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

Supporting Information

High Photoactive Black Phase Stability of $CsPbI_3$ Nanocrystals under Damp-heat Conditions of 85℃ and 85% Relative Humidity

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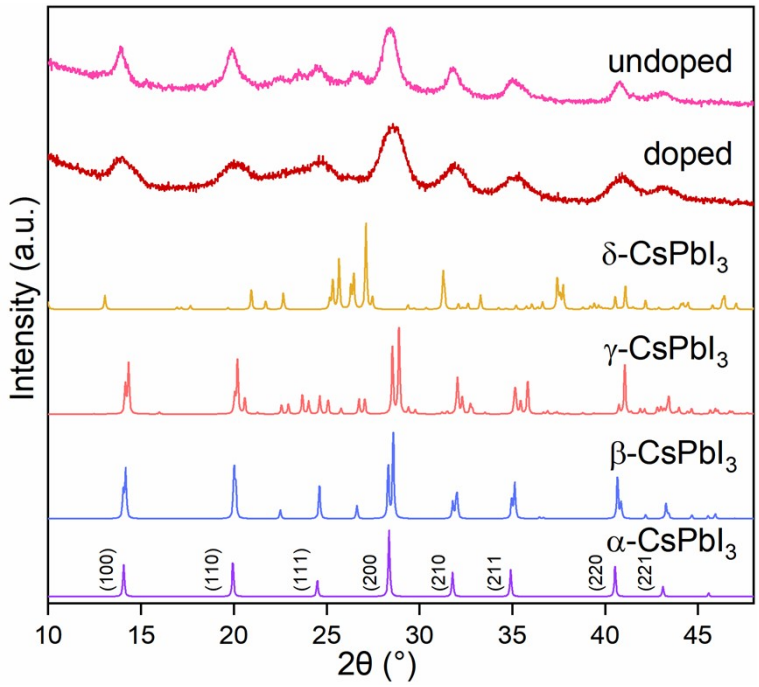

Figure S1. XRD pattern analysis of undoped and doped (Ni-3.65%) $CsPbI_3$ NCs.

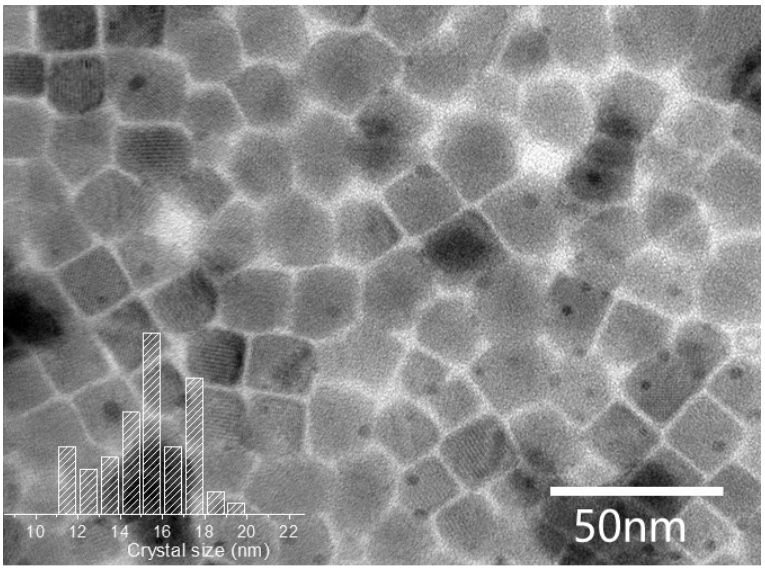

Figure S2. TEM image and size distribution statistics of undoped $CsPbI_3$ NCs.

