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Polymer Ligands Induced Remarkable Spectral Shifts in All-Inorganic Lead Halide Perovskite Nanocrystals

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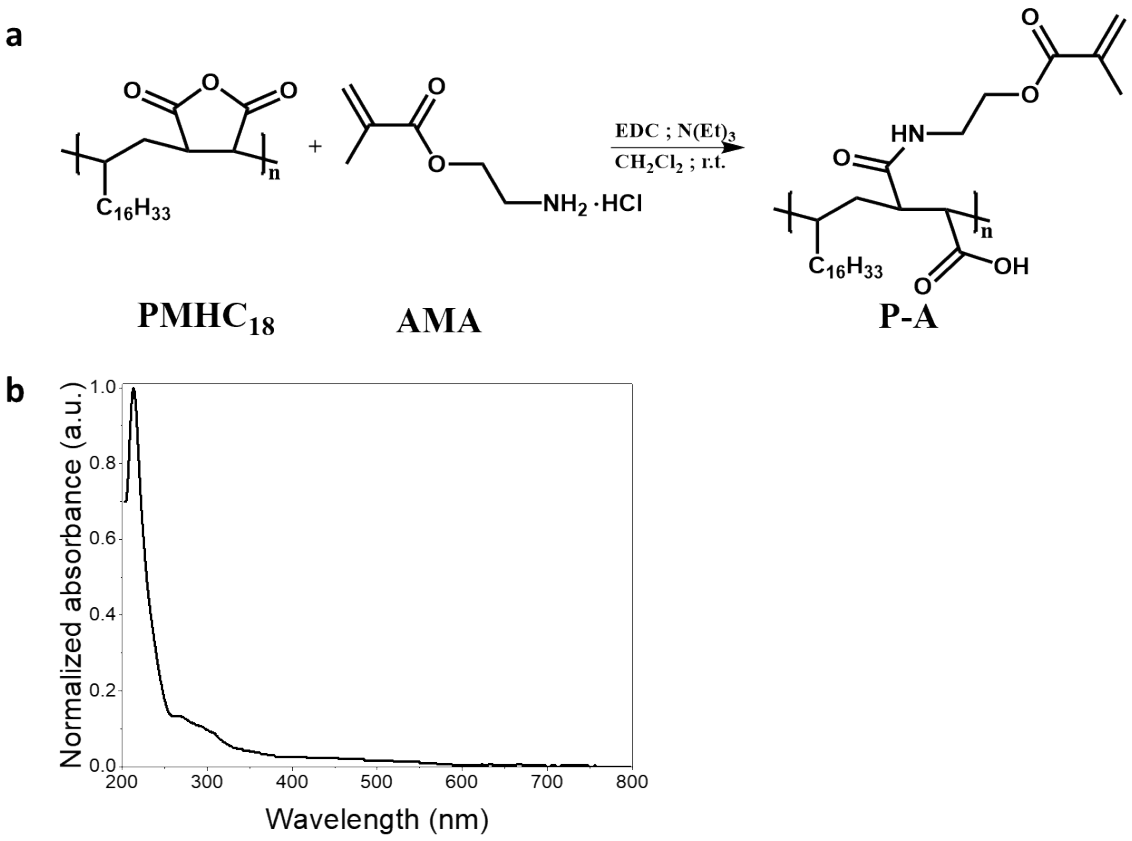


Figure S1. Further details of P-A. a, Chemical reaction equation. b, UV-Vis absorbance of P-A, showing an optical band gap of ~5.17 eV.

