Copolymers based on trialkylsilylethynyl-phenyl substituted benzodithiophene building block for efficient organic solar cells

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Instruments

The NMR spectra were collected on a Bruker AVANCEIII 600 MHz spectrometer with tetramethylsilane (TMS) (δ 0 ppm) as an internal standard. The mass spectra (FT-MS) were conducted on a Thermo Fisher Scientific LTQ FT Ultra mass spectrometer. UV−vis absorption spectra were recorded using a Hitachi U-3000 spectrometer. XRD diffraction data was measured on Bruker D8 Advance. TGA curves were acquired through Netzsch STA449 F3 instrument. The electrochemical measurements were performed in a deoxygenated solution of tetra-n-butylammonium hexafluorophosphate (0.1 M) in CH_3CN with a CHI604E electrochemical workstation, wherein a Pt plate working electrode coated with samples, a Pt wire counter electrode, and a $Ag/AgNO_3$ reference electrode were applied. TEM images were obtained by a FEI Tecnai G^2 F 20 S-TWIN with an accelerating voltage of 200 kV.

Hole mobility measurement

Hole-only diodes were fabricated using the structure: ITO/PEDOT:PSS/blend/MoO_3/Ag. Mobilities were extracted by fitting the current density-voltage curves under dark using the

space-charge-limited current (SCLC) method. The J–V curves of the devices were plotted as $J^{0.5}$ versus V using the equation: $J = (9/8)\varepsilon_r\varepsilon_0\mu(V^2/L^3)$, where ε_0 is the permittivity of free space (8.85×10^{-12} F/m), ε_r is the dielectric constant of the polymer (assumed to be 3), μ is the hole mobility, V is the voltage drop across the device, and L is the average active layer thickness. $V = V_{appl} - V_{bi}$, where V_{appl} is the applied voltage to the device, and V_{bi} is the built-in voltage due to the difference in work function of the two electrodes ($V_{bi} = 0.4$ V).

Table S1 Influence of annealing temperature on the photovoltaic performance of PSCs based on $PW30_H$:IDIC with a D/A ratio of 1:1.5.

Polymer	Annealing temperature [°C]	V_{oc} [V]	J_{sc} [mA cm^{-2}]	FF [%]	PCE_{max} (PCE_{ave})[c] [%]
$PW30_H$	90	0.904	12.27	53.0	5.87 (5.80 ± 0.07)
	110	0.910	12.70	54.0	6.24 (6.00 ± 0.24)
	130	0.874	12.30	52.9	5.69 (5.60 ± 0.09)

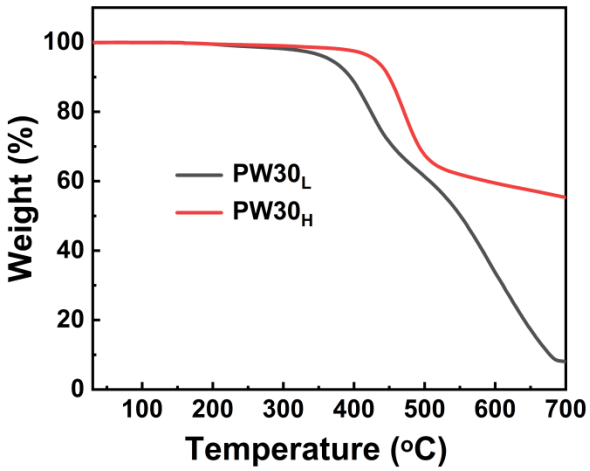

Fig. S1 Thermogravimetric analysis curves of the polymers $PW30_H$ and $PW30_L$.

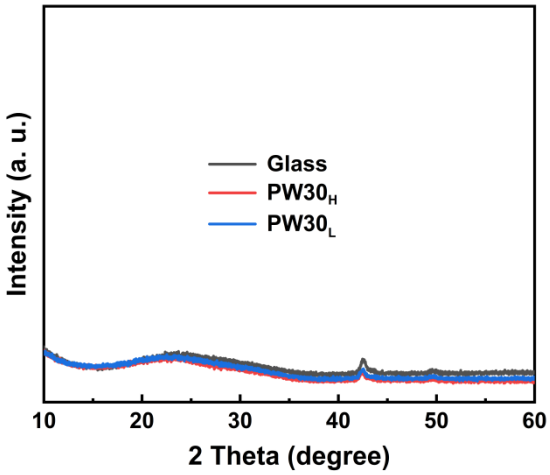

Fig. S2 XRD diffraction patterns of the films of $PW30_H$ and $PW30_L$ coated on glass.