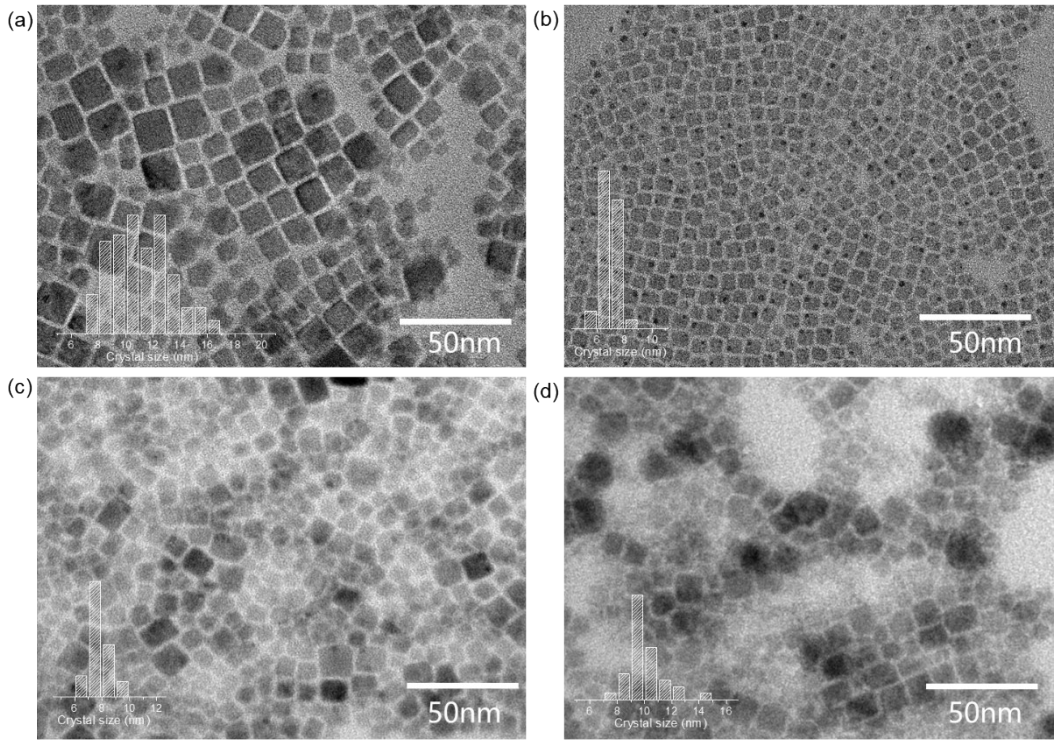

Figure S3. TEM images and size distribution statistics of (a) Ni-1.25%, (b) Ni-3.65%, (c) Ni-4.42%, (d) Ni-5.28% $CsPbI_3$ NCs.

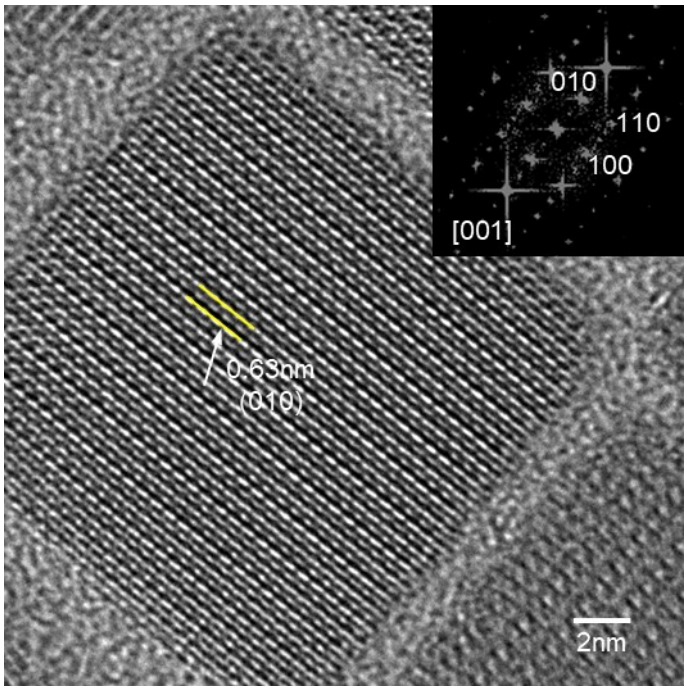

Figure S4. HRTEM image and corresponding FFT of Ni-1.25% $CsPbI_3$ NCs.