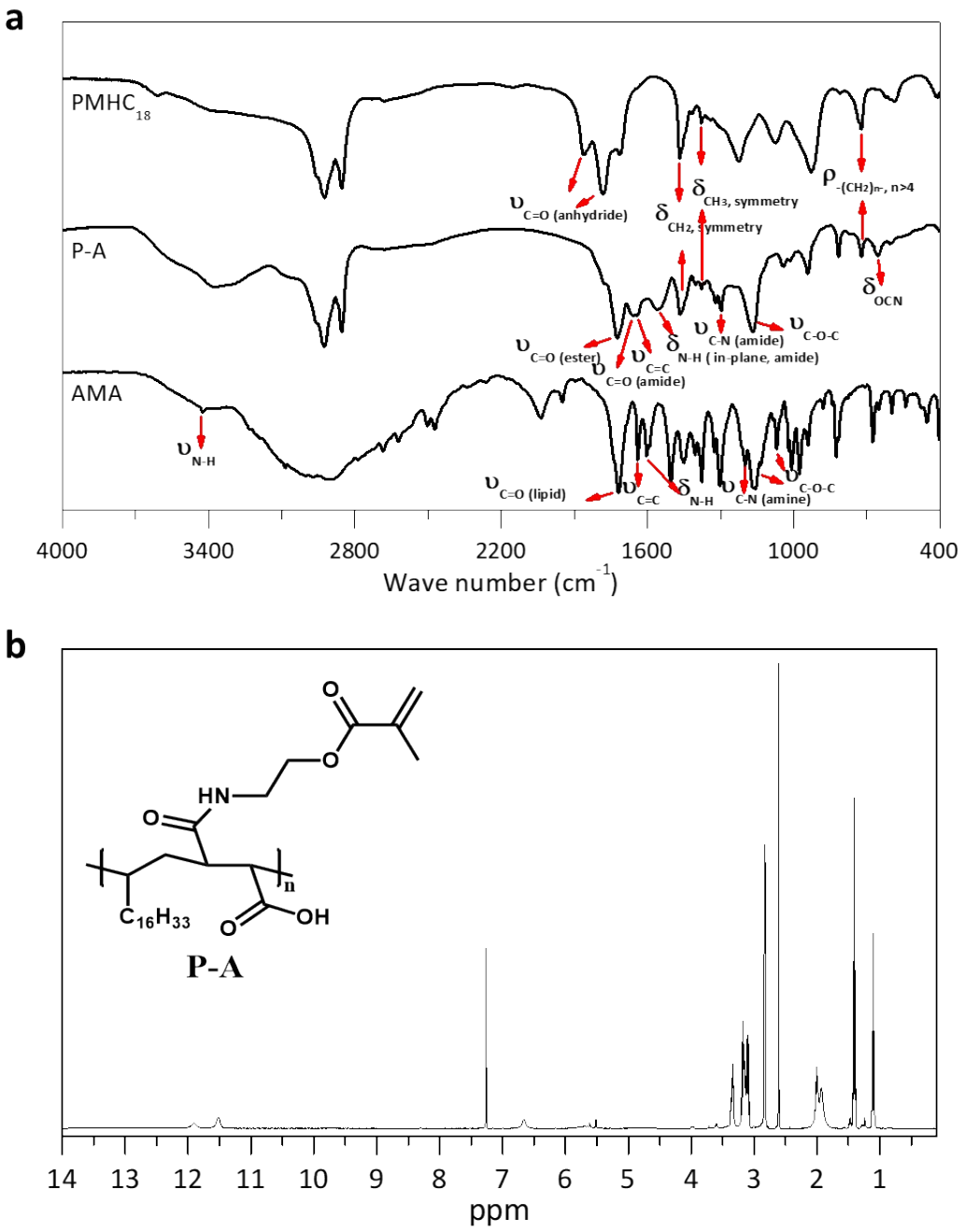


Figure S2. a, Fourier transform infrared spectroscopy (FTIR) of $PMHC_{18}$, AMA and P-A. b, ^{1}H NMR spectra of P-A (400 MHz, $CDCl_3$. The chemical shift signals at 11.9 ppm and 11.5 ppm came from hydrogen atoms on carboxylic acids in different chemical environments. It should be noted that active hydrogen on carboxyl and amide groups may not be detected due to heavy hydrogen exchange).

