Supporting Information

Morphologies of self-organizing regioregular conjugated polymer/fullerene aggregates in thin film solar cells

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The radius of gyration (R_g) of a PCBM aggregate can be determined from the scattering peak intensity, using the Guinier approximation

$$I(Q) = I(0)\exp\left(-\frac{Q^2 R_g{}^2}{3}\right) \qquad (1)$$

where $I(Q)$ is the scattering intensity; $I(0)$ is the zero-angle scattering intensity; Q is the scattering vector; and R_g is the radius of gyration of the PCBM clusters. Figure S3 presents plots of ln$I(Q)$ versus Q^2 that were fitted using Equation 1 (solid lines) in the low-Q range. The values of R_g can be extracted from the slopes ($-R_g{}^2/3$) of the fitted lines.

The out-of-plane electron and hole mobilities were determined by fitting the dark current density–voltage curves of the devices into the space-charge-limited current (SCLC) model, based on the equation

$$J = \frac{9}{8}\varepsilon_o \varepsilon_r \mu_{h(e)} \frac{V^2}{L^3}$$

where ε_o is the permittivity of free space, ε_r is the dielectric constant of the materials, $\mu_{h(e)}$ is the hole (electron) mobility, V is the voltage drop across the device, and L is the active layer thickness.

Figure S1 GISAXS pattern of the P3HT/PCBM blend film incorporating 55 wt% PCBM and a schematic representation of the device structure.

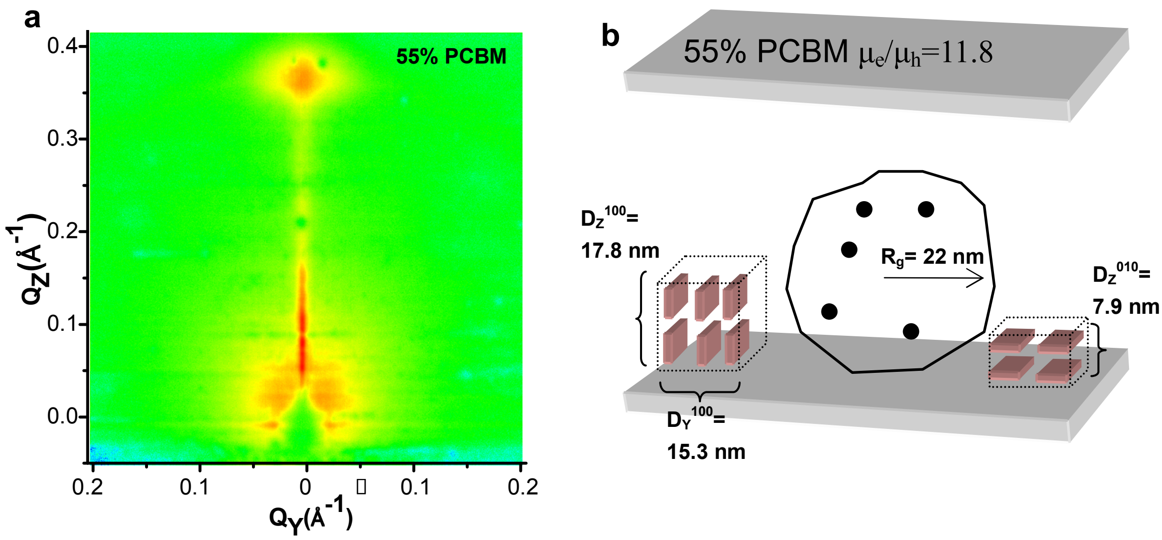


Figure S2 Profiles of azimuthal angles at $Q_{(100)}$, extracted from the GISAXS 2D pattern. Inset: Defining the spread angle of the P3HT chains on the substrates. When the P3HT molecules were aligned edge- and face-on to the substrates, the azimuthal angles were designated as 0 and 90°, respectively.