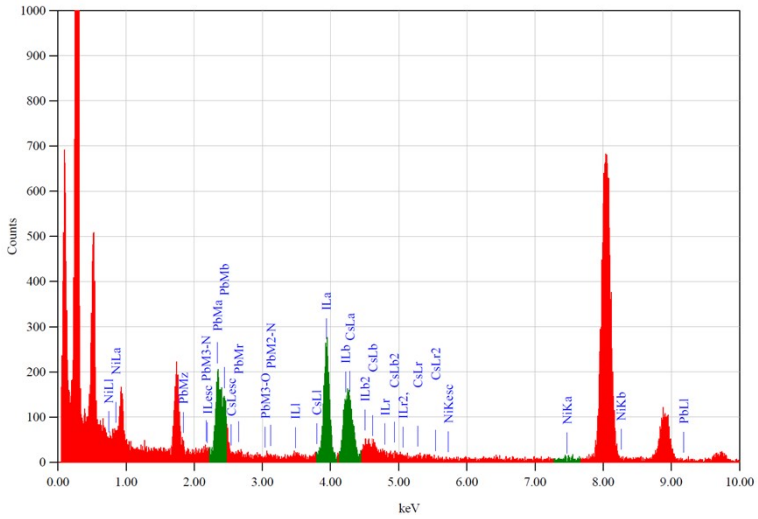

Figure S5. EDS spectrum of Ni-3.65% $CsPbI_3$ NCs.

