

Supporting Information

Bridging the Mesoscopic Blend Structure and Property to Macroscopic Device Performance by In-situ Optoelectronic Characterization

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Phase images of blend films with different P3HT-PCBM ratios

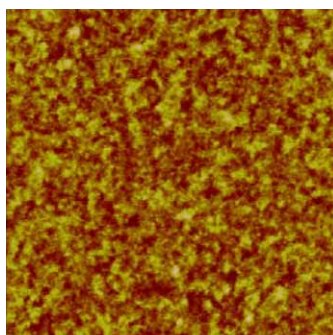


Fig S1. Tapping mode AFM ($5\ \mu\text{m} \times 5\ \mu\text{m}$) tomography images for pure P3HT.

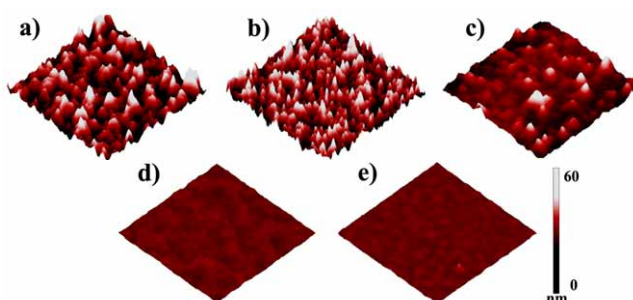


Fig S2. Tapping mode AFM ($10\ \mu\text{m} \times 10\ \mu\text{m}$) tomography images corresponding to Fig. 2 with different P3HT:PCBM ratios a) 3:1, b) 2:1, c) 1:1, d) 1:2, e) 1:3.

Table S1. Morphology details of PSCs with various P3HT:PCBM ratios

P3HT:PCBM	Domain depth (nm)	Rms (nm)	Domain shape (nm)
3:1	83.5	15.6	Strip
2:1	69.4	15.3	
1:1	57.8	8.11	Strip+Sphere
1:2	23.1	3.27	
1:3	14.6	1.48	Sphere

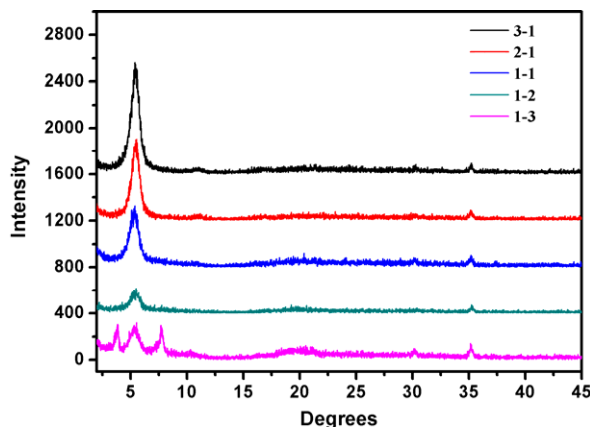


Fig 3. XRD images of P3HT:PCBM films fabricated by spin-coating and post processing.

EFM phase image analysis of the blend films

The phase shift over the sample, due to tip-sample capacitive coupling is:

$$\phi = -\frac{Q}{2k} C'(h) (V_{ip} - V_0)^2$$

Where Q and k represent the quality factor and the elastic constant of the cantilever, h is the distance between the tip and the sample surface. C is the capacitance of the tip-sample system. V_{ip} is the voltage applied to the tip and V_s is the local electrostatic potential on the sample surface. EFM can map out the phase shift of the cantilever, a lag between the drive frequency and the cantilever oscillation. This equation allows us to understand the phase changes over the blend films. From the formula, we can deduce $\Delta\phi$:

$$\begin{aligned} \phi_{P3HT} - \phi_{PCBM} &= -\frac{Q}{2k} C'(h) [(V_{ip} - V_{P3HT})^2 - (V_{ip} - V_{PCBM})^2] \\ &= -\frac{Q}{2k} C'(h) (V_{P3HT} - V_{PCBM})(V_{P3HT} + V_{PCBM} - 2V_{ip}) \\ &= -\frac{Q}{2k} C'(h) (\phi_{P3HT} - \phi_{PCBM})(\phi_{P3HT} + \phi_{PCBM} - 2\phi_{ip}) \end{aligned}$$

According to the energy level tested previously, the work function of P3HT and PCBM in the blend system were 4.39 eV and 4.44 eV,^{1,2} and the work function of Pt-Ir is about 5.7-6.1. Hence, $V_{P3HT} - V_{PCBM} > 0$ and $V_{P3HT} + V_{PCBM} - 2V_{ip} < 0$. In EFM images, the brighter features indicate P3HT-rich regions, and the darker features represent PCBM-rich regions. Blend films containing different amounts of PCBM also prove this, increasing the content of PCBM results in the obvious increase of the darker spots.

