

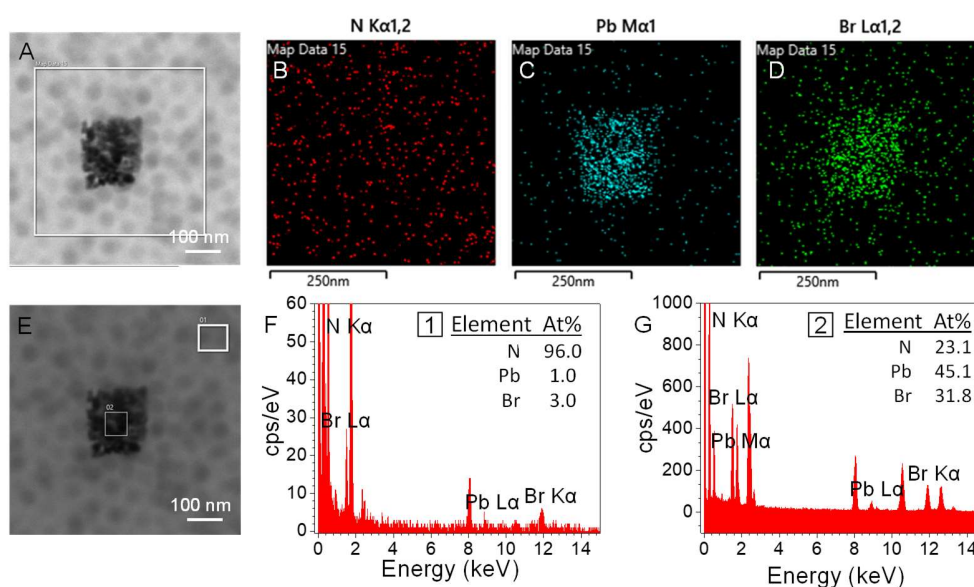
## SUPPORTING INFORMATION

### Room-Temperature Synthesis of Highly Luminescent Methylammonium Lead Bromide Nanocubes Encapsulated in Block Copolymer Micelles: Impact of Solvent Choice on Crystallization and Stability

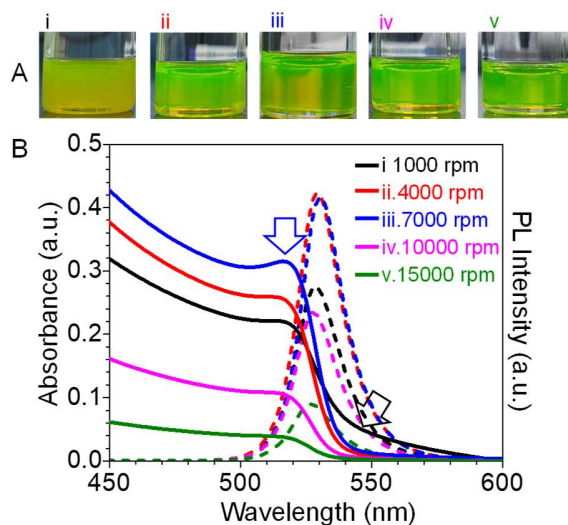
Belda Amelia Junisu, Ya-Sen Sun\*, Bo Cheng Zhao

*Department of Chemical Engineering, National Cheng Kung University, Tainan 701, Taiwan*

\*corresponding author: Y. S. Sun (Email: [yssun@gs.ncku.edu.tw](mailto:yssun@gs.ncku.edu.tw))



**Figure S1.** (A, E) TEM images, (B-D) EDS 2D maps of N, Pb, and Br elements, and (F, G) EDS 1D profiles. The data were collected from the dried state of a t-LHP<sub>7</sub> solution. The t-LHP<sub>7</sub> solution was prepared by dissolving 10 mg PbBr<sub>2</sub> in 1 mL TMB with 17.6 mg PS<sub>48.5</sub>-b-P2VP<sub>70</sub>, followed by stirring at room temperature for 7 days. The scanned positions are marked by white boxes in (A) and (E).

