Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

Air-Stable Cesium Lead Bromide Perovskite Nanocrystals *via* Post-Synthetic Treatment with Oleylammonium Bromides

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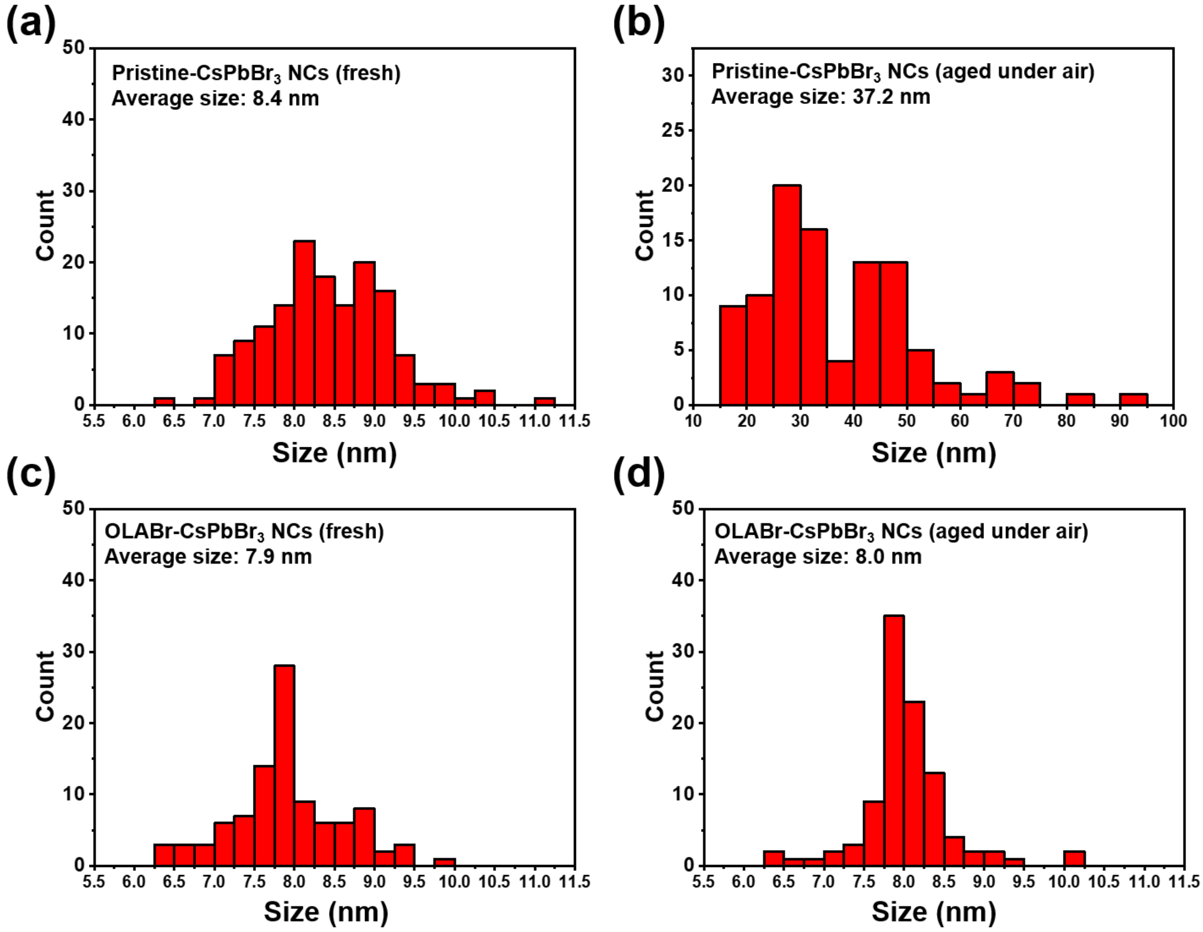

Fig. S1 Size histograms of (a) fresh pristine-$CsPbBr_3$ NCs and (b) air-exposed pristine-$CsPbBr_3$ NCs. Average sizes of (a) and (b) are 8.4 and 37.2 nm, respectively. Size histograms of (c) fresh OLABr-$CsPbBr_3$ NCs and (d) air-exposed OLABr-$CsPbBr_3$ NCs. Average sizes of (c) and (d) are 7.9 and 8.0 nm, respectively.