Surface potential characterization of the blend films with different P3HT-PCBM ratios

The topography, corresponding surface potential images in dark and under 532 nm illumination, and the statistic potential contrast distribution were concluded in this part.

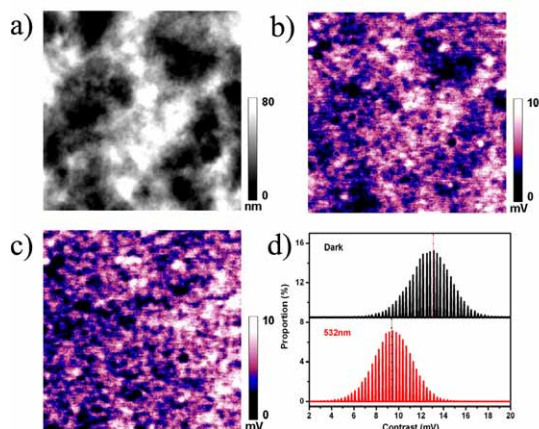


Fig S4. KPFM images ($5\ \mu\text{m} \times 5\ \mu\text{m}$) of the P3HT:PCBM sample with 3:1. a) Topography, b) SP image in dark, c) SP image under illumination at 532 nm, d) Histogram distribution of the surface potential contrast in dark and under illumination at 532 nm.

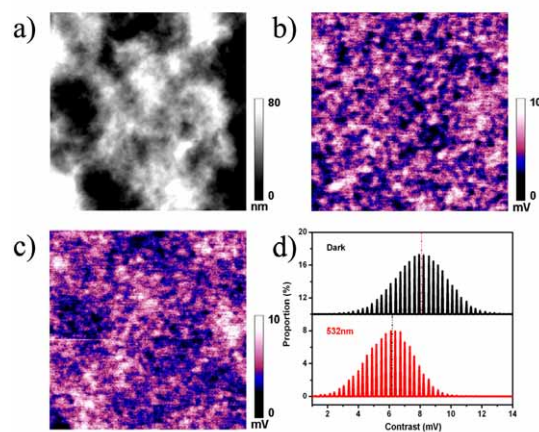


Fig S5. KPFM images ($5\ \mu\text{m} \times 5\ \mu\text{m}$) of the P3HT:PCBM sample with 2:1. a) Topography, b) SP image in dark, c) SP image under illumination at 532 nm, d) Histogram distribution of the surface potential contrast in dark and under illumination at 532 nm.

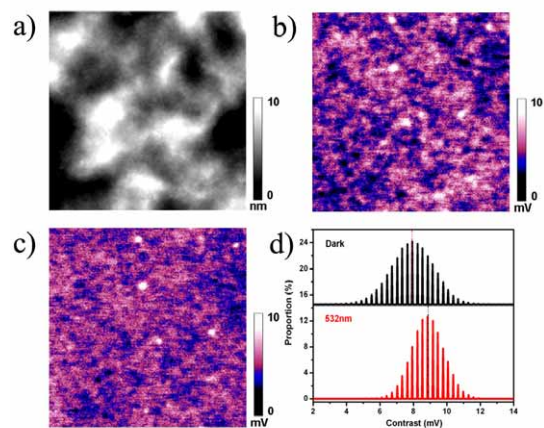


Fig S6. KPFM images ($5\ \mu\text{m} \times 5\ \mu\text{m}$) of the P3HT:PCBM sample with 1:2. a) Topography, b) SP image in dark, c) SP image under illumination at 532 nm, d) Histogram distribution of the surface potential contrast in dark and under illumination at 532 nm.

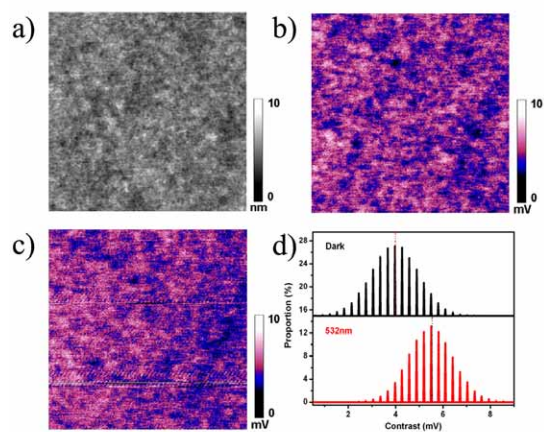


Fig S7. KPFM images ($5\ \mu\text{m} \times 5\ \mu\text{m}$) of the P3HT:PCBM sample with 1:3. a) Topography, b) SP image in dark, c) SP image under illumination at 532 nm, d) Histogram distribution of the surface potential contrast in dark and under illumination at 532 nm.

References

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- 2 M. Lenes, F. B. Kooistra, J. C. Hummelen, I. Van Severen, L. Lutsen, D. Vanderzande, T. J. Cleij and P. W. M. Blom, *J. Appl. Phys.*, 2008, **104**, 114517.