

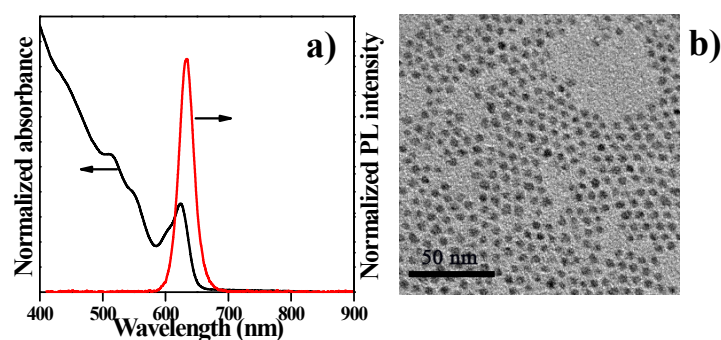
# Optimizing the deposition of CdSe colloidal quantum dots on TiO<sub>2</sub> film electrode *via* capping ligand induced self-assembly approach

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**Fig. S1** (a) UV-vis, PL and (b) TEM of OAm-capped CdSe QD

**Table S1** The details of photovoltaic performance of solar cells based on different pH of CdSe QD aqueous solution in the absence of free ligand

pH	$V_{oc}$ (V)	$J_{sc}$ (mA/cm <sup>2</sup> )	FF	PCE (%)
8	0.623	5.36	0.644	2.15
	0.607	5.13	0.639	1.99
	0.612	5.20	0.650	2.07
	0.609	5.32	0.675	2.20
	0.613	5.30	0.658	2.14
9	0.610	11.69	0.632	4.51
	0.616	11.92	0.656	4.82
	0.620	11.85	0.649	4.77
	0.613	12.06	0.638	4.72
	0.609	11.99	0.642	4.69
10	0.612	14.12	0.639	5.52
	0.602	14.07	0.626	5.30
	0.611	14.02	0.641	5.49
	0.617	13.92	0.657	5.64
	0.617	14.05	0.635	5.50
11	0.612	14.89	0.642	5.85
	0.613	14.92	0.632	5.78
	0.604	14.83	0.661	5.92
	0.615	14.79	0.646	5.88
	0.604	14.80	0.642	5.74
12	0.616	15.36	0.649	6.14
	0.613	15.23	0.632	5.90
	0.618	15.10	0.645	6.02
	0.607	15.48	0.650	6.11
	0.614	15.33	0.634	5.98

**Table S2** Details of Photovoltaic performance of solar cells based on different concentrations of free MPA ligand at pH 12.0

MPA (M)	$V_{oc}$ (V)	$J_{sc}$ (mA/cm <sup>2</sup> )	FF	PCE (%)
0	0.615	14.97	0.639	5.88
	0.606	15.20	0.653	6.01
	0.608	14.97	0.647	5.89
	0.619	15.40	0.630	6.01
	0.610	15.52	0.637	6.03
	0.619	15.63	0.652	6.30
	0.617	15.66	0.657	6.35
	0.05	0.622	15.64	0.640
0.619		15.60	0.652	6.30
0.614		15.63	0.644	6.18
0.618		15.94	0.669	6.59
0.616		15.97	0.650	6.39
0.1		0.618	15.85	0.663
	0.617	15.86	0.658	6.44
	0.620	15.93	0.660	6.52
	0.616	15.89	0.669	6.55
	0.612	15.82	0.655	6.34
0.3	0.616	15.95	0.662	6.50
	0.618	15.88	0.668	6.56
	0.624	15.82	0.653	6.44

**Table S3** Details of photovoltaic performance of solar cells based on different pH of CdSe QD solution in the presence of 0.1 M free MPA ligand