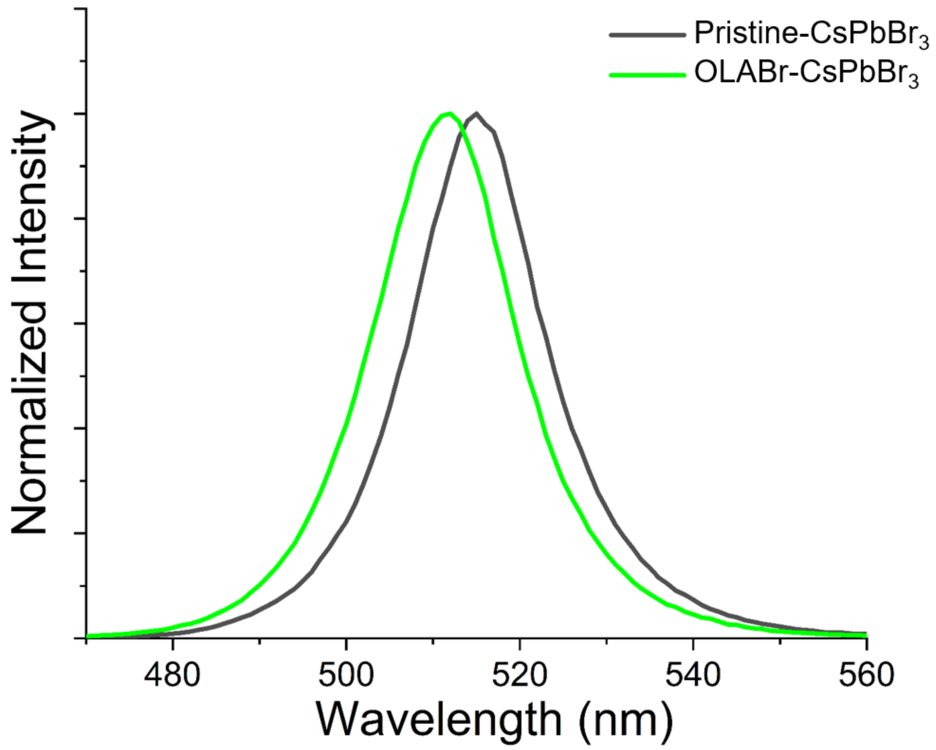

Fig. S2 Normalized PL spectra of (black) pristine-$CsPbBr_3$ NCs (λ_{peak} = 516 nm) and (green) OLABr-$CsPbBr_3$ NCs (λ_{peak} = 512 nm). A blue shift (~4 nm) was observed upon oleylammnoium bromide post-treatment.

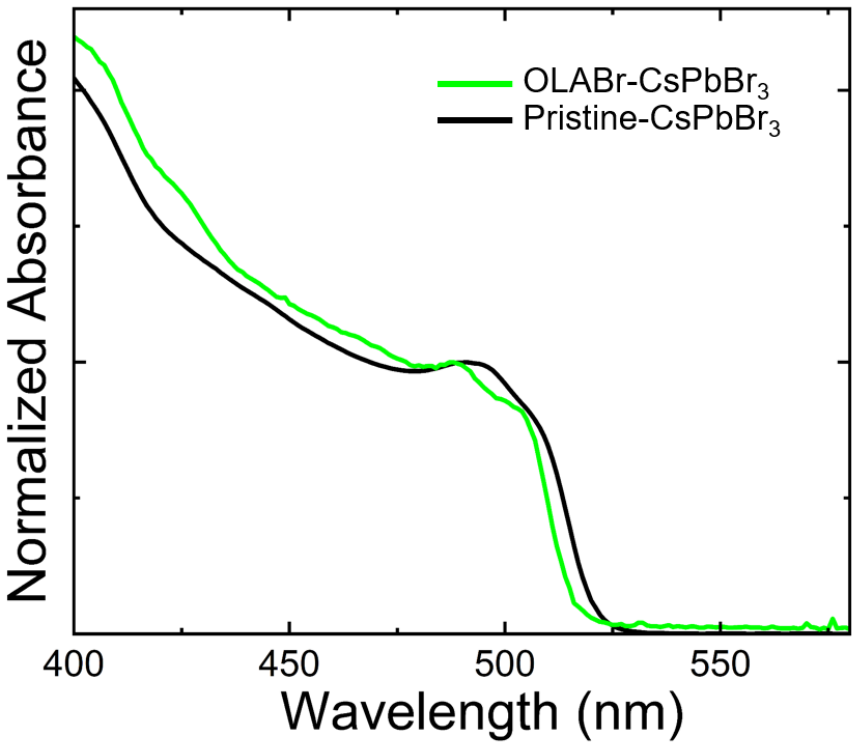

Fig. S3 Normalized absorption spectra of (black) pristine-$CsPbBr_3$ NCs and (green) OLABr-$CsPbBr_3$ NCs.

