Supplementary Information (SI) for ChemComm.

Synthesis of pure-red-emission perovskite quantum dots with high color purity by A-site cation exchange with lecithin at room temperature

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1. Materials and Methods

1.1 Chemicals

We used the following chemicals without any further purification, such as methylamine acetate (MAAc, TCI, >97.0%), cesium acetate (TCI, >98.0%), formamidine acetate (FAAc, TCI, >98.0%), lead (II) iodide (PbI_2, TCI, >98%), n-octylammonium iodide (TCI, >98.0%), dimethyl carbonate (TCI, >98%), oleic acid (OAc, Sigma-Aldrich, >90%), oleylamine (OAm, Fujifilm Wako), ethyl acetate (EtOAc, Fujifilm Wako, >99%), toluene (Fujifilm Wako, >99.5%), tri-n-octylphosphine (TOP, Kanto Chemical, >95%), dimethyl sulfoxide-d_6 (Kanto Chemical), and polymethyl methacrylate (PMMA, Fujifilm Wako).

1.2 Preparation of precursor solutions of PeQDs

All procedures were conducted inside a glove box.

MA-oleate precursor was prepared by loading MAAc (82.0 mg) along with OAc (2.0 mL) into a 9 mL glass vial and dissolving by stirring at 25±3 °C. Cs-oleate precursor was prepared by loading CsAc (172.8 mg) along with OAc (2.0 mL) into a 9 mL glass vial and dissolving by stirring at 70±3 °C.

Pb and I precursor solutions were prepared by loading PbI_2 (115.3 mg) and OAmI (96.4 mg) with OAm (0.201 mL), OAc (0.155 mL), and EtOAc (1.25 mL) into a 9 mL glass vial and dissolved by stirring at 25±3 °C.

1.3 Synthesis of $MA_xCs_{1-x}PbI_3$ PeQDs

All the following procedures, except centrifugation, were conducted inside a glove box.

The Pb precursor solution (1.53 mL), ethyl acetate (0.75 mL), and TOP (0.09 mL) were added to a 9 mL glass vial and stirred at room temperature at 1,500 rpm. Subsequently, the MA precursor solution (0.24 mL) was injected into the mixture using a gas-tight syringe and stirred for 10 min at room temperature. Thereafter, the Cs precursor solution (0.12 mL) was successively injected with a gas-tight syringe, followed by an additional 10 min of stirring. The resulting suspension was divided into four microtubes (0.65 mL each) and centrifuged at 16,500 rpm for 2 min each. After discarding the supernatant, 2 mL of toluene was added to each microtube, and the precipitates were redispersed via ultrasonication. The dispersions were then centrifuged at 16,500 rpm for 3 min, and the supernatants were collected for

further evaluation.

1.4 Procedure of A-site cation exchange

All of the following procedures, except for centrifugation, were conducted inside the glove box.

FAAc (110 mg) was placed in a 9 mL glass vial, followed by the addition of a PeQDs dispersion (3 mL, 3 mg/mL by weight). The mixture was stirred at 1,500 rpm at 25 ± 3 °C. Subsequently, TOP (0.01 mL) and oleic acid (0.004 mL) were added successively, and the solution was stirred for 1 h. In the lecithin-containing system, lecithin 0.5 M ethyl acetate solution (0.01 mL) was added immediately before the injection of oleic acid. After stirring, dimethyl carbonate (2 mL) was added, and the resulting suspension was divided into four microtubes (1.2 mL each) and centrifuged at 16,500 rpm for 1 min each. The supernatant was discarded, and 0.5 mL of toluene was added to each microtube to redisperse the precipitates via ultrasonication. The dispersions were centrifuged again at 16,500 rpm for 1 min, and the supernatants were filtered through a plastic syringe equipped with a membrane filter before collection for further evaluation.

