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Supporting information

Structure and crystallinity in water dispersible photoactive nanoparticles for organic solar cells

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Transmission electron microscopy

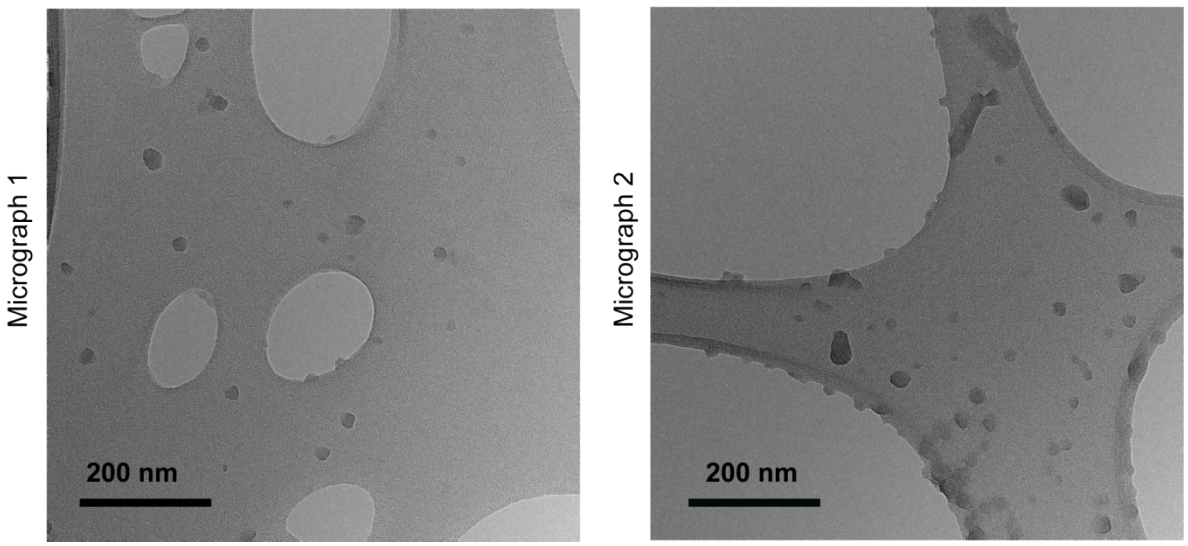

Figure S1: Representative raw TEM images acquired by imaging a droplet of the sample dispersed on a TEM copper grid with a holey carbon film. From the acquired TEM images, particle sizes were measured by manually outlining the particle perimeters, using the software ImageJ and converting the measured projected particle areas to particle diameters using a circular approximation.