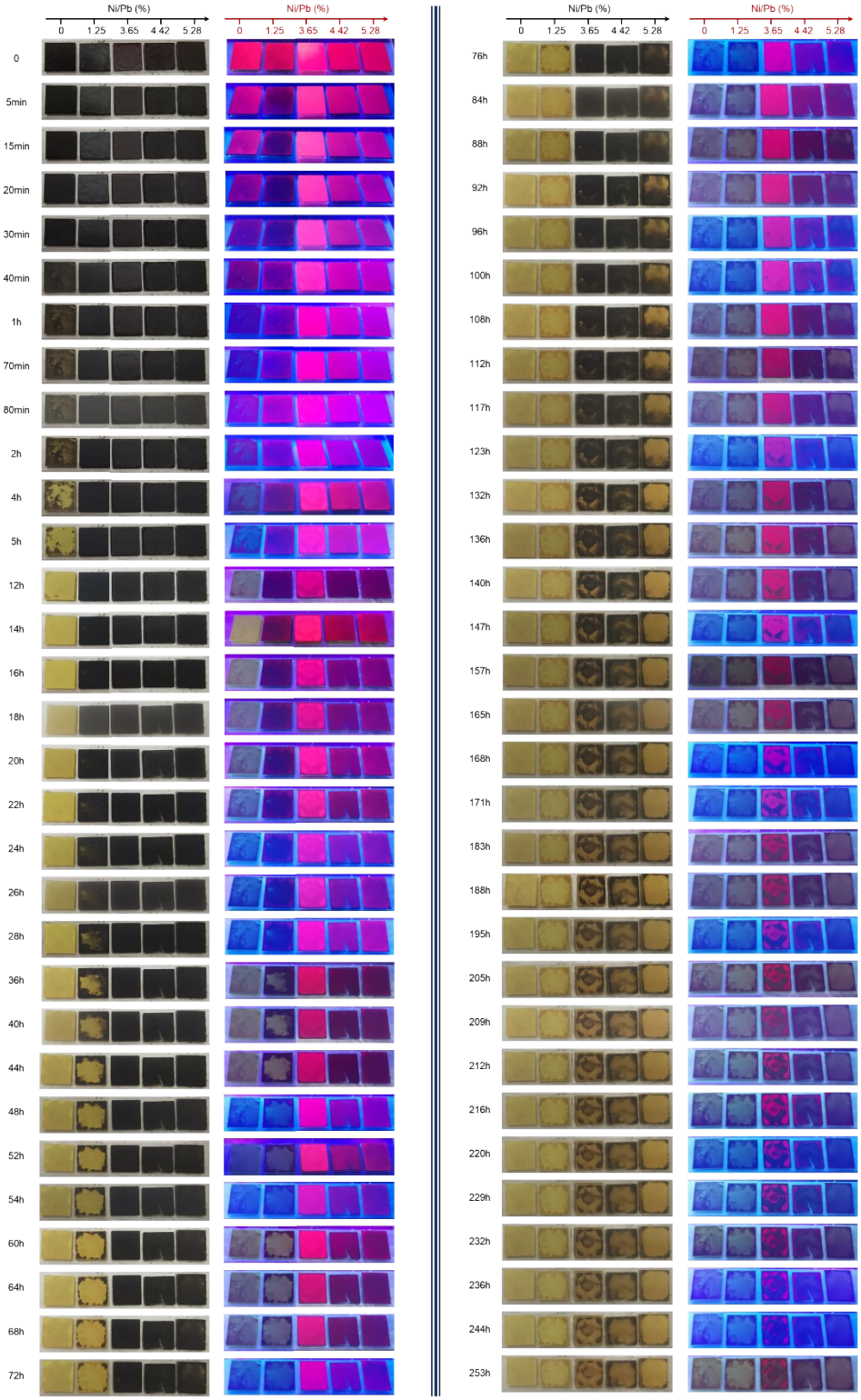

Figure S6. Full spectrum of the 85℃/85% RH damp-heat stability test of undoped and doped $CsPbI_3$ NCs films.

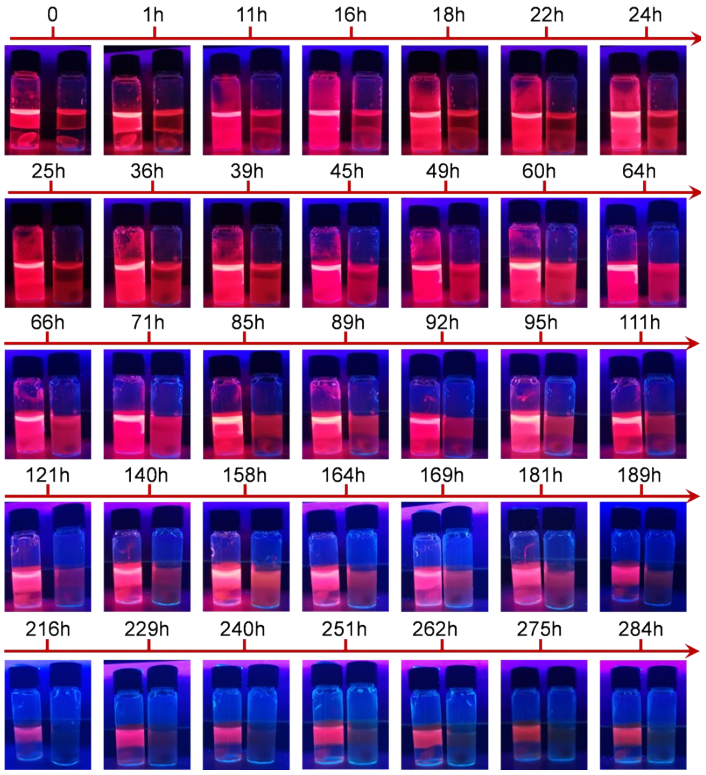

Figure S7. The stability of doped (Ni-3.65% $CsPbI_3$ NCs, left) and undoped (right) $CsPbI_3$ NCs solutions mixed with equal volume of water, the solutions were intensely sloshed by stirrers in the whole test process.