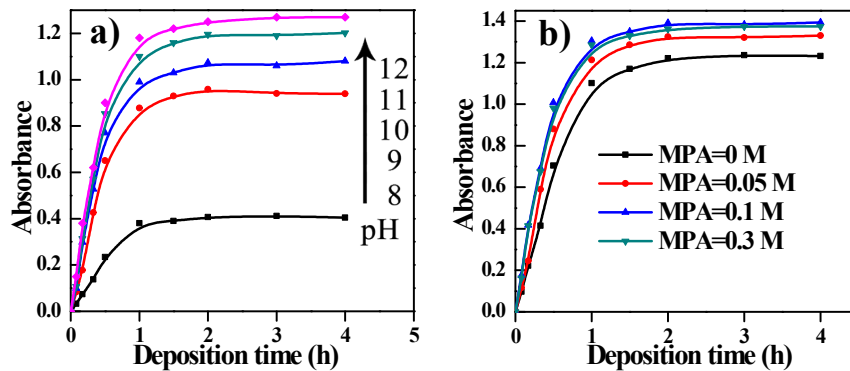
pH	$V_{oc}$ (V)	$J_{sc}$ (mA/cm <sup>2</sup> )	FF	PCE (%)
8	0.613	15.98	0.656	6.42
	0.627	15.99	0.654	6.56
	0.616	15.89	0.654	6.41
	0.610	15.97	0.652	6.36
	0.620	15.98	0.645	6.40
9	0.613	15.90	0.654	6.38
	0.615	15.89	0.667	6.52
	0.626	15.98	0.649	6.50
	0.614	15.91	0.658	6.43
	0.621	15.95	0.649	6.43
10	0.618	15.86	0.660	6.47
	0.605	15.92	0.662	6.38
	0.622	15.94	0.659	6.54
	0.630	15.98	0.652	6.56
	0.619	15.96	0.660	6.52
11	0.618	15.90	0.657	6.46
	0.620	15.88	0.659	6.49
	0.616	15.86	0.659	6.44
	0.620	15.97	0.652	6.47
	0.617	15.95	0.650	6.40
12	0.616	15.95	0.659	6.47
	0.620	15.98	0.662	6.56
	0.619	15.96	0.658	6.50
	0.617	15.87	0.650	6.37
	0.615	15.92	0.649	6.38

**Table S4** Details of photovoltaic performance of solar cells based on different deposition temperatures

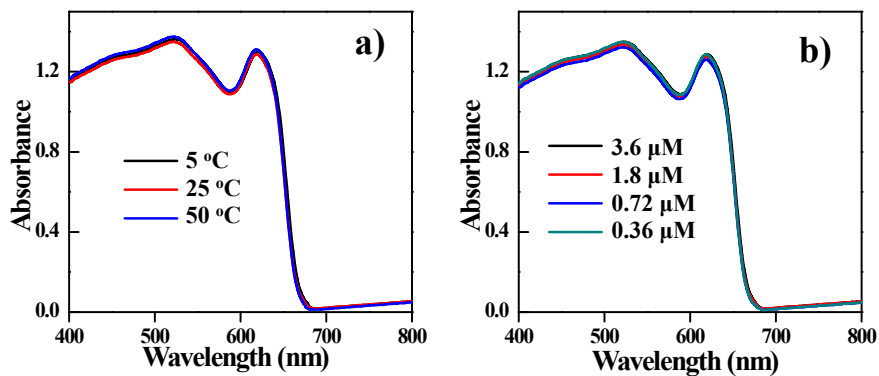
Temperature (°C)	$V_{oc}$ (V)	$J_{sc}$ (mA/cm <sup>2</sup> )	FF	PCE (%)
5	0.617	15.97	0.639	6.30
	0.621	15.98	0.651	6.46
	0.621	15.88	0.652	6.43
	0.623	15.96	0.645	6.42
	0.615	15.88	0.660	6.45
25	0.619	15.91	0.650	6.57
	0.616	15.96	0.645	6.34
	0.617	15.80	0.648	6.32
	0.616	15.94	0.647	6.35
	0.618	15.93	0.659	6.49
50	0.616	15.95	0.648	6.37
	0.613	15.96	0.641	6.27
	0.613	15.89	0.658	6.41
	0.619	15.91	0.664	6.54
	0.612	15.90	0.659	6.41

**Table S5** Details of photovoltaic performance of solar cells based on different concentrations of CdSe QD solution

Concentration ( $\mu\text{M}$ )	$V_{oc}$ (V)	$J_{sc}$ ( $\text{mA}/\text{cm}^2$ )	FF	PCE (%)
3.6	0.620	15.95	0.664	6.56
	0.616	15.88	0.663	6.49
	0.616	15.80	0.660	6.42
	0.619	15.85	0.639	6.27
	0.618	15.89	0.663	6.51
1.8	0.610	15.99	0.662	6.46
	0.616	15.92	0.656	6.43
	0.620	15.85	0.649	6.38
	0.613	15.96	0.662	6.48
	0.619	15.99	0.660	6.53
0.72	0.612	15.92	0.669	6.52
	0.622	15.97	0.646	6.42
	0.619	15.92	0.641	6.32
	0.617	15.92	0.657	6.45
	0.617	15.95	0.655	6.45
0.36	0.606	15.94	0.650	6.28
	0.617	15.72	0.666	6.46
	0.619	15.85	0.669	6.56
	0.620	15.85	0.649	6.38
	0.616	15.80	0.647	6.30



**Fig. S2** Temporal evolution of the absorbance at first excitonic absorption peak of CdSe-sensitized TiO<sub>2</sub> films deposition under QD aqueous solution with (a) different pH values, (b) different MPA concentrations



**Fig. S3** (a) UV-vis absorption spectra of CdSe-sensitized films which contains only transparent layer prepared under different absorption temperatures and (b) UV-vis absorption spectra of CdSe-sensitized films which contains only transparent layer prepared under different concentrations of CdSe QD solution