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Supplementary Information

Highly efficient vapor-deposited organic photovoltaic cells based on a simple bulk heterojunction

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1. Characterization of Indium Tin Oxide (ITO) Substrates:

Morphology:

Atomic Force Microscopy (AFM) experiments were carried out on two batches of ITO substrates and the results are shown in Figure 1. ITO batch A was used for all the device optimization experiments and ITO batch B was only used for charge extraction efficiency measurements in Fig. 4a. Based on a 4 μm^2 image, the root mean square roughness (R_{ms}) is calculated to be 2.06 nm for batch A and 3.52 nm for batch B.

Sheet Resistance:

Sheet resistance was measured using the four-point probe method and calculated using Equation 1. The values are listed in Table 1. No significant difference in sheet resistance is observed for these two batches of ITO.

$$R_{sheet} = \frac{\pi}{\ln 2} \cdot \frac{I}{V} \qquad \text{Equation 1}$$

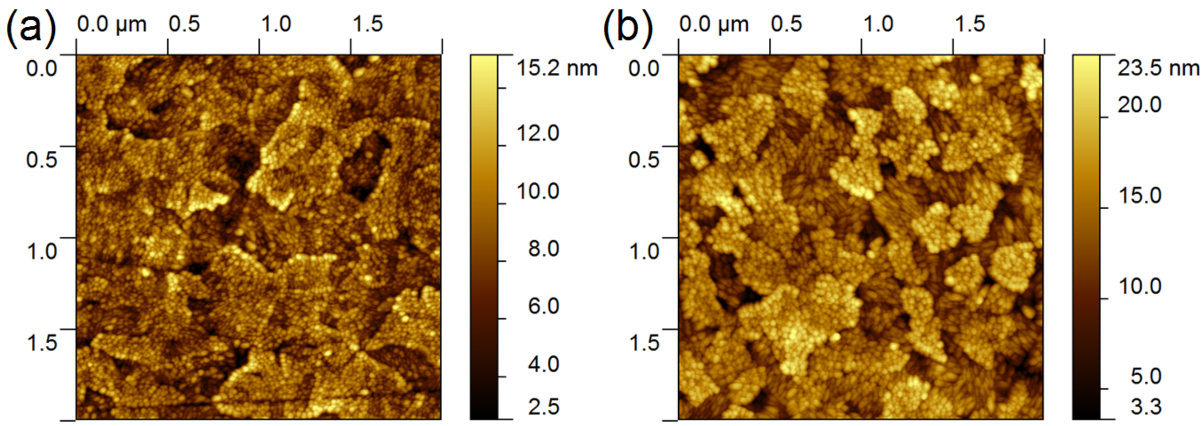

Figure 1: Atomic force microscopy images for ITO batch A (a) and B (b).

Device Performance:

The optimized device structure (70 nm DTDCPB:C_{70} = 1:2) was grown on both batches of ITO. All operating parameters are summarized and plotted in Figure 2. Devices fabricated on ITO batch B exhibit higher fill factor (FF), lower short-circuit current (J_{SC}) and lower open-circuit voltage (V_{OC}) than devices on ITO batch A, but the overall efficiency stays roughly the same. The reduction of V_{OC} can be explained by the larger R_{ms} observed in ITO batch B. A rougher ITO substrate may lead to a less uniform organic film grown on top of it, possibly causing local hot spots with high dark current which reduces V_{OC}.

Series resistance of devices grown on different batches of ITOs are calculated by fitting the dark current with generalized Shockley equations and listed in Table 1.[1] Devices grown on ITO batch B show a >40 % reduction in series resistance when compared to devices grown on ITO batch A, albeit the two batches of ITO show roughly the same sheet resistance according to the four-point probe measurement. ITO morphology may play a role in determining R_s. The difference in R_s will eventually impact FF, with ITO batch B (with lower R_s) showing higher FF.

Table 1: Morphological and electrical parameters for two batches of ITO substrates

ITO Batch	R_{ms} (nm)	Sheet resistance (Ω/□)	Fitted R_s (Ωcm^2)
A	2.06	9.12±0.53	0.79±0.06
B	3.52	8.99±0.39	0.46±0.03

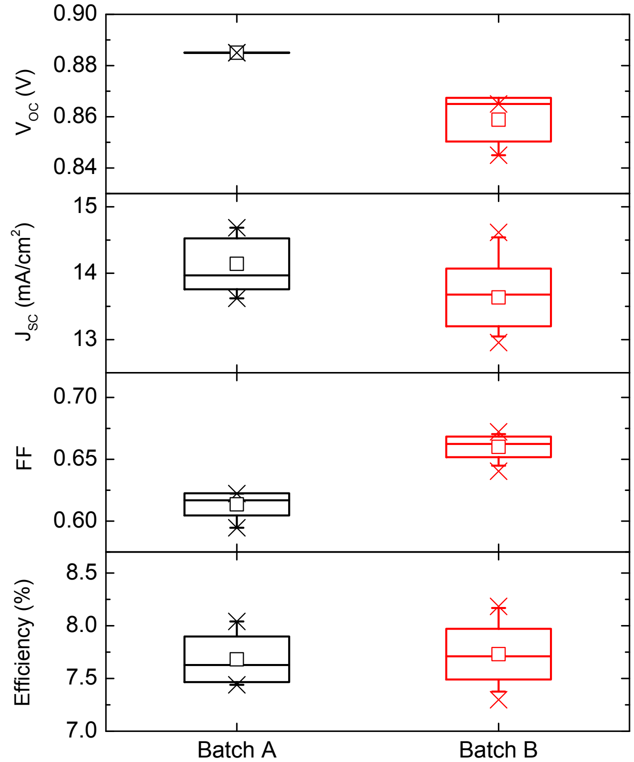

Figure 2: Operating parameters for devices fabricated on different batches of ITO, shown as a 5-95 whisker plot and a box plot of standard deviation. The □ indicates the mean value, and the × indicates the maximum or minimum value.

