Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information for:

Supermolecule-assisted synthesis of perovskite nanorods with high PLQY for standard blue emission

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Materials

Lead(II) bromide ($PbBr_2$, 99%), oleic acid (OAc, 85%), oleylamine (OAM, 80~90%), N,N-dimethylformamide (DMF, anhydrous, 99.8%), octylamine (OA, 99%), octadecene (ODE, 90%), β-cyclodextrin (β-CD, 99%), α-cyclodextrin (α-CD, 99%), and γ-cyclodextrin (γ-CD, 99%) were purchased from Aladdin. Toluene (AR) was purchased from Tianjin Yuanli Chemical Co., LTD. Methyl acetate (MeOAc, 99%, AR) was purchased from Macklin.

Synthesis of $CsPbBr_3$ NC

$CsPbBr_3$ NC was synthesized by ligand-assisted reprecipitation method as reported before. The precursor solution was formed by mixing oleylamine (OAM), dried oleic acid (OAc), CsBr, $PbBr_2$ and DMF at room temperature. Then the precursor solution was swiftly injected into toluene. The $CsPbBr_3$ NC was separated via centrifugation at 4000 rpm for 5 min followed by 12500 rpm for 5 min.

Synthesis of CD@$CsPbBr_3$ NRs

Firstly, the precursor solution was formed by mixing oleylamine (OAM), dried oleic acid (OAc), CsBr, $PbBr_2$ and DMF at room temperature and stirred until dissolved. Then, proportional CD was added to precursor solution. The clear solution precursor solution was injected to toluene to grow $CsPbBr_3$ NRs. The crude nanoparticles were separated by centrifugation 12500 rpm for 5min and then $CsPbBr_3$ NRs was injected into toluene and centrifuge at 4000 rpm for 5 min in the follow purification process.

Instruments

The UV-vis absorption spectra were recorded on a MAPADA UV-1800PC spectrophotometer. The PL spectra and PLQYs were recorded by a Horiba Fluorolog system (Horiba-F4600) with a Xe lamp as the excitation source and a Quanta-Phi integrating sphere. The X-Ray diffraction spectra were measured with the XRD Bruker D8-focus with Cu Kα (λ = 1.5406 Å) radiation source. The transmission electron microscopy images of the NCs and NRs were recorded on a TEM (JEM-200F) at 200 kV. The samples for measurements were suspended on carbon-coated Cu grids. The XPS spectra and elemental composition was detected by a PHI 5000 Versa Probe X-ray photoelectron spectroscope (ULVAC-PHI, America).

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Table S1. The summary of PLQY, average lifetime (τ_{ave}), radiative (τ_r) and nonradiative (τ_{nr}) recombination lifetime, radiative (k_r) and nonradiative (k_{nr}) decay rates, slow (τ_1) and fast (τ_2) decay lifetime and their weighting factors (f_1 and f_2) of the $CsPbBr_3$ NC and $CsPbBr_3$ NRs with different kinds of CD and various CD:Pb^{2+} ratios in the precursor solution.

	f_1	f_2	τ_1(ns)	τ_2(ns)	τ_r(ns)	τ_{nr}(ns)	τ_{avg}	QY(%)	k_r	k_{nr}
$CsPbBr_3$	0.13	0.87	24.7	2.8	9.4	14.4	5.7	60.5	0.106	0.069
β-CD:$PbBr_2$=1:5	0.06	0.94	13.2	3.3	5.2	15.7	3.9	75.2	0.192	0.063
β-CD:$PbBr_2$=1:4	0.05	0.95	12.3	3.8	4.7	42.4	4.2	90.1	0.213	0.024
β-CD:$PbBr_2$=1:3	0.06	0.94	10.8	3.4	6.5	9.2	3.8	58.8	0.154	0.109
α-CD:$PbBr_2$=1:5	0.05	0.95	13.7	3.5	9.5	6.6	3.9	40.9	0.105	0.152
α-CD:$PbBr_2$=1:4	0.05	0.95	12.9	3.4	9.4	7.0	3.9	42.5	0.106	0.143
α-CD:$PbBr_2$=1:3	0.04	0.96	14.8	3.8	10.4	7.0	4.2	40.3	0.096	0.143
γ-CD:$PbBr_2$=1:5	0.03	0.97	9.7	3.2	4.3	23.2	3.6	84.5	0.233	0.043
γ-CD:$PbBr_2$=1:4	0.04	0.96	14.3	3.3	4.3	27.8	3.7	86.7	0.233	0.034
γ-CD:$PbBr_2$=1:3	0.05	0.95	14.7	3.0	4.8	14.1	3.6	74.5	0.208	0.071