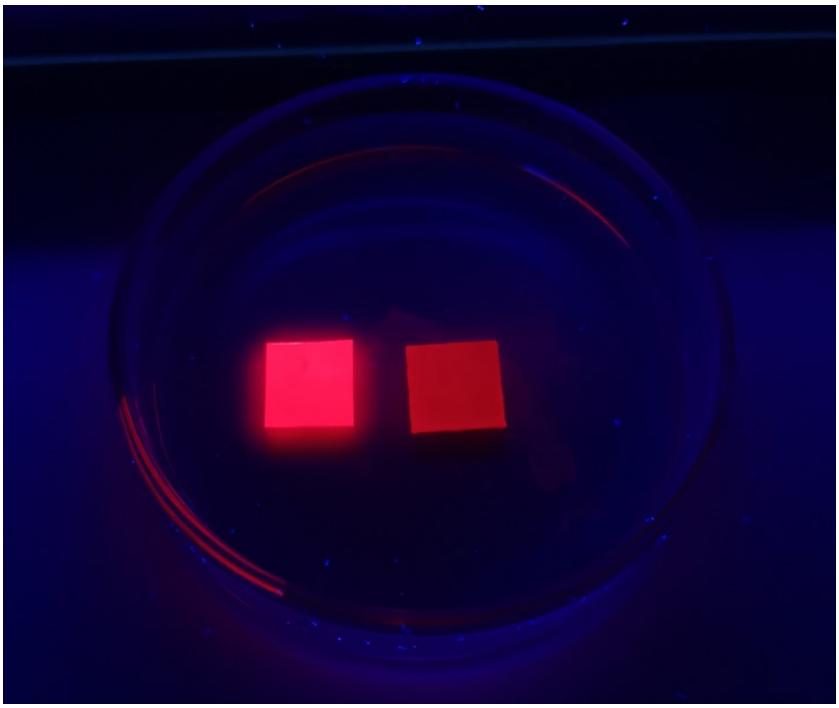

Figure S8. Doped (Ni-3.65% $CsPbI_3$ NCs, left) and undoped (right) $CsPbI_3$ NCs films soaking in the water.

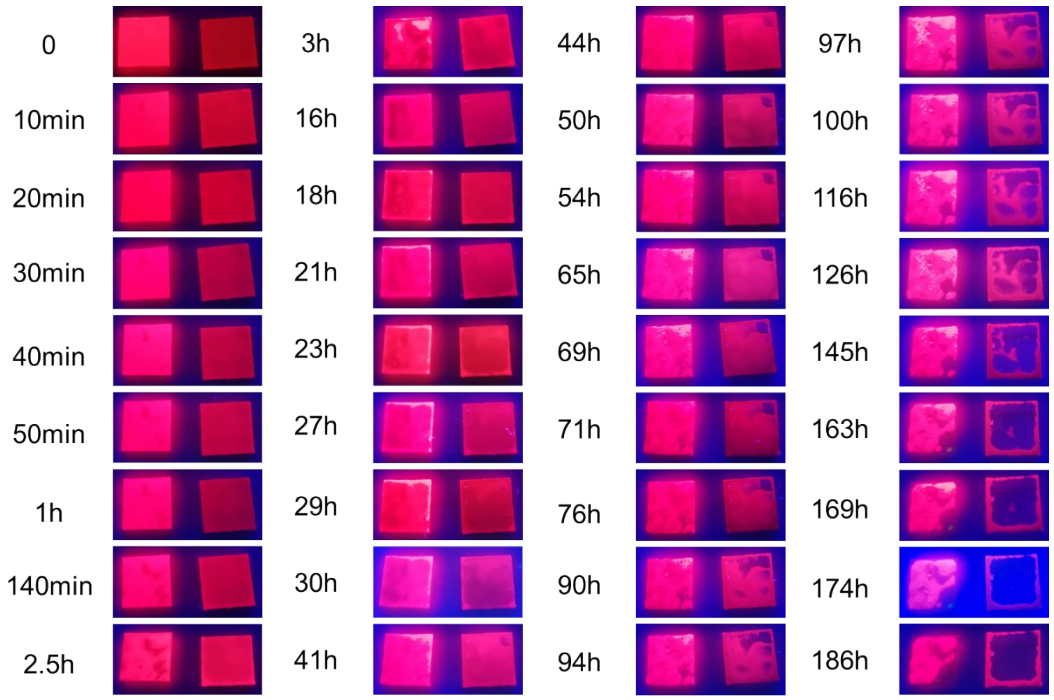

Figure S9. The stability of doped (Ni-3.65% $CsPbI_3$ NCs, left) and undoped (right) $CsPbI_3$ NCs films soaking in water.

