Supplementary Information

Impact of defect states on capacitance voltage characteristics of space charge limited organic diodes, and determination of defect states

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Figures

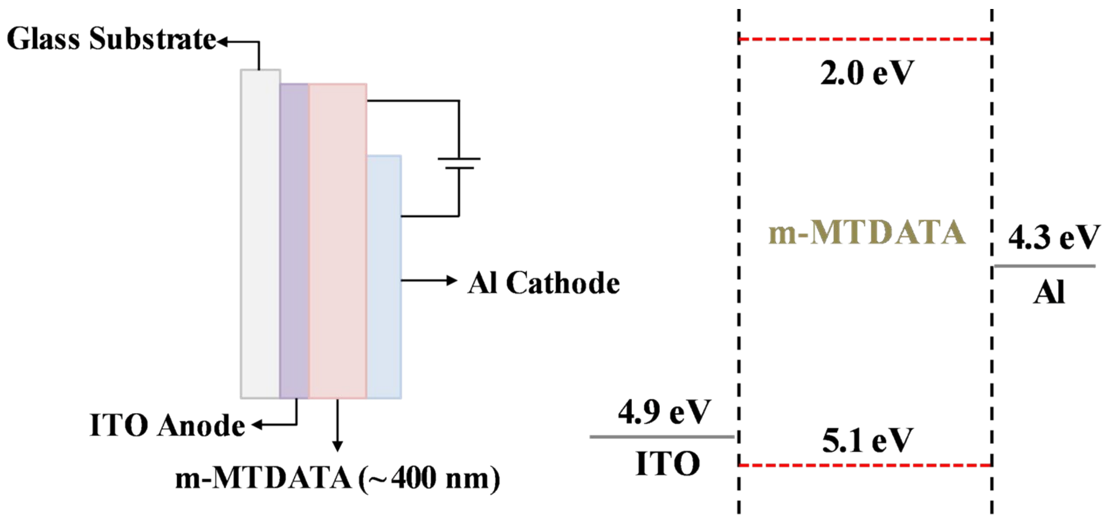

Figure S1: Schematic of (a) device structure and (b) corresponding energy level diagram.

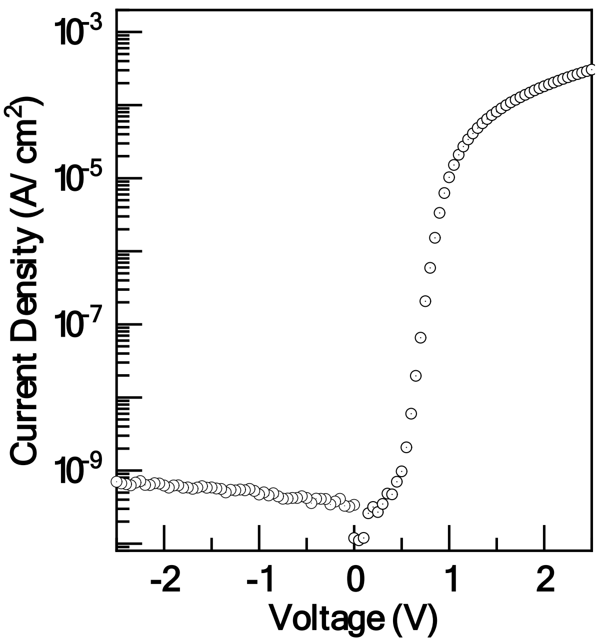

Figure S2: Experimental J-V characteristics of 400 nm thick m-MTDATA organic diodes. Note that the rectification ratio is observed more than five orders of magnitudes.