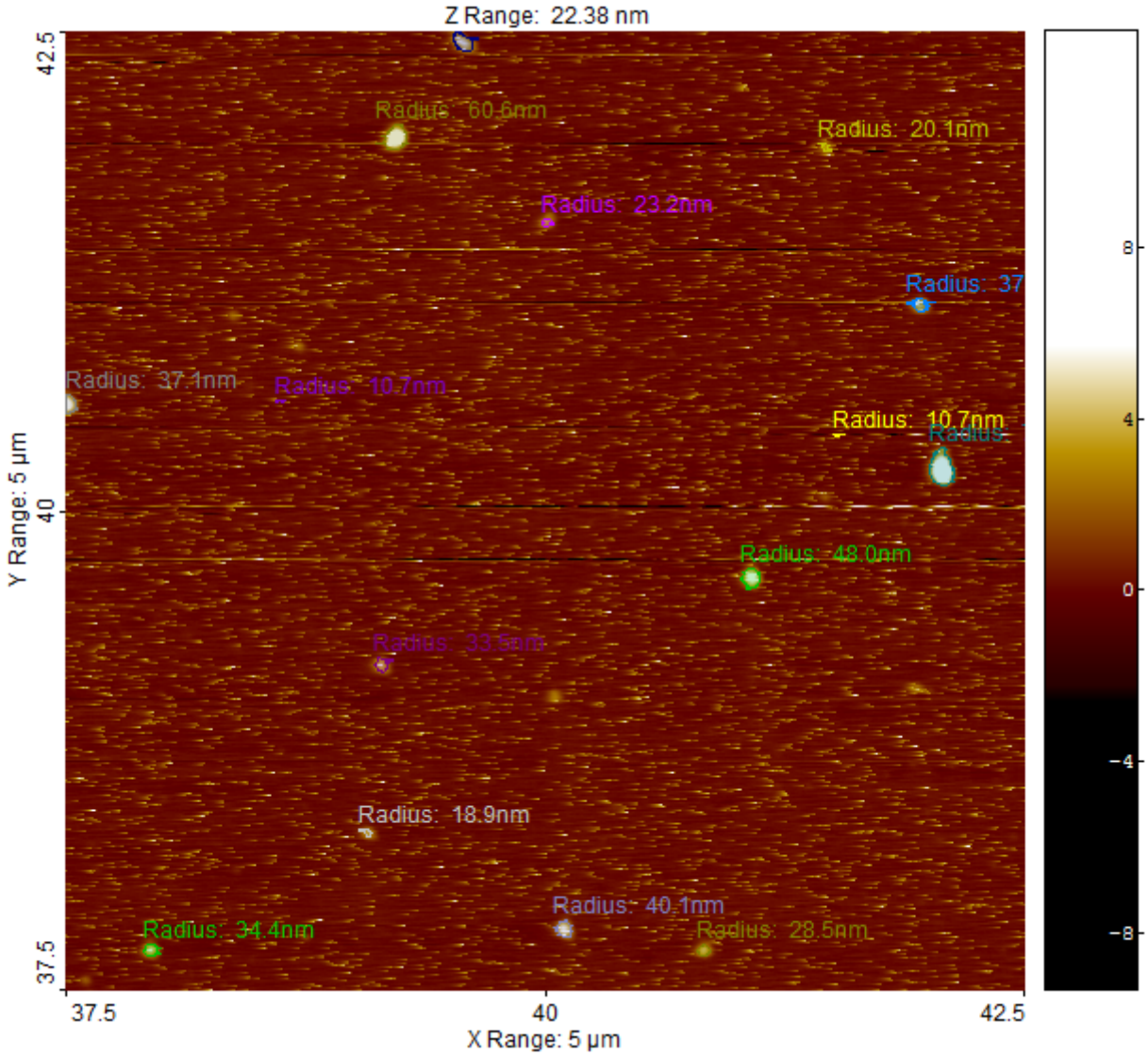

Figure S2: Representative raw AFM image acquired by imaging a droplet of the sample dispersed on mica. Particle heights and radii were extracted from the acquired AFM images with the SPIP 6.2.6 software using an automated thresholding routine.

