Supporting Information

High Efficiency BODIPY Based Organic Photovoltaics

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Optical Field Modeling

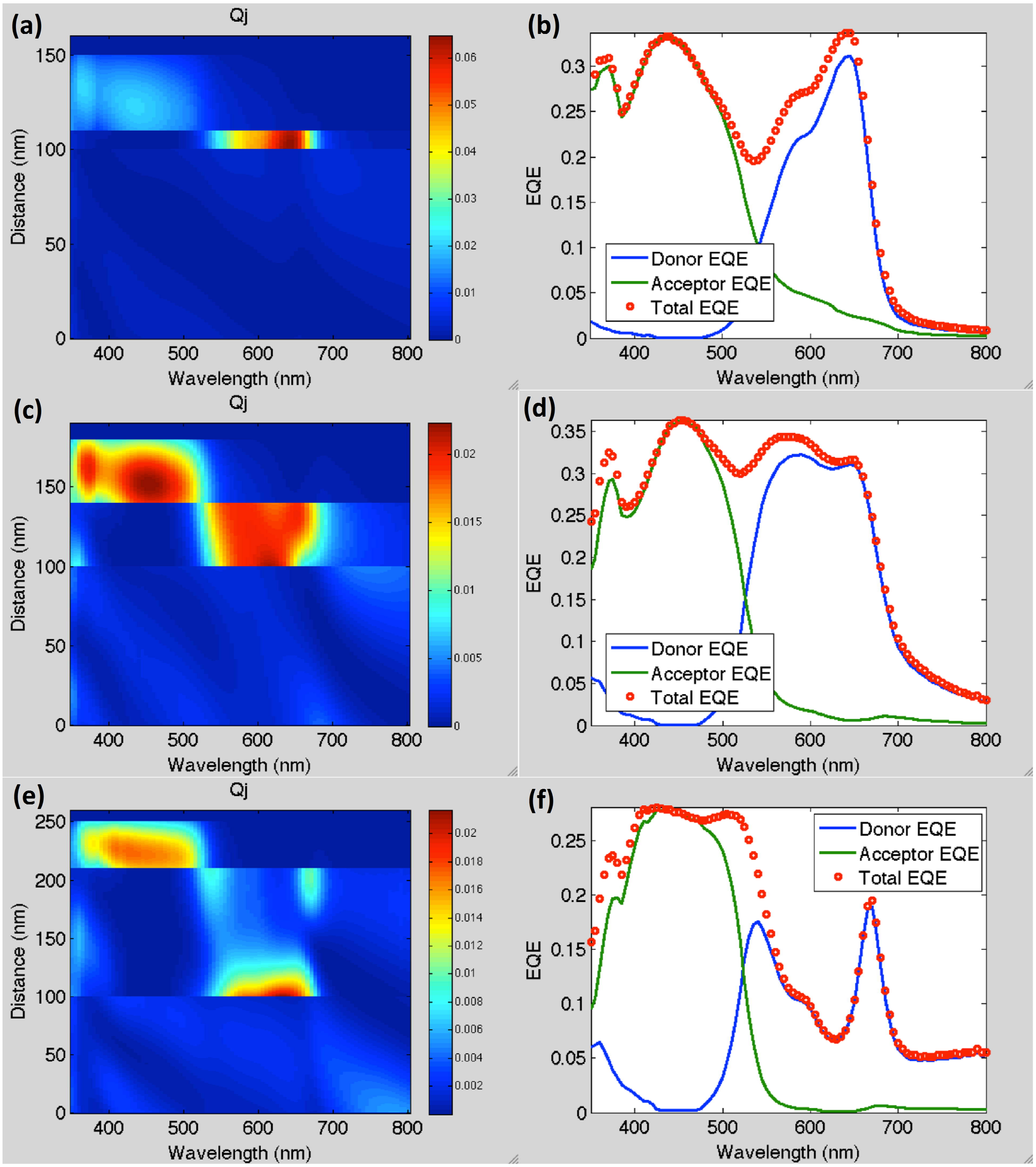

Figure S1. Representative absorbed power, Q_j, from modeled optical field of device stack ITO (100 nm)/bDIP (*X* nm)/C_{60} (40 nm)/BCP (10 nm)/Al for bDIP thickness *X* = (a) 10 nm, (c) 40 nm, and (e) 110 nm. Distance of 0 nm on y-axis is taken as the ITO/glass interface. Modeled EQE spectra of analogous devices with bDIP thickness *X* = (b) 10 nm, (d) 40 nm, and (f) 110 nm. The individual contributions are shown from bDIP (donor-blue), C_{60} (acceptor-green), and combined response (total-red).