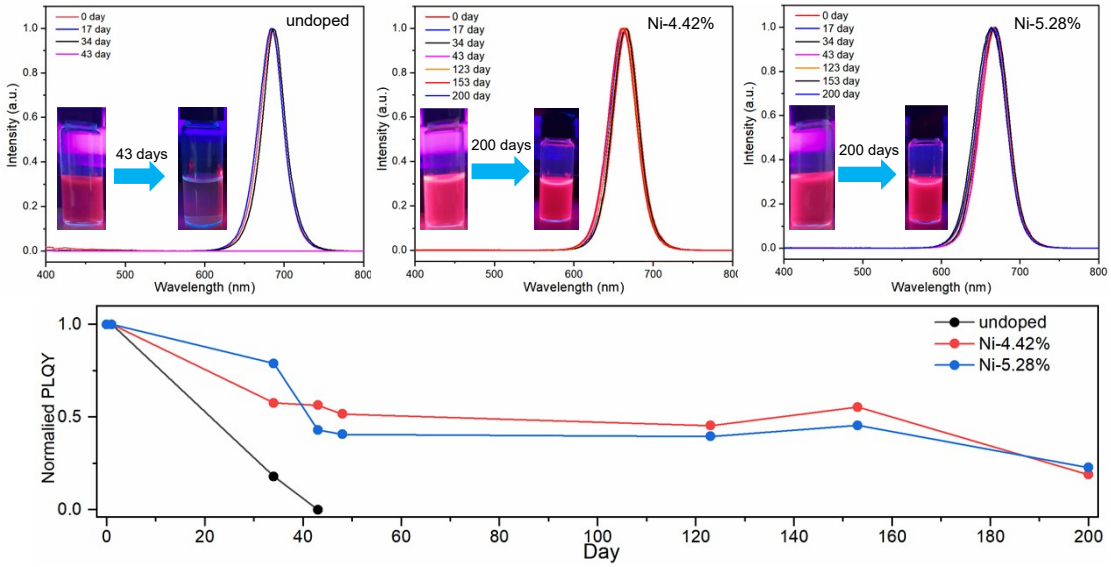

Figure S10. The stability of doped and undoped $CsPbI_3$ NCs solutions under ambient condition.

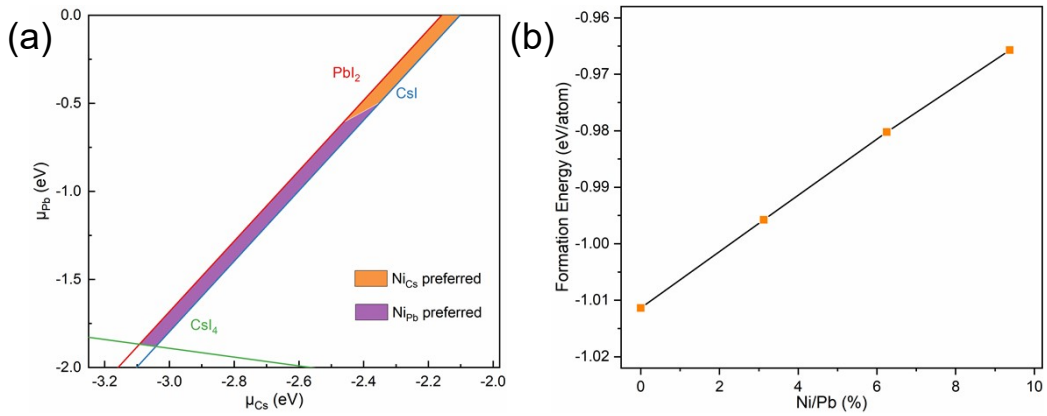

Figure S11. DFT calculation results. (a) Stability regions of Cs, Pb, and I compounds against Cs and Pb chemical potentials. The shaded region is the stability region for the synthesis of $CsPbI_3$, and the different patterns indicate whether the formation of Ni_{Cs} or Ni_{Pb} is preferred. The formation of Ni_i is not favored over the whole region. (b) Crystal formation energies of $CsPbI_3$ with different Ni/Pb doping concentrations.

