Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

DDAB-Assisted Synthesis of Iodine-Rich $CsPbI_3$ Perovskite Nanocrystals with Improved Stability in Multiple Environments

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SI1. Characterization of perovskite nanocrystals

Optical properties of perovskite NCs were studied over a period of at least 60 days. Figure S1b shows PL spectra of DDAB-capped NCs. No significant change in PL peak position and in optical linewidth is observed. The relative quantum yield of $CsPbI_3$ NCs was obtained by comparing it with the standard sample of rhodamine 6G (QY = 95% in ethanol). And QY was calculated as follows:

$$QY_x = QY_R \frac{I_x}{I_R} \frac{OD_R}{OD_x} \frac{n_x^2}{n_R^2}$$

where *R* indicates standard rhodamine 6G sample, *x* is test samples, *I* is integrated PL intensity, *OD* is absorbance, and *n* is the refraction coefficient of the solvent.

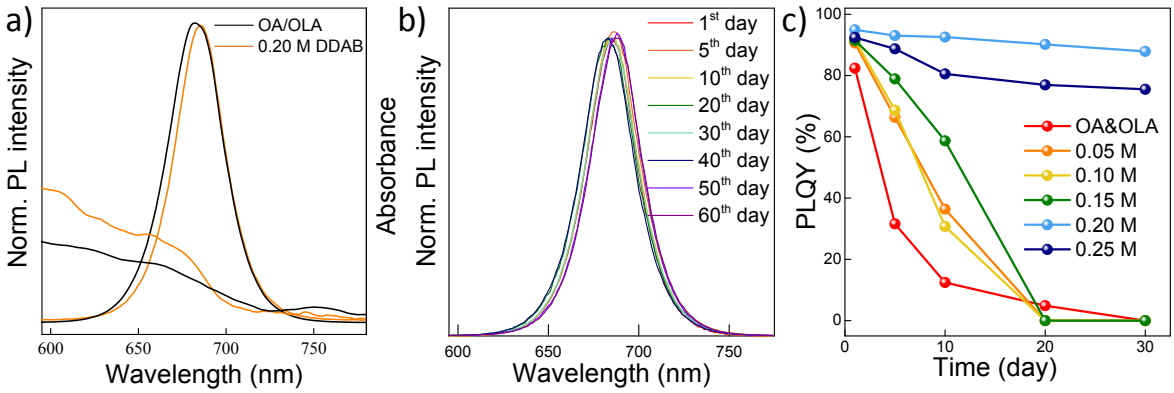

Figure S1 a) Room temperature PL and absorbance spectra of OA/OLA and DDAB-capped perovskite nanocrystals measured on the 1st day after synthesis. **b)** Room temperature PL of DDAB-capped NCs measured over 60−day period. **c)** The PLQY of perovskite nanocrystals prepared with OA/OLA and different concentrations of DDAB as a function of time.

Morphological properties of the synthesized nanocrystals were assessed by TEM. Representative TEM images are shown in the Figure S2. Table S1 summarizes results of optical and morphological characterization.