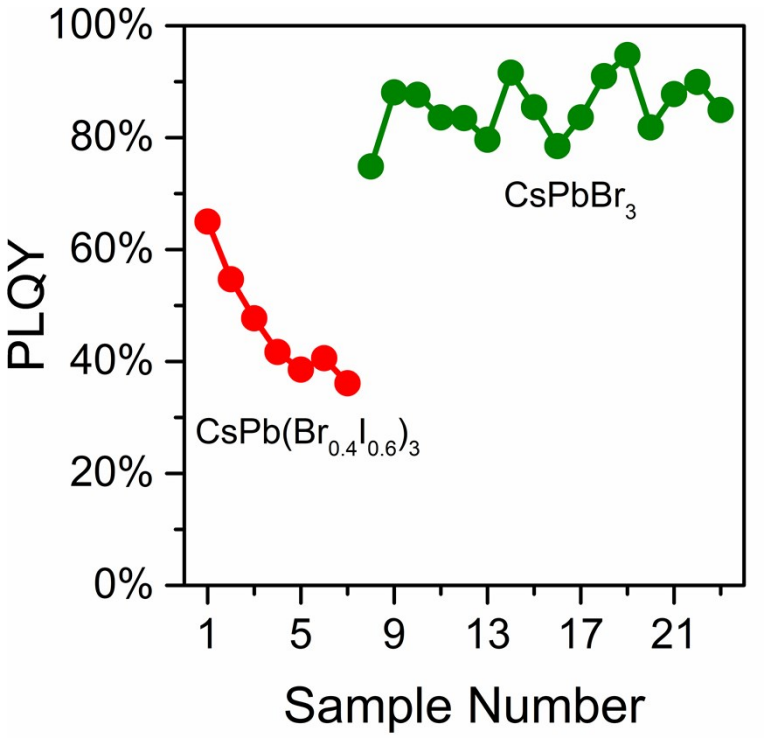


Figure S3. The trend of PLQY of samples.

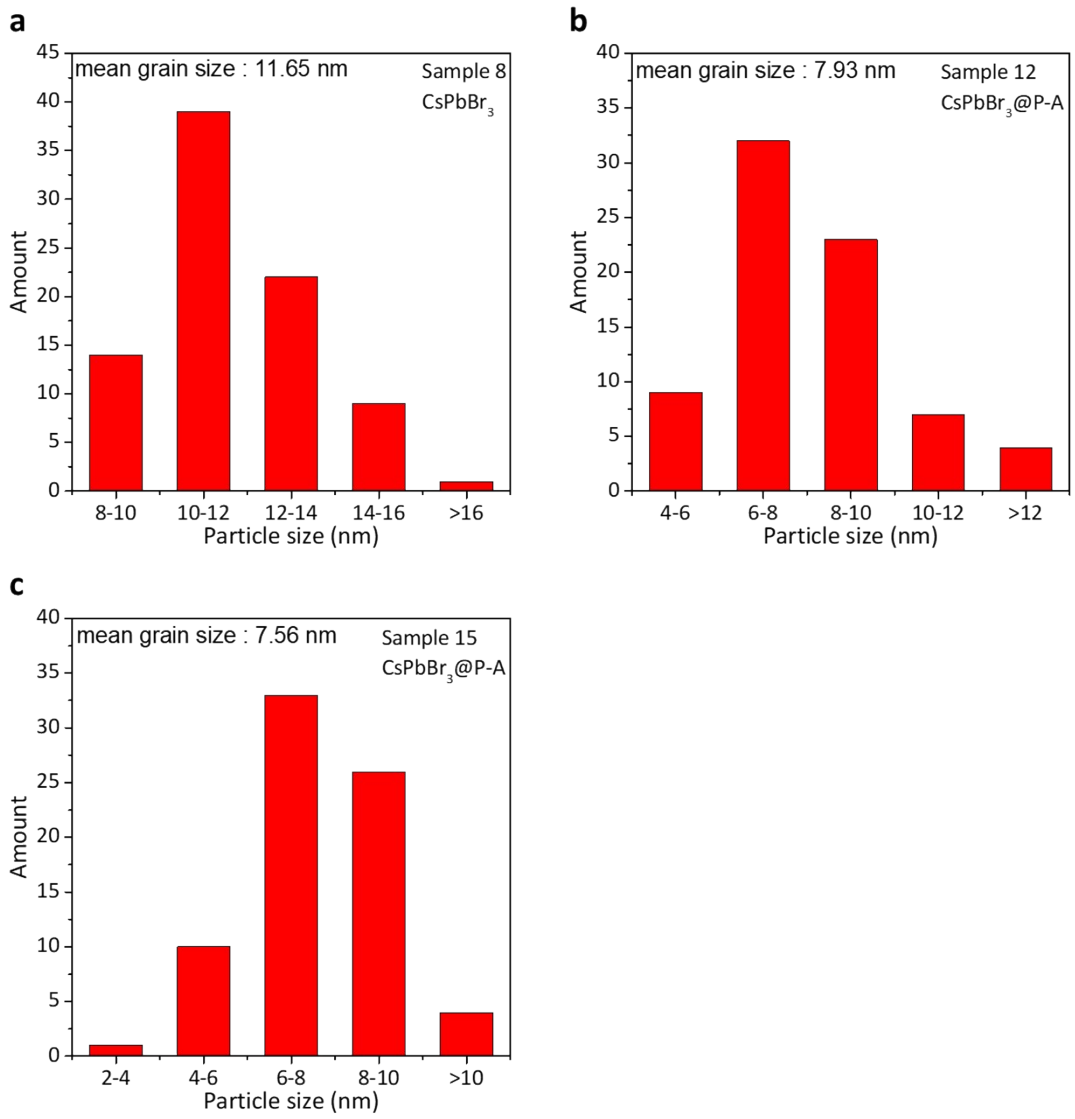


Figure S4. a, b, c, Size distribution histograms of Sample 8, 12 and 15 respectively.