The decay transients can be fitted using a biexponential decay function[1, 2] given by Eq. (1):

$$I(t) = A_1 exp(-t/\tau_1) + A_2 exp(-t/\tau_2) \quad (1)$$

The average lifetimes (τ_{avg}) is calculated according to Eq. (2), where τ_i and f_i are the lifetime and lifetime weighted fractional intensity of each component of the multi exponential fit:

$$\tau_{avg} = \sum f_i \times \tau_i \quad (2)$$

The radiative recombination lifetime (τ_r), nonradiative recombination lifetime (τ_{nr}), radiative decay rate (k_r) and nonradiative decay rate (k_{nr}) are given by Eq. (3):

$$QY = k_r/(k_r + k_{nr}) = {}^1/_{\tau_r}/\left({}^1/_{\tau_r} + {}^1/_{\tau_{nr}}\right) = {}^{\tau_{nr}}/(\tau_{nr} + \tau_r) \quad (3)$$

Table S2. The XPS measured element contents of $CsPbBr_3$ NC and β-CD@$CsPbBr_3$ NR with 1:4 mole ratio of β-CD and $PbBr_2$. The error is the standard deviations of the mean of three batches.

Element	C1s	N1s	O1s	Br3d	Cs3d5	Pb4f7
$CsPbBr_3$	33.85±3.35	1.47±0.32	63.66±5.08	0.51±0.20	0.24±0.18	0.27±0.16
β-CD@$CsPbBr_3$	24.20±4.11	0.37±0.25	74.11±6.27	0.52±0.29	0.31±0.15	0.40±0.20

Table S3. The summarized diameter and length of NRs. The error is the standard deviations of the mean of 100 NRs.

NRs	Length (nm)	Diameter (nm)
β-CD:$PbBr_2$=1:5	17.8±1.5	3.5±0.2
β-CD:$PbBr_2$=1:4	18.3±1.7	3.6±0.1
β-CD:$PbBr_2$=1:3	20.1±1.1	3.6±0.1
α-CD:$PbBr_2$=1:4	22.1±1.6	3.5±0.1
γ-CD:$PbBr_2$=1:4	17.8±2.0	3.6±0.2

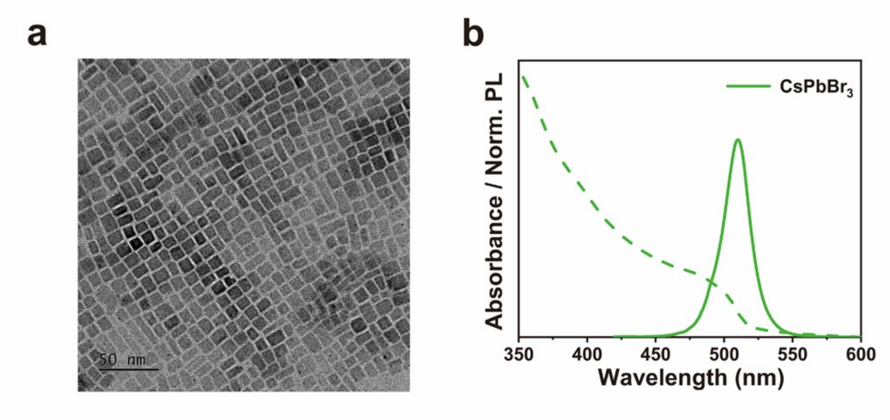

Figure S1. (a) TEM image and (b) UV-vis absorption and PL spectra of $CsPbBr_3$ NC.

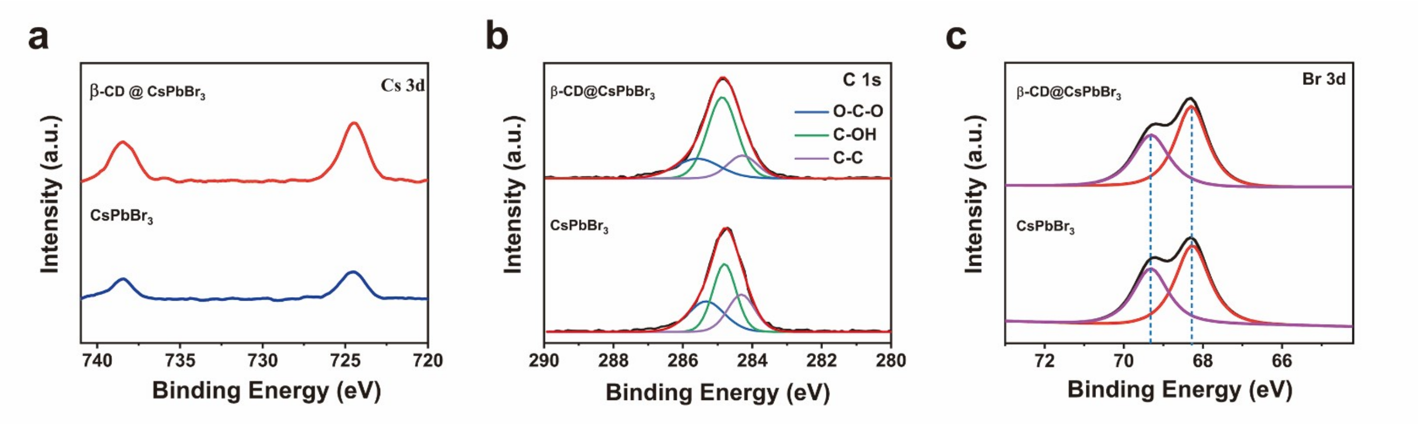

Figure S2. XPS spectra with elements (a) Cs 3d, (b) C 1s and (c) Br 3d of $CsPbBr_3$ NC and β-CD@$CsPbBr_3$ NR with 1:4 mole ratio of β-CD and $PbBr_2$.

