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Correlating three-dimensional morphology with function in PBDB-T:IT-M non-fullerene organic solar cells

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GISAXS modeling

To quantify and compare the phase separation in the non-fullerene photovoltaic blends, the 1D GISAXS profiles were fitted using a universal model expressed in Equation 1 using the fitting software SasView (Version 3.1.2). The first term of the equation is the so-called Debye−Anderson−Brumberger (DAB) term, where q is the scattering wave vector, A_1 is an independent fitting parameter, and ξ is the average correlation length of the PBDB-T domain. The second term represents the contribution from fractal-like aggregations of IT-M. Here, P(q, R) is the form factor of IT-M. S(q, R, η, D) is the fractal structure factor, which describes the interaction between primary particles (defined as 4 nm in our fitting) in this fractal-like aggregation system, with R the mean radius of primary IT-M aggregates, and η the correlation length of the fractal-like structure. The average correlation length of the clustered IT-M phases can be defined by the Guinier radius (R_g) of the network, where $R_g = \sqrt{\left(\frac{D(D+1)}{2}\right)}\eta$.

$$I(q) = \frac{A_1}{[1+(q\xi)^2]^2} + A_2\langle P(q, R)\rangle S(q, R, \eta, D) + B \qquad (1)$$

$$S(q) = 1 + \frac{\sin[(D-1)\tan^{-1}(q\eta)]b \pm \sqrt{b^2-4ac}}{(qR)^D} \frac{D\Gamma(D-1)}{\left[1+\frac{1}{(q\eta)^2}\right]^{(D-1)/2}} \qquad (2)$$

Caculation of donor:acceptor ratio from XPS measurements

XPS data were obtained using a Kratos Axis Supra (Kratos Analytical, Manchester, UK) having a monochromated Al Kα source. All spectra were recorded using a charge neutralizer to limit differential charging. The main carbon peak is referenced to 284.5 eV. Depth profiles of different samples were generated by Minibeam 6 gas cluster ion source rastering a 2.5 kV Ar_{500}^{+} cluster beam over a 3 mm x 3 mm area giving a typical sample current of 5.53 nA. The data was fitted using CASA XPS with Shirley backgrounds using the Kratos sensitivity factor library. To identify PBDB-T and IT-M, we first measured the PBDB-T and IT-M pure films to identify the content of C, N, O, and S atoms in pure PBDB-T and IT-M films. Afterwards, we identify the C, S, O content in PBDB-T as C_{PBDB-T} wt%, S_{PBDB-T} wt%, O_{PBDB-T} wt%, and the C, S, O, N content in IT-M as C_{IT-M} wt%, S_{IT-M} wt%, O_{IT-M} wt%, N_{IT-M} wt%. We then measured PBDB-T:IT-M blend films and identified the C, N, O, S content as (C from blend) wt%, (N from blend) wt%, (O from blend) wt%, (S from blend) wt%. Since IT-M contain N atom but PBDB-T does not has N atom, we therefore use N atom to calculate the IT-M content in the PBDB-T:IT-M blend films. The content of C, O, S comes from IT-M can be calculated as:

(C from IT-M) wt% = (N from blend film) wt% * C_{IT-M} wt% / N_{IT-M} wt%,

(O from IT-M) wt% = (N from blend film) wt% * O_{IT-M} wt% / N_{IT-M} wt%,

(S from IT-M) wt% = (N from blend film) wt% * S_{IT-M} wt% / N_{IT-M} wt%.