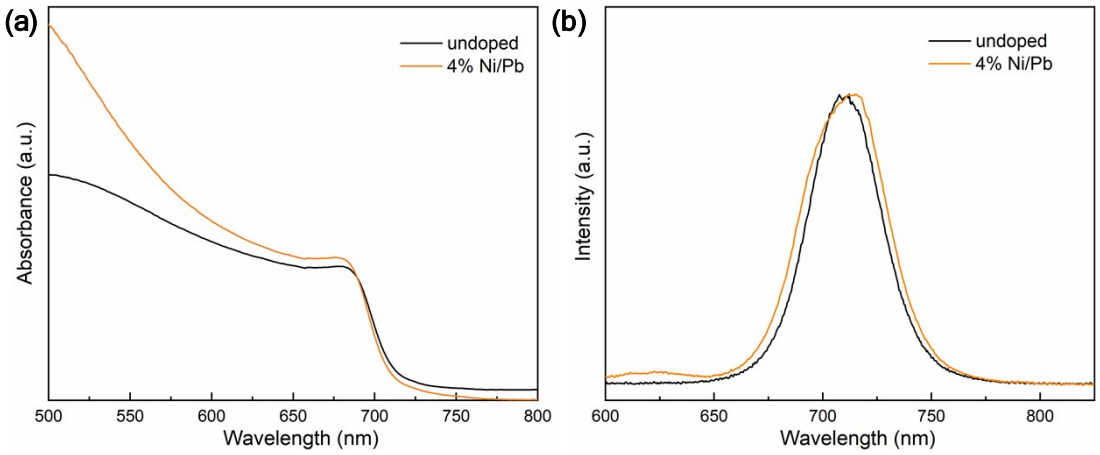

Figure S12. Absorption spectrum (a) and photoluminescence (PL) spectrum (b) of the undoped $CsPbI_3$ and Ni^{2+} doped $CsPbI_3$ (4% Ni/Pb) bulk films.

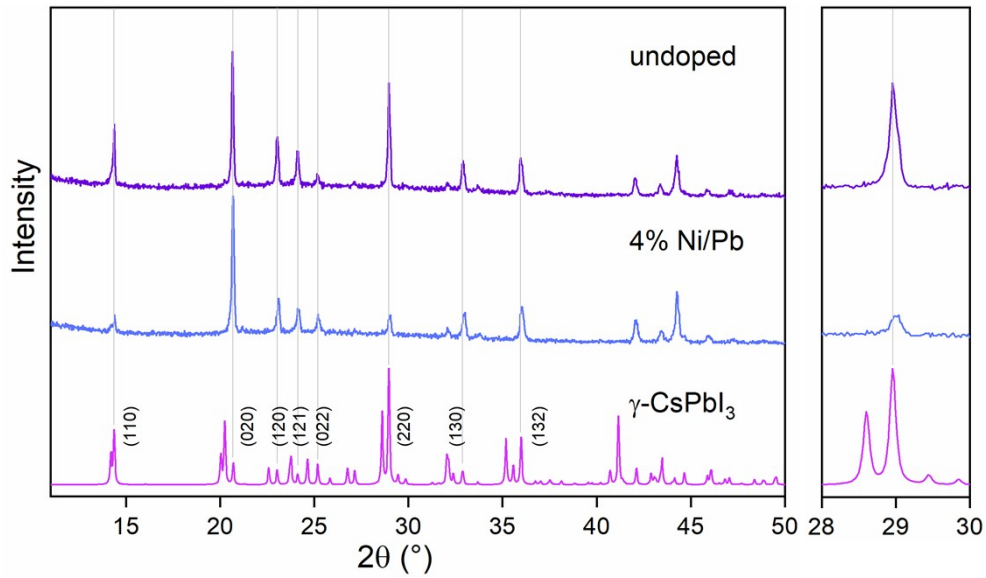

Figure S13. XRD pattern of the undoped $CsPbI_3$ and Ni^{2+} doped $CsPbI_3$ (4% Ni/Pb) bulk films.