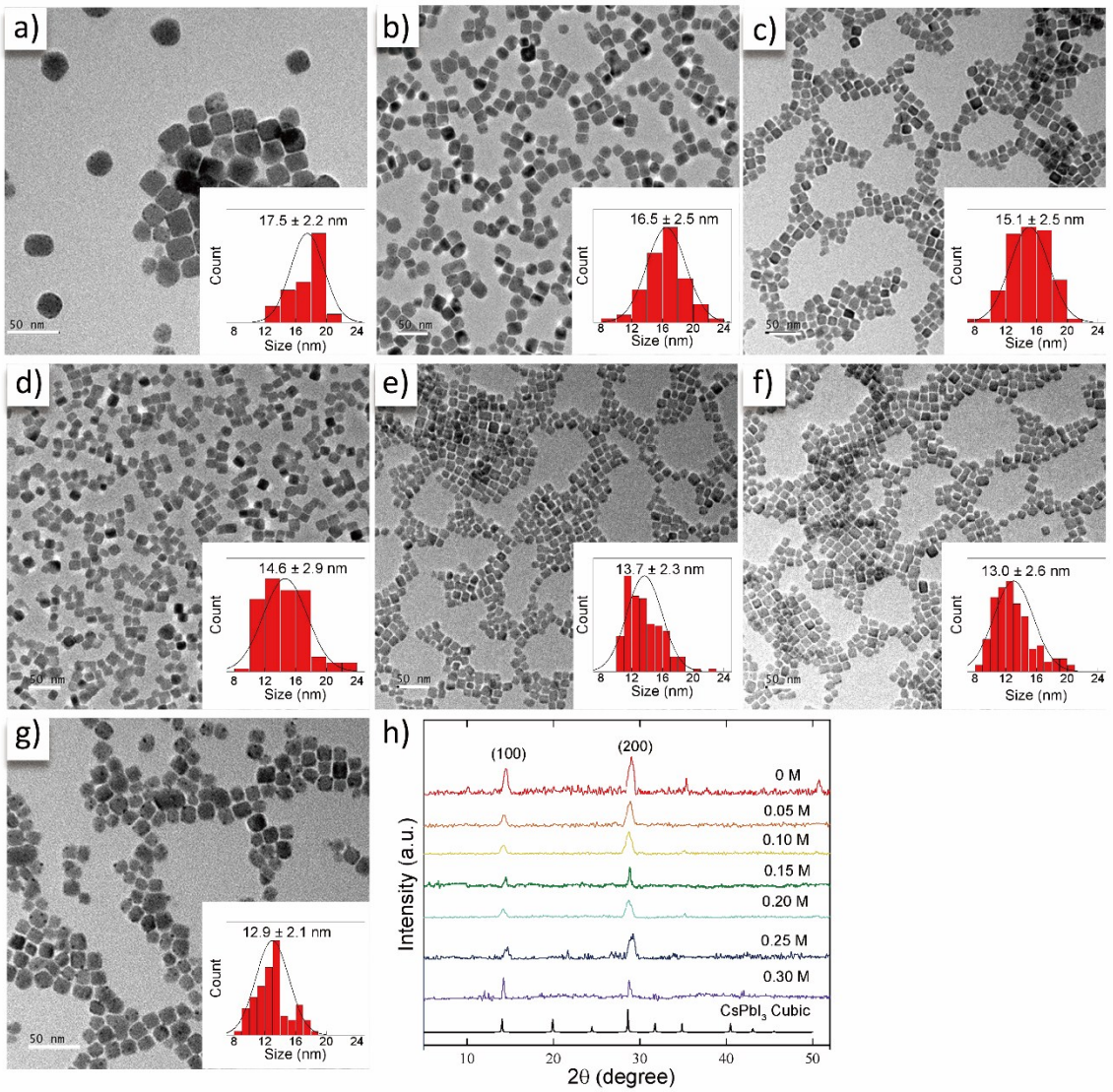

Figure S2 TEM images of $CsPbI_3$ NCs prepared with different concentrations of DDAB **a)** 0 M, **b)** 0.05 M, **c)** 0.10 M, **d)** 0.15 M, **e)** 0.20 M, **f)** 0.25 M, **g)** 0.30 M. **h)** XRD patterns of $CsPbI_3$ NCs films obtained by different concentration of DDAB.

Table S1 Optical properties and sizes of $CsPbI_3$ NCs synthesized by different concentrations of DDAB and OA/OLA.

Samples (DDAB concentration, M)	PL Peak (nm)	FWHM (nm)	PLQY (%)	Particle size (nm)
OA&OLA	680	39	82.4	11.9 ± 2.4
0 M	691	35	91.4	17.5 ± 2.2
0.05 M	690	36	90.6	16.5 ±2.5
0.10 M	688	36	91.7	15.1 ± 2.5
0.15 M	687	39	91.5	14.6 ± 2.9
0.20 M	686	37	95	13.7 ± 2.3
0.25 M	680	38	92.4	13.0 ± 2.6
0.30 M	677	40	88.3	12.9 ± 2.1

Composition of the NCs was analyzed by XPS (Figure S3) and confirmed presence of DDAB (0.2M) and formation of I-rich nanocrystals.

Figure S3 a) EDX and **b)** XPS spectra of DDAB-capped $CsPbI_3$ NCs.