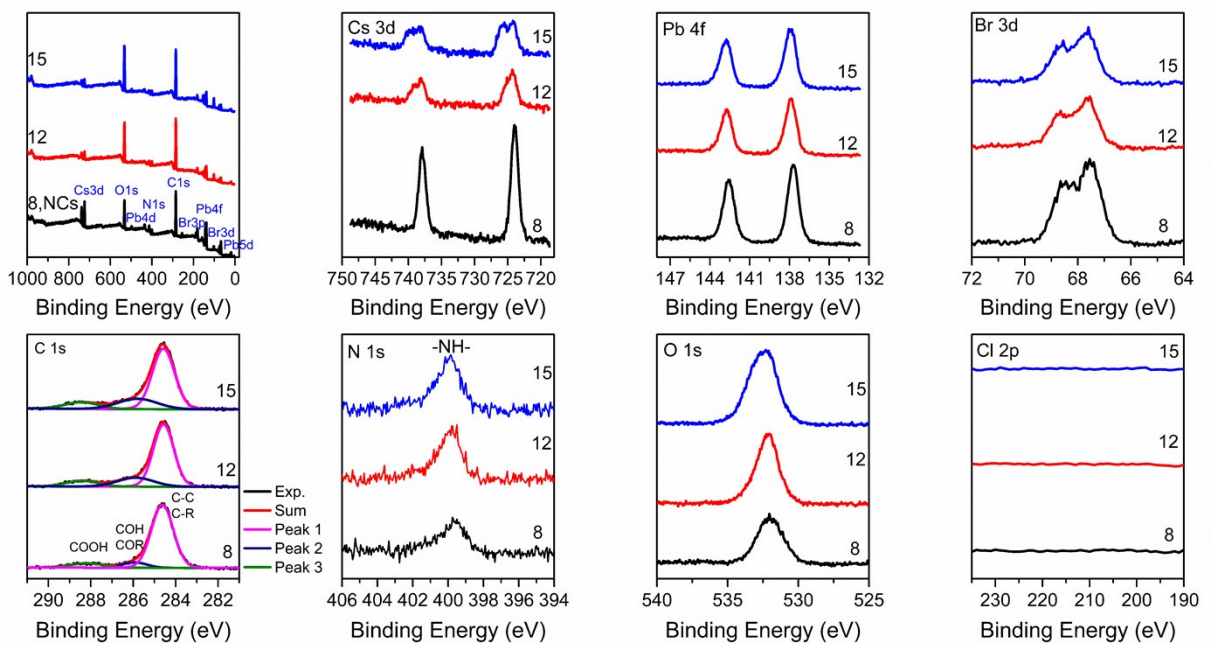


Figure S5. Total spectra and Cs 3d, Pb 4f, Br 3d, C 1s, N 1s, O 1s and Cl 2p core level spectra of Sample 8, 12, 15.