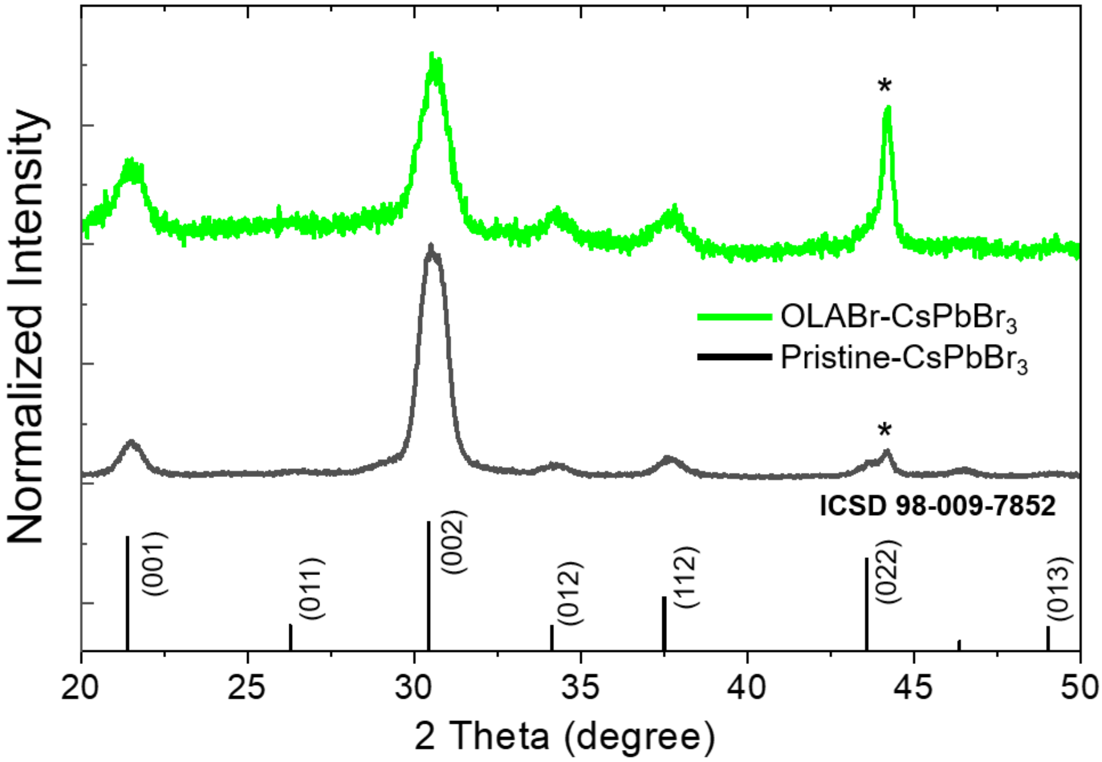

Fig. S4 XRD patterns of (black) pristine- and (green) OLABr-$CsPbBr_3$ NCs with reference patterns (ICSD 98-009-7852). Asterisk corresponds to the scattering peak from the sample holder.