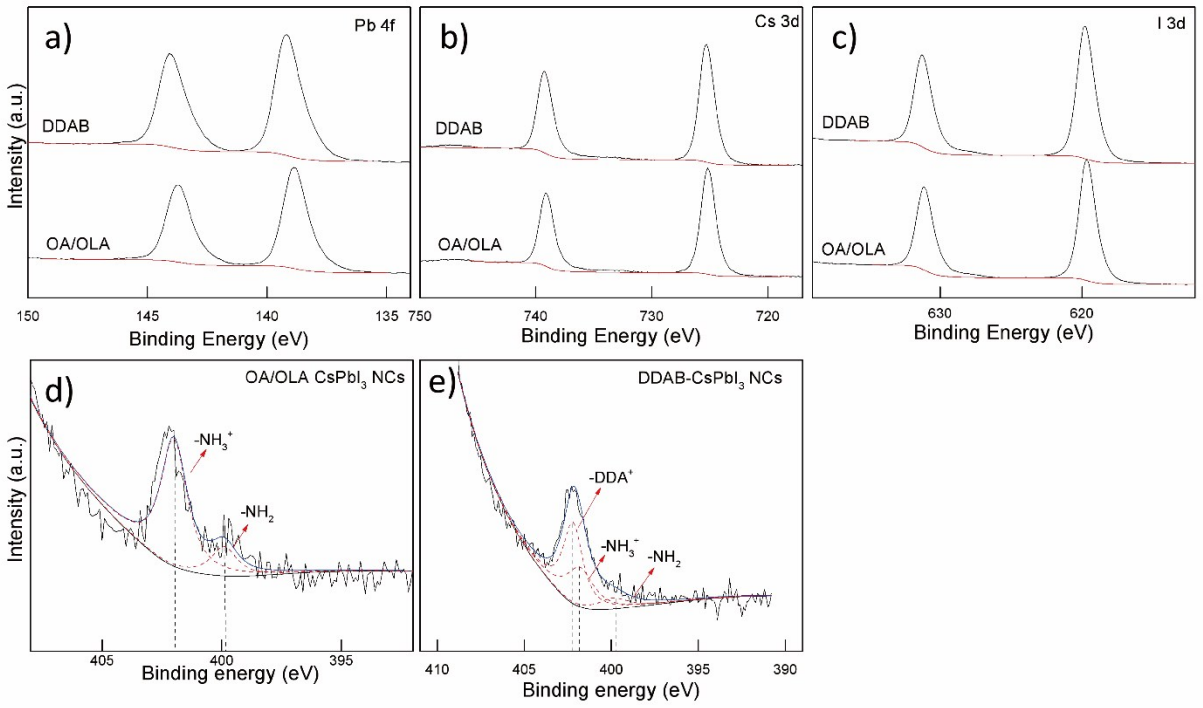

Figure S4 XPS spectra of **a)** Cs 3d, **b)** Pb 4f, **c)** I 4d, **(d-e)** N1s of OA&OLA $CsPbI_3$ NCs and DDAB-capped $CsPbI_3$ NCs.

SI2. Optical stability of $CsPbI_3$ NCs in different environments

To evaluate the thermal stability, DDAB-capped $CsPbI_3$ NCs and OA/OLA $CsPbI_3$ NCs were uniformly spin-coated on ITO glasses. The samples were heated up to 160 °C. The PL intensity of NC films was recorded at by a portable spectrometer (Ocean optics, with 365nm excitation).

The photostability was measured by exposing solutions of DDAB-capped $CsPbI_3$ NCs and OA/OLA $CsPbI_3$ NCs to UV light (with 365nm excitation) for up to 1 hour. The PL intensity was measured every five minutes.

Stability against polar solvents was evaluated in a dark room. 10 μL of water or ethanol were added to 500 μL of NC solution. The PL intensity was continuously monitored over 1 hour (Figure S4).

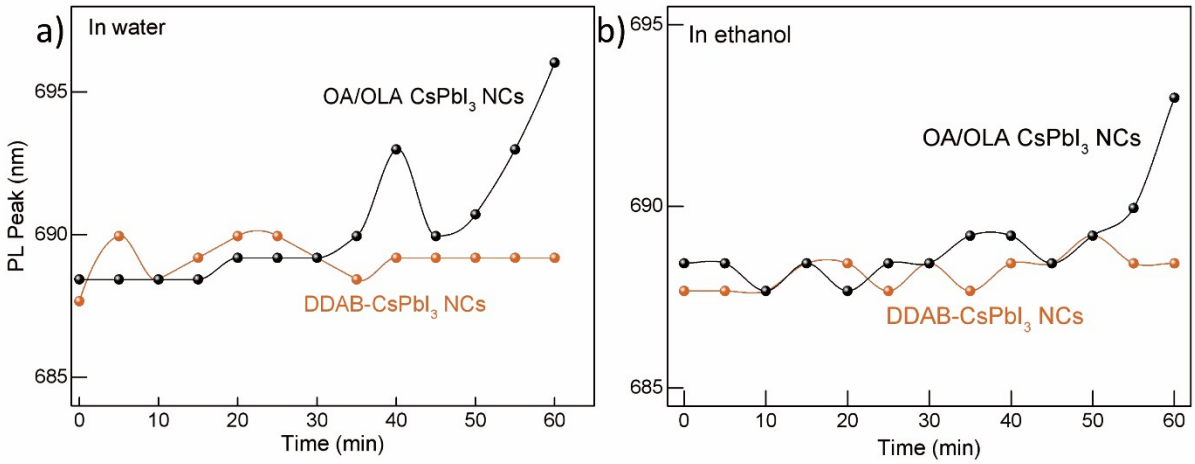

Figure S5 The PL peak of OA&OLA $CsPbI_3$ NCs and DDAB-capped $CsPbI_3$ NCs in **a)** water and **b)** in ethanol as a function of time.

SI3. Comparison of optical stability of different perovskite nanocrystals

Ligands strongly affect the density of surface defects and optical stability of the perovskite nanocrystals[1-7]. The Table S2 summarizes published results and compares them with the results achieved in our work.

Table S2 Survey of ligands in the literature showing increased stability of $CsPbI_3$ NCs.

Year	Ligand	Time Stability (days)	Thermal Stability	Stability against Polar Solvent	Photo stability	Application	Ref.
2017	TOP	30	/	/	/	/	[1]
2017	TMPPA	20	/	/	/	/	[2]
2018	IDA	15	/	/	/	QLED EQE=5.02%	[3]
2018	DPPA	6	/	/	/	Solar cells PCE=2%	[4]
2019	AET	/	/	√	√	Photodetectors	[5]
2019	TMSI	105	√	/	No enhancement	QLED EQE=1.8%	[6]
2019	IDA	50	/	/	√	GaN-LED	[7]
2019	DDAB	60	√	√	√	QLED EQE=1.25%	Our work

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