

Supplementary Information

Atomic Characterization of Byproduct Nanoparticles on Cesium Lead Halide Nanocrystals using High-resolution Scanning Transmission Electron Microscopy

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More SAED results are illustrated in Figure S1, to further verify the existence of both PbBr_2 NPs and CsPb_2Br_5 NPs.

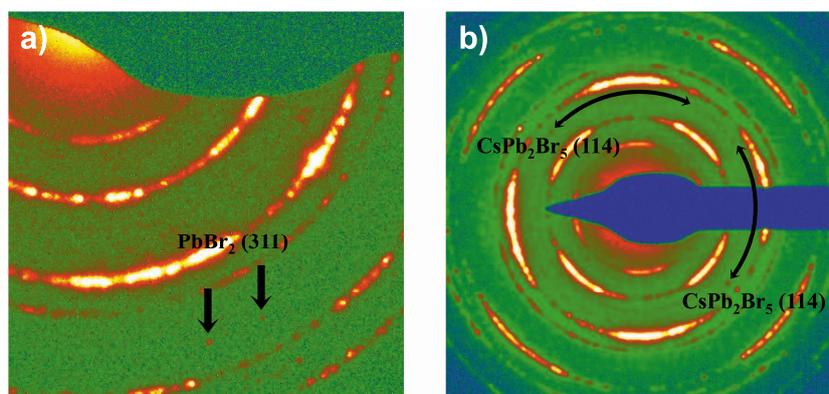


Figure S1. SAED patterns from two $0.48 \mu\text{m}^2$ areas of the NPs on the CsPbBr_3 NCs. Arrowed spots and arcs can be identified as from PbBr_2 NPs and CsPb_2Br_5 NPs, excluding the main diffraction rings or arcs belonging to various CsPbBr_3 planes.

As shown in Figure S1a, excluding the bright diffractive rings belonging to various CsPbBr_3 planes, additional spots indicated with arrows can be indexed as PbBr_2 (311) plane. Also, in Figure S1b, additional spots and arcs indicated with arrows can be indexed as CsPb_2Br_5 (114) plane. Therefore, we finally prove the existence of both PbBr_2 and CsPb_2Br_5 NPs on the CsPbBr_3 NCs through SAEDs.

Table S1. Interplanar spacings of CsPbBr₃, PbBr₂ and CsPb₂Br₅ respectively

CsPbBr ₃ (PDF#75-0412)				PbBr ₂ (PDF#31-0679)				CsPb ₂ Br ₅ (PDF#25-0211)			
d (Å)	I(f)	I(v)	hkl	d (Å)	I(f)	I(v)	hkl	d (Å)	I(f)	I(v)	hkl
5.874	43.1	21.6	1 0 0								
4.153	98.3	69.5	1 1 0	4.105	56.0	40.0	1 2 0				
3.391	21.2	18.4	1 1 1	4.032	31.0	22.0	2 0 0	3.800	10.0	8.0	2 1 0
				3.751	73.0	57.0	1 1 1				
				3.102	50.0	47.0	1 2 1				
				3.081	55.0	52.0	2 2 0				
				3.071	56.0	53.0	2 0 1				
				2.958	23.0	23.0	1 3 0				
2.937	100.0	100.0	2 0 0	2.924	100.0	100.0	2 1 1				
2.626	18.5	20.7	2 1 0	2.641	90.0	100.0	0 3 1	2.685	45.0	51.0	3 1 0
2.398	39.3	48.1	2 1 1								
2.076	64.1	90.6	2 2 0								

As shown in Table S1, most low index planes of PbBr₂ and CsPb₂Br₅ are overlapped with those of CsPbBr₃. Thus, in the SAED patterns, most diffractive signals from PbBr₂ and CsPb₂Br₅ are difficult to discern from the background of those from CsPbBr₃, leaving only few spots or weak arcs in between, which can be identified as from PbBr₂ and CsPb₂Br₅. Therefore, fewer diffraction spots corresponding to PbBr₂ and CsPb₂Br₅ are found in the SAED patterns compared with the large number of NPs observed in STEM-HAADF images.

EDS results of the NPs on a carbon film are illustrated in Figure S2 and Table S2, revealing the chemical information of the free NPs.

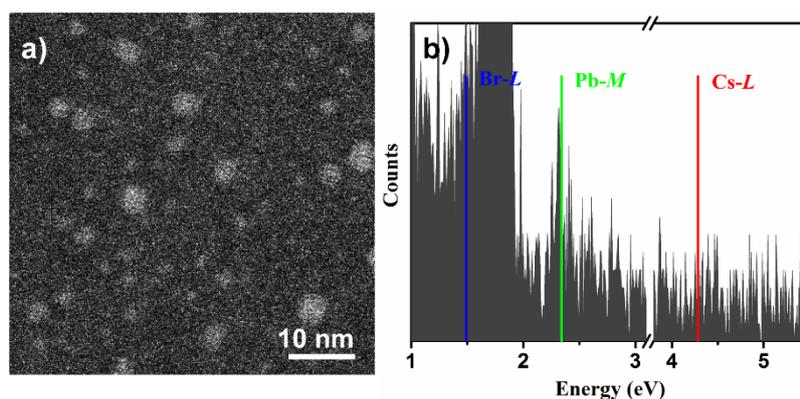


Figure S2. (a) A STEM-HAADF image of the NPs on a carbon film. (b) An integrated EDS spectrum acquired from the region as shown in (a).

Table S2. Atomic percentages of Cs, Pb and Br for a region with the NPs on a carbon film.

Element	Series	Norm. at. %
Cs	L	0
Pb	M	54.5
Br	L	45.5

As shown in Figure S2, both Br-L and Pb-M peaks can be clearly identified, whereas Cs-L peak is absent. Furthermore, quantitation has also been carried out and is shown in Table S2. Therefore, we conclude that the free NPs contain both Br and Pb, but lack Cs.