1.5 Procedure of fabrication of polymer film

All solution preparations were performed in a glovebox. A PMMA solution (10wt%) was prepared by dissolving PMMA (6.7 g) in toluene (70 mL). Subsequently, 26.5 mL of the PMMA solution was mixed with 3 mL of the PeQDs dispersion (2 mg/mL) to obtain a resin solution. The resulting solution was spray-coated onto a polyethylene terephthalate substrate and dried under heating to fabricate a film with dimensions of 2 × 2.5 cm^2 and a thickness of approximately 100 μm, which was used for further characterization.

1.6 Characterization Methods

X-ray diffraction (XRD) patterns of the samples were obtained from out-of-plane and in-plane diffraction measurements using a Rigaku Smart Lab (Cu Kα radiation at 45 kV and 200 mA). The samples were observed by a JEOL JEM-2100F transmission electron microscope (TEM) (accelerating voltage of 200 kV). The visible absorption spectra of the samples were obtained using a JASCO V-670 spectrophotometer (detection wavelength

range of 300–800 nm). Photoluminescence (PL) spectra and photoluminescence quantum yield (PLQY) of the samples were obtained using a JASCO FP-8000 luminescence spectrometer (excitation wavelength of 400 nm). PLQY was determined using a JASCO ILF-835 100 mm φ integral sphere system with a Xe lamp as the excitation source (wavelength: 400 nm). The crystal size was measured using dynamic light scattering (DLS: NANOTRAC FLEX / Microtrac Bell). The binding energy of the PeQDs was evaluated using an X-ray photoelectron spectroscopy (XPS) instrument (Thermo Fisher Scientific Theta). The measured samples were cast onto ITO glass substrates and dried for several hours in a vacuum. The elemental composition of the PeQDs was analyzed using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (SEM-EDX: Scanning Electron Microscope-Energy Dispersive X-ray Spectroscopy, JSM-IT800 / JEOL). The measurement samples were prepared by casting a PeQD dispersion onto a silicon substrate and drying it for several hours in a vacuum oven. Measurements were performed under the following conditions: acceleration voltage, 15 kV; working distance, 10 mm.

2. Result and discussion

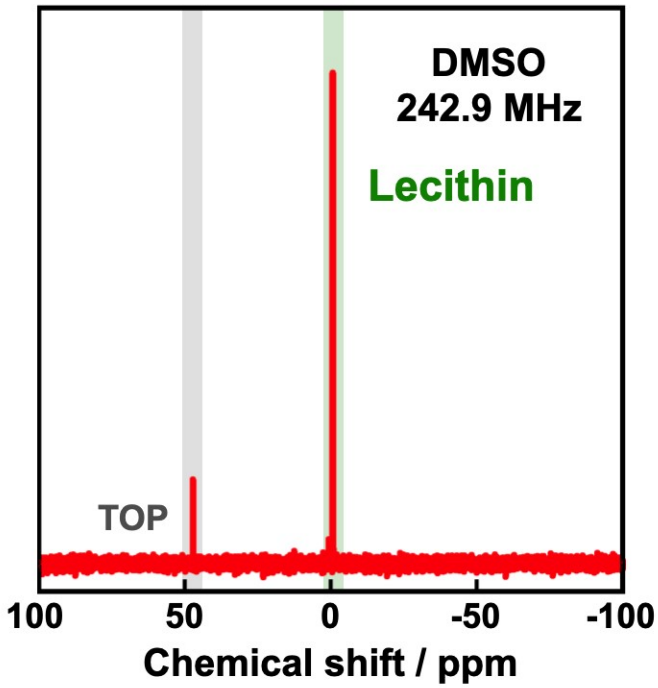

Fig. S1 ^{31}P-NMR spectroscopy of lecithin in PeQDs after A-site cation exchange w/ lecithin**.**

