Electronic Supplementary Information

Easily accessible conjugated pyrene sulfonates as cathode interfacial materials for polymer solar cells

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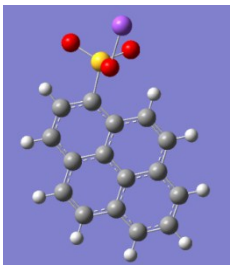
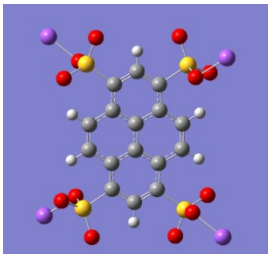
Table S1.The optimized geometry and the dipole moments obtained from DFT calculations of PyS and PyTS.

Chemical structure	Optimized geometry	Dipole moment (Debye)
PyS		4.8549
PyTS		0.0045

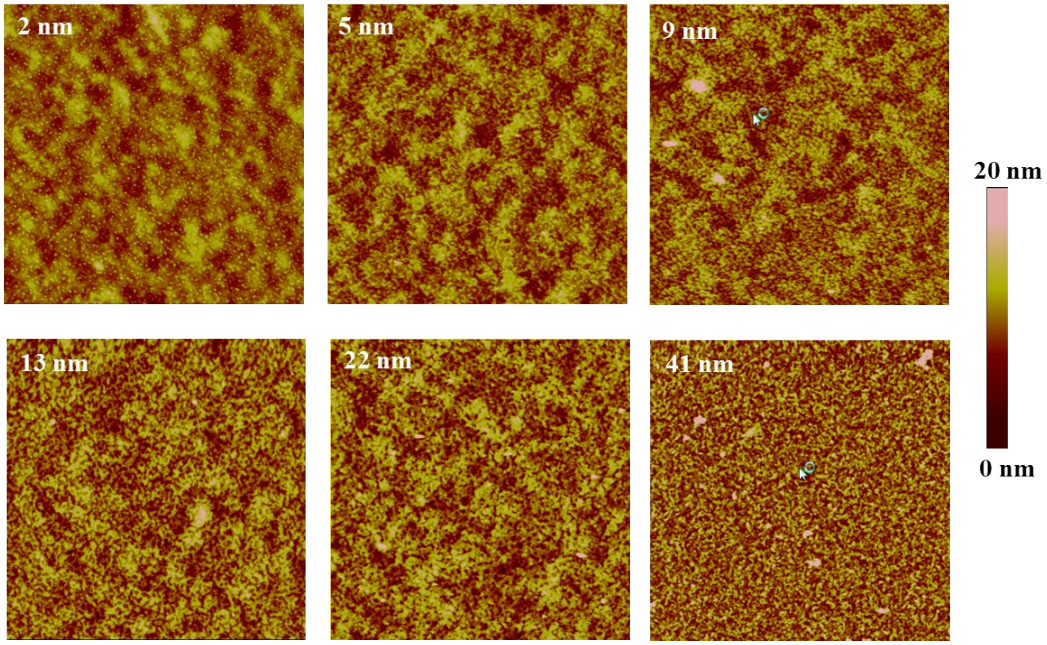


Figure S1: Surface topographic AFM images (5μm×5μm) of different thicknesses of PyS spin-coated on surface of PBDTTT-C:$PC_{71}BM$ blend films.