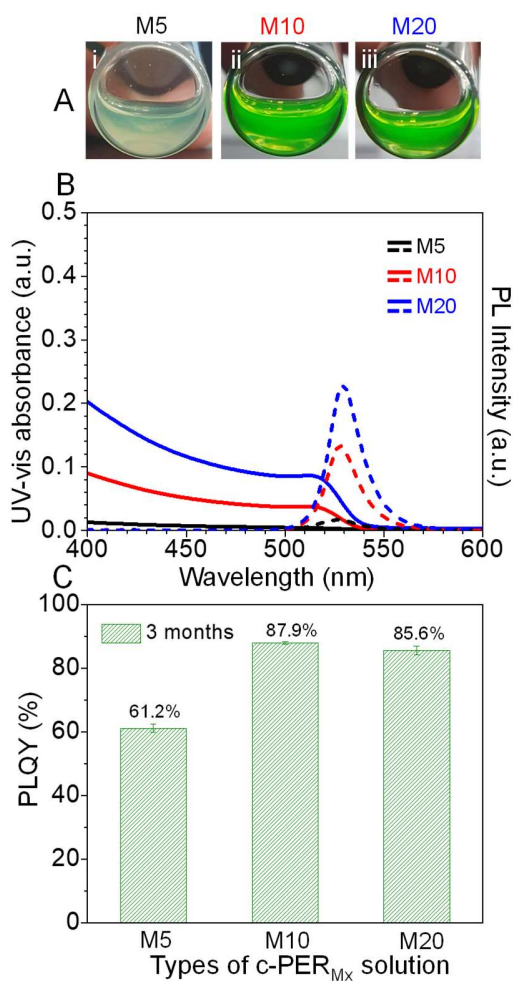


**Figure S2.** (A) Photos and (B) UV-Vis absorbance and PL spectra of c-PER<sub>M20</sub> supernatants. The c-PER<sub>M20</sub> supernatants were obtained by centrifuging t-PER<sub>M20</sub> solutions at various speeds: (i) 1000, (ii) 4000, (iii) 7000, (iv) 10000, and (v) 15000 rpm.

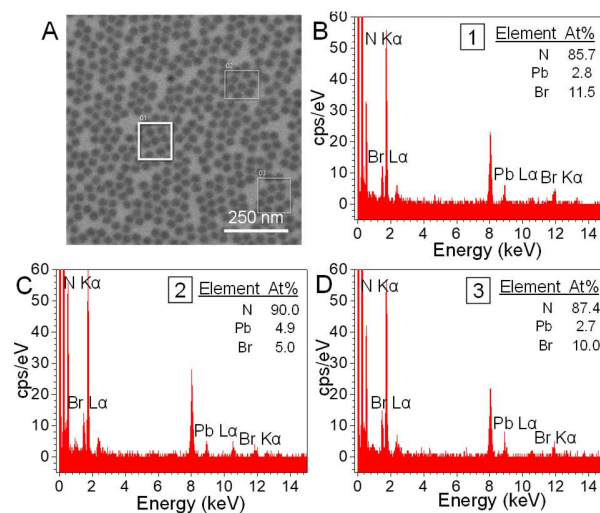
To investigate this effect, t-PER<sub>M20</sub> solutions were centrifuged at various speeds (1000, 4000, 7000, 10000, and 15000 rpm), and the resulting c-PER<sub>M20</sub> solutions were characterized using UV-vis absorbance and PL spectroscopy. At a centrifugation speed of 1000 rpm, the c-PER<sub>M20</sub> solution appeared turbid (Figure S2A<sub>i</sub>) and exhibited an absorption edge at ~520 nm, followed by a diffuse tail between 540–580 nm (Figure S2B<sub>i</sub>, titled black arrow). The turbidity and diffuse tail indicate that the low centrifugation speed failed to completely remove microcrystals with a low PL property.

Increasing the speed to 7000 rpm produced a clearer solution (Figure S2A<sub>iii</sub>), showing a sharper, more intense absorption peak at ~520 nm and an intense PL at ~530 nm. This sharp absorption edge at 7000 rpm (Figure S2B<sub>iii</sub>, blue arrow) suggests the formation of uniform, high-quality MAPbBr<sub>3</sub> nanocrystals. However, higher centrifugation speeds (such as 10000 and 15000 rpm) removed not only microcrystals but also encapsulated MAPbBr<sub>3</sub> nanocrystals. Beyond 7000 rpm, both the quality and quantity of nanocrystals decreased, as evidenced by diminishing peak intensity (see Figure S2B<sub>iv-v</sub>). This result indicates that the high centrifugation speeds likely disrupted the encapsulation efficiency and led to the excessive removal of encapsulated MAPbBr<sub>3</sub> nanocrystals.

