Supporting Information

Influence of Film Formation Kinetics on the Dispersion of Colloidal Quantum Dots in Organic Small Molecule Matrices

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1. FCC Colloidal Paracrystal Model

1.1. Model Description

To fit the 1D GISAXS data, we employ a face-centered cubic (FCC) lattice with paracrystalline distortion as outlined in previous works.[1–3] The FCC paracrystal models (as implemented in SasView version 6.0.0) calculates the scattering intensity $I(q)$ as:

$$I(q) = \frac{scale}{V_p} V_{lattice} F(q) Z(q) + background$$

where scale is the volume fraction of spheres in the sample, V_p is the volume of the primary particle, $V_{lattice}$ is a volume correction for the crystal structure, $F(q)$ is the form factor of the sphere (normalized), and $Z(q)$ is the paracrystalline structure factor for an FCC structure.[4,5]

GIXS data in this work is not calibrated to an absolute intensity scale. As such, the 'scale' and 'background' terms represent a convolution of instrumental factors, sample thickness, sample transmission and baseline offsets. They are included to improve fit quality but have no standalone physical meaning.

For an FCC array of spheres with radius R and nearest-neighbour centre-to-centre distance D the lattice parameter a (the cubic unit cell edge length) is given by:

$$a = \sqrt{2D}$$

And the lattice volume correction (the occupied volume of the lattice) for an FCC structure is:

$$V_{lattice} = \frac{8\pi R^3}{3\sqrt{2}D^3}$$

The paracrystalline distortion is introduced through the disorder parameter g, which defines the standard deviation of the lattice spacing ($\Delta a = gD$) and describes the degree of structural disorder in the superlattice, where g is a fractional distortion based on the nearest neighbor distance.[5]

In the context of QD–organic semiconductor blends, the fitted lattice parameter should be interpreted as a nominal average interparticle spacing within locally ordered domains rather than a true crystallographic constant. For PbS QDs with core radius $R \sim 22$ Å and typical ligand shell lengths of 10–20 Å, an ideal close-packed FCC lattice would yield D values of 60–80 Å. Deviations from this range and reductions in the fitted lattice parameter correspond to increased disorder and diminished long-range QD ordering.

1.2 Simulated FCC 1D Profiles

To better visualize the effect of the disorder parameter on QD ordering, the FCC paracrystal models for QDs with a radius of 22 Å are presented in Supplementary **Figure S1**. Here, highly ordered QDs are characterized by low disorder parameters corresponding to a highly aggregated FCC arrangement. In contrast, weakly ordered QD arrangements are characterized by low disorder parameters where a value of 1.0 corresponds to a random QD arrangement described by a scattering model of spheres with hard-sphere interactions.

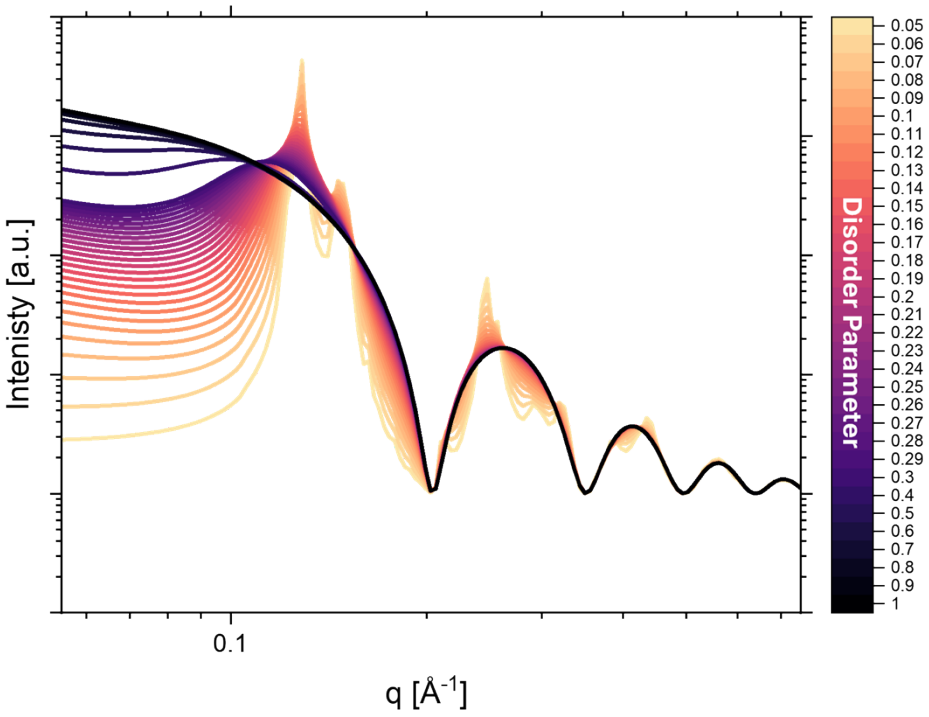

Figure S1: *The effect of the disorder factor on the packing of QDs using the FCC paracrystal model. Simulations were produced in SasView software,*[4] *with the following fixed parameters: scale = 1, background = 1, QD radius = 22 Å, QD particle SLD = 50.30×10^{-6} Å^{-2} and solvent SLD = 10 ×10^{-6} Å^{-2}.*