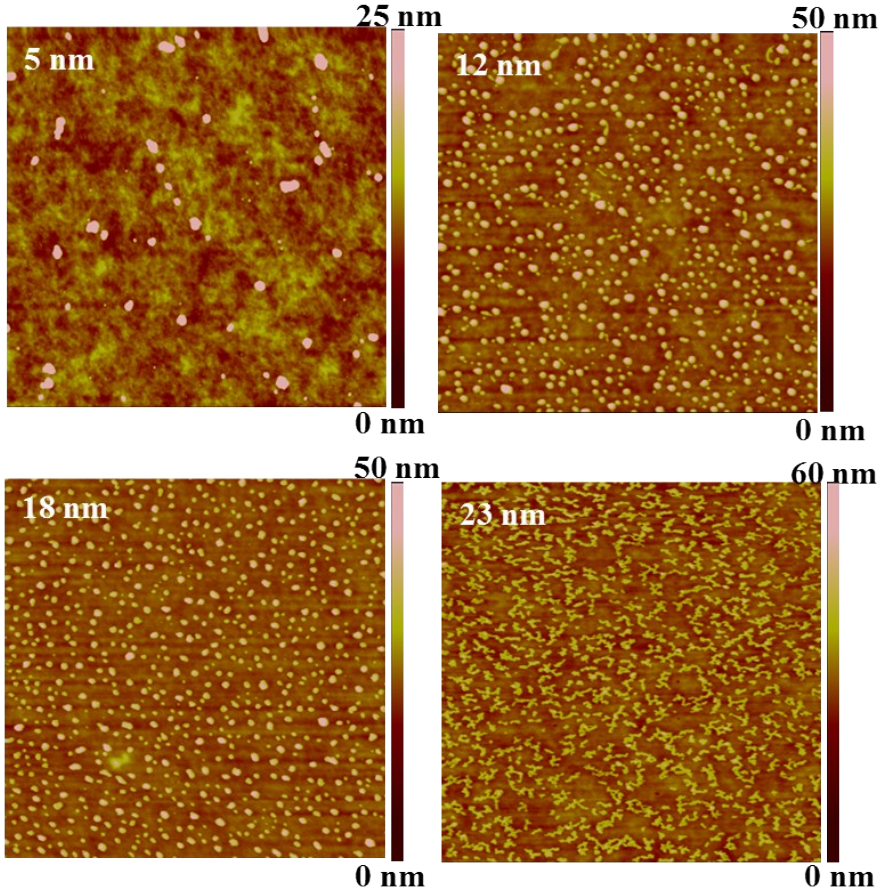


Figure S2: Surface topographic AFM images (5μm×5μm) of different thicknesses of PyTS spin-coated on surface of PBDTTT-C:$PC_{71}BM$ blend films.

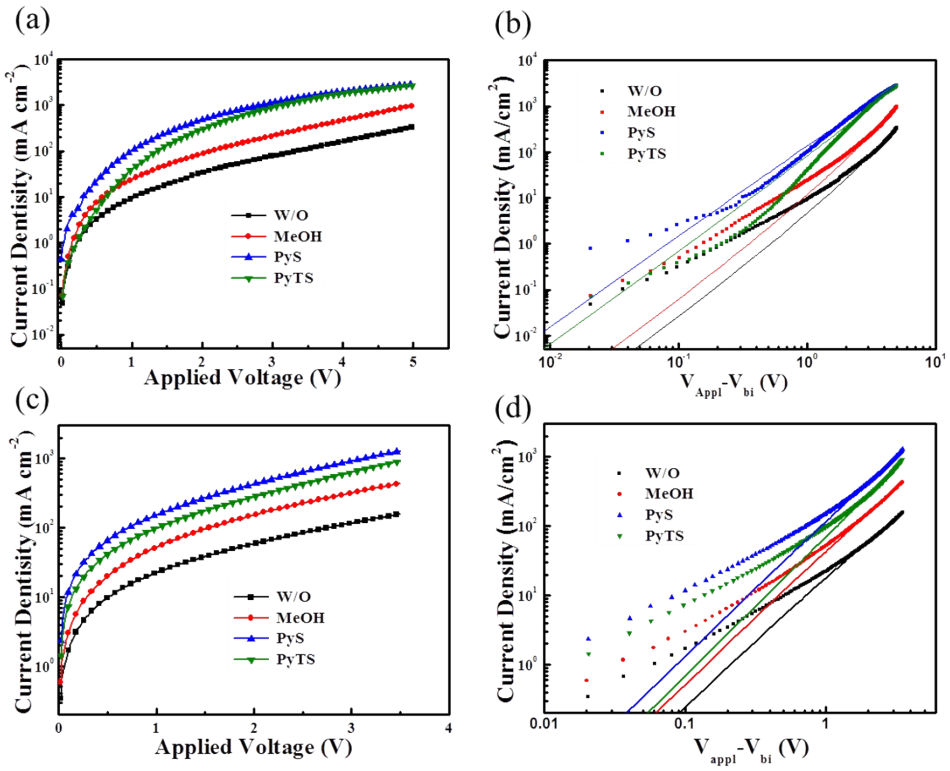


Figure S3. The experimental current density-applied voltage (J-V) curves of electron-only devices (a) and hole-only devices (c). Fitting results of electron-only devices (b) and hole-only devices (d) from Mott-Gurney law that includes field dependent mobility, given by $J = \frac{9}{8}\varepsilon_0\varepsilon_r \mu \frac{(V - V_{bi})^2}{L^3} \exp(\beta \sqrt{\frac{(V - V_{bi})}{L}})$.

