Mode based on a Series of Suspension Concentration.

Concentration	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
	0.622	15.05	0.648	6.06
	0.606	14.97	0.660	5.99
13.3 μM	0.617	15.01	0.657	6.08
	0.613	14.82	0.652	5.92
	0.612	15.07	0.655	6.04
Average	0.614 ± 0.008	14.98 ± 0.16	0.654 ± 0.006	6.02 ± 0.10
	0.615	14.97	0.656	6.04
	0.622	15.18	0.655	6.19
26.6 μM	0.626	15.00	0.646	6.07
	0.618	15.19	0.658	6.18
	0.614	15.28	0.653	6.13
Average	0.619 ± 0.007	15.12 ± 0.16	0.654 ± 0.008	6.12 ± 0.08
	0.610	14.89	0.651	5.91
53.2 μM				
	0.599	14.99	0.653	5.86

	0.596	14.69	0.663	5.80
	0.603	14.69	0.649	5.75
	0.606	14.82	0.659	5.92
Average	0.603 ± 0.007	14.82 ± 0.17	0.655 ± 0.008	5.85 ± 0.10
	0.596	14.10	0.626	5.26
	0.591	14.40	0.626	5.33
106.4 μM	0.588	14.00	0.633	5.21
	0.583	14.43	0.646	5.43
	0.576	14.33	0.641	5.29
Average	0.587 ± 0.011	14.25 ± 0.25	0.634 ± 0.012	5.30 ± 0.13

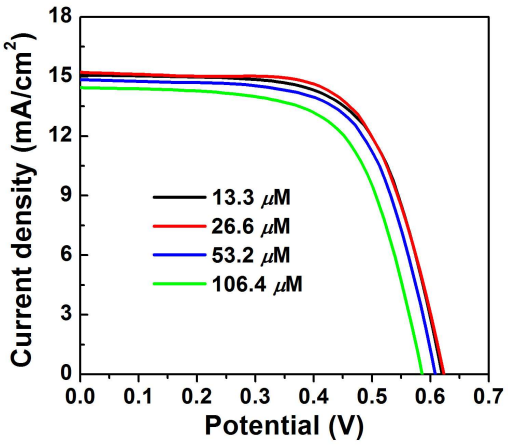

Figure S12. *J-V* curves of champion CdSe QDSCs *via* DA mode based on a series of QD suspension concentration.

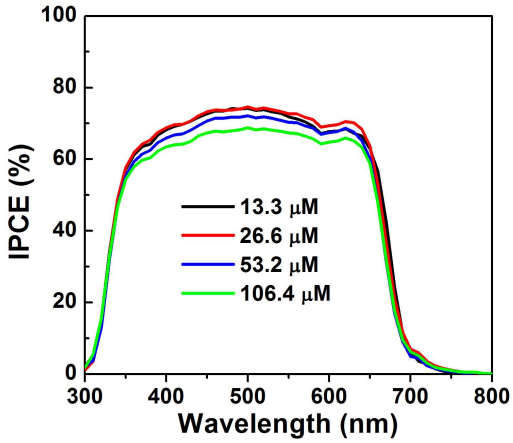

Figure S13. Comparison of IPCE of QDSCs *via* DA mode based on a series of QD suspension concentration.

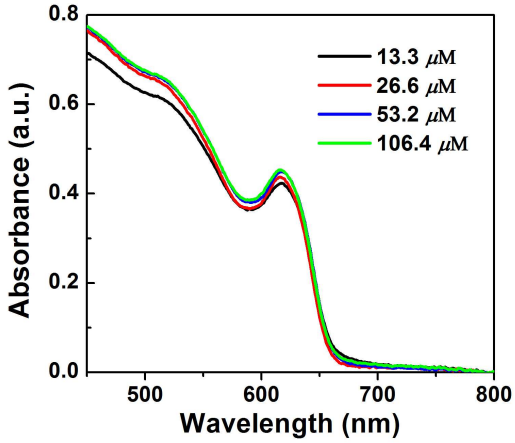

Figure S14. UV-vis absorption spectra of CdSe QD sensitized TiO_2 films *via* DA mode at a series of suspension concentration. The results deducted the absorbance of blank TiO_2 film.

Table S5. Details of Photovoltaic Performance of Solar Cells *via* CLIS Mode based on a Series of Suspension Concentration.

