Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Supporting Information

Influence of Fluorine Substituents on the Film Dielectric Constant and Open-circuit Voltage in Organic Photovoltaics

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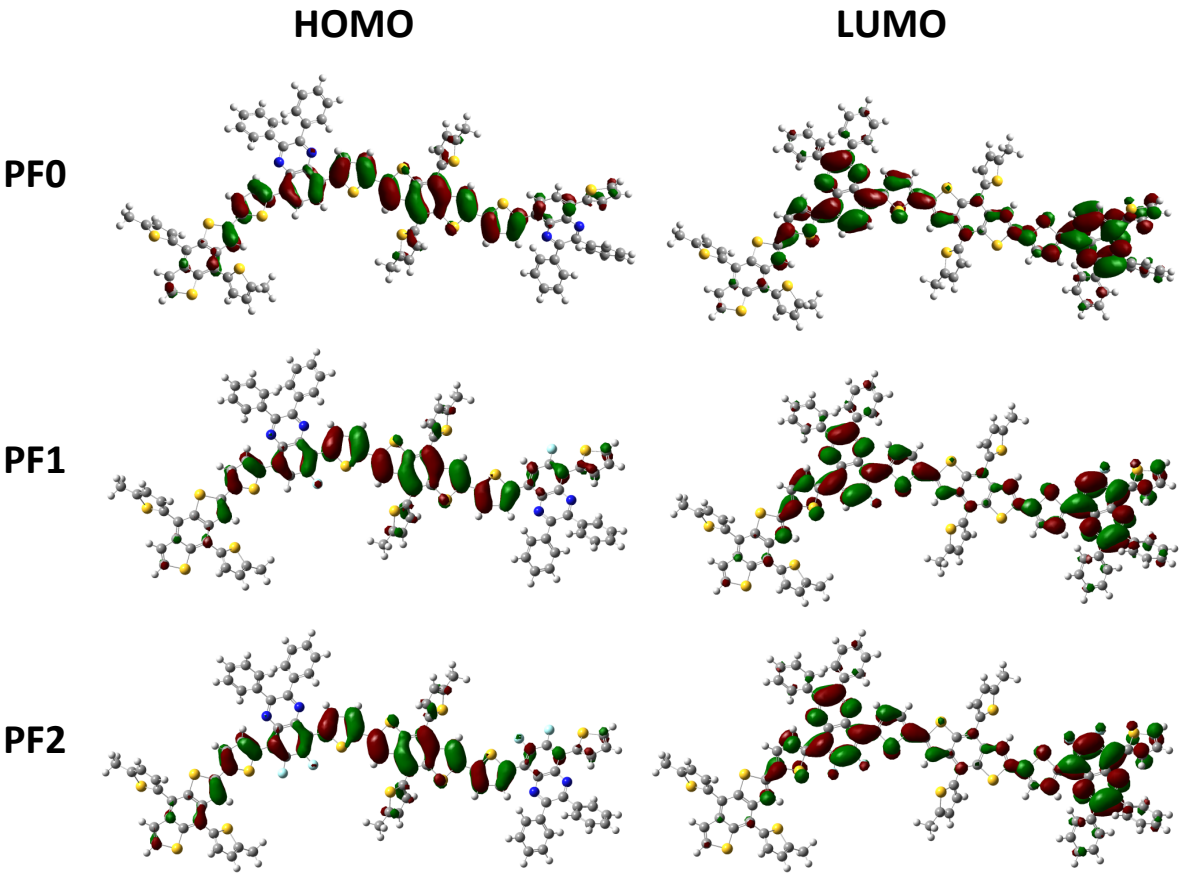

Figure S1 Optimized structures and calculated frontier orbitals for **P0F**, **P1F** and **P2F**.

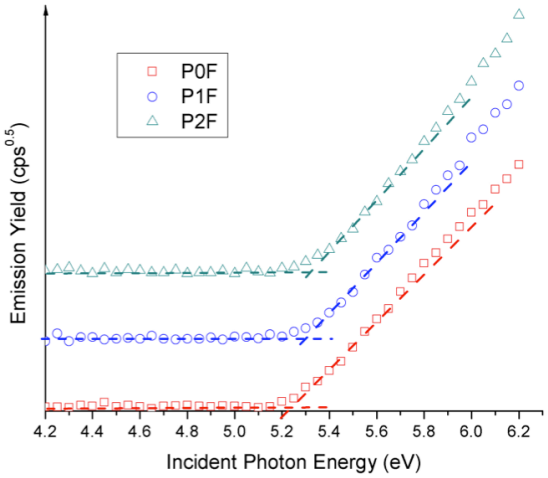

Figure S2 Photoelectron spectroscopy in air of **P0F**, **P1F** and **P2F** films (the dash lines were added to help visualize the curve onsets, $HOMO_{P0F}$=-5.23 eV, $HOMO_{P1F}$=-5.30 eV and $HOMO_{P2F}$=-5.31 eV).

Dark Current Density and Modified Shockley Equation Fitting

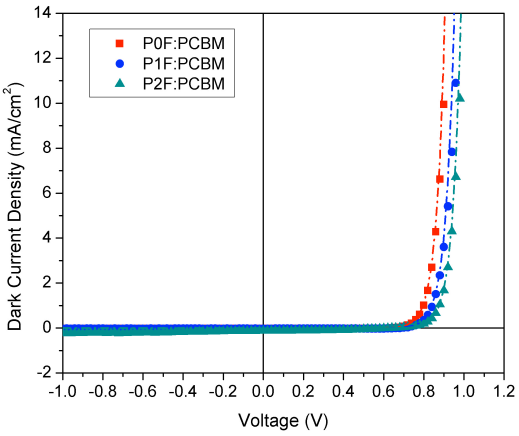

Figure S3 *J-V* characteristics of ITO/PEDOT:PSS/polymer:$PC_{61}BM$/Ca/Al under dark (Scatter) and simulation (Dot dash line) fitted according to the modified Shockley equation.

