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Supporting information

A new donor-acceptor molecule with uniaxial anisotropy for efficient vacuum-deposited organic solar cells

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Synthetic procedures:

General Methods: All chemicals and reagents were used as received from commercial sources without purification. Solvents for chemical synthesis were purified by distillation. All chemical reactions were carried out under an argon or nitrogen atmosphere.

Synthesis of 5-[*N*,*N*-Bis(phenylamino)phenyl]-5'-dicyanomethylidenemethyl -3,3'-diphenylsilylene-2,2'-bithiophene (TPDCDTS). A mixture of **1** (1.03 g, 1.66 mmol), malononitrile (220 mg, 3.32 mmol), and basic aluminum oxide (830 mg) in toluene (40 mL) was stirred and heated at 70 ^{o}C for 1 h. After cooling to room temperature, the aluminum oxide residue was removed by filtration and thoroughly washed with toluene. The solvent of the filtrate was removed by rotary evaporation, and the crude product was purified by column chromatography on silica gel with ethyl acetate/dichloromethane/hexane (v/v/v, 1 : 2 : 10) as eluent to afford **TPDCDTS** as a black solid (800 mg, 72% yield). M.p. 294 ^{o}C (DSC); IR (KBr) ν 3052, 3027, 2216, 1592, 1514, 1488, 1384, 1255, 1114, 926, 830 cm^{-1}; ^{1}H NMR (CD_2Cl_2, 400 MHz) δ 7.82 (s, 1H), 7.80 (s, 1H), 7.65 (d, J = 7.2 Hz, 4H), 7.52-7.47 (m, 5H), 7.41 (t, J = 7.2 Hz, 4H), 7.30 (t, J = 7.8 Hz, 4H), 7.13-7.03 (m, 8H); ^{13}C NMR (CD_2Cl_2, 100 MHz) δ 162.8, 152.5, 150.6, 148.7, 148.2, 147.4, 146.5, 142.7, 141.2, 137.3, 135.7, 131.4, 130.1, 129.8, 128.8, 127.2, 125.6, 125.4, 124.1, 123.0, 115.3, 114.7, 73.8; HRMS (m/z, FAB^{+}) Calcd for $C_{42}H_{27}N_3S_2Si$ 665.1416, found 665.1416.

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OPVs device fabrication and testing:

Organic compounds including synthesized **TPDCDTS**, and purchased fullerene C_{60} or C_{70} and 2,9-Dimethyl-4,7-Diphenyl-1,10-Phenanthroline (BCP) were subject to purification once by temperature-gradient sublimation before use in this study. The organic and metal oxide thin films and metal electrodes were deposited on indium tin oxide (ITO) coated glass substrates in a high vacuum chamber with base pressure ~ $1x10^{-6}$ Torr. The sheet resistance of ITO is ~ 15Ω/sq. The deposition was performed at rate of 2-3 Å with the substrate held at room temperature. Thicknesses were monitored using a crystal oscillator during deposition and were verified later with spectroscopic ellipsometry. The active area of the cells had an average size of 2.5-5 mm^2. Devices were encapsulated using a UV-cured sealant (*Everwide Chemical Co., Epowide EX*) and a cover glass under the dry nitrogen atmosphere after fabrication and were measured in air. Current density-voltage characteristics were measured with a SourceMeter *Keithley* 2636A under illumination of AM1.5G solar light from a xenon lamp solar simulator (*Abet Technologies*). The incident light intensity was calibrated as $100mW/cm^2$. The external quantum efficiency spectra were taken by illuminating chopped monochromatic light with a continuous-wave bias white light (from halogen lamp) on the solar cells. The photocurrent signals were extracted with lock-in technique using a current preamplifier (*Stanford Research System*) followed by a lock-in amplifier (*AMETEK*). The EQE measurement is fully computer controlled and the intensity of monochromatic light is carefully calibrated with optical power meter (*Ophir Optronics*). Organic films for absorption, photoelectron spectroscopy and ellipsometry measurements were vacuum deposited on fused silica substrates. Absorption measurements were performed with *Shimadzu* spectrophotometer. The HOMO values of thin films were acquired with a photoelectron spectrometer (*Riken Keiki Co. Ltd.*). Ellipsometry measurements were carried out with *J. A. Woollam Inc. V-VASE* variable-angle spectroscopic ellipsometer.