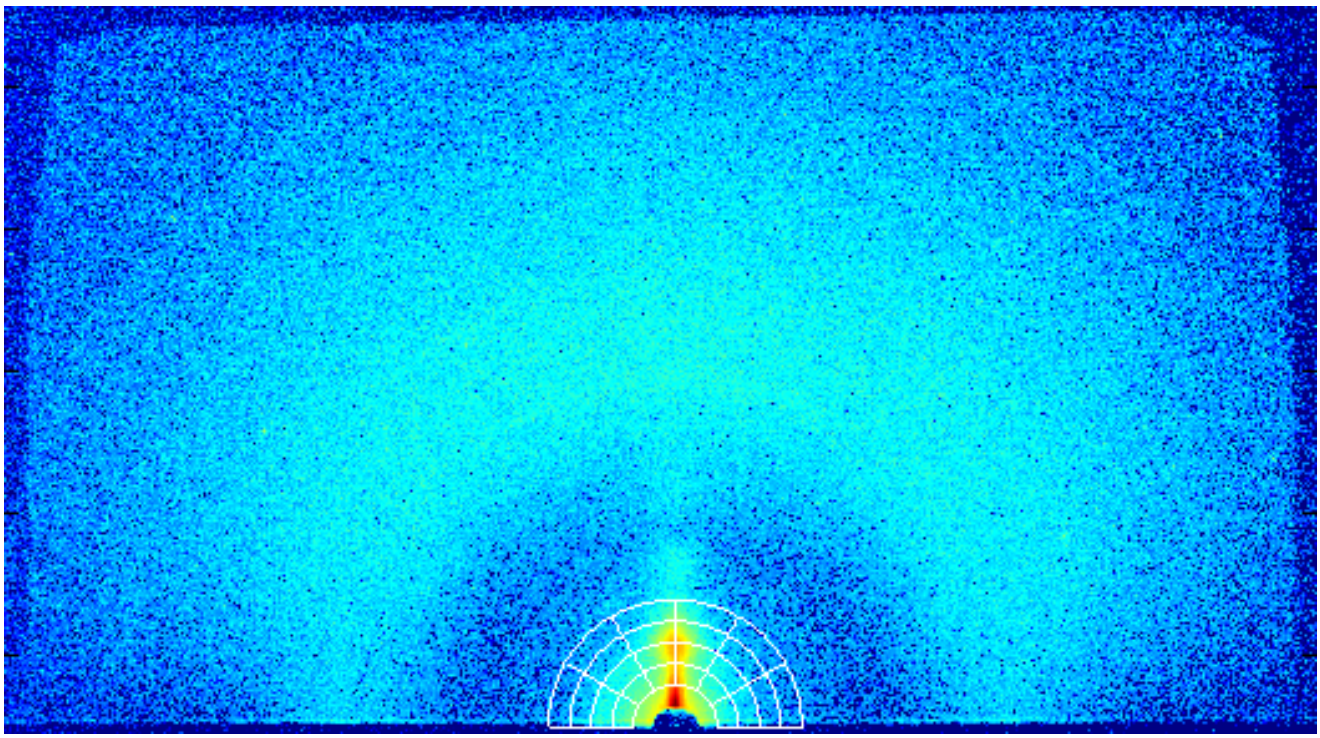

Figure S3A: Example raw GIWAXS data of nanoparticles spin-coated on glass and annealed for 5 minutes, showing the azimuthal integration region from 0.2 $Å^{-1}$ to 0.6 $Å^{-1}$ around the P3HT *100* reflection.

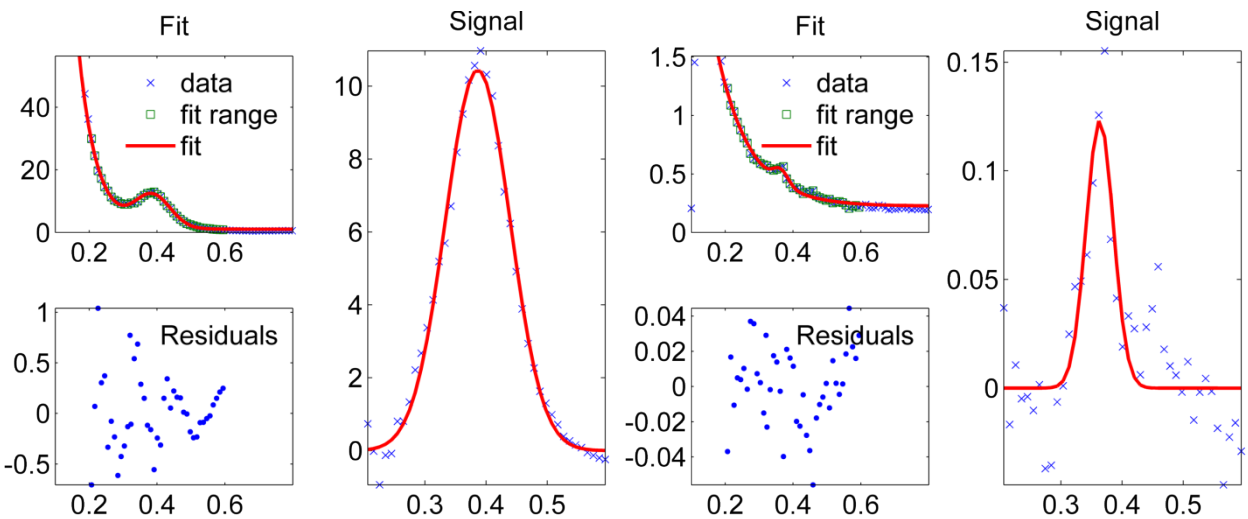

Figure S3B: Corresponding fits of integrations out-of-plane, from 87.5° to 92.5° (left) and in-plane, from 160° to 180° (right) used to derive peak widths at half maximum for the Scherrer estimation of domain sizes.

SDS estimate

The total volume, V, and area, A of the particles was found from TEM particle size distribution in the following way

$$A = \sum_i w_i \, 4 \, \pi \, r_i^2$$

$$V = \sum_i w_i \frac{4}{3} \pi \, r_i^3$$

where w_i was the relative fraction of particles with $r_{i.}$

The conversion to mass of SDS, m_{sds}, was done using the molar surface density, σ_{sds}, and the molar mass of SDS M_{sds}

$$m_{sds} = A \, \sigma_{sds} \, M_{sds}$$

An upper estimate of σ_{sds} was optained from σ_{sds} reported for latex particles[1]

The mass of P3HT:PCBM, m_{np}, was determined using the mass density of a 1:1 mixture of P3HT and PCBM, ρ_{np}

$$m_{np} = V \, \rho_{np}$$

The SDS mass fraction of the total mass was found to be 18 %.