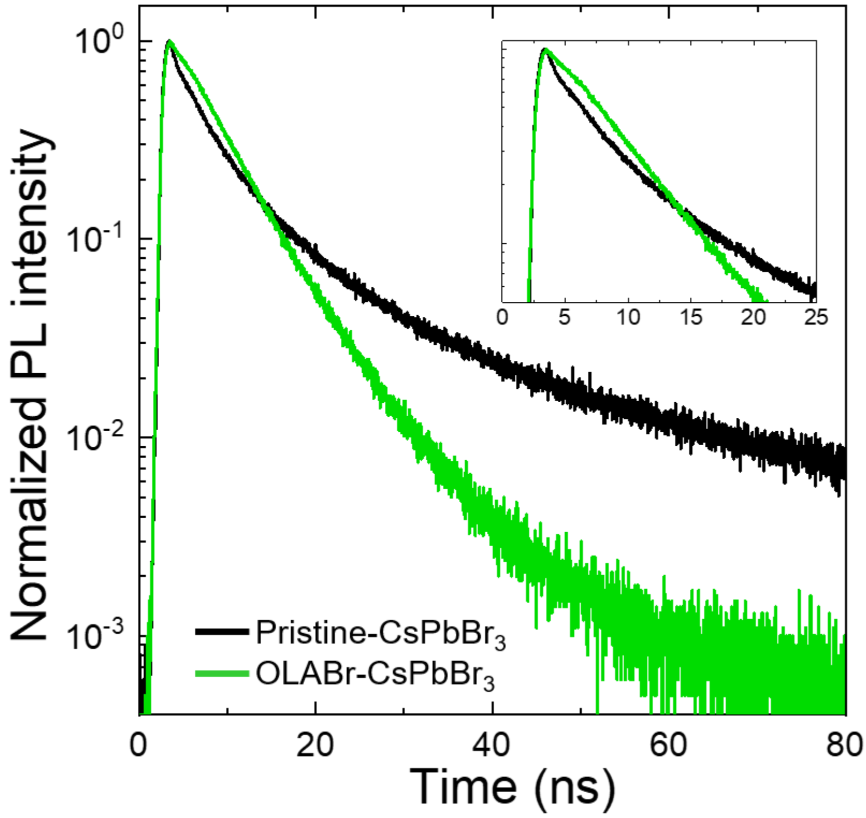

Fig. S5 Time-resolved photoluminescence data of (black) pristine-$CsPbBr_3$ NCs and (green) OLABr-$CsPbBr_3$ NCs.

Table S1. Summary of the effects of post-synthetic treatment on PL QY and stability reported in other studies.

Compound	PL QY (Before treatment)	PL QY (After treatment)	Reported stability enhancement	Ref.
$CsPbBr_3$	75%	95%	Air stability, thermal stability, UV stability, stability against polar solvent.	1
$CsPbBr_3$	69.8±2%	97±2%	Air stability, UV stability, stability against polar solvent.	2
$CsPbBr_3$	50.91%	99.34%	Air stability, UV stability, stability against polar solvent.	3
$CsPbBr_3$	72%	89%	N.A.	4
$CsPbBr_3$	54%	98%	Air stability	5
$CsPbI_3$	87%	~100%	Air stability, thermal stability	6
$CsPbI_3$	52.3%	82.4%	air stability, phase stability	7
$CsPbBr_3$	70%	81%	Photo-stability	8
$CsPbBr_3$	-	-	Phase stability, stability against polar solvent	9
$CsPbI_3$	80±5%	95±2%	Air stability	10
$CsPbI_3$	34%	89%	Thermal stability, device stability	11
$CsPbBr_3$	92±2%	99±2%	Air stability, UV stability	12
$CsPbI_3$	22%	51%	UV stability, phase stability, stability against polar solvent	13
$CsPbBr_3$	54%	83%	N.A.	14
$CsPbBr_3$	73%	100%	UV stability, thermal stability, stability against polar solvent	15
$CsPbBr_3$	49%	71%	N.A	16
$CsPbBr_3$ $CsPbI_3$	80% 80%	93% 95%	N.A	17
$CsPbCl_3$ $CsPbBr_3$	<10% 60-80%	~100% ~100%	N.A	18
$CsPbI_3$	-	~80%	Thermal stability, air stability	19
$CsPbBr_3$ $CsPbI_3$ $CsPbCl_3$	-	~90% 55% 65%	Air stability	20
$CsPbI_3$	27±3%	96±2%	Air stability	21