Afterwards, we used (C from blend) wt%, (O from blend) wt%, (S from blend) wt% to deduce (C from IT-M) wt%, (O from IT-M) wt%, (S from IT-M) wt% to obtain the (C from PBDB-T) wt%, (O from PBDB-T) wt%, and (S from PBDB-T) wt%. Furthermore, we use (C from PBDB-T) wt%, (O from PBDB-T) wt%, (S from PBDB-T) wt% to check the accuracy of our results. The appearance of Ti atoms marks the appearance of the TiO_2 layer during depth profiling. The S atoms in PEDOT:PSS consist those from the thiophene unit in PEDOT and those from the sulfonate unit in PSS, whilst the S 2p of PEDOT and PSS locates at 165 and 169 eV respectively. The appearance of S atoms from the PSS unit marks the appearance of the PEDOT:PSS layer during depth profiling. As the ratio of S atoms from PEDOT and those from PSS is fixed, we can then determine the total S atoms contributed by PEDOT:PSS. Then the S atoms from PBDB-T can be obtained by subtracting the total S atoms by S atoms contributed by IT-M and PEDOT:PSS. All film thicknesses after etching were confirmed using a Dektak 150 stylus profilometer.

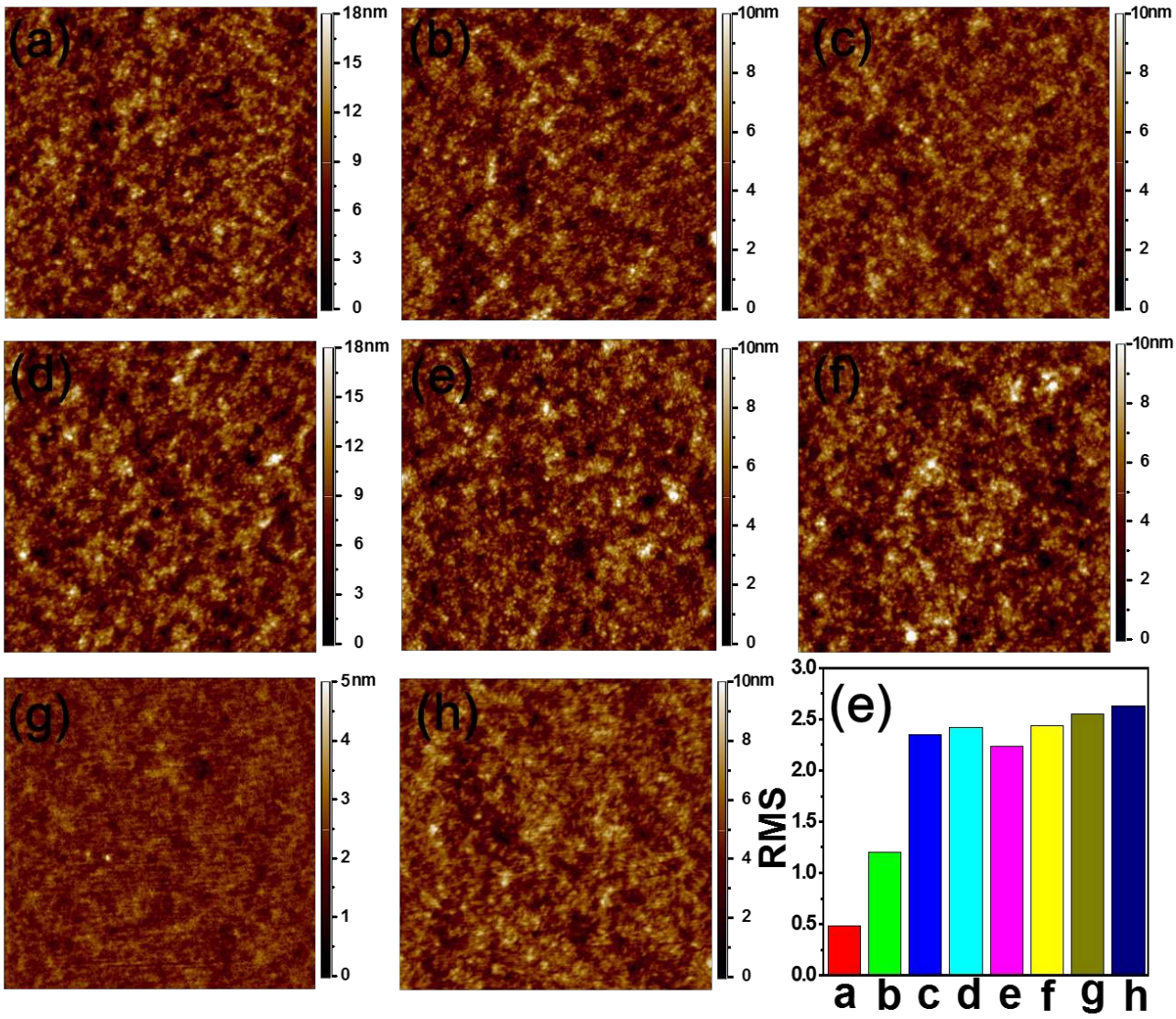

Figure S1 SPM topographic images of PBDB-T:IT-M films cast on (a, b, c) PEDOT:PSS and (d, e, f) TiO_2 substrates with (a, c) none annealing, (b, d) 80℃ annealing, (c, f) 160℃ annealing. (g) and (f) are SPM topographic images of pure PBDB-T and IT-M films. (e) The RMS surface roughness of images a-h.

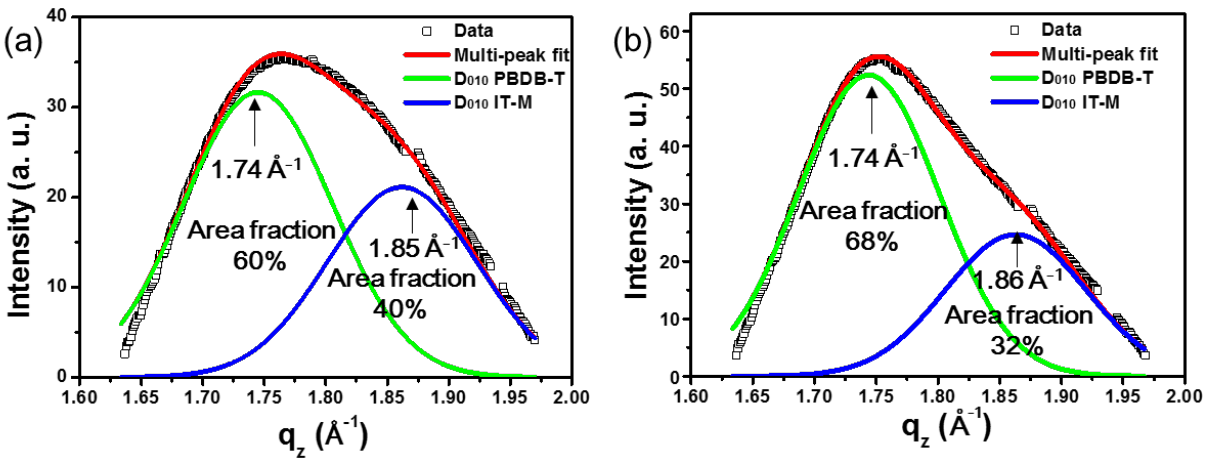

Figure S2. Multi-Peak fitting results of the OOP (010) peaks of PBDB-T:IT-M (a) upon 80 °C thermal annealing and (b) upon 160 °C thermal annealing.

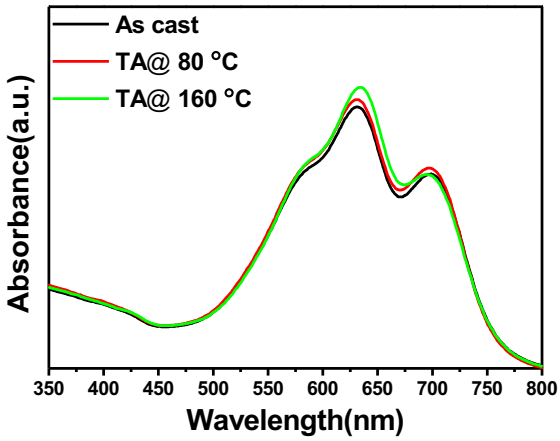

Figure S3. Absorption spectra of PBDB-T:IT-M with different annealing temperature.