NMR

The Landfester nanoparticles were scanned using ^{1}H NMR shown in figure 1. A clear water peak is observed but no chloroform signal is found.

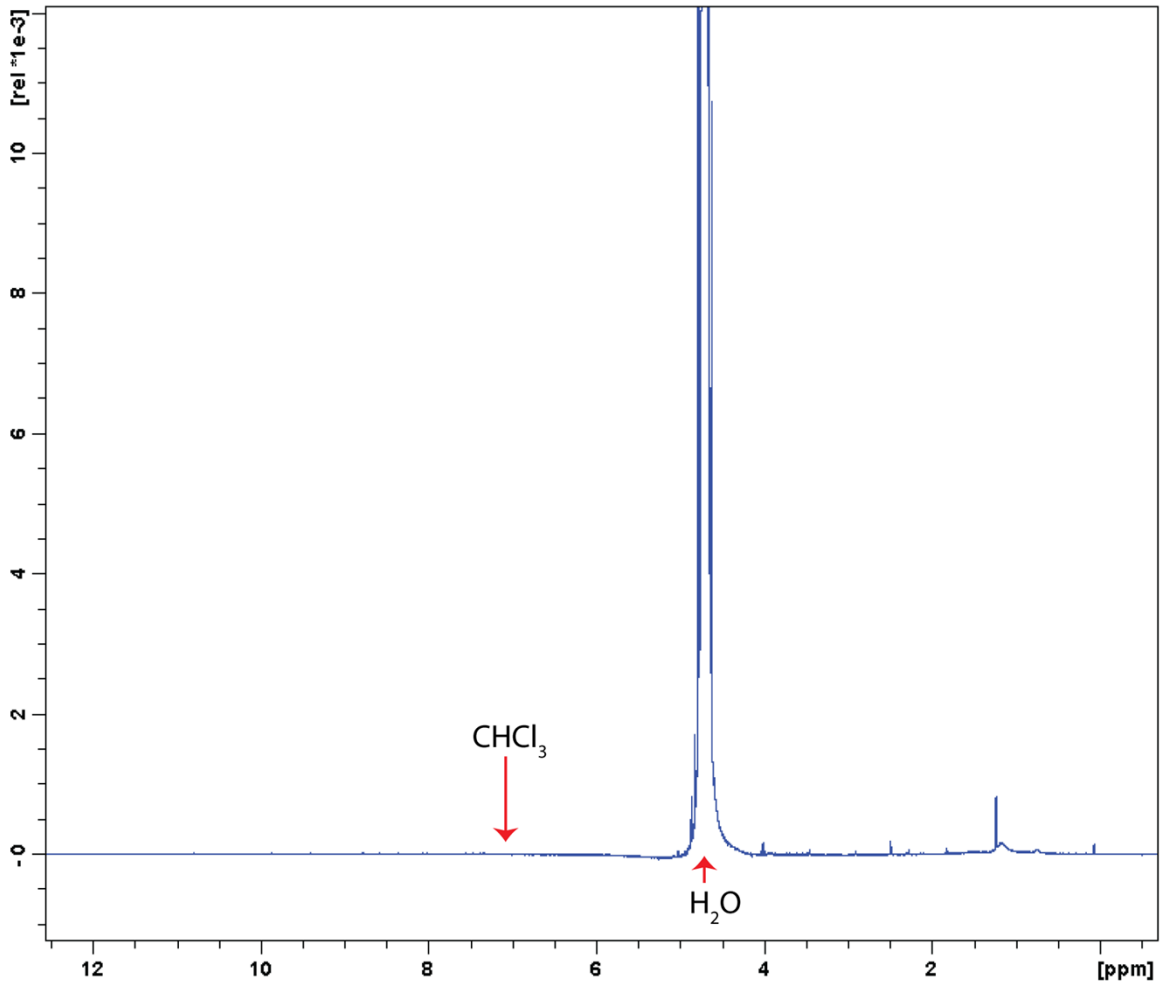

Figure S4. NMR scan of P3HT:PCBM 1:1 Landfester particles dispersed in water.

