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Supporting Information

Influences of non-fullerene acceptor fluorination on three-dimensional morphology and photovoltaic properties of organic solar cells

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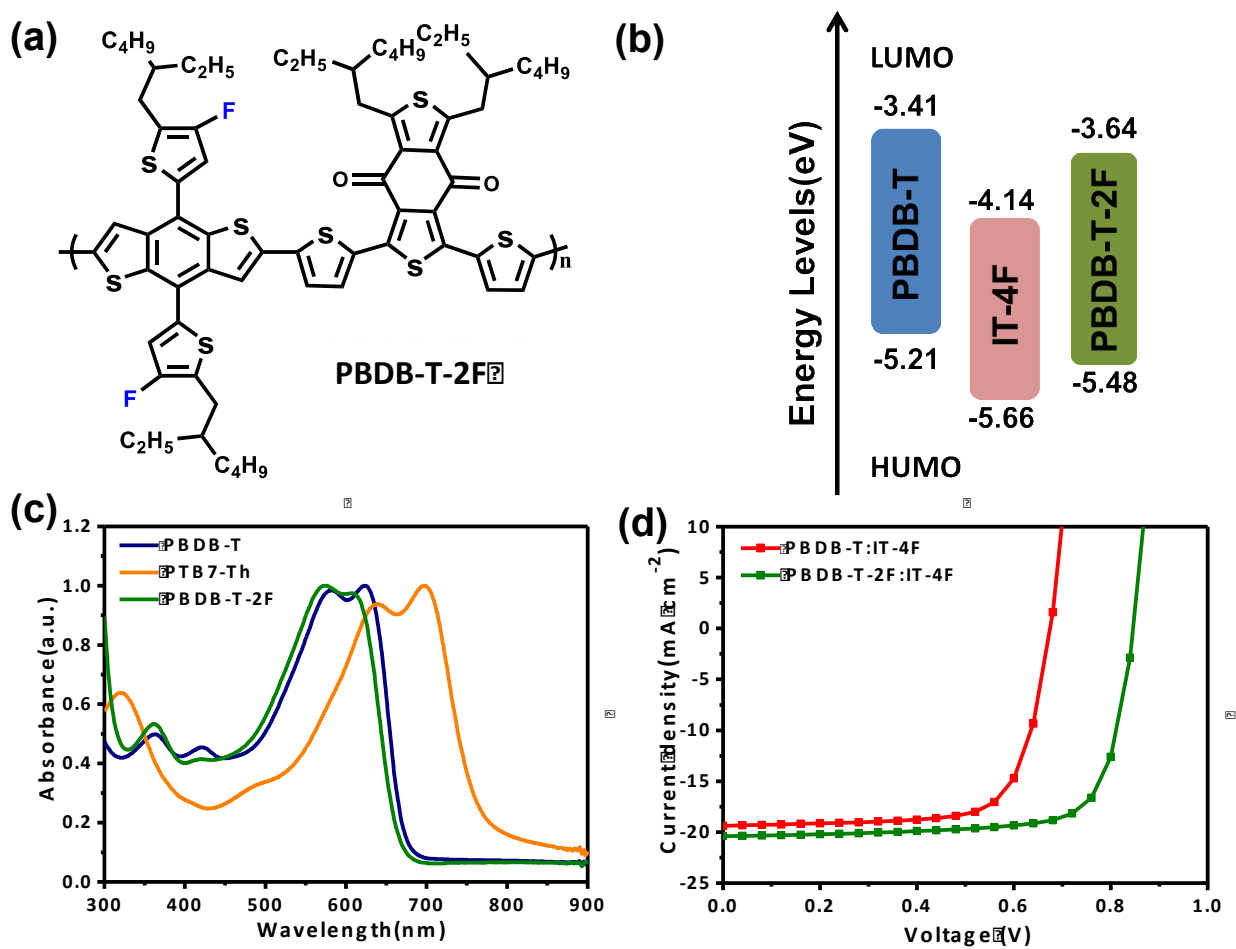


Figure S1 (a) Chemical structure of PBDB-T-2F. (b) Energy level diagram of donors (PBDB-T, PBDB-T-2F) and IT-4F. (c) Absorbance of donors (PBDB-T, PTB7-Th, PBDB-T-2F). (d) J-V characteristics of our best performing PBDB-T:IT-4F and PBDB-T-2F:IT-4F OSCs.

