Supporting Information

Rational design of diketopyrrolopyrrole-based oligomers for high performance small molecular photovoltaic materials via extended framework and multiple fluorine substitution

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Experimental Section

SCLC device fabrication and characterization:
The structures of hole only and electron only device are ITO/PEDOT/donor materials: PC_{71}BM/MoO_{3}/Al and ITO/ZnO/PFN/ donor materials: PC_{71}BM/Ca/Al, respectively.
The mobility was determined by fitting the dark current to the model of the filed-independent space charge limited current (SCLC) according to the Mott-Gurney law,
given by \( J = \frac{9}{8} \varepsilon_0 \varepsilon_r \mu \frac{V^2}{L} \) for hole only device and \( J = \frac{9}{8} \varepsilon_0 \varepsilon_r \mu \frac{V^2}{L} \) for electron only device.

Where \( J \) is the current density, \( \varepsilon_0 \) is the permittivity of free space, \( \varepsilon_r \) is the relative permittivity of the material, \( \mu \) is the mobility, \( V \) is the applied voltage, and \( L \) is the thickness of the active layer.

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permittivity of the material, $\mu_h$ is the hole mobility, $\mu_e$ is the electron mobility, $L$ is the film thickness of the active layer, and $V$ is the effective voltage which is determined by subtracting the built-in voltage ($V_{bi}$) from the applied voltage ($V = V_{app} - V_{bi}$). The hole and electron mobility can be directly calculated from $J-V$ curves.

**Figure S1.** Current density-voltage ($J-V$) characteristics of devices based on DPPBIT4F blend with PC$_{71}$BM (different blend ratio and before/after solvent treatment).
**Figure S2.** Current density-voltage (J-V) characteristics of devices based on DPPBIT blend with PC_{71}BM (different blend ratio and before/after solvent treatment).

**Figure S3.** Absorption spectra of DPPBIT: PC_{71}BM (1:1, 1:2, and 1:3, w/w) blend films with or without CH$_2$Cl$_2$ vapor annealing.
Figure S4. EQE plots of devices based on DPPBIT4F blend with PC$_{71}$BM (1:1, 1:2, and 1:3, w/w) after CH$_2$Cl$_2$ vapor annealing.

Figure S5. The $J-V$ plots of the devices with a configuration of ITO/PEDOT/donor materials: PC$_{71}$BM/MoO$_3$/Al for hole only device (a) and ITO/ZnO/PFN/ donor materials: PC$_{71}$BM/Ca/Al for electron only device (b) before and after CH$_2$Cl$_2$ vapor annealing, respectively.
Copies of $^1$H and $^{13}$C NMR, and MALDI-TOF MS Spectra

$^1$H NMR spectrum for compound 4
$^{13}$C NMR spectrum for compound 4.
$^1$H NMR spectrum for compound 7
$^{13}$C NMR spectrum for compound 7.
$^1$H NMR spectrum for DPPBIT
$^{13}$C NMR spectrum for **DPPBIT**.
$^1$H NMR spectrum for DPPBIT4F
$^{13}$C NMR spectrum for DPPBIT4F.
MALDI-TOF mass spectrum of DPPBIT.
MALDI-TOF mass spectrum of **DPPBIT4F**.