2. Dependence of Device Performance on Active Area:

Typical current density-voltage characteristics of devices with the following structure: 10 nm MoO_x/70 nm DTDCPB:C_{70} (1:2)/10 nm BCP/100 nm Al, and an active area of 0.785 mm^2 and 9 mm^2 are plotted in Figure 3. Device operating parameters extracted from the plot are listed in Table 2, containing both the measured and spectral mismatch corrected J_{SC} and efficiency. The large-area device shows lower V_{OC} and J_{SC} but a higher FF, overall the efficiency stays roughly the same.

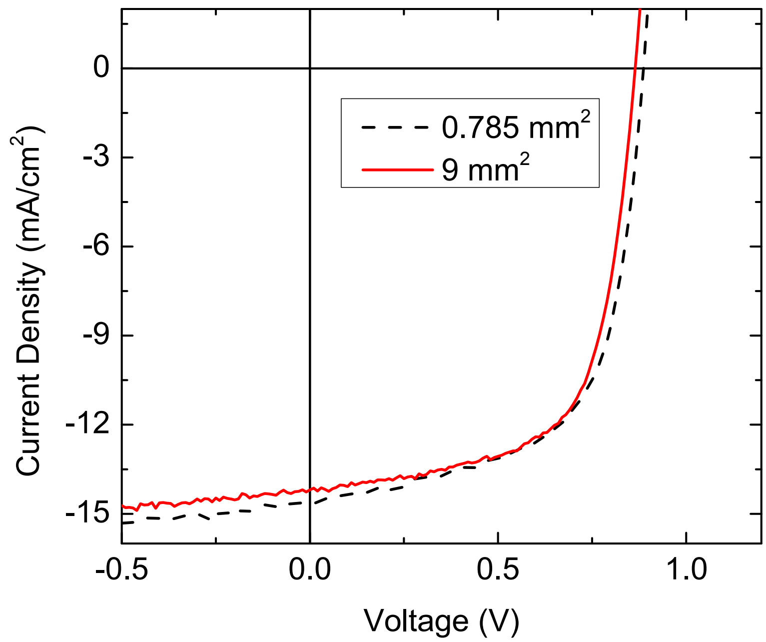

Figure 3: Comparison of device performance between large-area device and small-area device under simulated AM 1.5G illumination at 100 mW/cm^2.

Table 2: Operating parameters for devices with two different active areas

Device Area (mm^2)	**V_{OC} (V)**	**J_{SC} (mA/cm^2)**	**J_{SC} Corrected (mA/cm^2)**	**FF**	**Efficiency (%)**	**Efficiency Corrected (%)**
0.785	0.89	14.6	14.8	0.62	8.0	8.2
9	0.86	14.2	14.4	0.65	7.9	8.1

3. MoO_x film characterization:

A 10-nm-thick MoO_x film was deposited on Silicon wafer at a rate of 0.05 nm/s and a base pressure of $<8\times10^{-7}$ Torr via thermal evaporation. The MoO_x film contains mostly Mo^{6+} as measured by X-ray photoelectron spectroscopy, as shown in Figure 4.

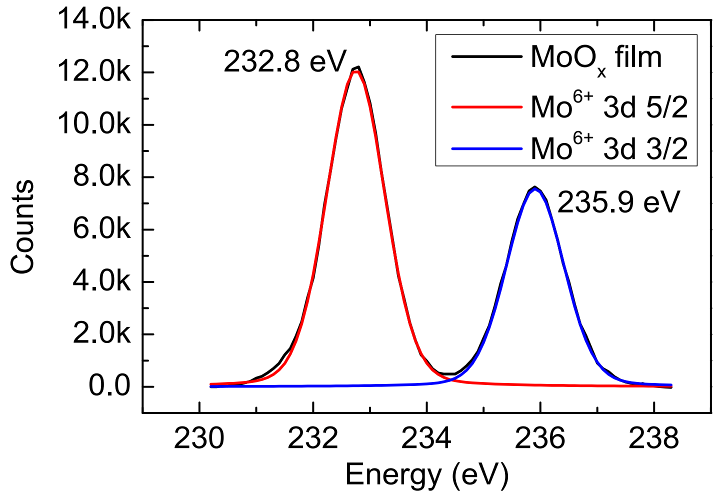

Figure 4: XPS spectrum of MoO_x deposited via thermal evaporation method.

References:

1. B. P. Rand, D. P. Burk and S. R. Forrest, *Phys Rev B*, 2007, **75**, 115327.