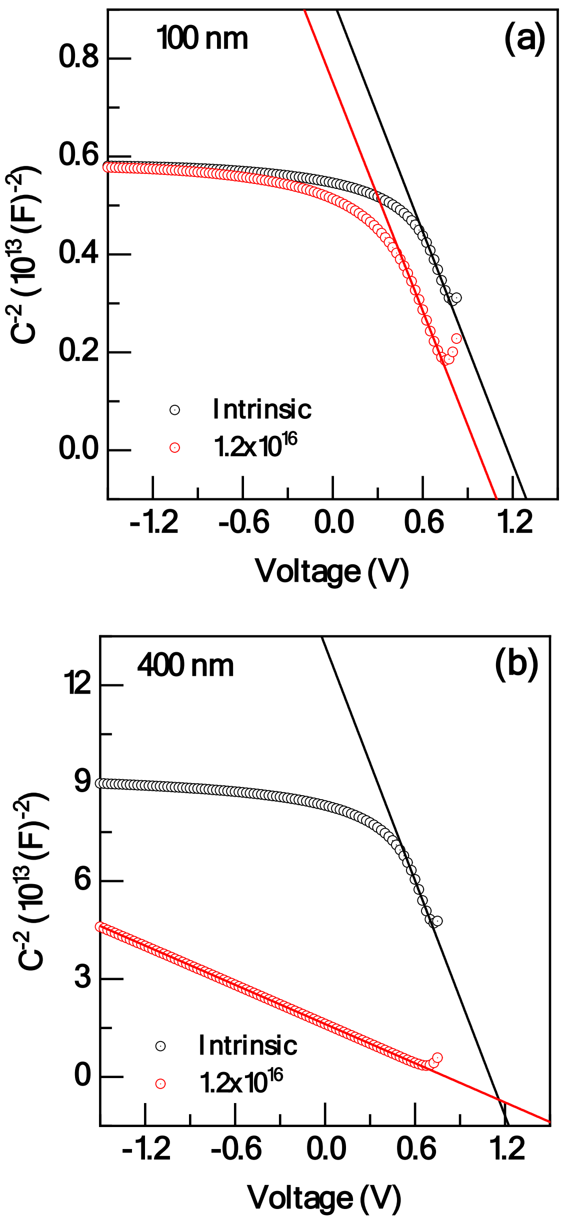

Figure S3: Mott-Schottky plots for simulated C-V characteristics considering two different defect densities with active layer thicknesses (a) 100 nm and (b) 400 nm. It should be noted that rise of capacitance is associated with diffusive carrier storage in the bulk region for thinner sample (100 nm) whereas voltage dependent depletion width variation for thicker sample particularly in presence of defect states. Indeed, a linear regime is observed for all cases. However, it remains very narrower in terms of voltage range and the slope value does not change even with introduction of defect states in the thinner devices. In contrary, the linear regime becomes wider and the slope value varies significantly corresponding to the defect density for thicker devices.

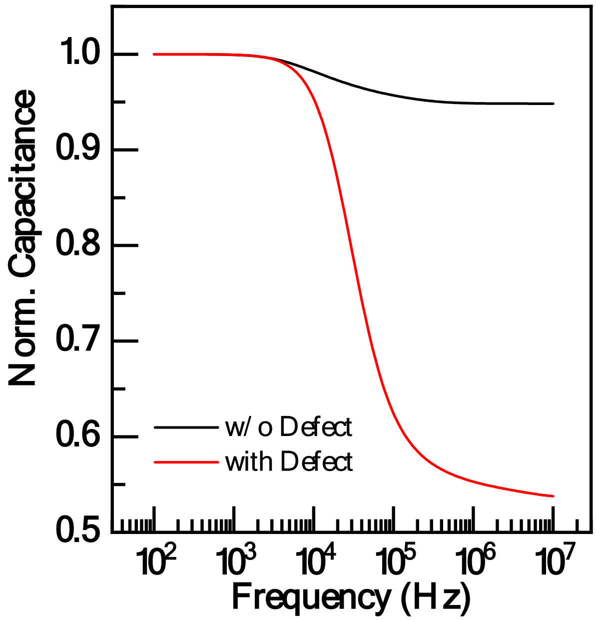

Figure S4: Simulated zero bias C-F characteristics with and without defect samples. The Gaussian shape of defect DOS is placed at 0.3eV above the valence band and the holes mobility is considered 2×10^{-4} $cm^2V^{-1}s^{-1}$ for both cases. Note that the curve is normalized with low frequency capacitance value. Indeed, the defect response is limited by the mobility.

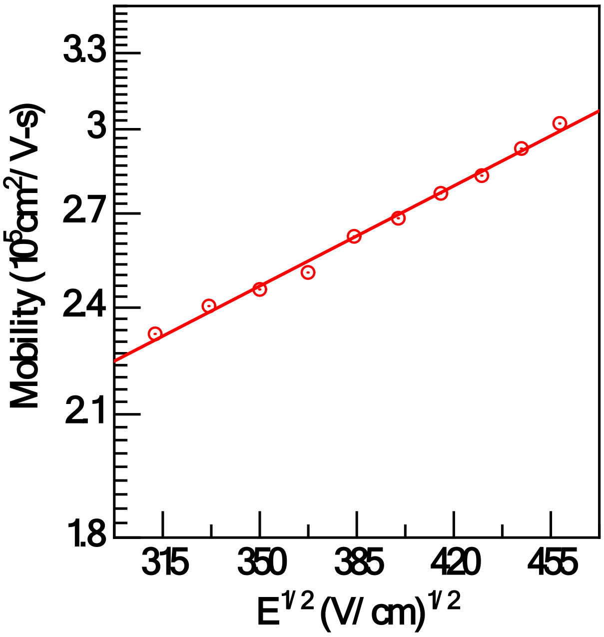

Figure S5: Poole-Frenkel (P-F) plot of mobility calculated from the frequency dependent imaginary part of impedance measurement [1] for m-MTDATA based SCL diode. The data fits excellently as a straight line. The y-axis intercept yields the zero-field mobility and the slope corresponds to the P-F coefficient which is found to be 1.32×10^{-5} $cm^2V^{-1}s^{-1}$ and 1.8×10^{-3} $cm^{1/2}V^{-1/2}$, respectively.