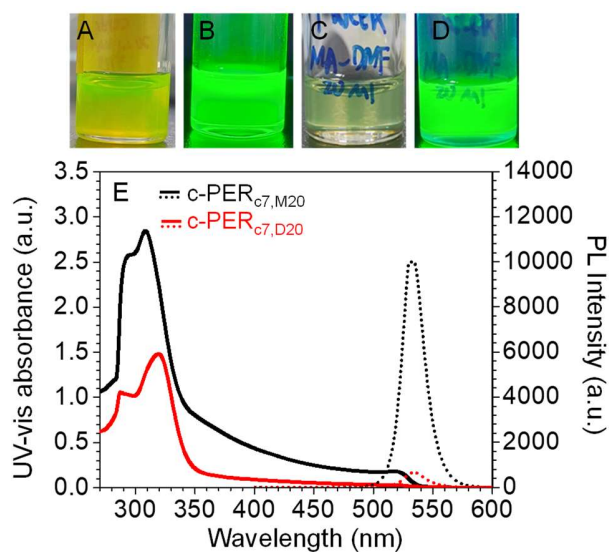
These results indicate that centrifugation speed was optimized at 7000 rpm to ensure the complete removal of microcrystals (consisting of unreacted  $\text{PbBr}_2$  and/or  $\text{MAPbBr}_3$  microcrystals) from the  $\text{t-PER}_{\text{M}20}$  solutions. Insufficient centrifugation left residual microcrystals, while excessive centrifugation risked disrupting micelle encapsulation efficiency.



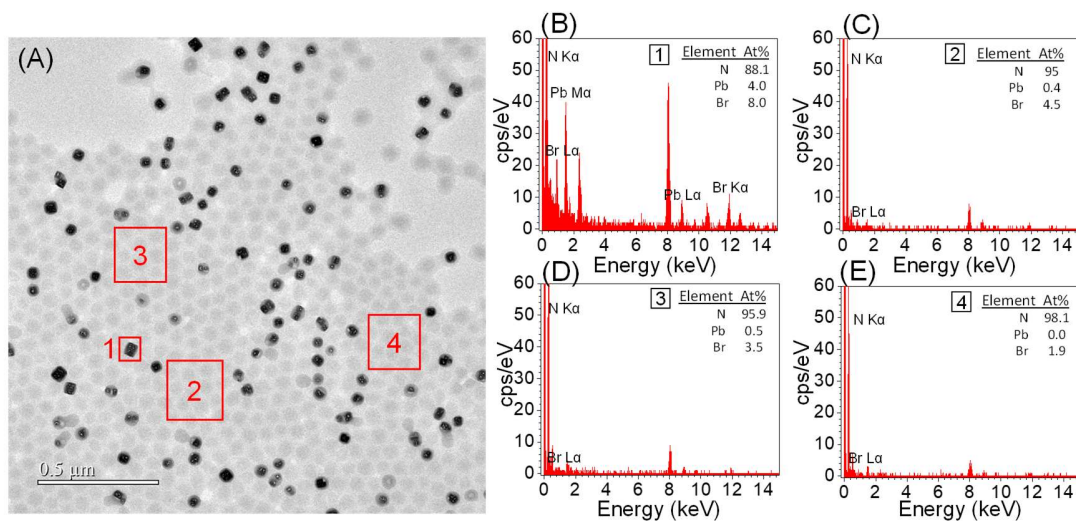
**Figure S3.** (A) Photos, (B) UV-vis and PL spectra, and (C) PLQY of the  $\text{c-PER}_{\text{M}x}$  solutions after being stored in an ambient environment for 3 months. No precipitates exist in the (i)  $\text{c-PER}_{\text{M}5}$ , (ii)  $\text{c-PER}_{\text{M}10}$  and (iii)  $\text{c-PER}_{\text{M}20}$  solutions.



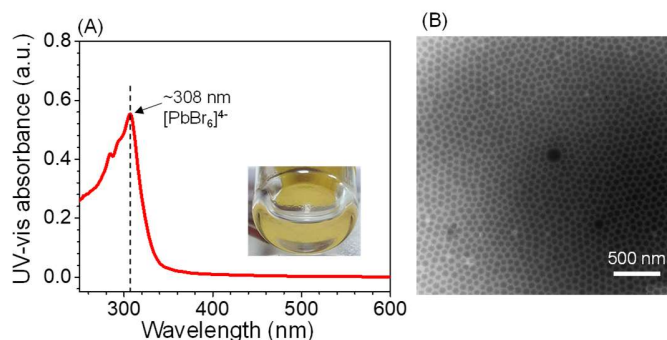
**Figure S4.** (A) TEM and (C-E) EDS 1D profiles of the c-PER<sub>D20</sub> solution in a dried state. The scanned positions for the EDS 1D profiles are marked in (A).