Cyclic voltammogram of TPDCDTS:

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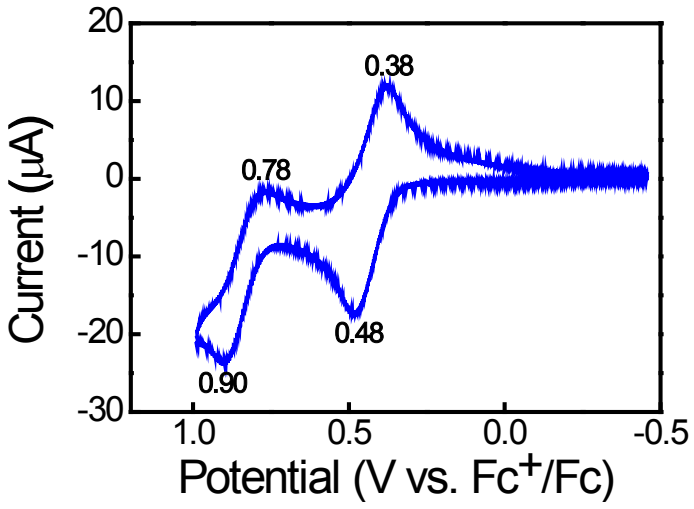

Fig. S1 Cyclic voltammogram of **TPDCDTS**; 0.1 M Bu_4NPF_6 in CH_2Cl_2 was used as supporting electrolyte. A glassy carbon electrode was used as the working electrode; scan rate: 100 mV/s.

Device structure and energy level diagram of TPDCDTS:fullerene PMHJ solar cells:

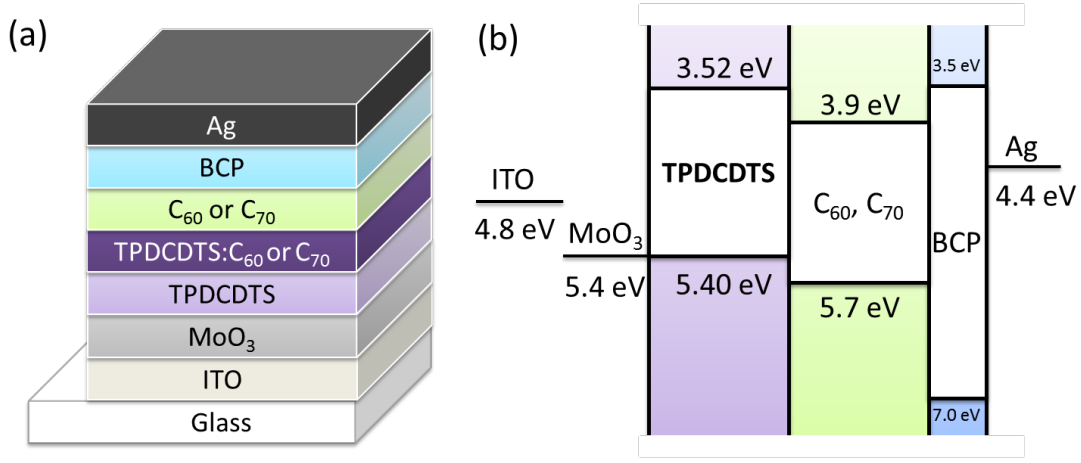

Fig. S2 (a) Device structure and (b) energy level diagram of **TPDCDTS**:fullerene PMHJ solar cells with MoO_3 as HTL.

