Electronic Supplementary Material (ESI) for Nanoscale.

In-situ inclusion of thiocyanate for highly luminescent and stable $CH_3NH_3PbBr_3$ perovskite nanocrystals

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Experimental

Materials

All reagents were used as received without further purification: $PbBr_2$ (99%, Sigma-Aldrich), $Pb(SCN)_2$ (99.5%, Sigma-Aldrich), CH_3NH_3Br (Dyesol), oleylamine (OLA, 80-90%, Accuchem), oleic acid (OA, Analytical Reagent, Accuchem), N,N-dimethylformamide (DMF, 99.8%, Sigma-Aldrich), toluene (99.7%, Sigma-Aldrich).

Preparation of $CH_3NH_3PbBr_3$ NCs

Colloidal $CH_3NH_3PbBr_3$ NCs were prepared with the LARP technique according to the literature after minor modification.[10] For in-situ inclusion of thiocyanate, first, two precursor solutions, solution A ($PbBr_2$:CH_3NH_3Br = 1:1 (mole ratio), in 4 mL DMF, 0.04 M Pb^{2+}) and solution B ($Pb(SCN)_2$:CH_3NH_3Br = 1:3 (mole ratio), in 4 mL DMF, 0.04 M Pb^{2+}) were separately prepared in a N_2-filled glovebox. The two solutions were stirred at room temperature for 30 min before mixing. Then, solution A and solution B were blended and the volume of A/B was 1 mL/0 mL, 0.8 mL/0.2 mL, 0.6 mL/0.4 mL, 0.4 mL/0.6 mL, 0.2 mL/0.8 mL and 0 mL/1 mL, respectively. Subsequently, the blended solution was blended with 20 μL OLA and 0.5 mL OA to obtain the precursor solution. Finally, the precursor solution was quickly injected into 10 mL 60 °C toluene under vigorous stirring. After centrifugation at 8000 rpm for 10 min to discard the insoluble precipitates, the bright $CH_3NH_3PbBr_3$ colloidal nanocrystal solution was obtained. For convenience, these samples were labeled as SCN-0%, SCN-20%, SCN-40%, SCN-60%, SCN-80% and SCN-100%, respectively.

Characterizations

The X-ray diffraction (XRD) patterns were measured on a Philips X-Pert X-ray diffractometer using a Cu Kα radiation source (λ = 1.54056 Å). To avoid the aggregation or recrystallization of $CH_3NH_3PbBr_3$ NCs in the drying process, the samples for XRD measurements are prepared using the freeze drying method in our experiments. A JEOL-JEM 2100F transmission electron microscopy (TEM) machine operating at an acceleration voltage of 200 kV was used to analyze the particle size and morphology of $CH_3NH_3PbBr_3$ NCs and TEM-based X-ray energy-dispersive spectroscopy (EDS) was carried out to analyze the chemical elements. Steady state and time-resolved photoluminescence (PL) spectra were measured on a F-380 fluorescence spectrometer. Ultra-visible (UV-vis) absorption spectra were taken on a UV-6100 UV-vis spectrophotometer. X-ray photoelectron (XPS) spectroscopy were carried out at a ULVAC-PHI (PHIQUANTERA-II SXM) machine with Al Kα as the X-ray source. Photoluminescence quantum yield (PLQY) was tested using an FLS920 spectrometer equipped with an integrating sphere from Edinburgh Instruments. Fourier Transform infrared spectroscopy (FTIR) was recorded using a Nicolet iS50.