**Figure S5.** (A-D) Photos, (E) UV-Vis absorbance (solid lines) and PL (dotted lines) spectra of fresh c-PER<sub>c7,M20</sub> and c-PER<sub>c7,D20</sub> solutions. Photos of B, D were taken under exposure of UV light ( $\lambda=365$  nm).



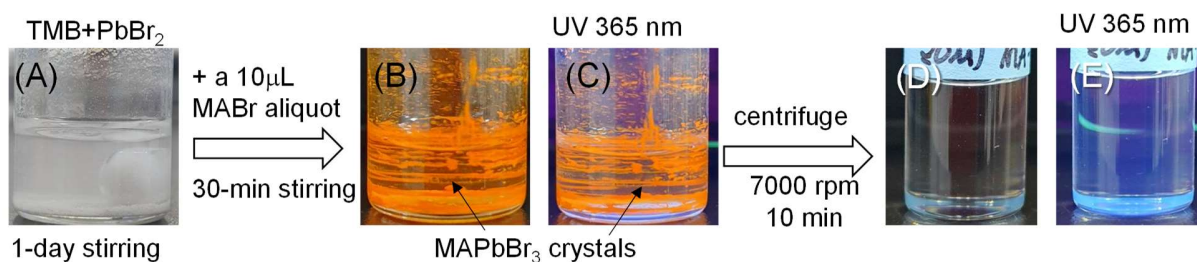
**Figure S6.** (A) HR-TEM image and (B-E) EDS elemental analysis of the dried state of the fresh c-PER<sub>c7,M20</sub> solution in dried state. The recorded areas are highlighted by red squares. Atomic compositions of N, Pb and Br elements are shown in (B-E).



**Figure S7.** (A) UV-vis absorption spectrum and (B) TEM image of the c-PER<sub>c7,M20</sub> solution with prolonged storage at room temperature. Inset of image (A): the photo of the c-PER<sub>c7,M20</sub> solution.

Figure S7A show a sharp peak at  $\sim 308$  nm. This band corresponds to the absorbance of  $[\text{PbBr}_6]^{4-}$  octahedral clusters. The absorbance of cubic  $\text{MAPbBr}_3$  crystals disappeared, indicative of crystal degradation during the prolonged storage. Due to crystal degradation, the color of the c-PER<sub>c7,M20</sub> solution completely fades to form a transparent solution with no precipitates (inset of Figure S7A). The dried state of the c-PER<sub>c7,M20</sub> solution displays a morphology of spherical

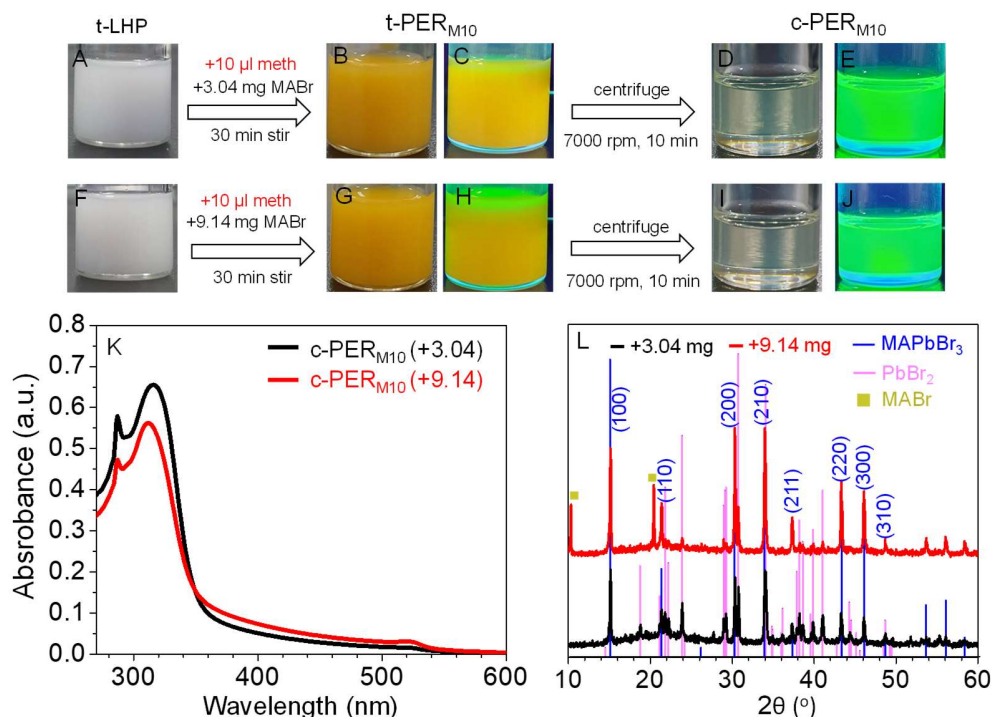
micelles without MAPbBr<sub>3</sub> nanocubes. This result indicates that the MAPbBr<sub>3</sub> nanocubes are completely degraded.