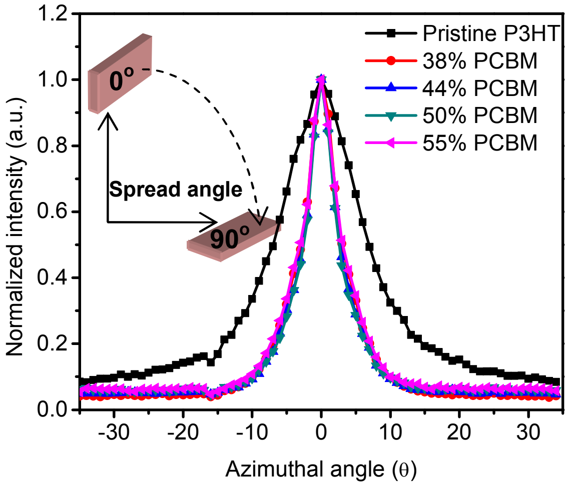
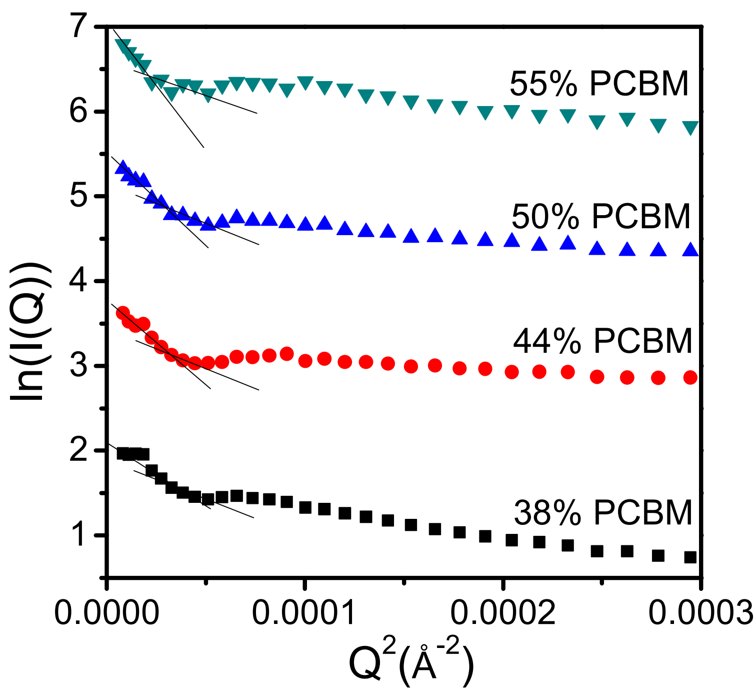
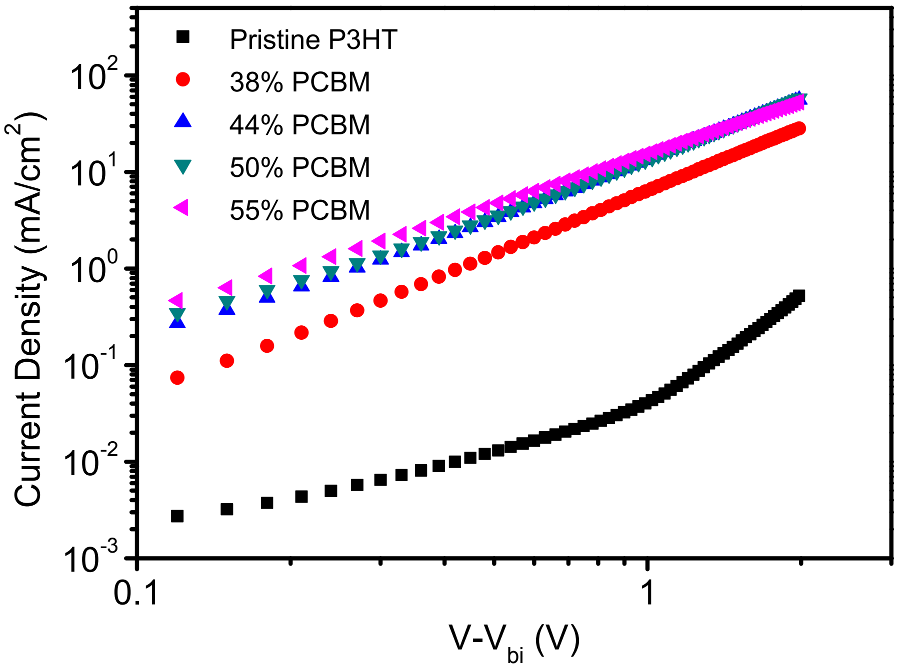