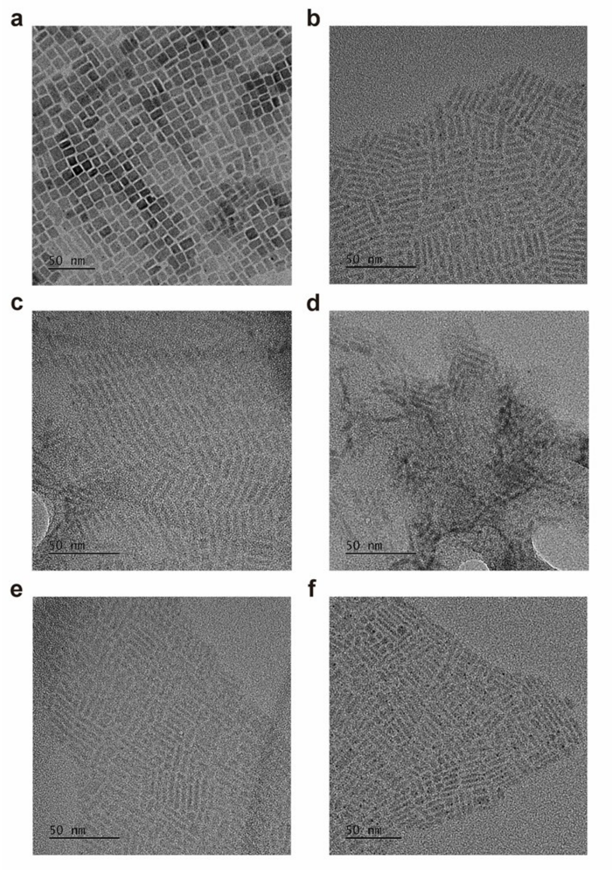

Figure S3. TEM of (a) $CsPbBr_3$ NC, (b) β-CD@$CsPbBr_3$ NR with 1:4 ratio of β-CD:Pb^{2+}, (c) β-CD@$CsPbBr_3$ NR with 1:5 ratio of β-CD:Pb^{2+}, (d) β-CD@$CsPbBr_3$ NR with 1:3 ratio of β-CD:Pb^{2+}, (e) α-CD@$CsPbBr_3$ NR with 1:4 ratio of α-CD:$Pb^{2+}$and (f) γ-CD@$CsPbBr_3$ NR with 1:4 ratio of γ-CD:Pb^{2+}.

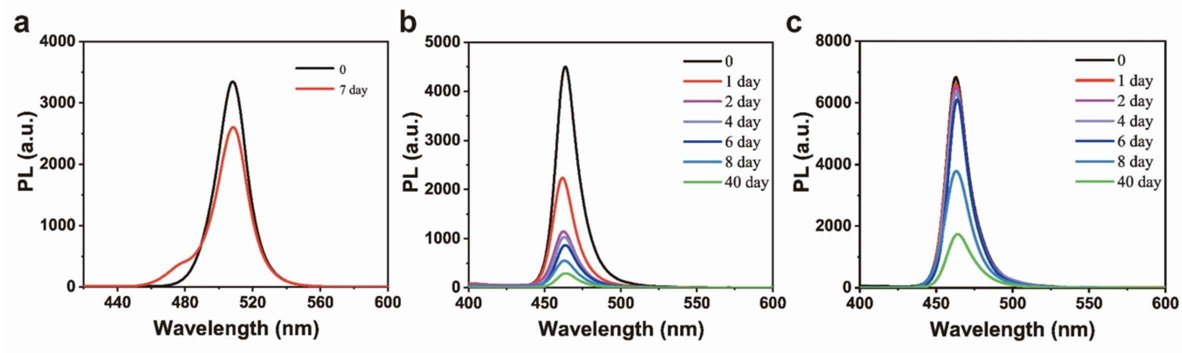

Figure S4. Time dependence of PL of colloidal nanostructures in toluene at ambient atmosphere (relative humidity; 30-40%). (a) $CsPbBr_3$ NC, (b) α-CD@$CsPbBr_3$ NR with 1:4 ratio of α-CD and $PbBr_2$ and (c) γ-CD@$CsPbBr_3$ NR with 1:4 ratio of γ-CD and $PbBr_2$.

Reference

1. C. Sun, Z. Gao, H. Liu, L. Wang, Y. Deng, P. Li, H. Li, Z.-H. Zhang, C. Fan and W. Bi, *Chemistry of Materials*, 2019, **31**, 5116-5123.

2. S. Zhang, H. Liu, X. Li and S. Wang, *Nano Energy*, 2020, **77**, 105302.