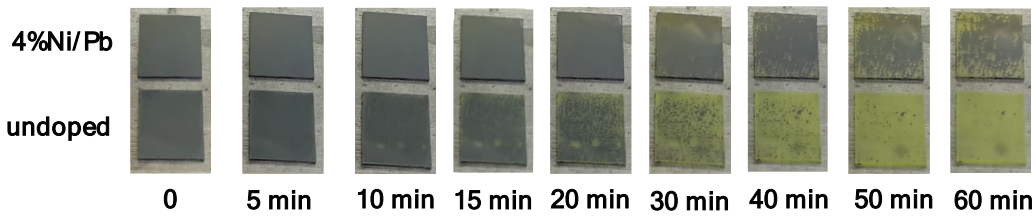

Figure S14. Stabilities of the Ni^{2+} doped $CsPbI_3$ (4% Ni/Pb) and undoped $CsPbI_3$ bulk films at 150 ℃ under the N_2 atmosphere.

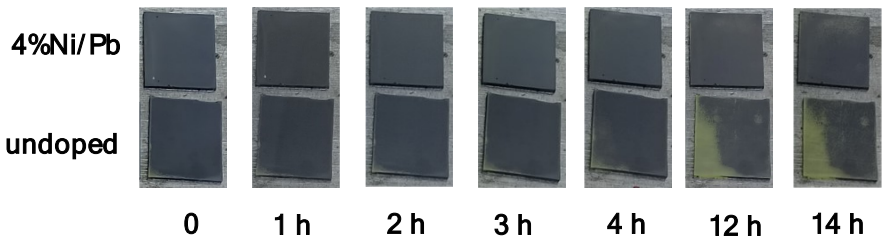

Figure S15. Stabilities of the Ni^{2+} doped $CsPbI_3$ (4% Ni/Pb) and undoped $CsPbI_3$ bulk film at 85 ℃ under the N_2 atmosphere.

Table S1. ICP-MS results of Ni doped $CsPbI_3$ NCs with different reaction temperature and NiI_2/PbI_2 loading ratio.

Samples	NiI_2/PbI_2	Reaction Temperatures (℃)	ICP-MS results (Ni/Pb)	Sizes (nm)
undoped	0:1	170	-	15.23
Ni-1.25%	1:1	170	0.0125:1	11.08
Ni-3.65%	3:1	170	0.0365:1	6.95
Ni-4.42%	3:1	185	0.0442:1	7.76
Ni-5.28%	3:1	200	0.0528:1	10.03

Table S2. Fitted TRPL decay results, average lifetimes (τ_{ave}), PLQYs, radiative (Γ_{rad}) and nonradiative ($\Gamma_{non\text{-}rad}$) decay rates of undoped and doped NCs. Crystal sizes were also given. The methods of calculation referenced previous study[1]. The bi-exponential function was used to fit the decay curves except Ni-3.65% $CsPbI_3$ NCs, because it sufficient to be fitted with a single-exponential function for Ni-3.65% $CsPbI_3$ NCs.

Samples	A1	τ1 (ns)	A2	τ2 (ns)	τave (ns)	PLQY (%)	Γrad (μs^{-1})	Γnon-rad (μs^{-1})	Sizes (nm)
undoped	0.66	22.97	0.33	106.34	81.08	0.31	3.88	8.45	15.23
Ni-1.25%	0.82	26.97	0.21	95.54	59.27	0.57	9.56	7.31	11.08
Ni-3.65%	1.03	18.94	0.00	0.00	18.94	0.88	46.31	6.50	6.95
Ni-4.42%	0.89	26.59	0.15	84.21	46.93	0.64	13.66	7.65	7.76
Ni-5.28%	0.84	28.62	0.19	94.78	57.34	0.59	10.24	7.20	10.03

1. Z.-J. Yong, S.-Q. Guo, J.-P. Ma, J.-Y. Zhang, Z.-Y. Li, Y.-M. Chen, B.-B. Zhang, Y. Zhou, J. Shu, J.-L. Gu, L.-R. Zheng, O. M. Bakr and H.-T. Sun, *J. Am. Chem. Soc.*, 2018, **140**, 9942-9951.