$CsPbBr_3$ **$CsPbI_3$** **$CsPbCl_3$**	- - -	99±1% 96±1% 70±2%	Air stability, UV stability	22
$CsPbI_3$	70.2%	96%	Air stability	23
$CsPbBr_3$	-	99%	Air stability, UV stability	24
$CsPbBr_3$	34.8%	32.3%	Air stability	25
$CsPbI_3$	28.6%	~100%	Stability against polar solvent	26
$CsPbBr_3$	54%	98%	Air stability	27
$CsPbBr_3$	~35%	~100%	Air stability, UV stability	28
$CsPbBr_3$	~25%	~99%	Air stability, UV stability	29
$CsPbBr_3$	~15%	~100%	UV stability, thermal stability	30
$CsPbBr_3$	74%	89%	Air stability	31
$CsPbBr_3$	70%	92%	Stability against polar solvent, UV stability	32
$CsPbBr_3$	65.89%	95.79%	Air stability	33
$CsPbBr_3$	85%	92%	Air stability	34
$CsPbBr_3$	65%	98%	Air stability, stability against polar solvent	35
$CsPbBr_3$	54.32%	82.77%	Air stability, thermal stability	36
$CsPbBr_3$	48±5%	90±7%	Air stability, thermal stability	37
$CsPbBr_3$	52%	74%	-	38
$CsPbBr_3$	-	~100%	Air stability, stability against polar solvent, thermal stability	39
$CsPbCl_3$ **$CsPbBr_3$** **$CsPbI_3$**	1.9% 75.5% 49.4%	5.8% 100% 97%	Air stability, UV stability, stability against polar solvent	40
$CsPbBr_3$	61%	76%	UV stability, stability against polar solvent	41
$CsPbBr_3$	-	83%	Air stability, stability against polar solvent, UV stability, thermal stability	42
$CsPbBr_3$	~68±8%	95±4%	Thermal stability	43
$CsPbBr_3$	56.7%	82.9%	UV stability, stability against polar solvent	44

$CsPbI_3$	60%	87.0%	N.A	45
$CsPbBr_3$	72%	~95%	Air stability, UV stability, thermal stability	46
$CsPbCl_3$ **$CsPbBr_3$**	11% 22%	88% 90%	Air stability, UV stability	47
$CsPbI_3$	63%	87%	Air stability	48
$CsPbI_3$	52%	93%	Air stability, UV stability	49
$CsPbBr_3$	-	92%	Air stability, thermal stability	50
$CsPbBr_3$	-	96.8%	N.A	51
$CsPbI_3$	52.3%	82.4%	Air stability, UV stability	52
$CsPbBr_3$	-	99.8%	Air stability, stability against polar solvent, thermal stability, UV stability	53
$CsPbBr_3$	60-80%	75-85%	Air stability	54
$CsPbBr_3$	54%	78%	Air stability, thermal stability	55
$CsPbBr_3$	-	Slightly higher	Air stability, stability against polar solvent, UV stability	56
$CsPbI_3$	-	Slightly higher	Air stability	57
$CsPbI_3$	-	63.7%	Air stability, UV stability, stability against polar solvent	58
$CsPbBr_3$	53%	85%	Air stability	59
$CsPbBr_3$	10.9%	24.2%	N.A	60
$CsPbI_3$	~90%	~100%	Air stability	61
$CsPbI_3$	-	80%	Air stability	62
$CsPbCl_3$	1-5%	~50%	Air stability, stability against polar solvent	63
$CsPbI_3$	-	Slightly higher	Air stability, stability against polar solvent	64
$CsPbI_3$	75%	96%	Air stability, thermal stability	65
$CsPbBr_3$	40%	98%	Air stability, thermal stability, UV stability	66
$CsPbBr_3$	-	>90%	Air stability, UV stability	67

$CsPbI_3$	61.8%	98.5%	Air stability, UV stability, thermal stability	68
$CsPbI_3$	60%	81%	Air stability	69

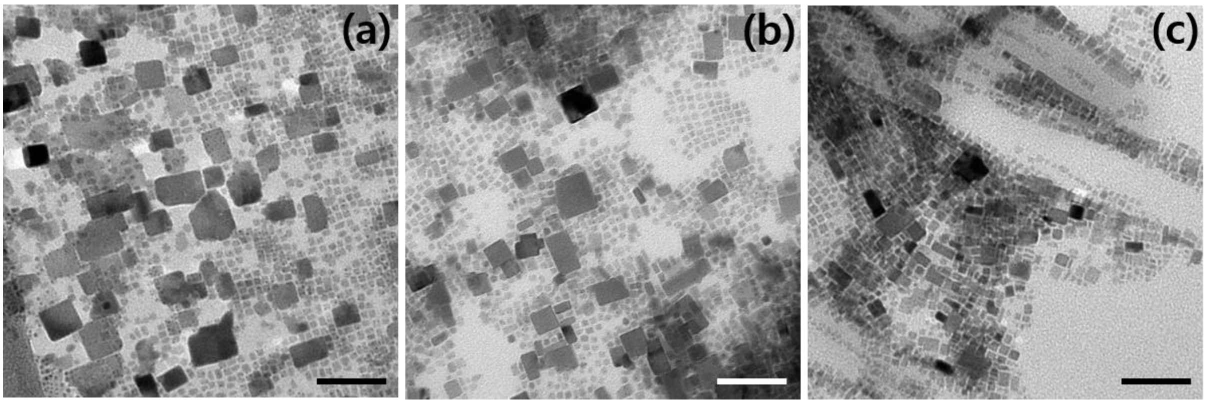

Fig. S6 TEM images of $CsPbBr_3$ NCs post-treated with (a) oleic acid, (b) oleylamine, and (c) $PbBr_2$ after exposure to air. Scale bars are 100 nm.