The ideality factor (n) and reverse saturation current density (J_0) were obtained by fitting the *J-V* characteristics of each device under dark with the modified Shockley equation:[1,2]

$$J_{dark}(V) = J_0\left\{\exp\left[\frac{e(V - J_{dark}(V)r_s}{nk_BT}\right] - 1\right\} \quad (1)$$

where J_{dark} is the dark current density, J_0 is the reverse-bias saturation current density, e the elemental electron charge, $r_s = R_s$ • area of device the specific series resistance, n the ideality

factor, k_B is the Boltzmann's constant and T the temperature. Furthermore, with n and J_0 obtained from fitting, V_{oc} of each device can be determined by:[2,3]

$$V_{OC} = \frac{nk_BT}{e}\ln\left[\frac{-J_{ph}(V_{OC})}{J_0}+1\right] \approx \frac{nk_BT}{e}\ln\left(\frac{J_{SC}}{J_C}+1\right) \quad (2)$$

Table S1 below summarizes the fitting results of important parameters.

Table S1 Parameters of device obtained by fitting *J-V* characteristics under dark with modified Shockley equation

	J_0 (mA/cm^2)	n	J_{sc} (mA/cm^2)	R_{sh} (kΩ)	V_{oc} (V)	
					Simulated	measured
P0F:PCBM	3.74×10^{-13}	1.54	6.37	20±4	0.835	0.832
P1F:PCBM	2.30×10^{-13}	1.58	6.52	19±3	0.878	0.872
P2F:PCBM	4.03×10^{-14}	1.51	6.84	22±3	0.912	0.914

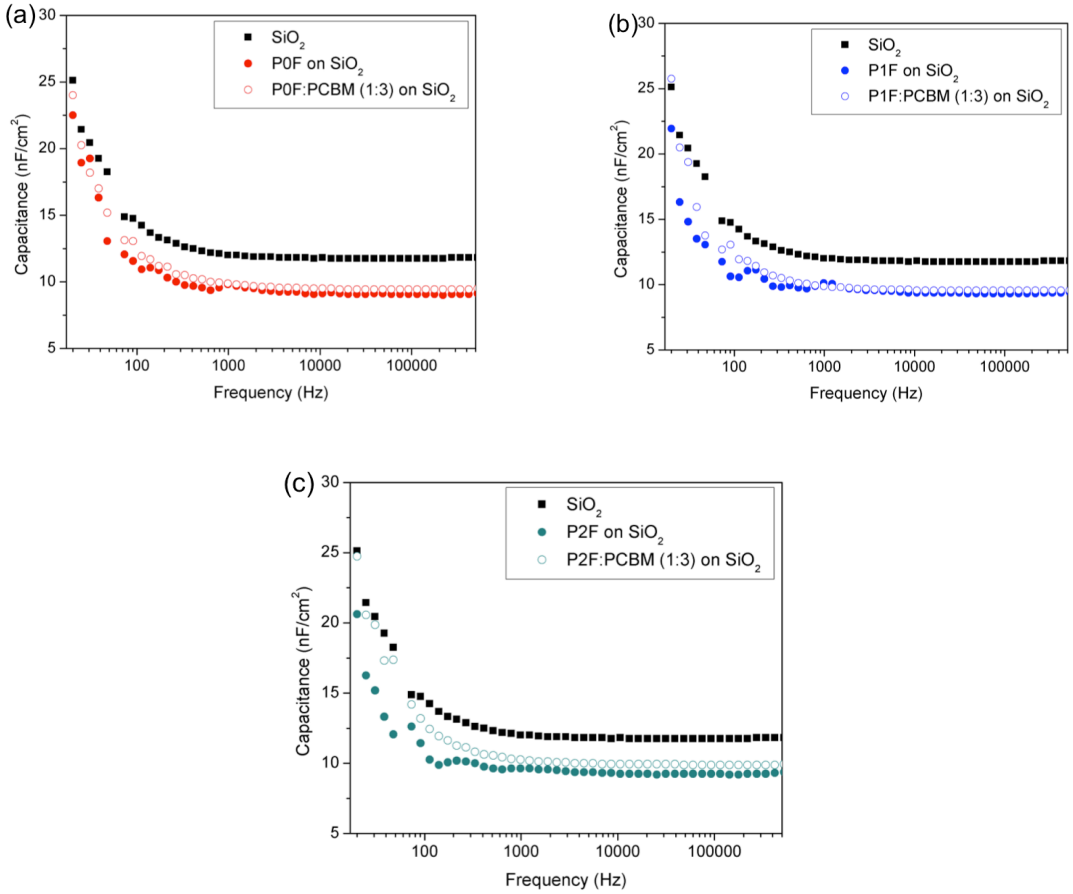

Figure S4 Capacitance measurement of (a) **P0F**, (b) **P1F** and (c) **P2F** pure and blends film on 300 nm SiO_2 layer.

Reference:

1. S. M. Sze and Ng, *Physics of semiconductor devices*, Wiley-Interscience, Hoboken, N.J., 2007.
2. J. Xue, S. Uchida, B. P. Rand, and S. R. Forrest, *Appl. Phys. Lett.*, 2004, **84**, 3013.
3. X. Tong, B. E. Lassiter, and S. R. Forrest, *Org. Electron.*, 2010, **11**, 705.