**Figure S8.** (A-E) Photos of one additional series of solutions during the synthesis of perovskites in the absence of PS-*b*-P2VP.

To investigate the roles of BCP and polar solvent in the crystallization of perovskite NCs, two sets of control experiments were conducted. These experiments aimed to determine the effect of BCP presence and methanol addition on the formation of perovskite NCs. In the first set, a BCP-free solution was prepared by dissolving 10 mg of PbBr<sub>2</sub> in 1 mL of TMB. This solution was stirred for 24 hours, followed by the addition of a 10 μL MABr/methanol aliquot. The mixture was then stirred for an additional 30 minutes and centrifuged at 7000 rpm for 10 minutes to separate supernatants and precipitates. During the synthesis, photos were taken. The photos are shown in Figure S8.





**Figure S9.** (A-J) photos of t-LHP, t-PER<sub>M10</sub>, c-PER<sub>M10</sub> solutions. (K) UV-vis absorbance spectra of the c-PER<sub>M10</sub> solutions. (L) WAXD profiles of precipitates that were separated from the t-PER<sub>M10</sub> solutions. Stick patterns in (L): orthorhombic PbBr<sub>2</sub> crystals (PDF #031-0679) and cubic MAPbBr<sub>3</sub> crystals (ICSD#26785). MABr crystals are highlighted by green squares.

Figure S9A-J shows photos of t-LHP, t-PER<sub>M10</sub>, and c-PER<sub>M10</sub> solutions prepared using an alternative process, respectively. In this process, MABr was not pre-dissolved in methanol. Instead, 10 μL of methanol was first added to each t-LHP solution, followed by 30 minutes of stirring. Then, 3.04 or 9.14 mg of MABr powder was added to the t-LHP solutions to prepared t-PER<sub>M10</sub> solutions, which were stirred for an additional 3 hours. After stirring, the t-PER<sub>M10</sub> solutions were centrifuged at 7000 rpm for 10 minutes to separate the supernatants from the precipitates. The supernatants were characterized using UV-vis absorbance spectroscopy (Figure S9K), and the precipitates were characterized using in-house WAXD (Figure S9L). Figure S9A-J shows that this alternative process produces t-PER<sub>M10</sub> and c-PER<sub>M10</sub> solutions with a similar appearance to the t-PER<sub>D</sub> and c-PER<sub>D</sub> solutions (Figures S9A-J and 2). Additionally, the UV-vis absorbance spectra

of the t-PER<sub>M10</sub> and c-PER<sub>M10</sub> solutions show a broad absorbance band at 325 nm, which is assigned to [PbBr<sub>3</sub>]<sup>-</sup> complexes. Increasing the amount of MABr powder did not improve the formation of MAPbBr<sub>3</sub> nanocubes in the c-PER<sub>M10</sub> supernatants. This result indicates that, with this procedure, adding MABr powders did not produce encapsulated MAPbBr<sub>3</sub> nanocubes dispersed in TMB with methanol but instead led to the formation of MAPbBr<sub>3</sub> microparticles, which primarily exist in the precipitates. Nevertheless, the MAPbBr<sub>3</sub> microparticles formed ineffectively in the precipitates. This explains why the precipitates exhibit diffractions corresponding to a mixture of orthorhombic PbBr<sub>2</sub> crystals, MABr crystals, and cubic MAPbBr<sub>3</sub> crystals (Figure S9L).