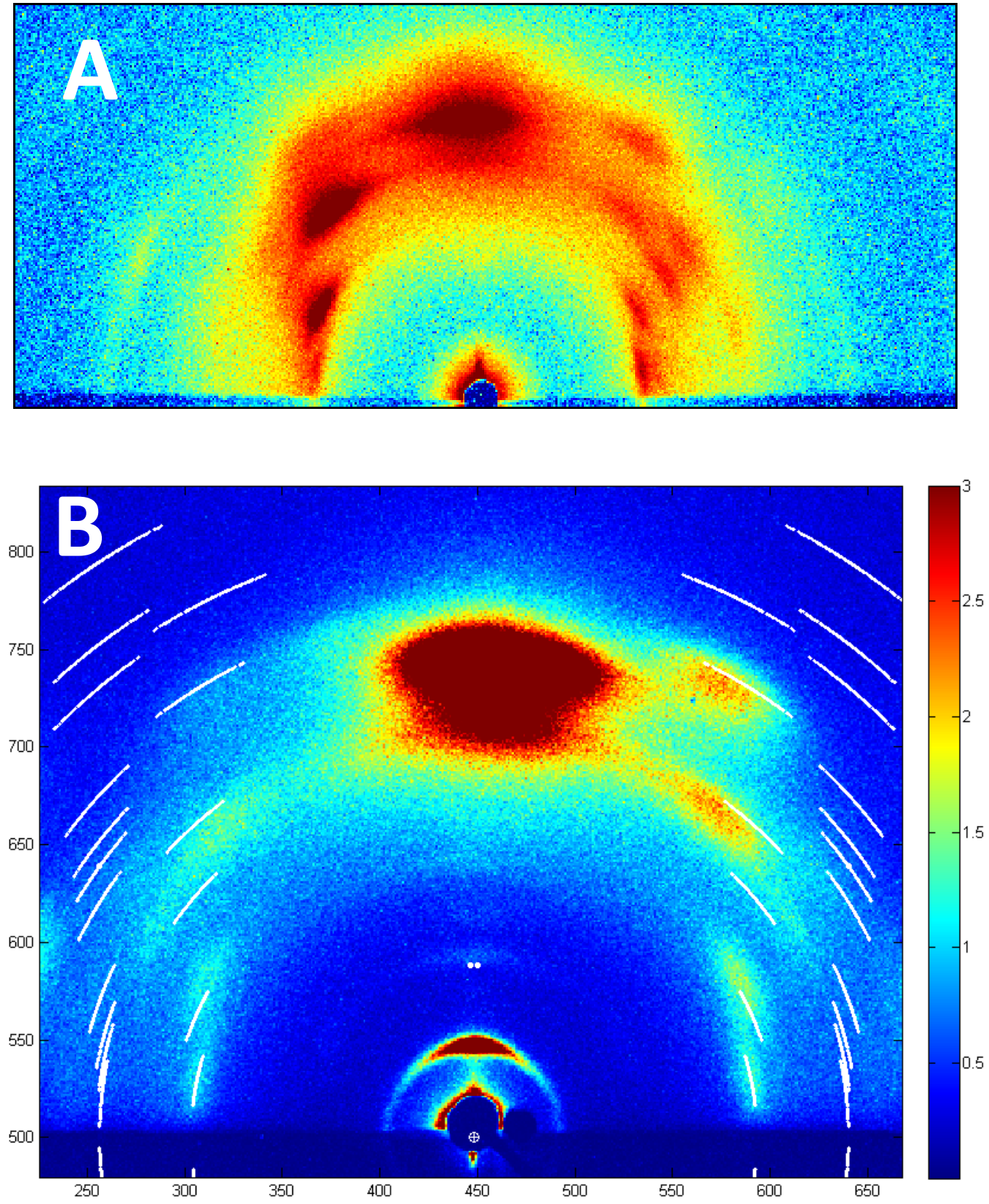

Figure S5 A) Raw WAXS data showing diffraction from a clean PET substrate B) Indexing of PET reflections using simDiffraction[2] assuming an orientation with *001* parallel with the surface normal.

Reflections at higher angles along the surface normal falls in the region of the Ewald sphere not probed with a small fixed incidence angle. P3HT *100* and *200* reflections are seen on the surface normal at lower angles.