Table S1 Photovoltaic parameters of OSCs measured at an illumination of AM 1.5 G, 100 mW cm⁻². The statistical data were obtained from over 15 individual devices.

Donor:Acceptor	FF	J _{sc}	Calculated J _{sc}	V _{oc}	PCE _{max} (PCE _{avg})
	[%]	[mA cm ⁻²]	[mA cm ⁻²]	[V]	[%]
PBDB-T:IT-4F	73.1	19.4	18.3	0.67	9.6 (9.2±0.5)
PBDB-T-2F:IT-4F	75.1	20.3	20.9	0.85	13.1 (12.8±0.4)

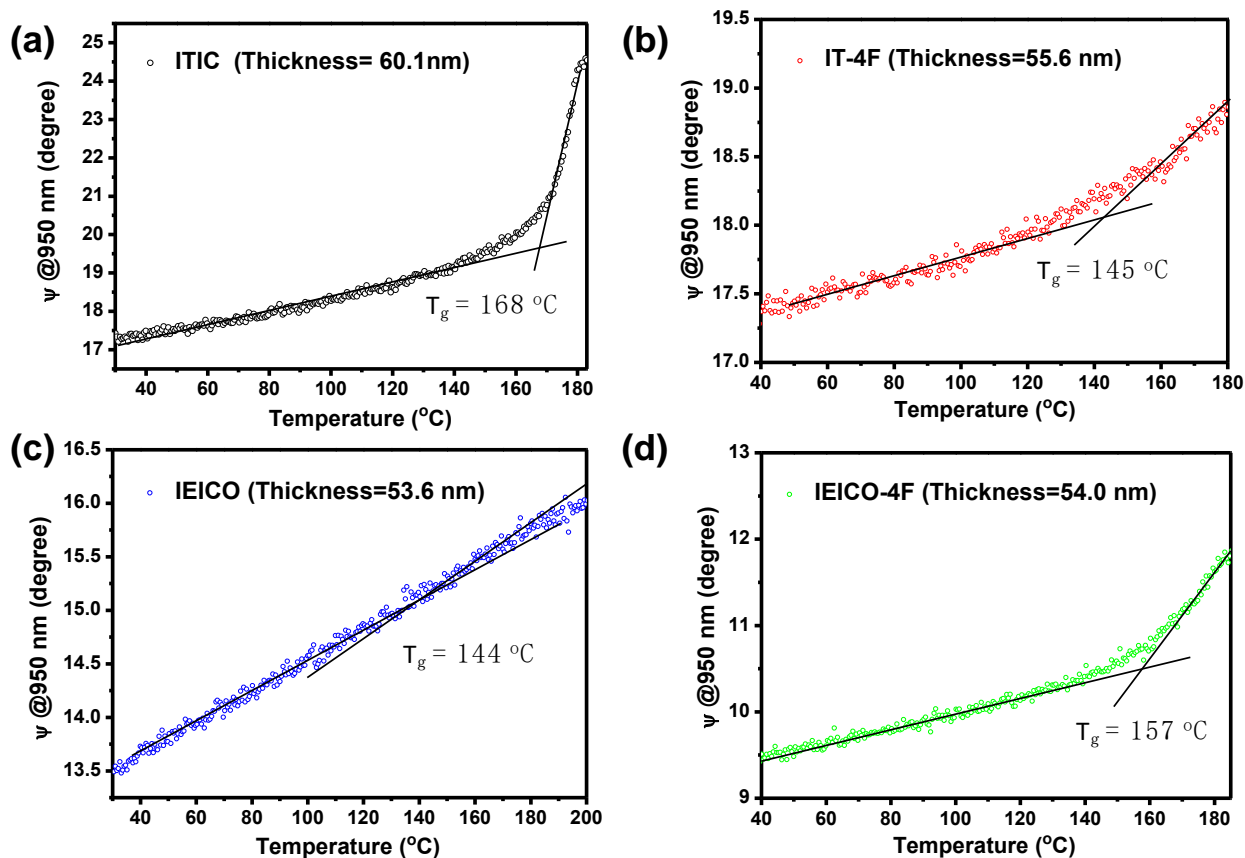
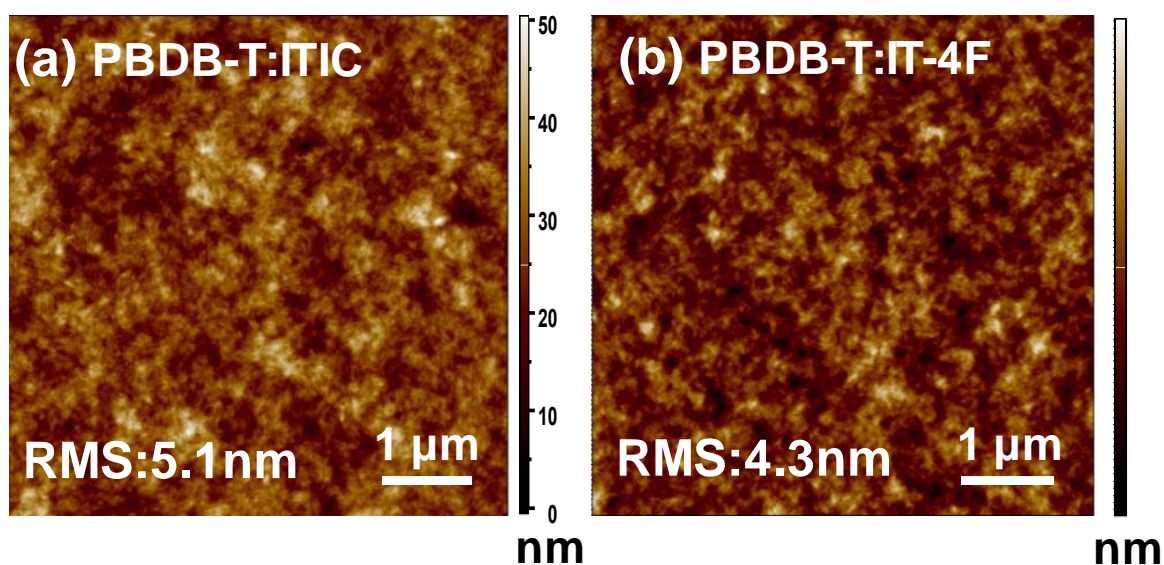