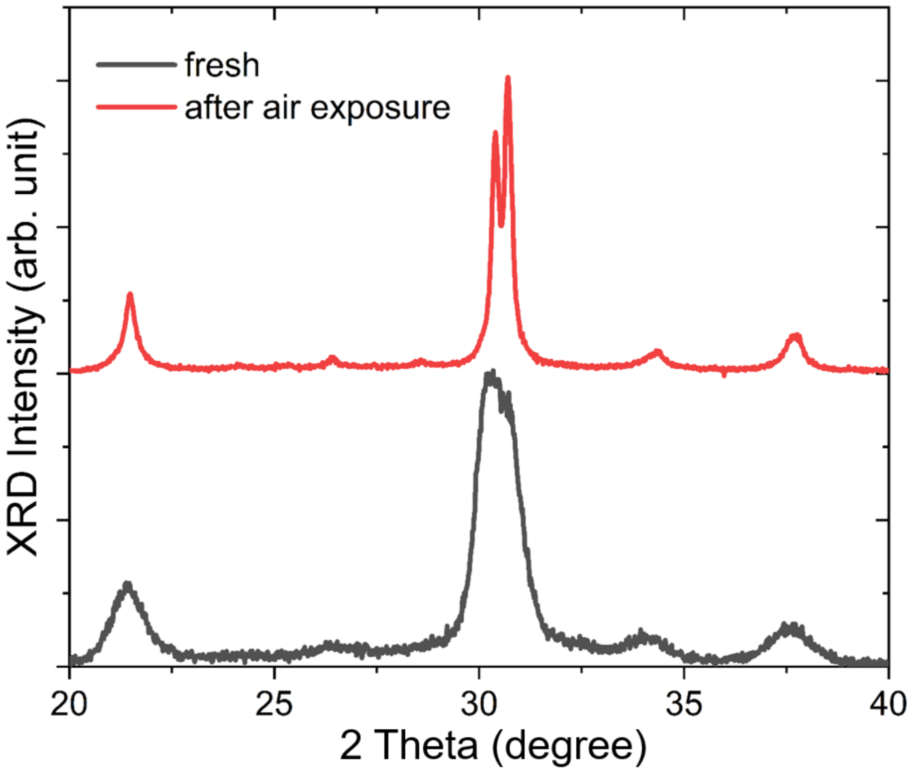

Fig. S7 XRD patterns of smaller size pristine-$CsPbBr_3$ NCs (λ_{PL} ~512 nm) before and after air exposure.