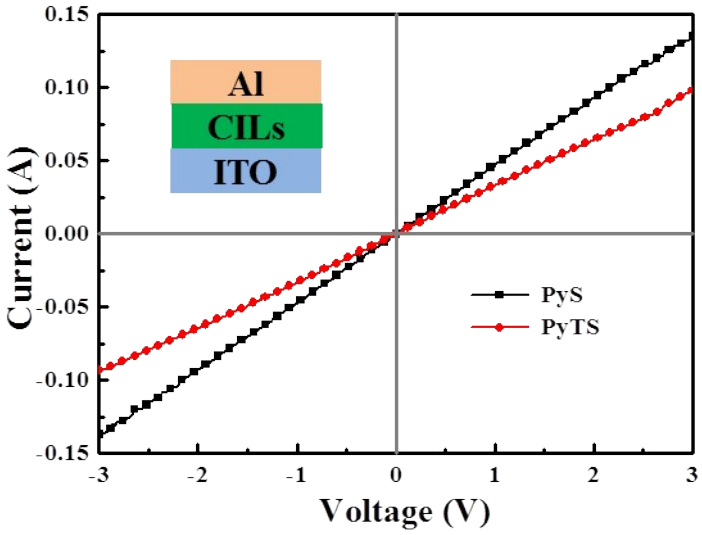


Figure S4. I–V curves of the conductivity measurements of PyS and PyTS with a configuration of ITO/CILs/Al. The thicknesses of the CILs are about 50 nm. The conductivities were calculated from Ohm's law at the linear regions.

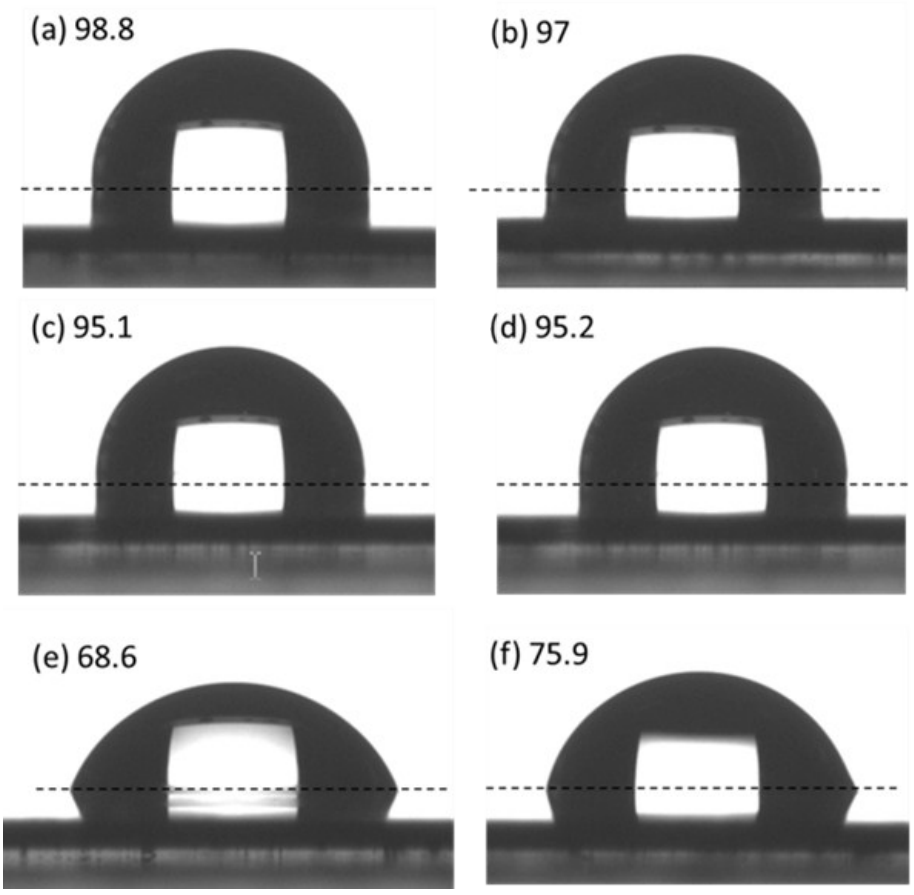


Figure S5. Photos of water droplets on the surfaces of (a) PBDTTT-C:$PC_{71}BM$ film, (b) PBDTTT-C:$PC_{71}BM$ film treated by methanol, a thin layer (5 nm) (c) and a thick layer (22 nm) (e) of PyS on PBDTTT-C:$PC_{71}BM$ film, a thin layer (12 nm) (d) and a thick layer (23 nm) (f) of PyTS on PBDTTT-C:$PC_{71}BM$ film.

As shown in Fig. S5, PBDTTT-C:$PC_{71}BM$ films before and after methanol treatment are highly hydrophobic. When a thin layer of PyS or PyTS was spin coated on the PBDTTT-C:$PC_{71}BM$ film, the surface becomes slightly hydrophilic. For a thick layer of PyS or PyTS on the active layer, the surface becomes hydrophilic.