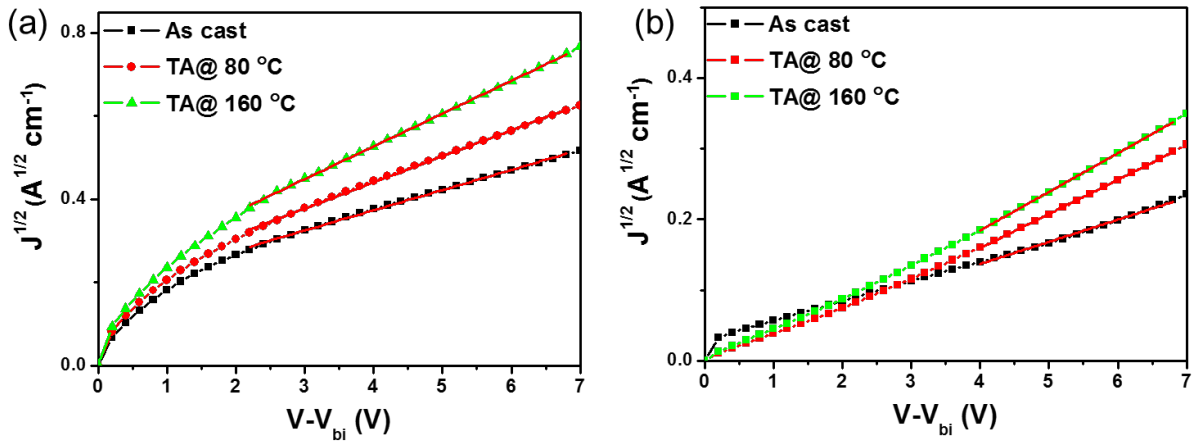

Figure S4. Root square plot of (a) electron current densities versus bias voltage of the ITO/TiO_2 /Active layer/Ca/Ag electron-only devices after different annealing treatments, and (b) hole current densities versus bias voltage of the ITO/PEDOT:PSS/Active layer/MoO_3/Ag hole-only devices.

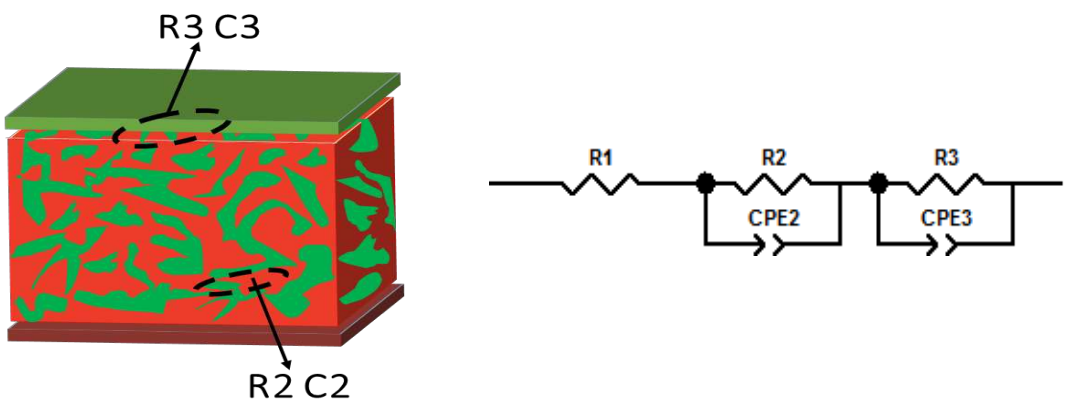

Figure S5. The equivalent circuit model to fit the impedance spectra.