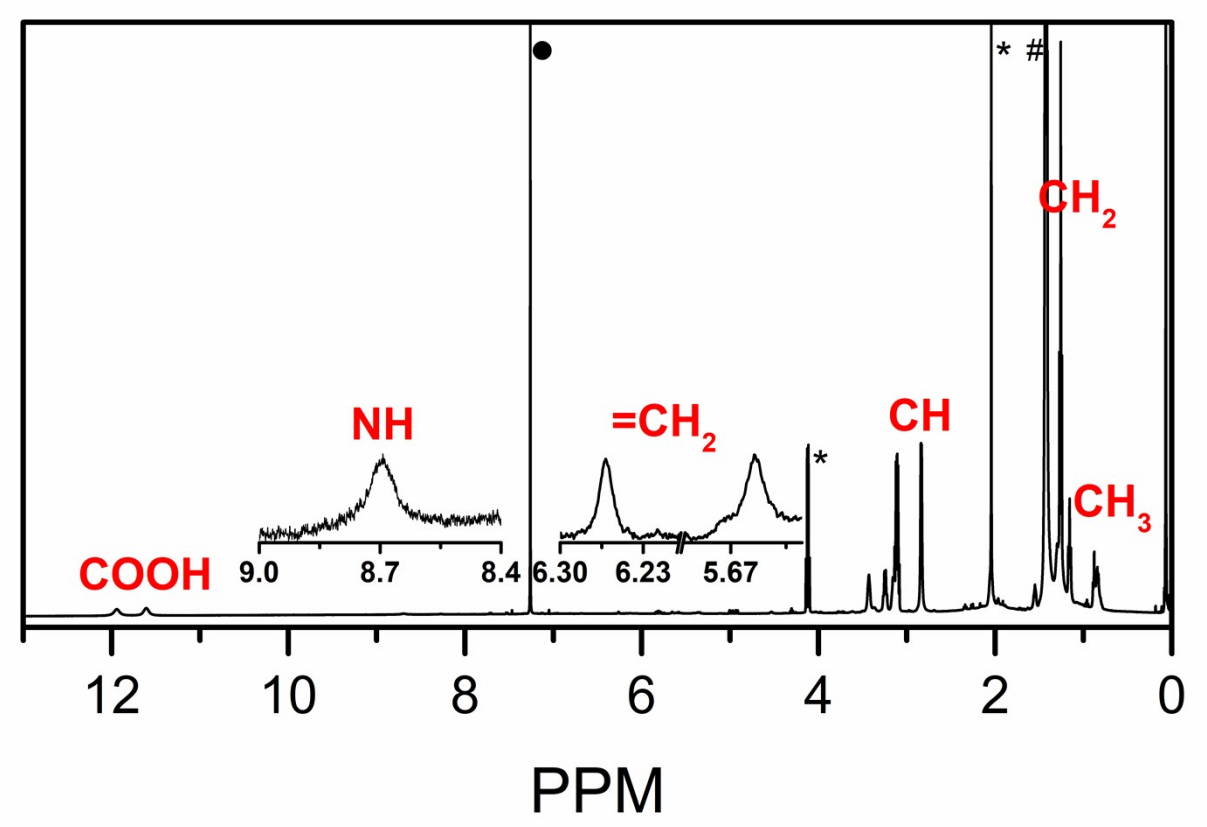


Figure S6. ^{1}H NMR spectra of NCs@P-A (500 MHz, $CDCl_3$). The spectrum can be assigned to the ligand P-A and solvents (* ethyl acetate, # cyclohexane and ● $CDCl_3$).

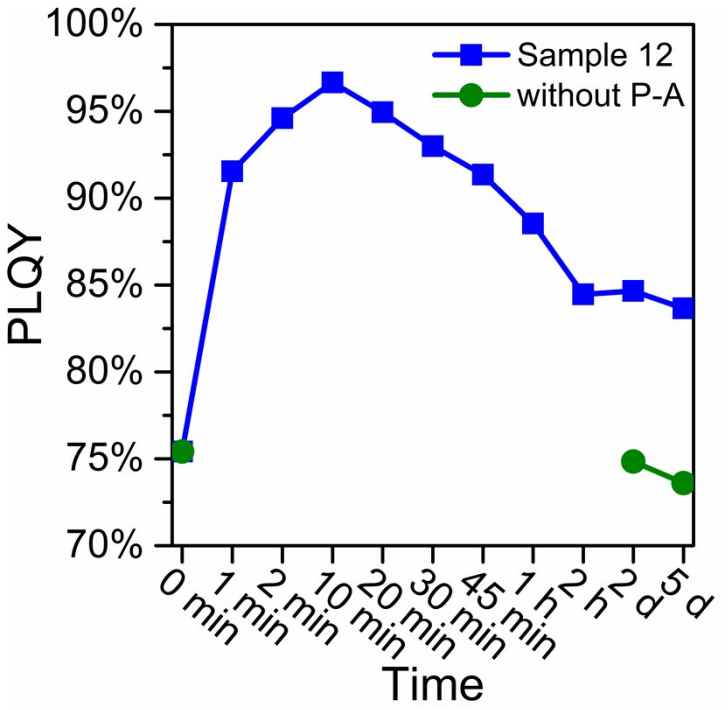


Figure S7. The trend of PLQY of sample 12 over time.