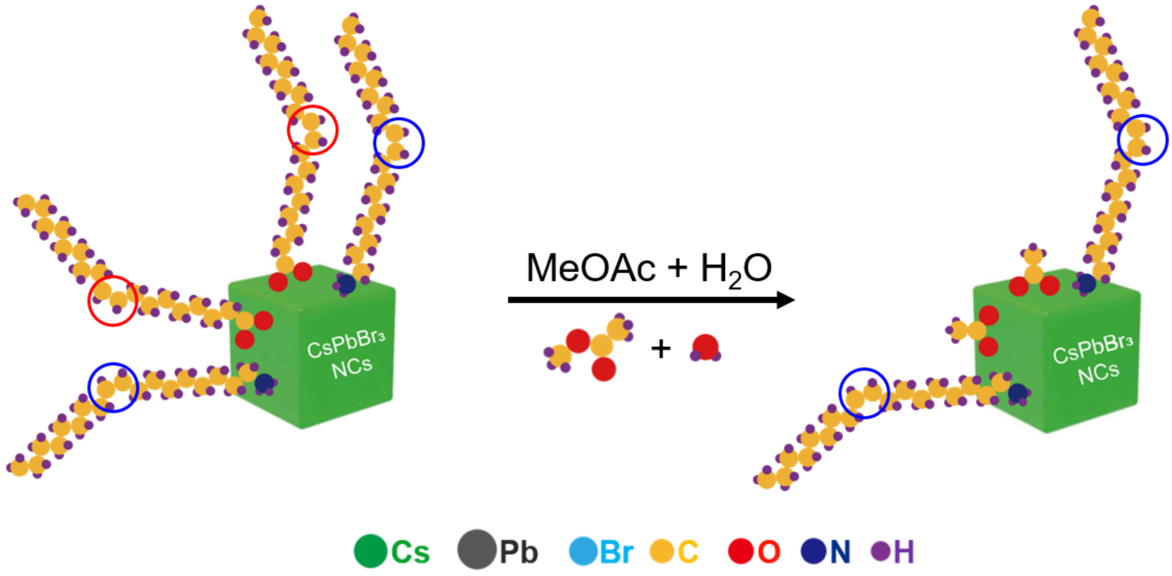

Fig. S8 Schematic of selective ligand exchange in $CsPbBr_3$ NCs employing methyl acetate (MeOAc).

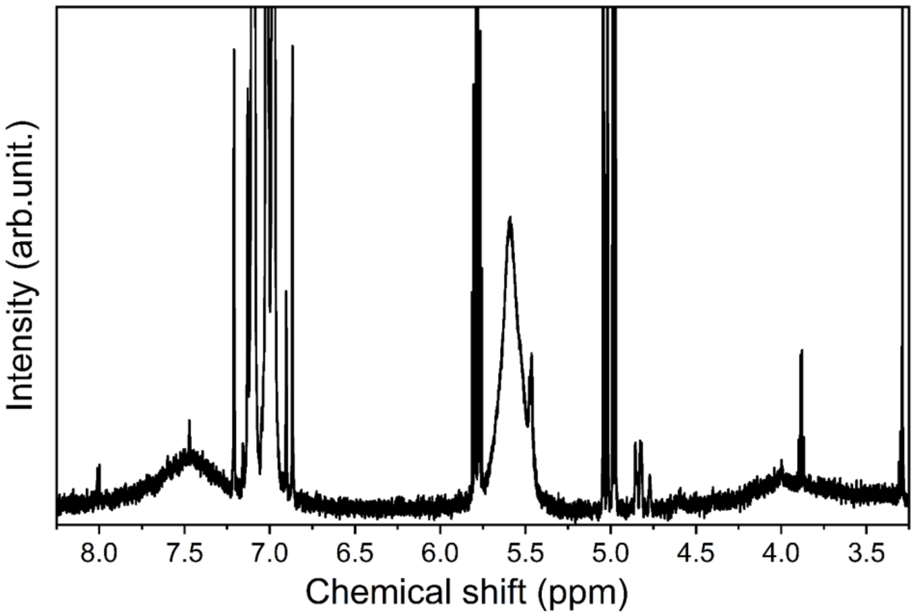

Fig. S9 ^{1}H-NMR spectra of pristine-$CsPbBr_3$ NCs after purification without MeOAc. Broad resonances around 7.5 ppm and 4.0 ppm can be assigned to weakly bound oleylammoniums.

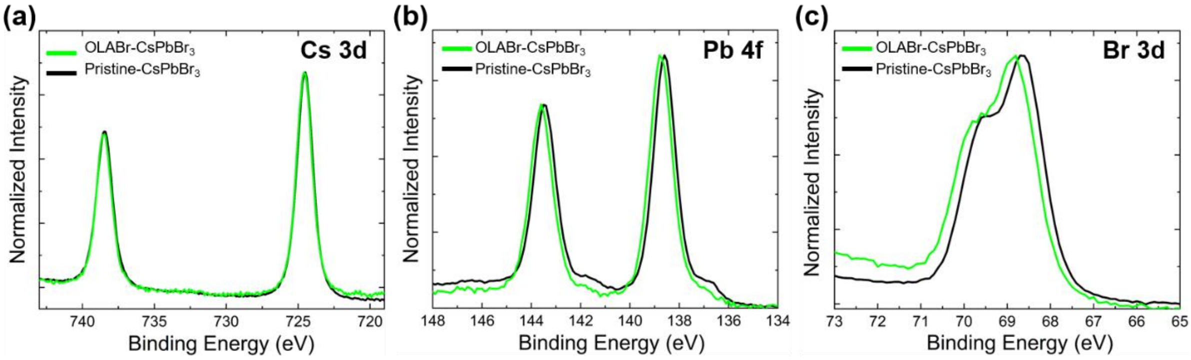

Fig. S10 Normalized XPS spectra of $CsPbBr_3$ NCs (black) before and (green) after treatment with oleylammonium bromide. Binding energy shift to high energy side of OLABr-$CsPbBr_3$ NCs in (b) and (c) supports the increase of Pb and Br compared to pristine-$CsPbBr_3$ NCs.