Concentration	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
	0.621	16.07	0.656	6.55
	0.621	15.99	0.656	6.51
25.5 μM	0.621	15.79	0.658	6.45
	0.614	15.83	0.660	6.41
	0.616	15.95	0.648	6.37
Average	0.619 ± 0.005	15.93 ± 0.14	0.657 ± 0.008	6.46 ± 0.09
	0.617	16.00	0.653	6.45
	0.613	16.03	0.660	6.49
102.0 μM	0.622	15.93	0.645	6.39
	0.613	16.07	0.647	6.37
	0.617	15.87	0.658	6.44
Average	0.616 ± 0.006	15.98 ± 0.11	0.653 ± 0.008	6.43 ± 0.06
	0.611	16.04	0.653	6.40
204.0 μM				
	0.615	15.99	0.643	6.32

	0.618	15.83	0.652	6.38
	0.621	16.01	0.651	6.47
	0.606	15.86	0.657	6.31
Average	0.614 ± 0.009	15.95 ± 0.12	0.651 ± 0.008	6.38 ± 0.09

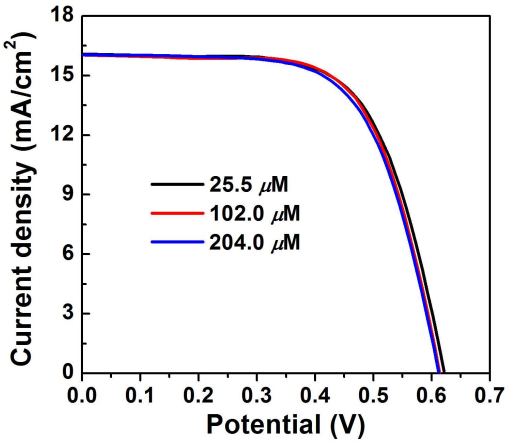

Figure S15. *J-V* curves of champion CdSe QDSCs *via* CLIS mode based on a series of suspension concentration.

Table S6. Details of Photovoltaic Performance of a Series of Optimized Solar Cells.

Photoanodes	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
	0.649	15.08	0.672	6.58
	0.649	14.97	0.684	6.65
DA-CdSe/ZnS/SiO_2	0.653	14.81	0.667	6.45
	0.638	14.95	0.682	6.50
	0.639	15.05	0.680	6.54
Average	0.646 ± 0.008	14.97 ± 0.16	0.677 ± 0.010	6.54 ± 0.11
	0.653	15.80	0.671	6.92
	0.647	15.90	0.670	6.89
DA-Mg^{2+}/CdSe/ZnS/ SiO_2	0.655	15.72	0.663	6.83
	0.655	15.98	0.661	6.92
	0.653	15.87	0.670	6.94
Average	0.653 ± 0.006	15.85 ± 0.13	0.667 ± 0.006	6.90 ± 0.07
	0.639	15.95	0.673	6.86
CLIS-CdSe/ZnS/SiO_2	0.646	15.88	0.667	6.84
	0.650	15.65	0.683	6.95

	0.641	15.74	0.674	6.82
	0.646	15.81	0.678	6.92
Average	0.644 ± 0.006	15.81 ± 0.16	0.675 ± 0.008	6.88 ± 0.07
	0.610	22.31	0.567	7.72
	0.600	22.56	0.580	7.85
DA-ZCISe/ZnS	0.613	22.21	0.563	7.67
	0.597	22.61	0.579	7.82
	0.594	22.56	0.583	7.81
Average	0.603 ± 0.010	22.45 ± 0.24	0.574 ± 0.011	7.77 ± 0.10
	0.622	24.84	0.585	9.04
	0.629	24.79	0.583	9.09
DA-Mg^{2+}/ZCISe/ZnS	0.619	25.13	0.573	8.91
	0.612	24.93	0.587	8.96
	0.616	25.06	0.591	9.12
Average	0.620 ± 0.009	24.95 ± 0.18	0.584 ± 0.011	9.02 ± 0.11
CLIS-ZCISe/ZnS	0.631	26.05	0.579	9.52

	0.640	25.97	0.582	9.67
	0.623	25.79	0.592	9.51
	0.638	26.03	0.580	9.63
	0.629	26.20	0.573	9.44
Average	0.632 ± 0.009	26.01 ± 0.22	0.581 ± 0.011	9.56 ± 0.12

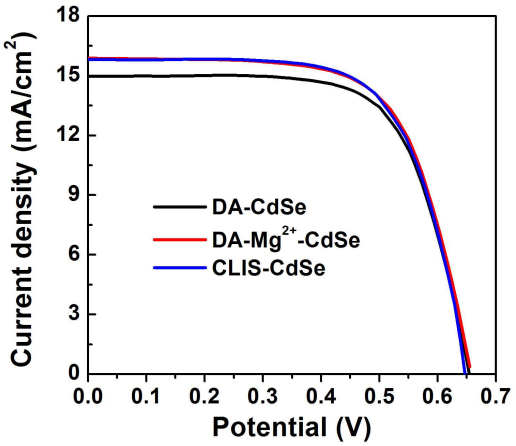

Figure S16. *J-V* curves of a series of optimized CdSe champion QDSCs.