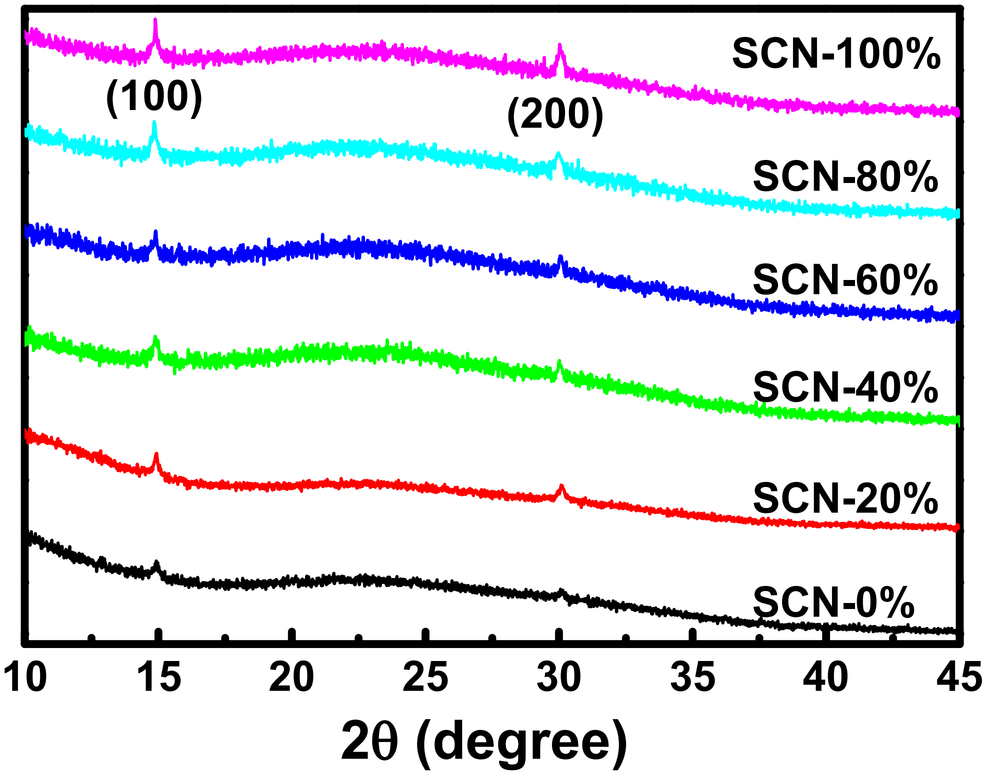

Figure S1. XRD patterns of the as-prepared $CH_3NH_3PbBr_3$ NCs using different amount of $Pb(SCN)_2$ (freeze dried sample).

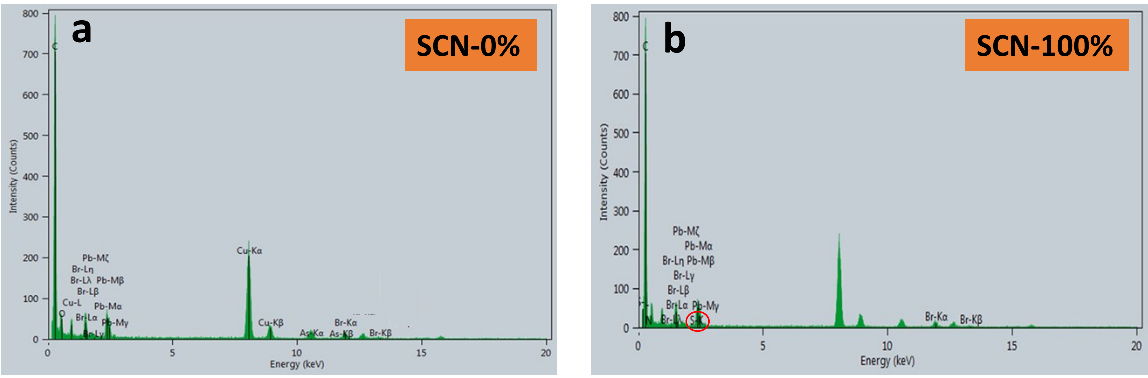

Figure S2. EDS spetra of SCN-0% and SCN-100% perovskite nanocrystals.

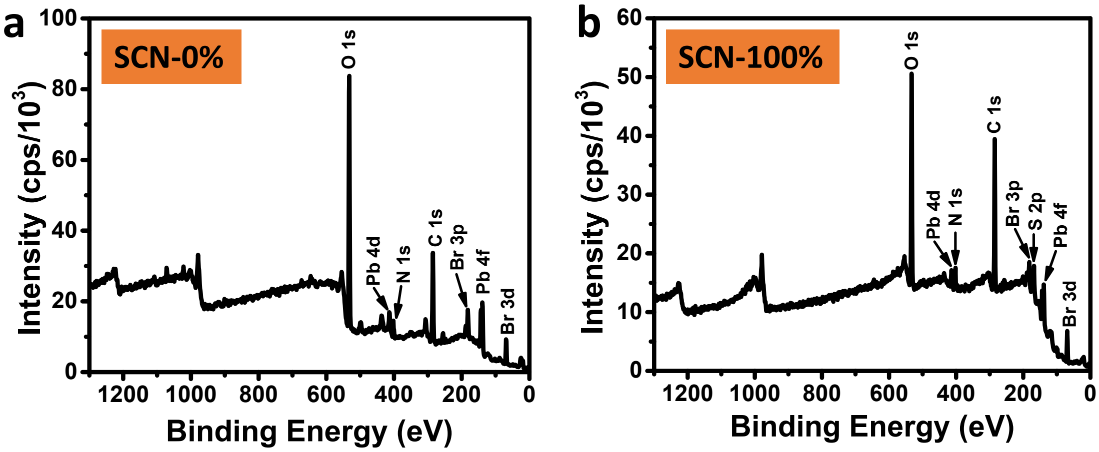

Figure S3. XPS survey scans of SCN-0% and SCN-100% perovskite NCs.