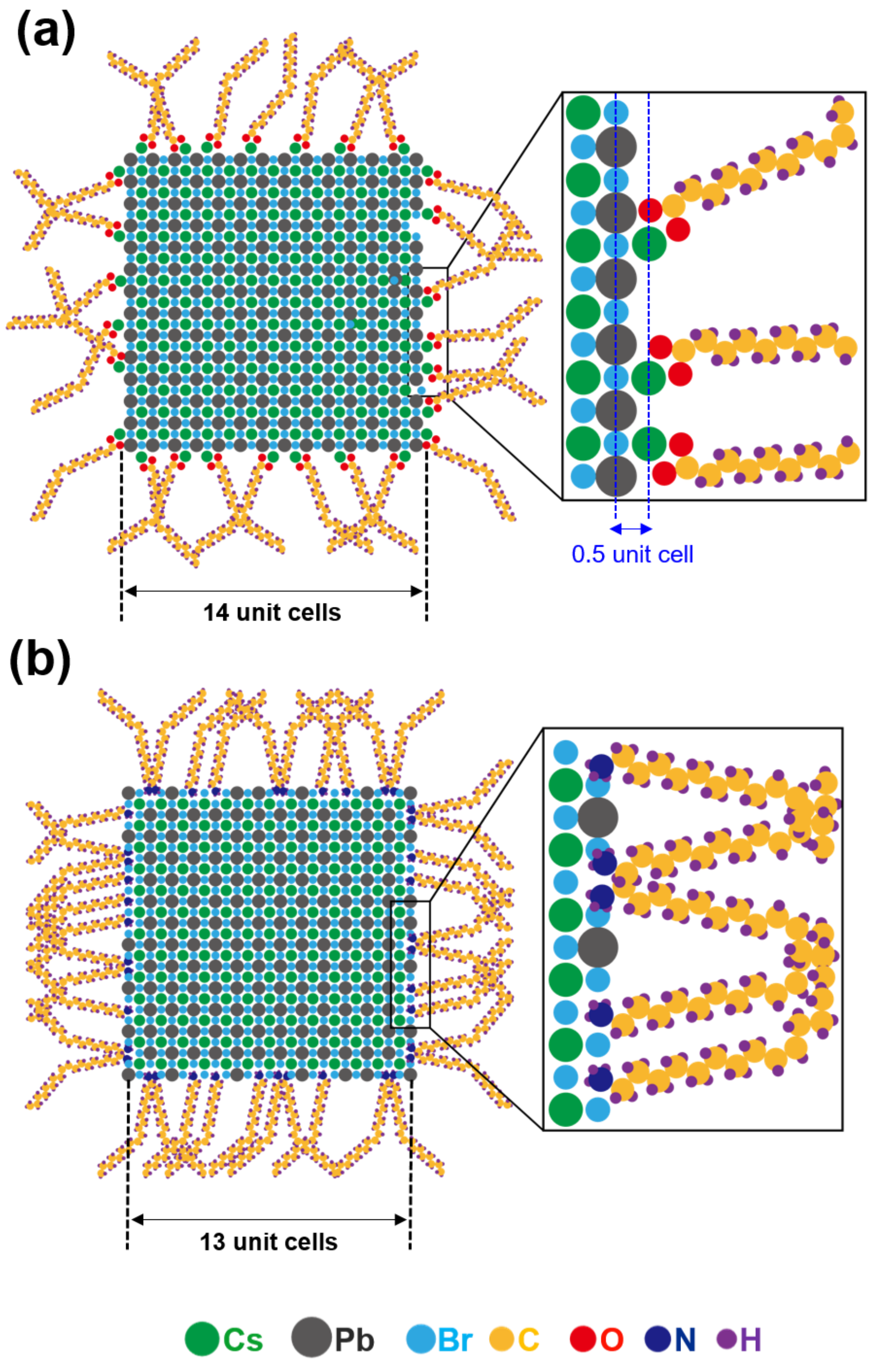

Fig. S11 $CsPbBr_3$ NC models ((a) pristine-$CsPbBr_3$ NC and (b) OLABr-$CsPbBr_3$ NC) proposed in our study. It is noted that the models are based on the NCs after purifications.

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