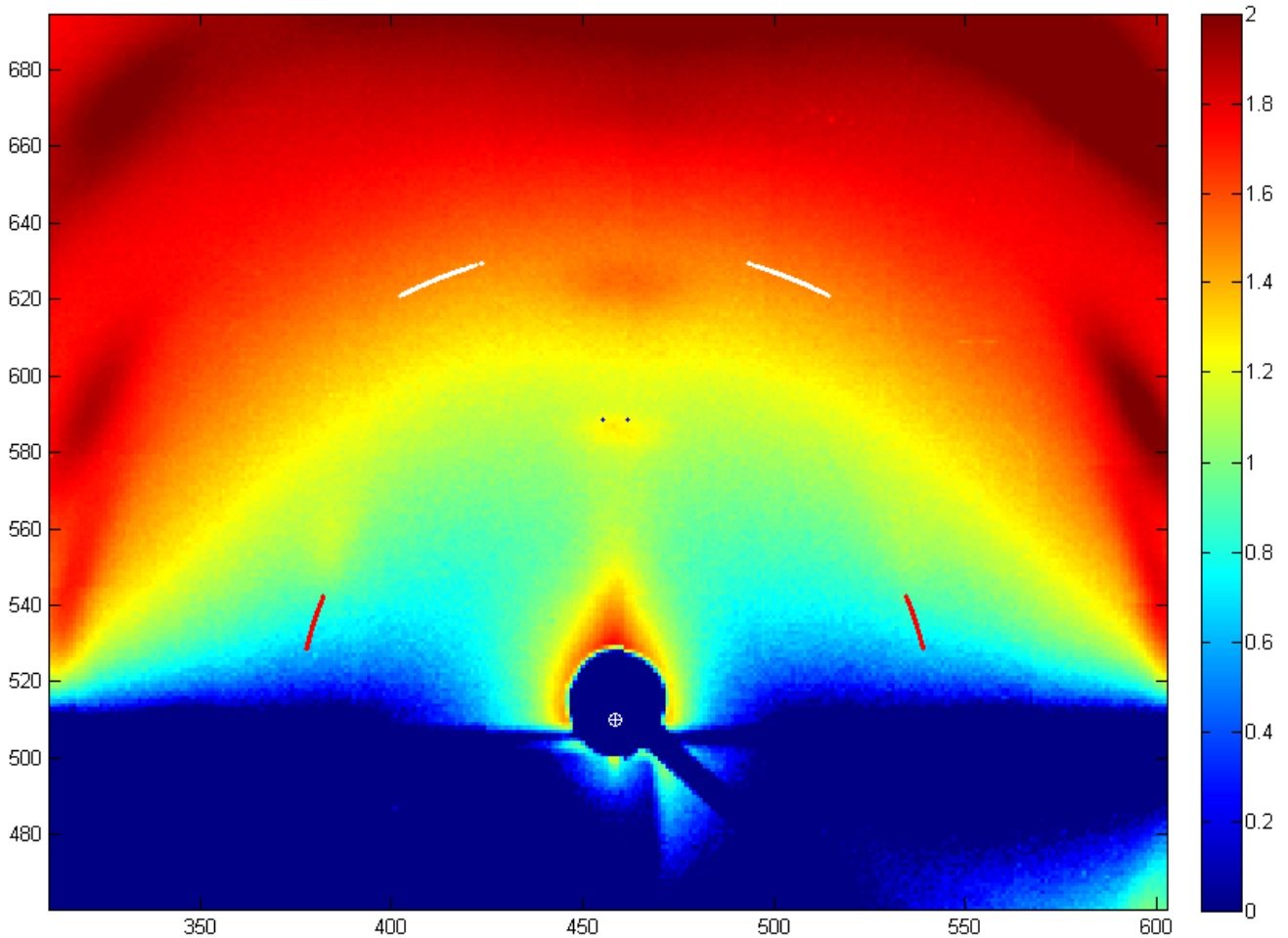

Figure S6 Indexing of PCBM reflections assuming a solvent-free structure[3]. Note that PCBM is known to crystallize in a variety of structures depending on coating methods, post-treatment and solvent content, most of them only tentatively described. The strongest low-angle reflections *11-1* (blue dots) and *002* (red dots) shows a reasonably good match for a preferred orientation with the *11-1* plane normal parallel with the surface normal. The *21-1* reflection is shown with white dots.

[1] Vale, H.M. and McKenna, T.F. (2005) Colloids Surfaces A Physicochem. Eng. Asp. **268**, 68–72

[2] D. W. Breiby, O. Bunk, J. W. Andreasen, H. T. Lemke, and M. M. Nielsen (2008) J. Appl. Crystallogr., **41**, 262–271

[3] Casalegno, M., Zanardi, S., Frigerio, F., Po, R., Carbonera, C., Marra, G., Nicolini, T., Raosa G. and Meille S.V. (2013) Chem. Commun., **49**, 4525-4527