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苝二酰亚胺：有机膦盐基双组份共混电子传输层及其开路电压接近 1.0 V 的非富勒烯聚合物太阳电池

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Perylenediimide: Phosphonium-Based Binary Blended Small-Molecule Cathode Interlayer for Efficient Fullerene-Free Polymer Solar Cells with Open Circuit Voltage to 1.0 V

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Materials and Instruments: All reagents were purchased from Sigma-Aldrich, Acros, Alfa Aesar or TCI, unless specified and used as received. The polymer PBDBT, and IDTBR were purchased from One Material. PDINO bought from LumTec Company (Taiwan) and QPPBr purchased from Acros. PEDOT:PSS (Baytron Clevios P VP AI 4083, Germany) was obtained from Heraeus Group. Ultraviolet photoelectron spectroscopy (UPS) experiments were performed on a Thermo Scientific ESCALab 250Xi spectrometer. The gas discharge lamp was used for UPS, with helium gas admitted and the He I (21.22 eV) emission line employed. The helium pressure in the analysis chamber during analysis was about 2×10^{-8} mbar. The data were acquired with −10 V bias. Absorption spectra were measured on a Hitachi U-3010 UV-Vis spectrophotometer and carried out at room temperature. The thickness of the solid films was measured using a Dektak Profilometer.

Sample preparations and characterizations: Film samples for measurements of absorption PBDBT, IDTBR, PDINO and QPhPBr were prepared atop of the silica substrate via the spin-coating method. For the experiments of UPS of the electron transporting layers (ETLs), the ETL was spin-coated atop the clear Al surface. The HOMO level of QPhPBr was determined using ultraviolet photoelectron spectroscopy (UPS) with the incident photon energy, $h\nu = 21.22$ eV. The HOMO energy is calculated with the equation $E_{\mathrm{HOMO}} = E_{\mathrm{cutoff}} - E_{\mathrm{onset}} - \mathrm{h}\nu$, E_{cutoff}, and the E_{onset} are got from the UPS data.

Table S1 Summarize device performance of PBDBT:IDTBR baesd OSCs with different weight ratios of binary mixture of PDINO:QPhPBr ETL.

ETL	V_{oc}/V	J_{sc}/(mA·cm^{-2})	FF/%	PCE/%
1:1	0.94	11.88	56.78	6.34
1:1.8	0.98	13.45	62.45	8.27
1:2	0.96	11.72	58.47	6.57
1:3	0.93	11.79	55.95	6.13

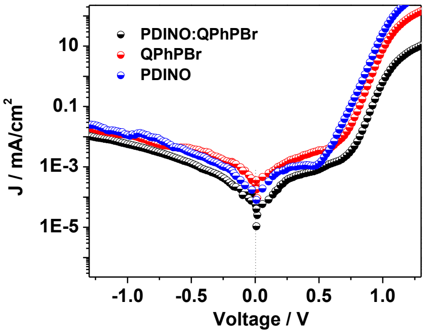

Fig. S1 ***J*–*V*** **Characteristics of PBDBT:IDTBR based device with different ETLs measured under dark conditions.**

Measurements of electron mobility by the space-charge limited current (SCLC) method: The electron-only devices were fabricated with a configuration of ITO/titanium (diisopropoxide) bis(2,4-pentanedionate) (TIPD)/blend/ETL/Al. The TIPD buffer layer was prepared by spin-coating a 3.5% (mass fraction) TIPD isopropanol solution onto the pre-cleaned ITO substrate and then baked at 150 °C for 10 min to convert TIPD into TOPD. [S1] Subsequently, the blend was spin-coated on it under the same condition as preparation of the optimal solar cell. The Al layer was thermally deposited on the top of the blend in vacuum. The Al layer was deposited at a speed of 0.1 nm·s^{-1}. The electron mobility was extracted by fitting the current density–voltage curves using the Mott-Gurney law, [S2, S3] Equation (1) $J_{\mathrm{SCL}} = 9\varepsilon\varepsilon_0\mu V^2/(8L^3)$ (1) where ε is the dielectric constant of the organic component, ε_0 is the permittivity of the vacuum (8.85419×10^{-12} F^{-1}m^{-1}), μ is the zero-field mobility, J is the current density, L is the thickness of the active layer, and $V = V_{\mathrm{app}} - V_{\mathrm{bi}}$, here V_{app} is the applied potential, and V_{bi} the built-in potential which results from the difference in the work function values of the cathode (in the electron-only device, $V_{\mathrm{bi}} = 0.4$ V). The electron mobility of the solar cell blend are deduced from the intercept value of $9\varepsilon\varepsilon_0\mu/(8L^3)$ by linearly plotting $\ln J$ *vs* $\ln V$ (the slope of $\ln V$ *vs* $\ln V$ is ≈ 2).

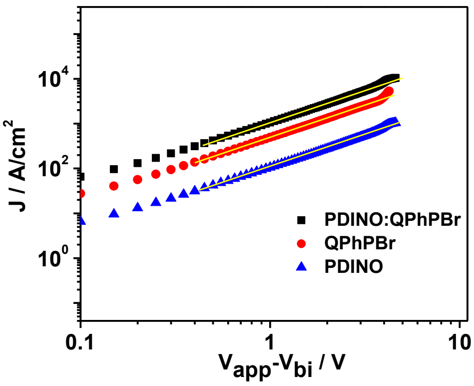

Fig. S2 Plots of J–V Obtained from the PBDBT:IDTBR based electron-only, which were estimated using the SCLC method.

Measurements of the hole mobility by the space-charge limited current (SCLC) method: The devices were fabricated with configuration of ITO/PEDOT:PSS/PBDBT:IDTBR (200 nm)/Au. The Au layer was deposited under a low speed (1 Å/10 s) to avoid the penetration of Au atoms into the active layer. The active layers were spin-coated with chlorobenzebe (CB) and dried. The hole mobility extracted by fitting the current density-voltage curves using the Mott-Gurney law.[S2, S3]

$$J_{\mathrm{SCL}} = 9\varepsilon\varepsilon_0\mu V^2 /(8L^3) \qquad (1)$$

where ε is the dielectric constant of the organic component, ε_0 is the permittivity of the vacuum (8.85419×10^{-12} F^{-1}m^{-1}), μ is the zero-field mobility, J is the current density, L is the thickness of the active layer, and V_{bi} the built-in potential which results from the difference in the work function of the anode and the cathode (in this device structure, V_{bi} = 0.2 V). Herein ε is 3. The results are shown in Fig. S3. The hole mobility of the solar cell blend are deduced from the intercept value of $9\varepsilon\varepsilon_0\mu/(8L^3)$ by linearly plotting ln$J$ *vs* ln$V$ (the slope of ln$J$ *vs* ln$V$ is ≈ 2) and calculated value as 2.74×10^{-4} cm^2 V^{-1} s^{-1}.

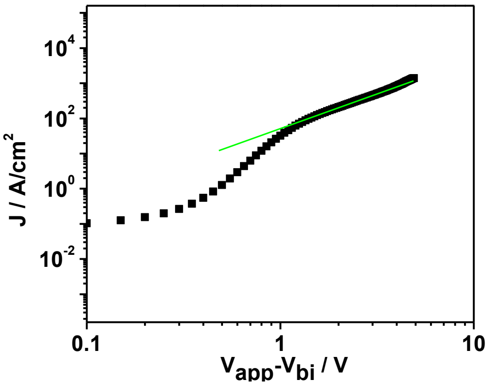

Fig. S3 Plots of J–V obtained from PBDBT:IDTBR based hole only device, which were estimated using the SCLC method.

References

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