

Raw data repository for the article:

Spatially resolved fluorescence of caesium lead halide perovskite supercrystals reveals quasi-atomic behavior of nanocrystals

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X-ray Data

The collection **X-ray_Data.zip** contains the raw data collected at P10 beamline at PETRA III and described in the main text, Figures 3 – 6, and in the Supporting Information, Sections S4 – S7, Figures S8 – S26.

Experimental Parameters:

X-ray energy: 13.8 keV

Beam size: $\sim 400 \times 400 \text{ nm}^2$ (h \times v)

Detector size: 2070×2167 pixels (h \times v)

Detector pixel size: $75 \times 75 \text{ }\mu\text{m}^2$

Sample-detector distance: 412 mm

Direct beam position: [1804.5, 1958] (h, v)

The experiment was performed in transmission geometry.

The detector as well as the sample were placed normal to the incident beam.

There are three compressed subfolders **Kapton_background.tar.xz**, **B18_27.tar.xz** and **B18_03.tar.xz** that contain files in HDF5 format.

Kapton_background.tar.xz contains 21 *.h5 files with detector images and a master file. The detector images were collected during a spatial scan of 21×21 points with a step of 500 nm. The sample was a **clean Kapton film**. Each *.h5 file corresponds to a horizontal row scan and contains 21 detector images. These images were used as a background and were subtracted from the data.

B18_27.tar.xz contains 25 *.h5 files with detector images and a master file. The detector images were collected during a spatial scan of 25×25 points with a step of 500 nm. The sample was a **Kapton film with a CsPbBr₂Cl supercrystal**. Each *.h5 file corresponds to a horizontal row scan and contains 25 detector images.

Results of analysis of this dataset are presented in the main text, Figures 3 – 6, and in the Supporting Information, Sections S4 – S6, Figures S8 – S21.

B18_03.tar.xz contains 441 *.h5 files with detector images and a master file. The detector images were collected during a spatial scan of 21×21 points with a step of 500 nm. The sample was a **Kapton film with a CsPbBr₂Cl supercrystal**. Each *.h5 file corresponds to a single spatial point and contains 1 detector image. The scanning was done in horizontal rows.

Results of analysis of this dataset are presented in the Supporting Information, Section S7, Figures S22 – S26.

Optical Data

The collection **Optical_Data.zip** contains the optical data described in this work, such as absorption and fluorescence spectra, photoluminescence and lifetime images, spatially resolved photoluminescence and time-correlated single photon counting (TCSPC) measurements of supercrystals. There are four compressed subfolders **Solution_Spectra.tar.xz**, **Supercrystals_Imaging.tar.xz**, **Supercrystals_SpatiallyResolved_PLspectra.tar.xz** and **Supercrystals_TCSPC.tar.xz**.

Solution_Spectra.tar.xz contains the data for the absorption and fluorescence of CsPbBr₂Cl and CsPbBr₃ nanocrystals in solution.

Results of analysis of this dataset are presented in the supporting information (Figure S1).

Supercrystals_Imaging.tar.xz contains the data for the photoluminescence and lifetime images of the supercrystals. The subfolder also contains the files CsPbBr₂Cl_SC1_ImageParameters.txt, CsPbBr₂Cl_SC2_ImageParameters.txt and CsPbBr₃_ImageParameters.txt, which provide information on acquisition parameters and size of the images. From here on CsPbBr₂Cl_SC1 refers to the CsPbBr₂Cl supercrystal first depicted in the main manuscript in Figure 1a, while CsPbBr₂Cl_SC2 refers to the CsPbBr₂Cl supercrystal first depicted in the supporting information in Figure S7a.

Results of analysis of this dataset are presented in the main text and the supporting information (Figures 1 – 2, Figures S2 – S7).

Supercrystals_SpatiallyResolved_PL Spectra.tar.xz contains the data for the spatially resolved photoluminescence measurements performed on the supercrystals.

The subfolder also contains the files CsPbBr₂Cl_SC1_SpectraParameters.txt, CsPbBr₂Cl_SC2_SpectraParameters.txt and CsPbBr₃_SpectraParameters.txt, which provide, among other things, information on the acquisition location of these spectra.

Results of analysis of this dataset are presented in the main text and the supporting information (Figure 1, Figures S6 – S7).

Supercrystals_TCSPC.tar.xz contains the SymPhoTime 64 workspaces for the TCSPC measurements performed on CsPbBr₂Cl and CsPbBr₃ supercrystals. Each workspace contains the measurement, the fitting progress file (FLIMFit.pqres), the IRF used for fitting, as well as a workspace logfile. The .pck, .ptu, pqres and .sptl files can be opened using Picoquants SymPhoTime 64 software package. The SymPhoTime 64 software can be freely obtained from PicoQuant GmbH.

Results of analysis of this dataset are presented in the main text and the supporting information (Figures 1 – 2, Figures S2 – S7).