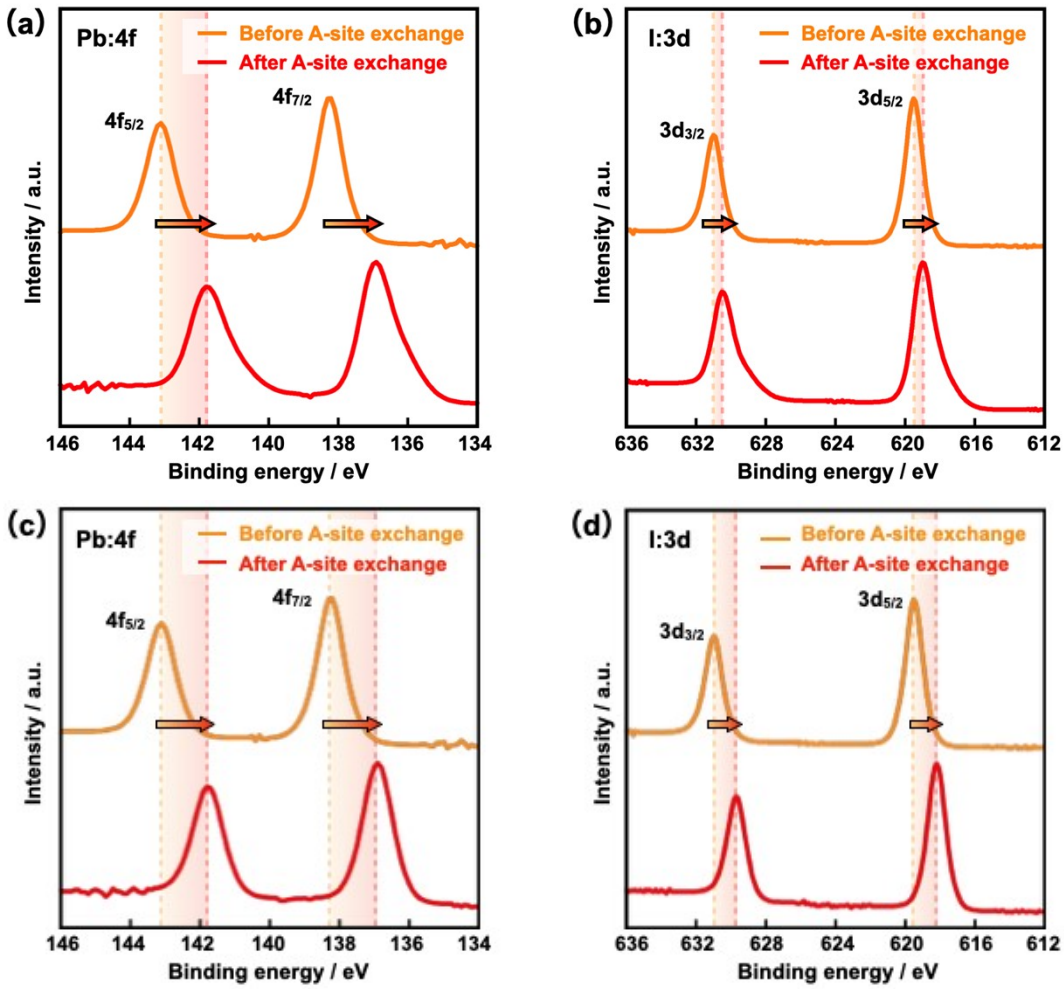

Fig. S2 XPS spectra of PeQDs before and after A-site cation exchange w/o lecithin. Survey spectra of Pb 4f and I 3d (a) and (b). XPS spectra of PeQDs before and after A-site cation exchange w/ lecithin. Survey spectra Pb 4f spectra and I 3d spectra (c), (d).