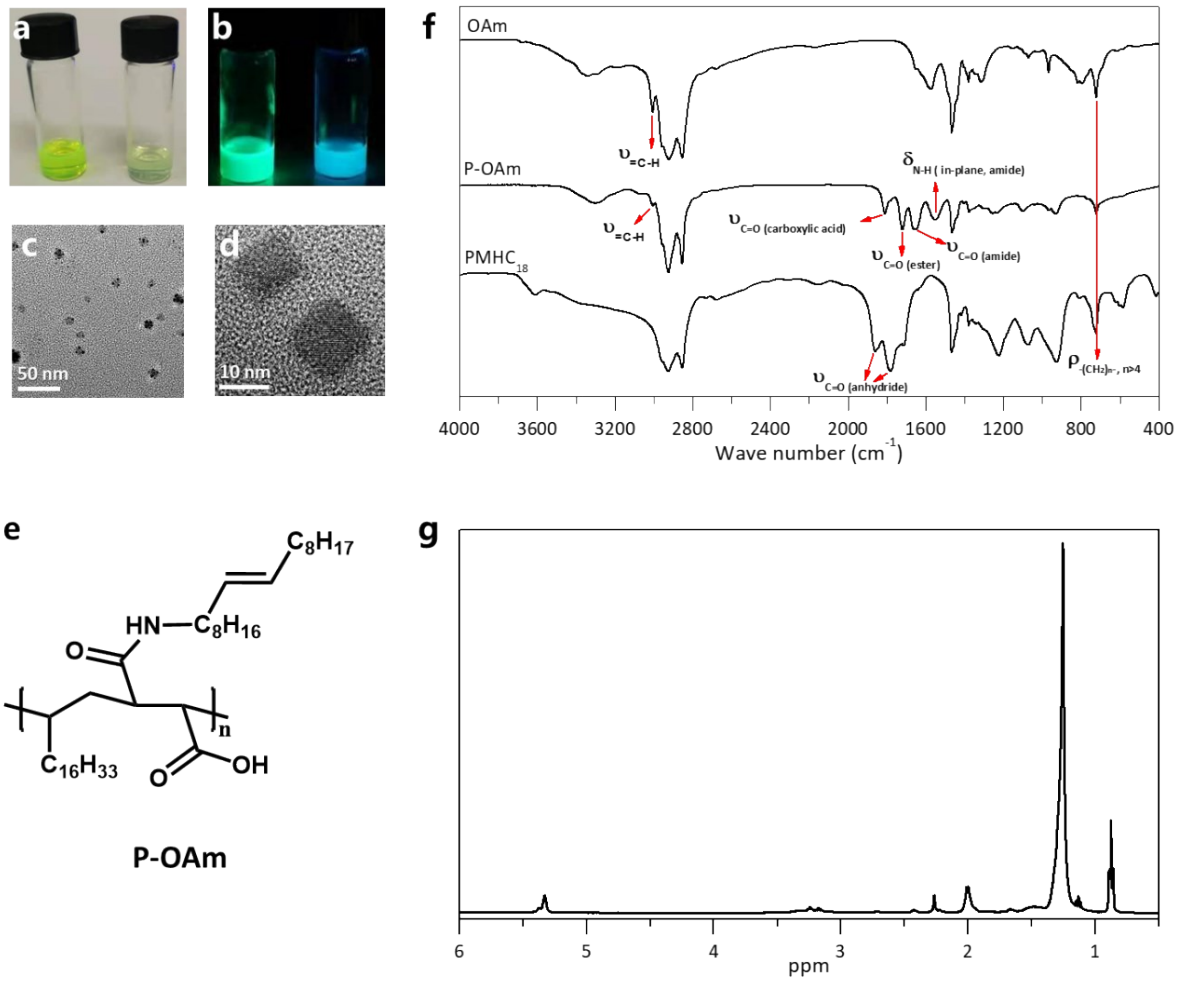


Figure S8. a, Photographs of $CsPbBr_3$ NCs colloidal solution (left) and $CsPbBr_3$ NCs@P-OAm solutions (right) under room light. b, Photographs of $CsPbBr_3$ NCs colloidal solution (left) and $CsPbBr_3$ NCs@P-OAm solutions (right) under UV illumination (λ_{EX} = 365 nm). c, d, TEM images of $CsPbBr_3$@P-OAm. e, Chemical structure of P-OAm. f, Fourier transform infrared spectroscopy (FTIR) of $PMHC_{18}$, OAm and P-OAm. g, ^1H NMR spectra of P-OAm (400 MHz, $CDCl_3$. It should be noted that active hydrogen on carboxyl and amide groups may not be detected due to heavy hydrogen exchange).