Figure S2 Ψ of (a) ITIC, (b) IT-4F, (c) IEICO, (d) IEICO-4F films as a function of temperature. The thickness of acceptor's films is fitted by the Cauchy model.



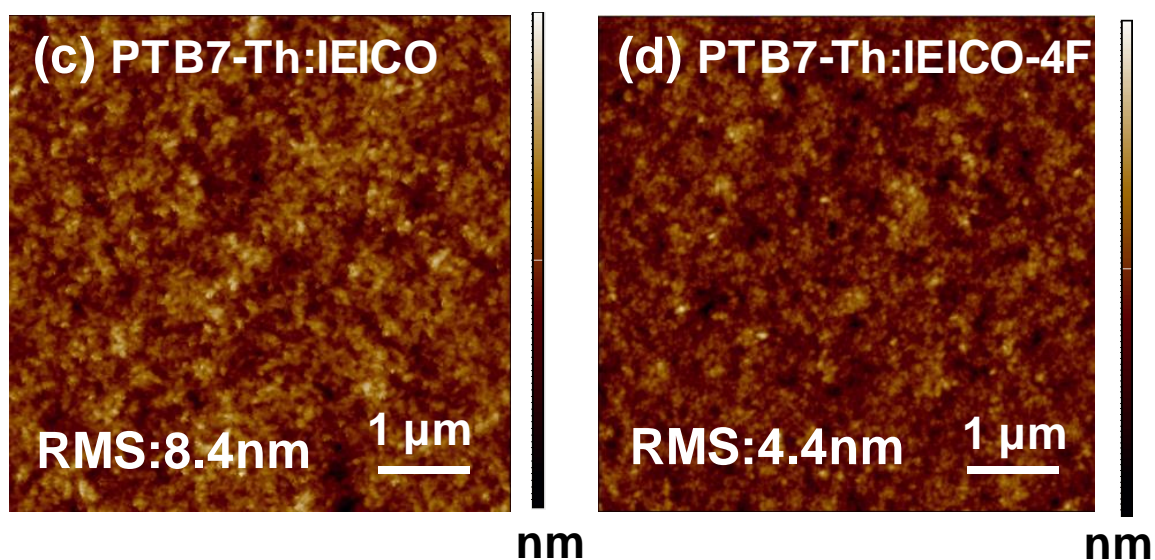


Figure S3 AFM height images (5 μm×5 μm) of (a) PBDB-T:ITIC, (b) PBDB-T:IT-4F, (c) PTB7-Th:IEICO and (d) PTB7-Th:IEICO-4F films.

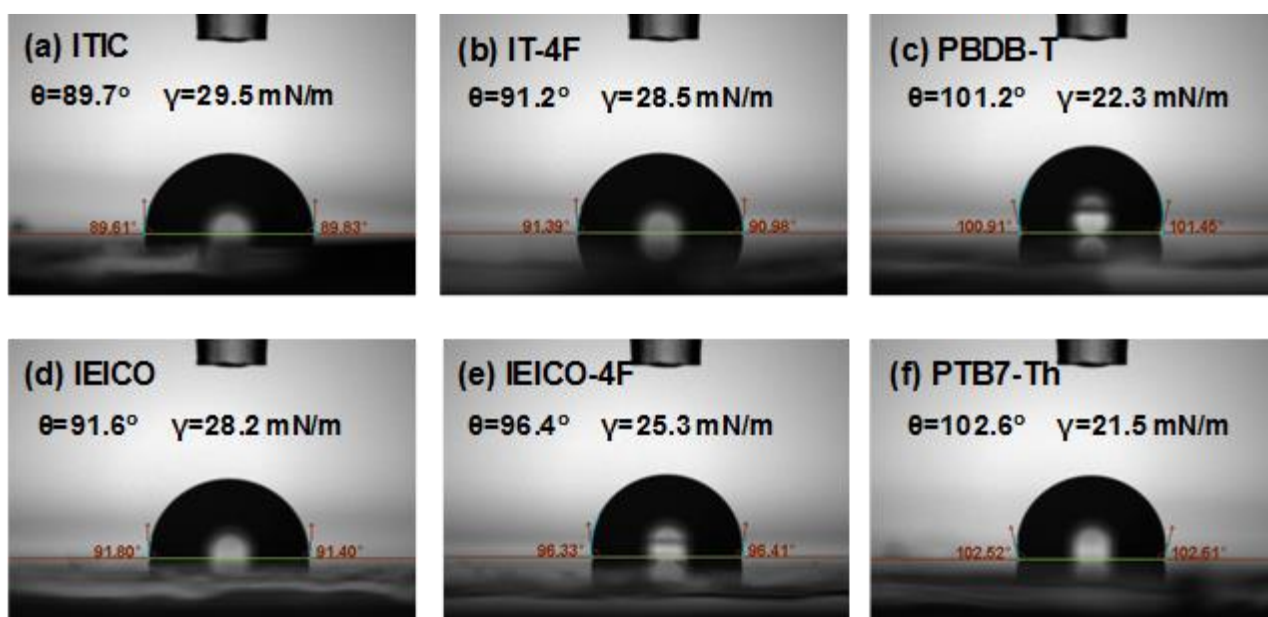


Figure S4 Water contact angles (θ) and surface energies (γ) of (a) ITIC, (b) IT-4F, (c) PBDB-T, (d) IEICO, (e) IEICO-4F and (f) PTB7-Th pure films.

