Raw data repository for the article:

Revealing the impact of polystyrene-functionalization of Au octahedral nanocrystals of different sizes on formation and structure of mesocrystals

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X-ray Data

The collection **Lapkin_Vartanyants_RawData.zip** contains the raw data collected at P23 beamline at PETRA III and described in the main text, Figures 3 – 5, and in the Supporting Information, Section S3, Figures S6 – S12.

Experimental Parameters:

X-ray energy: 8.32 keV
Beam size: ~10 × 30 um^2 (h × v)
Detector size: 516 × 1556 pixels (h × v)
Detector pixel size: 55 × 55 μm^2
Sample-detector distance: 1497 mm
Direct beam position: [306, 812] (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 five compressed subfolders **O1_data.tar.xz**, **O2_data.tar.xz**, **O3_data.tar.xz, O4_data.tar.xz** and **O5_data.tar.xz** corresponding to the samples O1 – O5 described in the paper.

The measured diffraction patterns are saved in the NeXus format. The detailed description of the format and a list of available software for opening the files can be found at http://www.nexusformat.org/. Essentialy these are HDF5 files and can be opened by the built-in libraries in MATLAB or Python.
Each of the subfolder contain 382 files with the names OX_000001.nxs – OX_000382.nxs. Each file corresponds to an angular position of the sample in the range from -5 to 185.5 degrees with the step of 0.5 degree and contains two diffraction pattern measured with the exposure time of 1 s.
File OX_background.nxs in each of the subfolder contain 10 diffraction patterns measured without the sample in the beam with the exposure time of 1 s and represent the background scattering from air and Kapton windows of the flight tube between the sample and the detector.