Optical field modeling for devices with varying bDIP thicknesses were performed with MATLAB software using transfer-matrix formalism reported in literature.[1-2] Representative samples are shown in Fig. S1. The modeled stacks have the structure: glass/ITO(100 nm)/bDIP (*X* nm)/C_{60} (40 nm)/BCP (10 nm)/Al, where X = 10 – 110 nm. Distance of 0 nm on y-axis is the glass/ITO interface and the maximum value is the BCP/Al interface. For thinner bDIP thicknesses shown in Fig. S1a and Fig. S1c , there are strong absorptions for photons between 550 and 700 nm. This correlates well with their corresponding EQE spectra in Fig. S1b and Fig. S1d, showing clear bDIP donor response from where it absorbs strongly. However, at higher bDIP thickness of 110 nm in Fig. S1e, there is a significant reduction in absorption for the majority of the bDIP film, resulting in a loss of bDIP photoresponse between 550 and 700 nm in the EQE, Fig. S1f. While the EQE spectra for the thinner devices match well with experimental results shown in Fig. 3d, there is clearly no loss in bDIP response for the 110 nm device experimentally. Thus, the optical interference effect on the modeled bDIP response does not present a good explanation for the experimental increase in J_{SC}.

Neutron Reflectivity Measurements

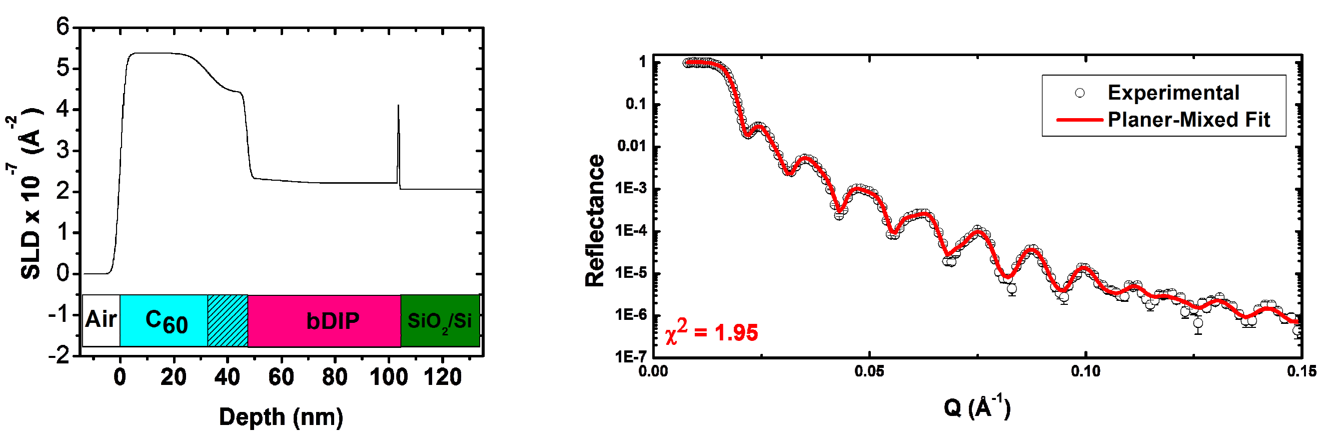

Figure S2. The three layer model film stack's SLD versus depth profile is shown (left). In this plot the air/C_{60} interface is taken as 0. The NR reflectance (black squares), with error bars, of the film stack: C_{60} (40 nm)/bDIP (60 nm)/SiO_2/Si is shown here (right). Overlaid on the data is the simulated reflectance spectrum and its χ^2 value of the intermixed three layer model (red). Despite the different thicknesses of bDIP and C_{60}, the thickness of intermixed layer remains relatively constant.

Layer	SLD (Å-2)	Thickness (nm)	Roughness (nm)
C_{60}	5.39×10^{-6}	33	3.9
Mixed Layer	4.41×10^{-6}	14	12
BDIP	2.23×10^{-6}	56	1.7
SiO_2	3.48×10^{-6}	0.5	0.3
Si	2.07×10^{-6}	∞	0.3

Table S1. Modeled SLD, thicknesses, and roughness of each component layer for a stack including a mixed C_{60}:bDIP layer as shown in Figure S1.

References

1. Pettersson, L. A. A.; Roman, L. S.; Inganas, O., Modeling Photocurrent Action Spectra of Photovoltaic Devices Based on Organic Thin Films. *J. Appl. Phys.* **1999,** *86*, 487-496.

2. Peumans, P.; Yakimov, A.; Forrest, S. R., Small Molecular Weight Organic Thin-Film Photodetectors and Solar Cells. *J. Appl. Phys.* **2003,** *93*, 3693-3723.