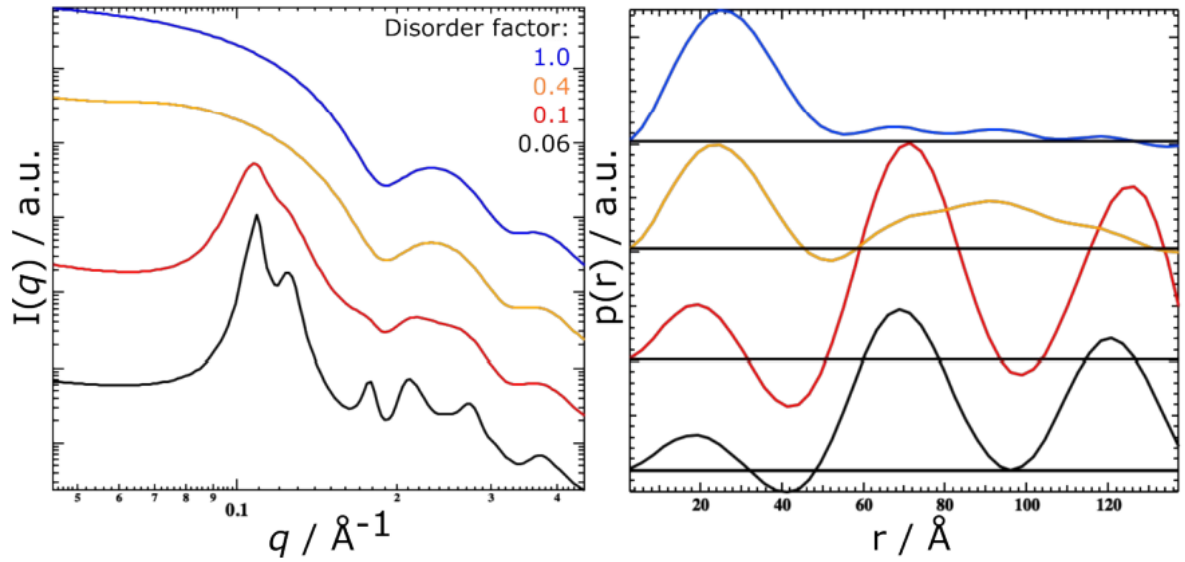

Figure S2: *The effect of disorder factor on the packing of quantum dots using the FCC paracrystal model, were a) shows simulated 1D scattering data and b) shows pair distance distribution function obtained from the simulated scattering data.*

This is further supplemented by illustrations of the effect of the disorder factor on the packing of quantum dots using the FCC paracrystal model for low (a), intermediate (b) and high disorder (c) factors.

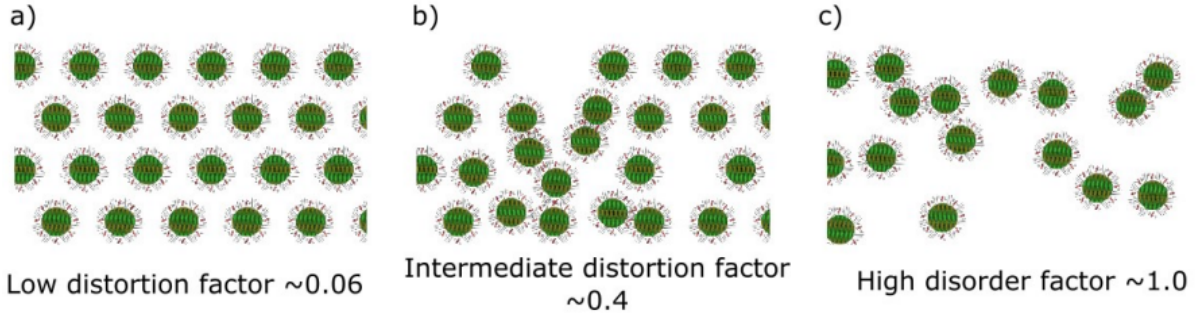

Figure S3: *Illustration of effect of disorder factor on the packing of quantum dots using the FCC paracrystal model for low (a), intermediate (b) and high disorder (c) factors.*

2. 1D GISAXS Fitting

Table S1: *Fit parameters of QD structures for TIPS-Tc:PbS-OA and TIPS-Tc:PbS-TET-CA OSC:QD blend films prepared by blade coating and spin-coating at speeds of 500 rpm, 1500 rpm and 6000 rpm. Data fitted using an FCC paracrystal model. The following parameters were fixed: QD radius = 22 Å, QD particle SLD = 50.30 $\times 10^{-6}$ Å^{-2} and solvent SLD = 10 $\times 10^{-6}$ Å^{-2}.*