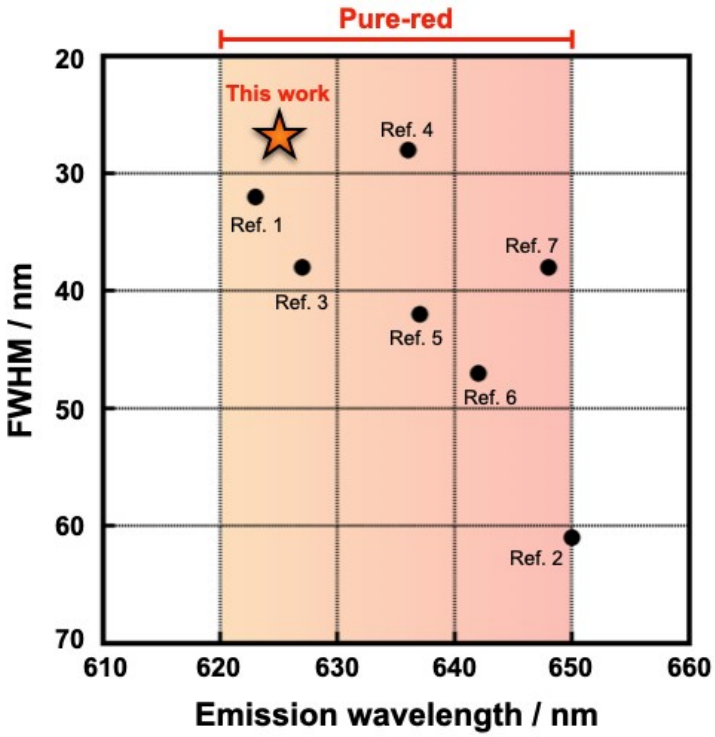

Fig. S3 Comparison of FWHM with previous works[1-7].

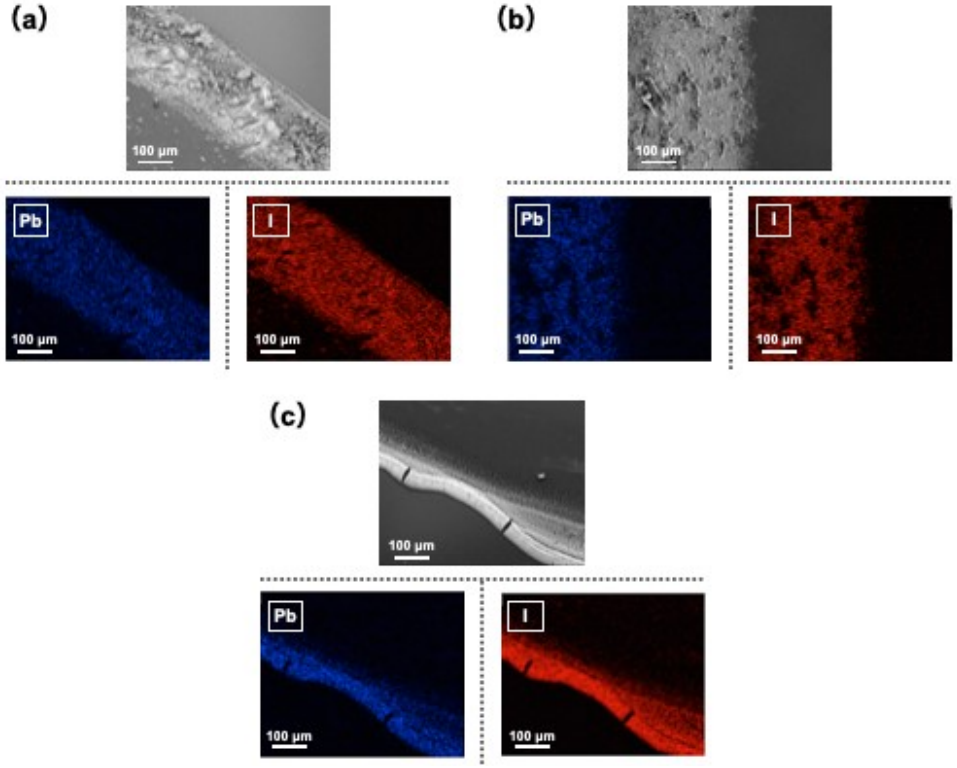

Fig. S4 Images of SEM-EDX mapping before and after A-site cation exchange w/o and w/ lecithin (a), (b), and (c).