Table S1. Sample number, concentration of P-A and peak position of $CsPb(Br_{0.4}I_{0.6})_3$ NCs.

No.	1	2	3	4	5	6	7
Concentration of P-A ($\times 10^{-3}$ mg/ml)	0	62.5	83.3	125	250	500	625
Peak position (nm)	646	634	630	622	611	609	551

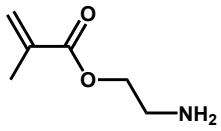
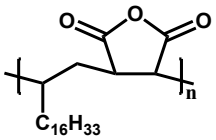
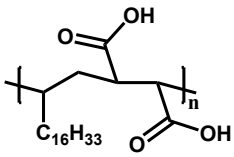
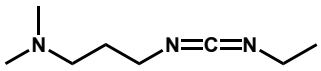
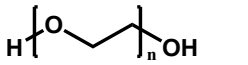
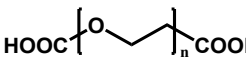
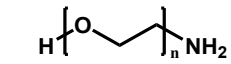
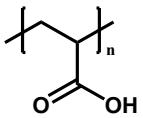
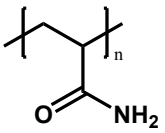
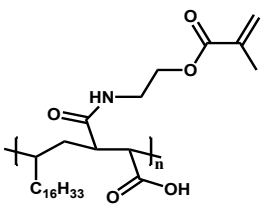
Table S2. Sample number, concentration of P-A and peak position of $CsPbBr_3$ NCs.

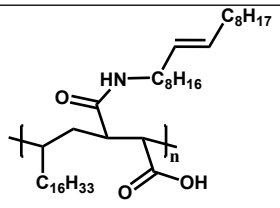
No.	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
Concentration of P-A ($\times 10^{-3}$ mg/ml)	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75
Peak position (nm)	519	514	506	501	497	491	484	481	476	472	464	460	457	452	449	446

Table S3. PL lifetime of sample 12 with time goes by. The monitored wavelength was the peak position. The PL decay curves have a tri-exponential form to investigate the exciton dynamics in the tailoring process. The intensity-weighted average exciton lifetime (τ_{avr}) was $f_1\tau_1 + f_2\tau_2 + f_3\tau_3$, where f_1, f_2 and f_3 are fractional intensities and τ_1, τ_2 and τ_3 are lifetimes.

time	τ_1/ns (f_1)	τ_2/ns (f_2)	τ_3/ns (f_3)	R^2	τ_{avr}/ns
0 min	2.18 (0.08)	8.10 (0.54)	28.32 (0.38)	0.9984	15.36
2 min	4.04 (0.14)	12.07 (0.55)	36.50 (0.31)	0.9985	18.55
10 min	1.48 (0.03)	8.24 (0.47)	27.74 (0.50)	0.9984	17.70
20 min	1.29 (0.03)	7.95 (0.48)	27.12 (0.49)	0.9985	17.13
30 min	1.23 (0.03)	7.69 (0.48)	26.48 (0.49)	0.9984	16.79
45 min	1.58 (0.03)	8.36 (0.52)	28.47 (0.45)	0.9984	17.24
1 h	2.44 (0.06)	8.47 (0.51)	27.97 (0.43)	0.9983	16.57
2 h	1.75 (0.04)	7.93 (0.50)	26.66 (0.46)	0.9984	16.23
5 d	1.49 (0.06)	8.31 (0.49)	33.04 (0.45)	0.9982	19.19

Table S4. The reactants and other polymers with amide and, or carboxylic acid bonds that added into the LHP NCs colloid solutions, the red cross means no, and the green hook means band gap adjustment.

Chemicals	Chemical structure	× or √
AMA		×
$PMHC_{18}$		×
$PMHC_{18}$ hydrolytic product		×
EDC		×
polyethylene glycol		×
		×
		×
polyacrylic acid		×
polyacrylamide		×
polyacrylamide + polyacrylic acid	–	×
[HOOC(-O-C-C-)$_n$COOH] + polyacrylamide	–	×
P-A		√

Chemicals	Chemical structure	× or √
P-OAm		√