OSC:QD Blend	Film Processing Conditions	Scale	Background	Lattice Constant [Å]	Disorder Parameter
TIPS-Tc:PbS-OA	Blade-coated	0.252 ± 0.002	0.432 ± 0.070	63.66 ± 0.04	0.120 ± 0.001
	Spin-coated 500rpm	1.000 ± 0.001	19.08 ± 0.07	62.84 ± 0.01	0.163 ± 0.001
	Spin-coated 1500rpm	0.385 ± 0.004	6.07 ± 0.23	57.83 ± 0.28	0.282 ± 0.004
	Spin-coated 6000rpm	0.155 ± 0.001	5.00 ± 0.07	57.24 ± 0.08	0.303 ± 0.001
TIPS-Tc:PbS-TET-CA	Blade-coated	0.249 ± 0.001	3.15 ± 0.05	58.59 ± 0.05	0.327 ± 0.001
	Spin-coated 500rpm	1.290 ± 0.006	7.47 ± 0.27	63.22 ± 0.04	0.154 ± 0.001
	Spin-coated 1500rpm	0.761 ± 0.001	55.64 ± 0.07	44.38 ± 0.02	0.451 ± 0.001
	Spin-coated	0.139 ± 0.007	8.89 ± 0.19	47.50 ± 1.08	0.440 ± 0.008

	6000rpm				

4. Polorised Optical Microscopy

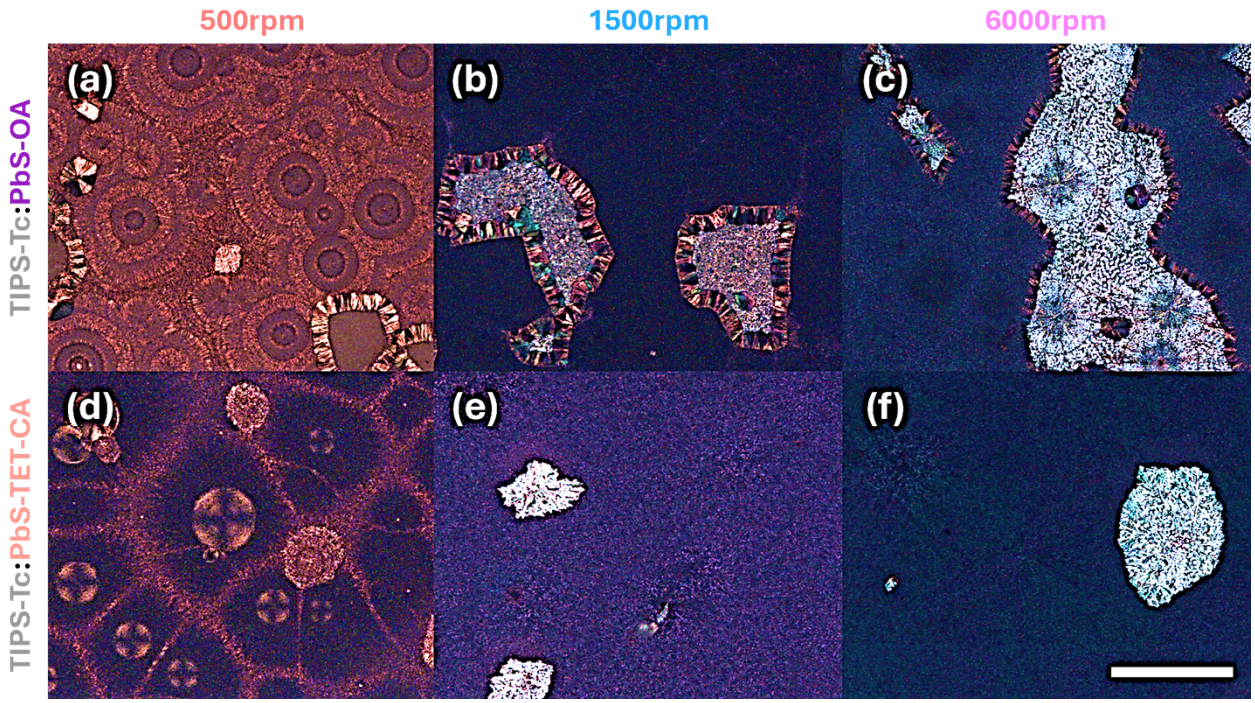

Figure S4*: Polarised optical microscopy (POM) images of spin-coated (a-c) TIPS-Tc:PbS-OA and (d-f) TIPS-Tc:PbS-TET-CA blend films prepared at spin speeds of 500rpm, 1500rpm and 6000rpm (500 µm scale bar).*

5. References

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https://www.sasview.org/docs/user/models/fcc_paracrystal.html.