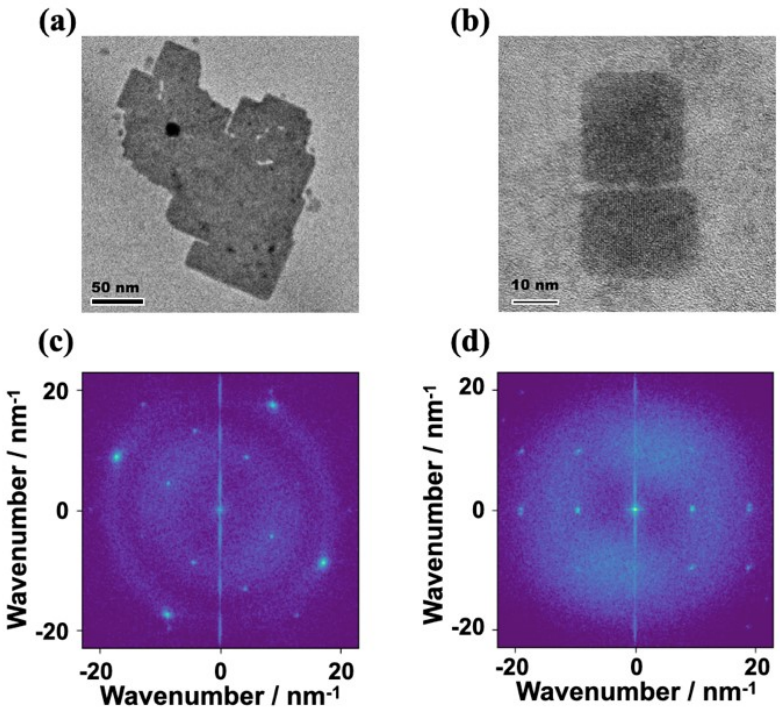

Fig. S5 TEM images of the PeQDs after A-site cation exchange w/o and w/ lecithin (a), (b). FFT patterns of the PeQDs after A-site cation exchange w/o and w/ lecithin (c), (d).

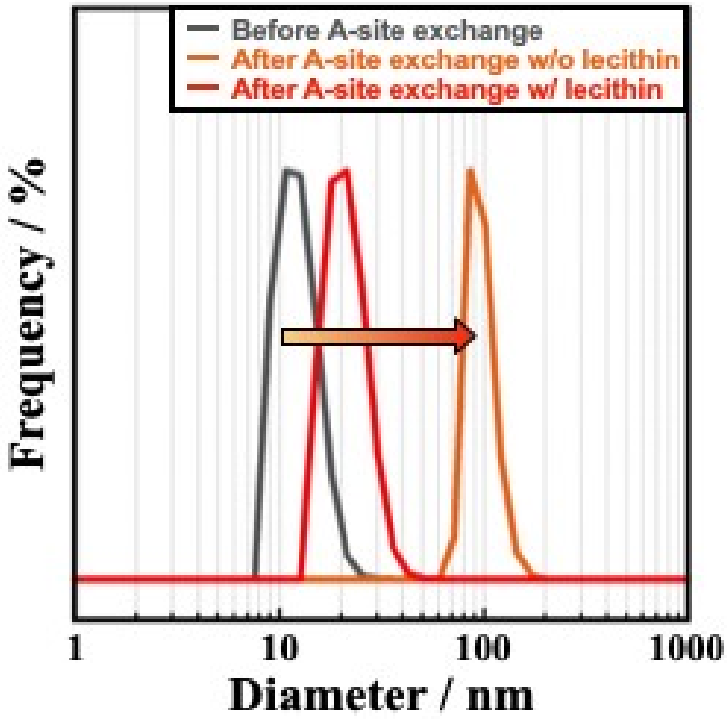

Fig. S6 Particle size distribution of PeQDs before and after A-site cation exchange w/o and w/ lecithin.

【Reference】

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