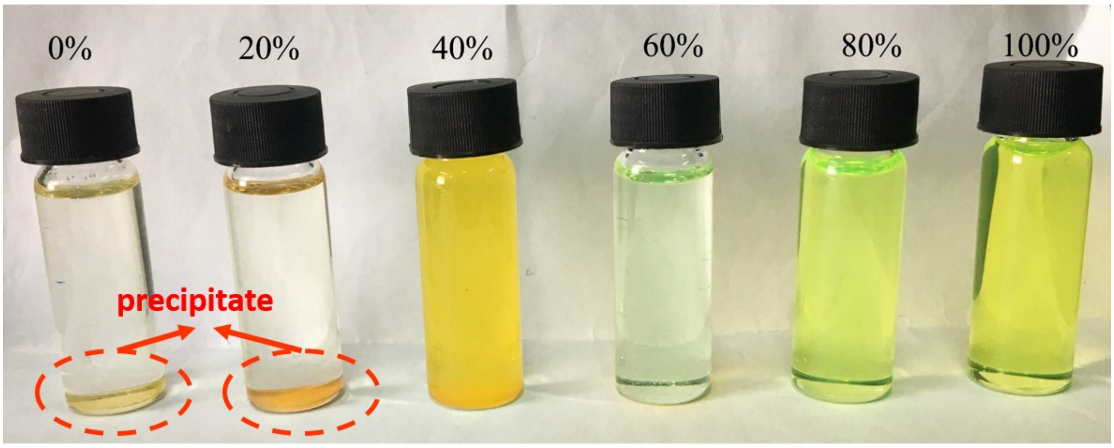

Figure S4. Photographic images of the aged $CH_3NH_3PbBr_3$ colloidal NCs after one month under the ambient light.

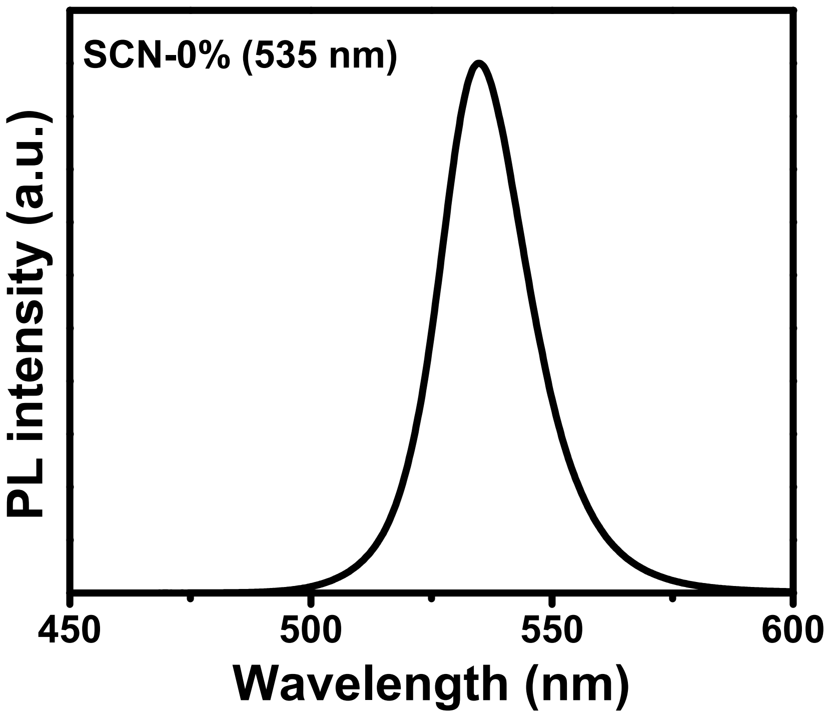

Figure S5. PL spectrum of the pristine $CH_3NH_3PbBr_3$ NCs (SCN-0% (535 nm)).