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Device characteristics of TPDCDTS:C_{60} PMHJ solar cells with different hole transport layers:

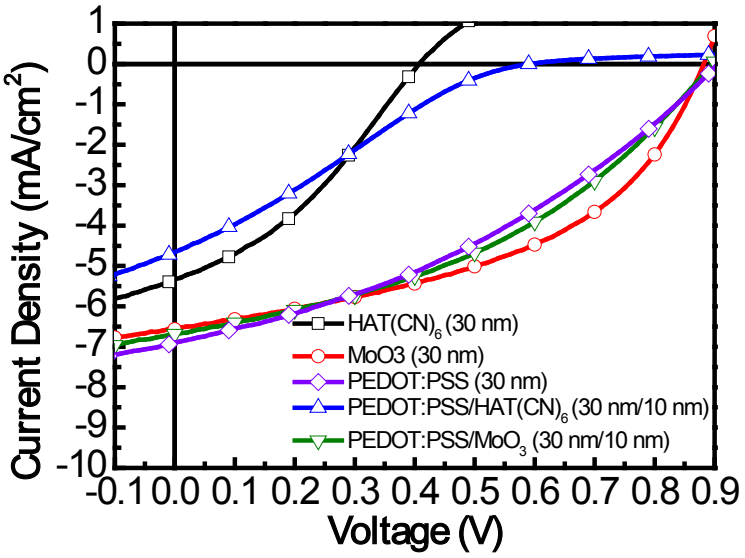

Fig. S3 J-V characteristics of **TPDCDTS**:C_{60} PMHJ solar cells. The device structures are: ITO/Hole transport layer/**TPDCDTS** (3 nm)/ **TPDCDTS**:C_{60} (1:1, 35 nm)/C_{60} (20 nm)/BCP (10 nm)/Ag (120 nm)

TABLE S1: Performance parameters of devices

Device	**V_{oc} (V)**	**J_{sc} (mA/cm^2)**	**FF**	**η_{PCE} (%)**
HAT(CN)$_6$	0.41	5.33	0.35	0.76
MoO$_3$	0.88	6.56	0.46	2.69
PEDOT:PSS	0.91	6.90	0.36	2.24
PEDOT:PSS/HAT(CN)$_6$	0.59	4.66	0.24	0.66
PEDOT:PSS/MoO$_3$	0.90	6.68	0.40	2.37

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Surface morphology of TPDCDTS and TPDCDTS:C_{70} (1:1)

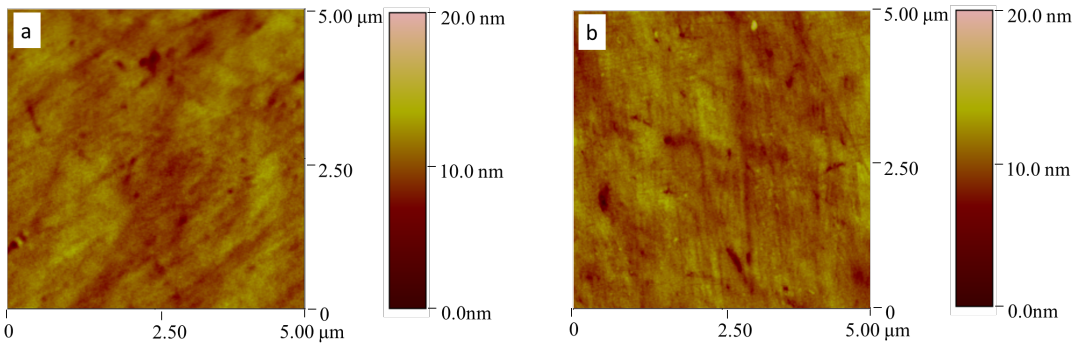

Fig. S4 Surface morphology of (a) **TPDCDTS** and (b) **TPDCDTS**:C_{70} (1:1) thin film obtained by atomic-force microscopy (AFM).

