Electronic Supplementary Material (ESI) for Energy & Environmental Science

Supporting Information

Modeling Geminate Pair Dissociation in Organic Solar Cells: High Power Conversion Efficiencies Achieved with Moderate Optical Bandgaps

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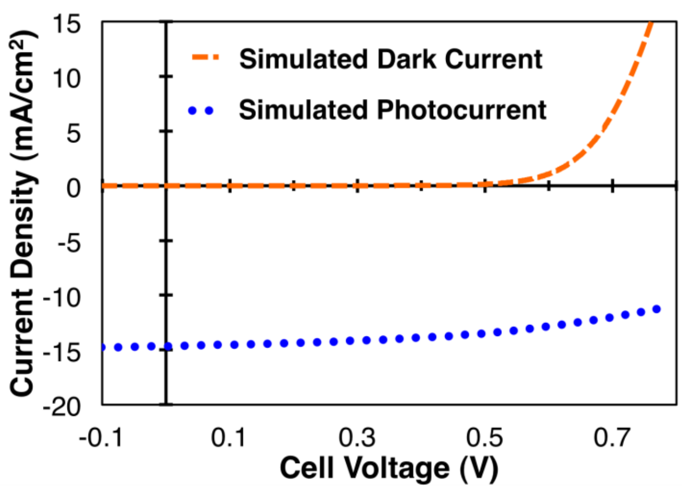

Figure SI1. Simulated Photocurrent and Dark Current. The photocurrent and dark current are calculated with the same parameters as Fig. 2 described in the main text. The net current is obtained by summing the dark and photocurrents.

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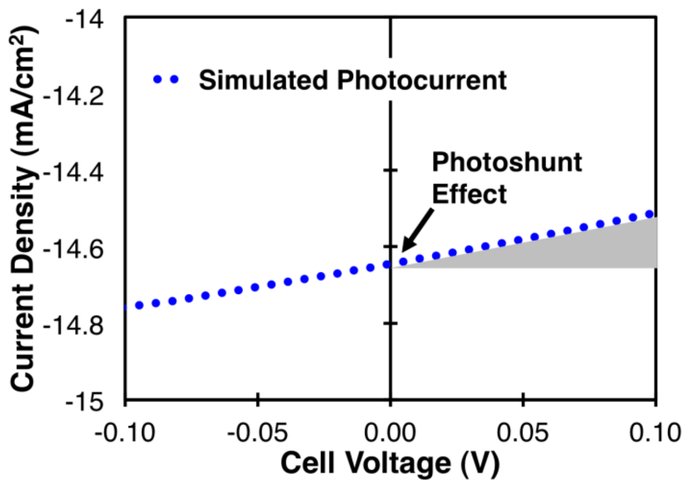

Figure SI2. Apparent Shunt Resistance. This figure shows the same photocurrent plotted in Fig. SI1, where the scale has been adjusted to highlight the apparent shunt effect. We note that this is effect arises from the field dependence of exciton dissociation described by our model, and should not be confused with the traditional diode sources of shunt resistance, such as pinholes.

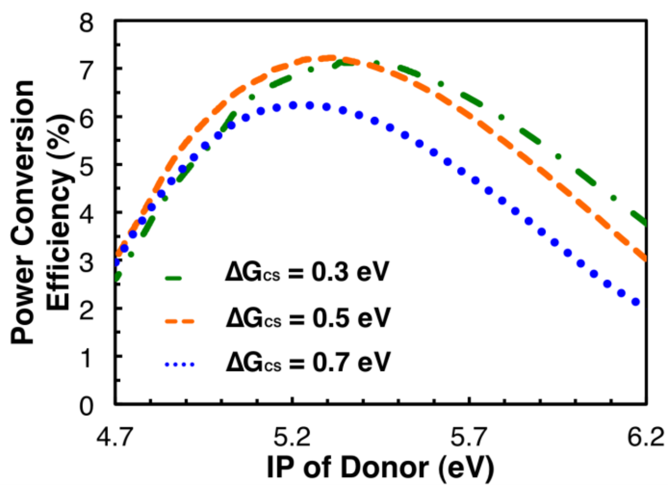

Figure SI3. Dependence of PCE on the IP of the Donor. PCE is calculated here assuming a constant ΔG_{CS} as indicated for each curve and an electron affinity of 4.0 eV for PCBM. Increasing IP yields an increased device voltage that benefits efficiency until the apogee. Past the maximum, further increases in voltage are offset by incomplete light absorption (current losses). Decreasing ΔG_{CS} also increases possible efficiencies up to a point. Further voltage gains from lowering ΔG_{CS} below the optimum are offset by incomplete exciton dissociation.