Figure S3 Plots of ln $I(Q)$ versus Q^2 for the GISAXS data of P3HT/PCBM films, measured with a large sample-to-detector distance of 3219 mm for an improved low-Q resolution. The data are fitted using the Guinier approximation (solid lines). Polydispersity effect of the PCBM aggregation is estimated using the two fitted lines for the upper- (R_g^1) and lower-limit (R_g^2); the fitted R_g values are summarized in the Table below. Averaged R_g values are used in the text.

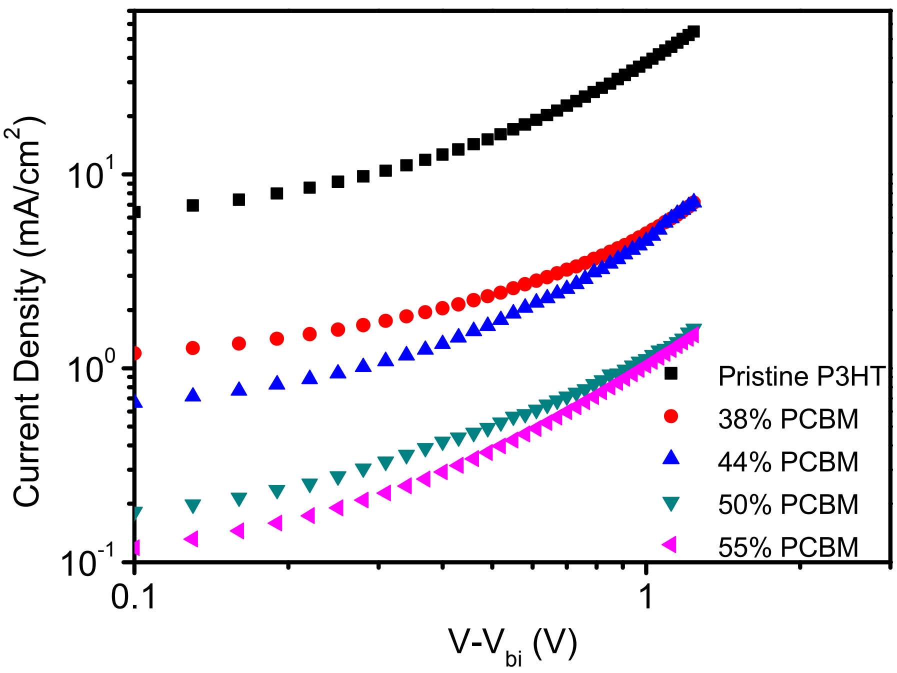


PCBM by weight in P3HT	R_g^1 (nm)	R_g^2 (nm)	$R_g^{average}$ (nm)
38%(1:0.6)	18.7	17.2	18.0
44%(1:0.8)	22.4	18.3	20.4
50%(1:1)	25.3	17.9	21.6
55%(1:1.2)	29.6	14.2	21.9

Figure S4: Dark *J–V* curves for (a) electron- and (b) hole-dominated carrier devices of P3HT/PCBM incorporating various PCBM loadings, annealed at 150 °C for 15 min.



(a)



(b)

Figure S5: Current density–voltage characteristics under illumination of devices incorporating P3HT films containing various weight percentages of PCBM, after annealing at 150 °C for 15 min.