TABLE S2: Surface roughness characteristics

Thin film	Rrms (nm)	Ra (nm)	Rmax (nm)
TPDCDTS	0.95	0.75	11.42
TPDCDTS:C_{70}	1.04	0.79	17.21

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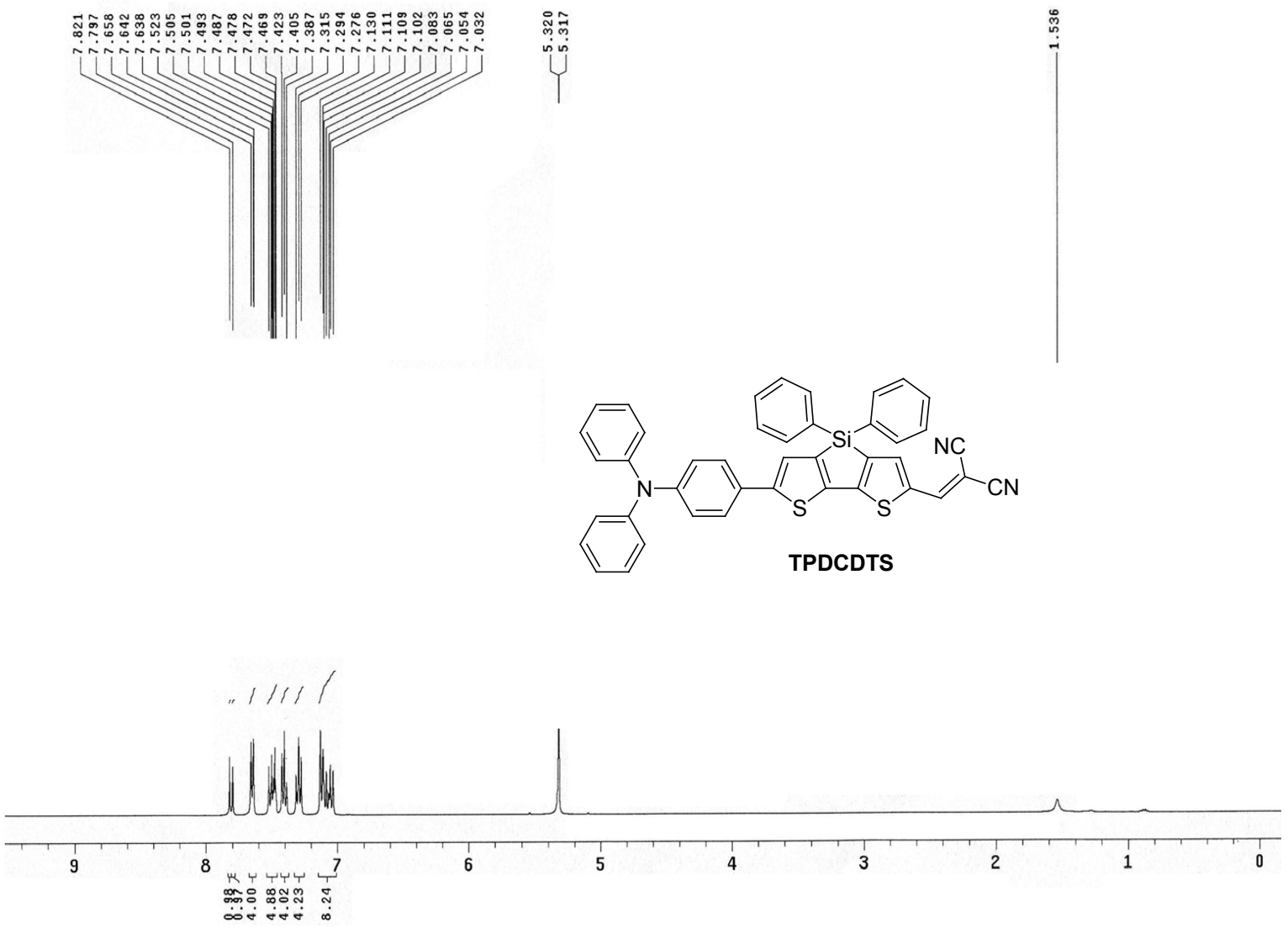

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