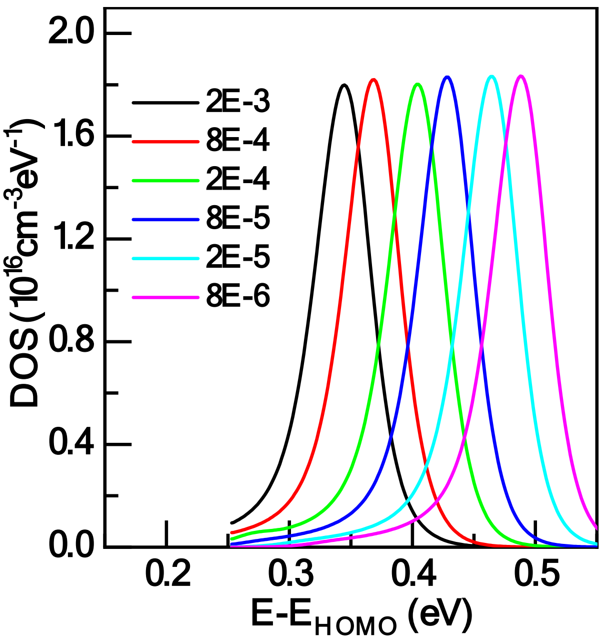

Figure S6: Defect DOS distributions extracted from the mobility dependent *C-f* curves given in Figure 4 assuming the value of ω_0 equal to 10^{12} s^{-1} [2,3]. Indeed, the defect density does not change with mobility variation, however the peak energy of defect DOS shifts towards the mid of energy gap with decrease of mobility value.

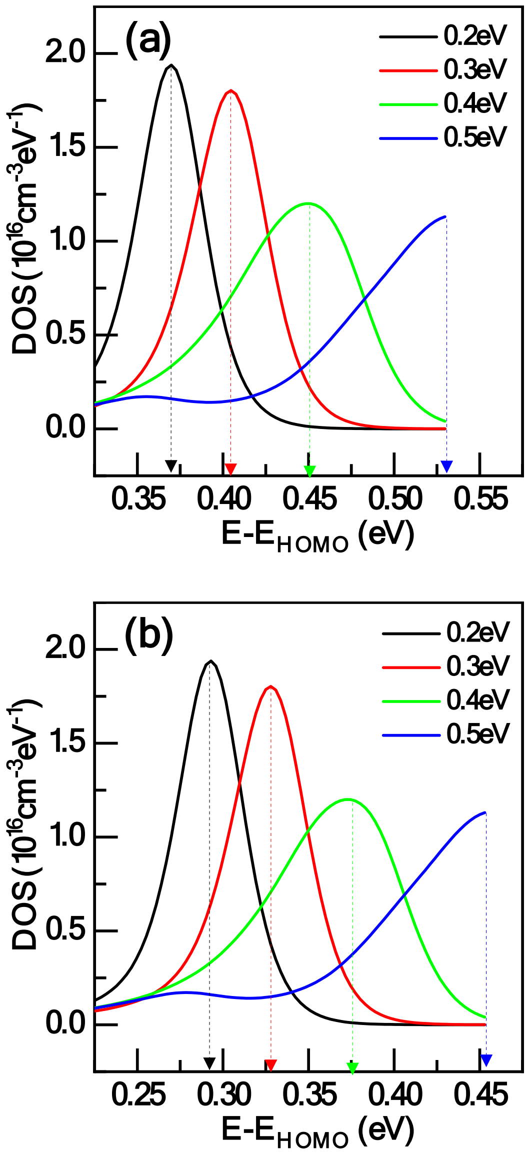

Figure S7: Defect DOS distributions extracted from the *C-f* curves obtained for varying Gaussian defect level between HOMO and midgap levels. Note that the value of ω_0 is assumed (a) mobility independent ($10^{12}s^{-1}$) and (b) mobility dependent. Indeed, the defect level very close to the input defect DOS when the value of ω_0 is considered mobility dependent.

References:

[1] D. C. Tripathi, A. K. Tripathi, and Y. N. Mohapatra, *Mobility Determination Using Frequency Dependence of Imaginary Part of Impedance (Im Z) for Organic and Polymeric Thin Films*, Appl. Phys. Lett. **98**, 1 (2011).

[2] P. P. Boix, G. Garcia-Belmonte, U. Muñecas, M. Neophytou, C. Waldauf, and R. Pacios, *Determination of Gap Defect States in Organic Bulk Heterojunction Solar Cells from Capacitance Measurements*, Appl. Phys. Lett. **95**, 233302 (2009).

[3] L. Xu, J. Wang, and J. W. P. Hsu, *Transport Effects on Capacitance-Frequency Analysis for Defect Characterization in Organic Photovoltaic Devices*, Phys. Rev. Appl. **6**, 1 (2016).