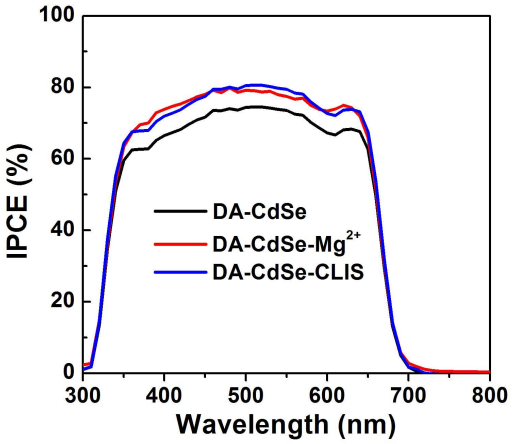

Figure S17. IPCE curves of a series of optimized CdSe champion QDSCs.

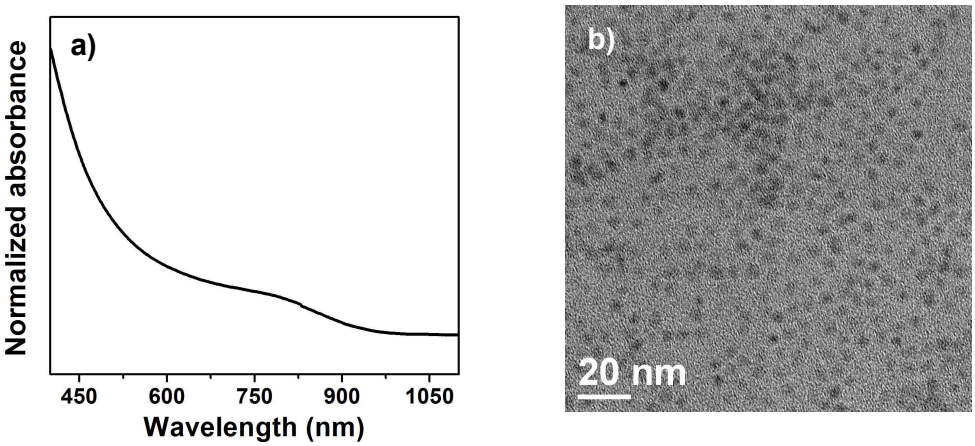

Figure S18. (a) UV-vis absorption spectrum of ZCISe QDs suspended in CH_2Cl_2. (b) TEM image of ZCISe QDs.

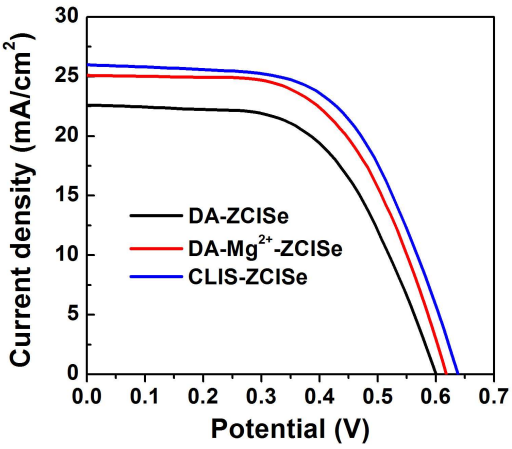

Figure S19. *J-V* curves of a series of optimized ZCISe champion QDSCs.

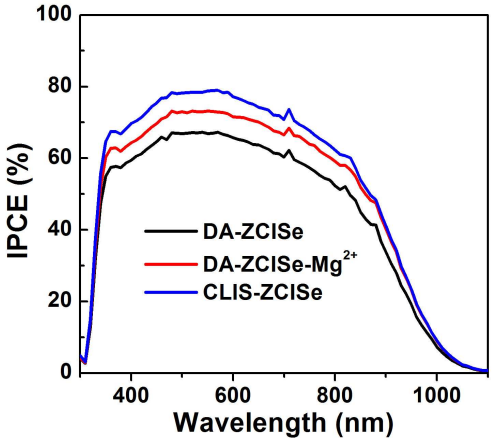

Figure S20. IPCE curves of a series of optimized ZCISe champion QDSCs.

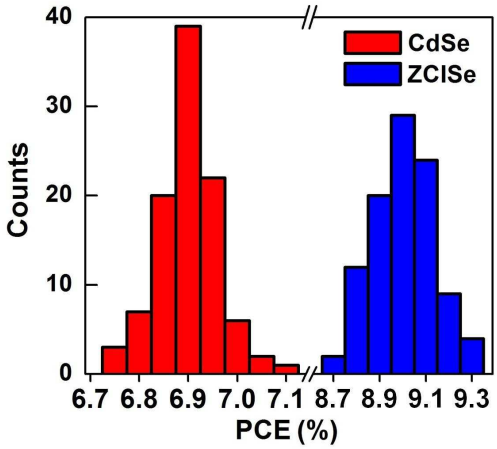

Figure S21. Histograms of device performance from a batch of 100 cell devices based on DA mode.