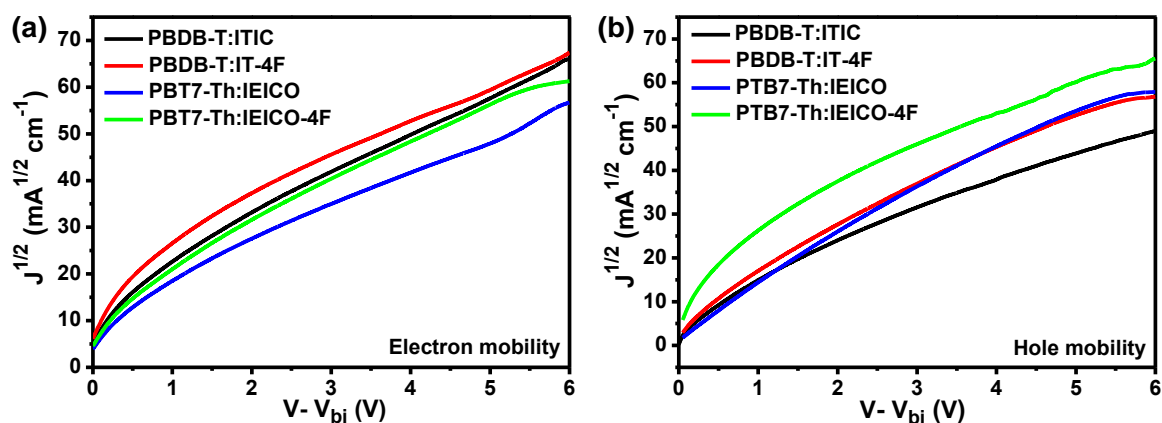


Figure S5 Root square plots of (a) electron densities versus voltage of the ITO/ZnO/Active layer/Ca/Ag electron-only devices and (b) hole densities versus voltage of the ITO/PEDOT:PSS/Active layer/MoO₃/Ag hole-only devices. A linear fit was applied in the voltage range from 0 to 6 V.

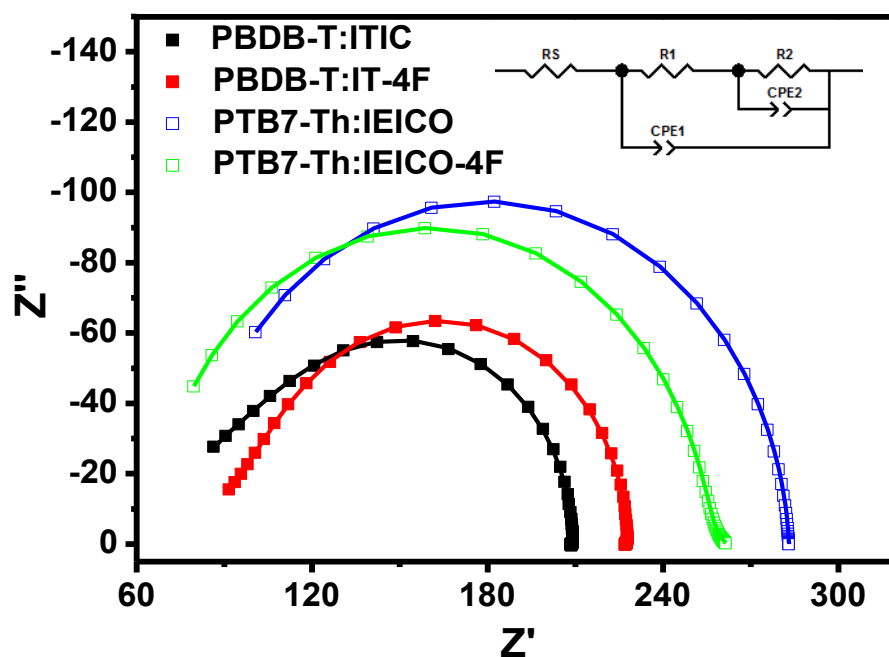


Figure S6 Nyquist plots of impedance spectra of various devices under 1 sun irradiation with an applied bias at V_{oc} .