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Supplementary Information

A perylene diimide electron acceptor with a triptycene core for organic solar cells

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General information

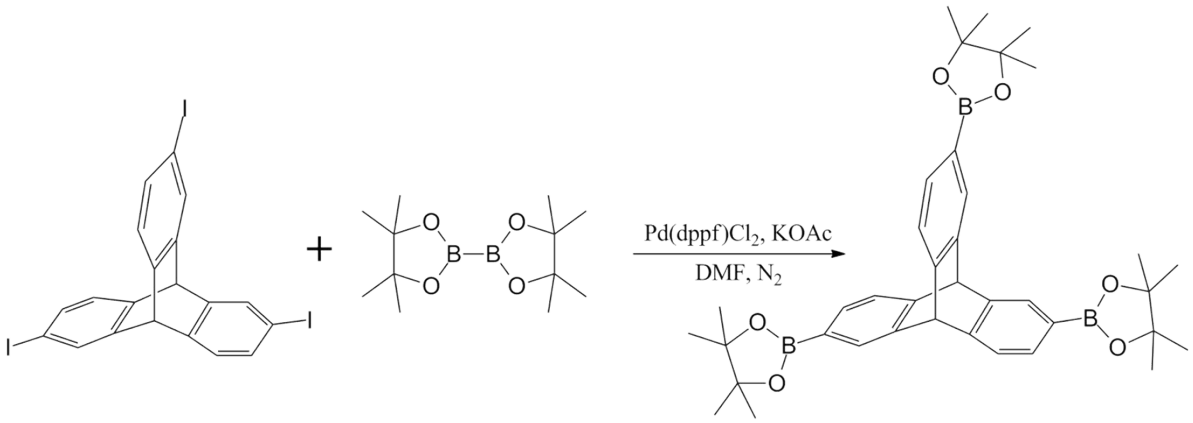
^{1}H NMR and ^{13}C NMR spectra were obtained on a Bruker Avance Ⅲ HD 400 MHz and 700 MHz nuclear magnetic resonance (NMR) spectroscope, respectively. HR-MALDI-TOF-MS (High resolution matrix assisted laser desorption/ionization time-of-flight mass spectrometry) were recorded on Shimadzu Biotech Axima Performance system and Bruker Autoflex Ⅲ instrument. UV-vis absorption spectra were recorded on a Shimadzu UV-2450 spectrophotometer. Cyclic voltammetry (CV) was performed with a CHI600A electrochemical workstation. All CV results were measured on the thin film in the 0.1 M $[nBu_4N]^+[PF_6]$ CH_3CN solution with a scan speed at 0.1 V s^{-1}. And a glassy carbon working electrode, the Ag/Ag^+ reference electrode, platinum(Pt) wire counter electrode were adopted in this system. The ferrocene/ferrocenium (Fc/Fc+) redox couple was used as an external standard. Thermogravimetric analysis (TGA) was carried out on a Shimadzu DTG-60 thermal balance under an nitrogen atmosphere at a heating rate of 10 ^{o}C/min. Differential scanning calorimetry (DSC) was recorded on a Shimadzu DSC-60 differential scanning calorimeter under protection of nitrogen at a heating and cooling rate of 10 ^{o}C/min. The charge transfer mobility of the blend films were measured using the space-charge-limited current (SCLC) method. The structures of the hole- and electron- only devices are ITO/ MoOx/ PTB7-Th: TP3/ MoOx/ Al and ITO/ Al/ PTB7-Th: TP3/Al, respectively. The SCLC is described by:

$$J=9\varepsilon_0\varepsilon_r\mu V^2/8d^3$$

Where $\boldsymbol{J}$ is the current density, $\boldsymbol{\varepsilon_0}$ is the permittivity of free space, $\boldsymbol{\varepsilon_r}$ is the relative permittivity of the material, $\boldsymbol{\mu}$ is the electron mobility, $\boldsymbol{V}$ (= V_{appl} - V_{bi}) is the voltage drop across the device and **d** is the thickness of the film.

Section 1: Synthesis

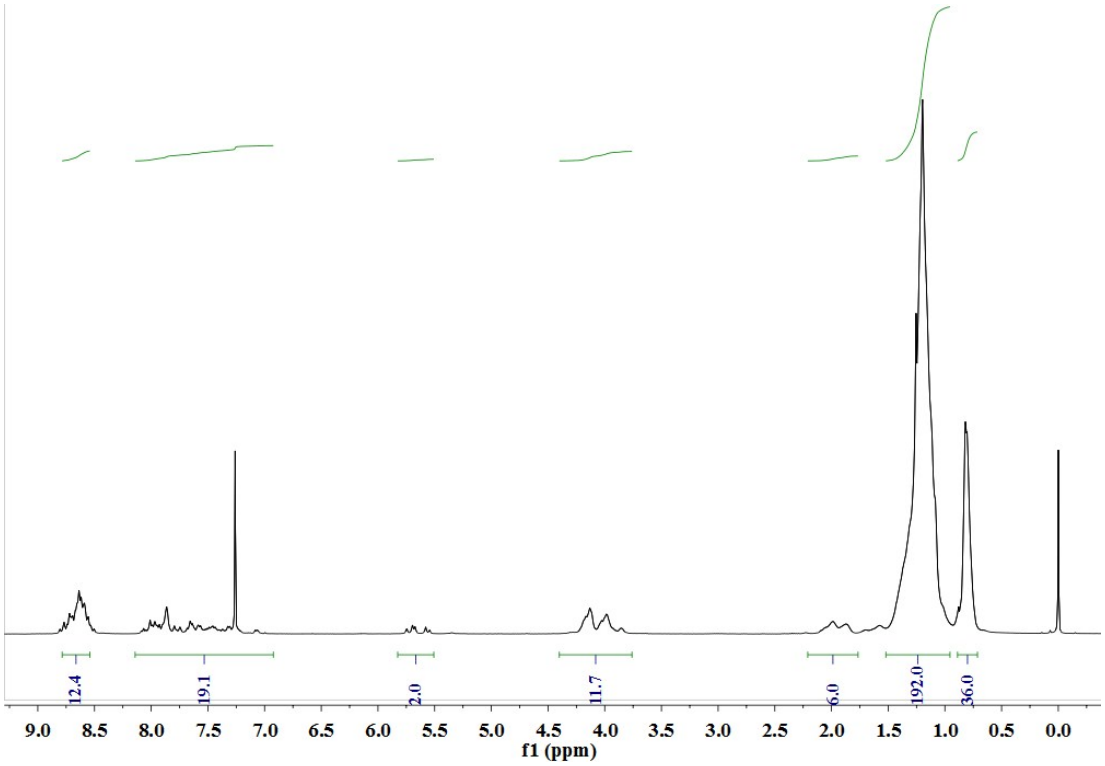
Synthesis of tri-boricester-triptycene **(TPC-B_3):**



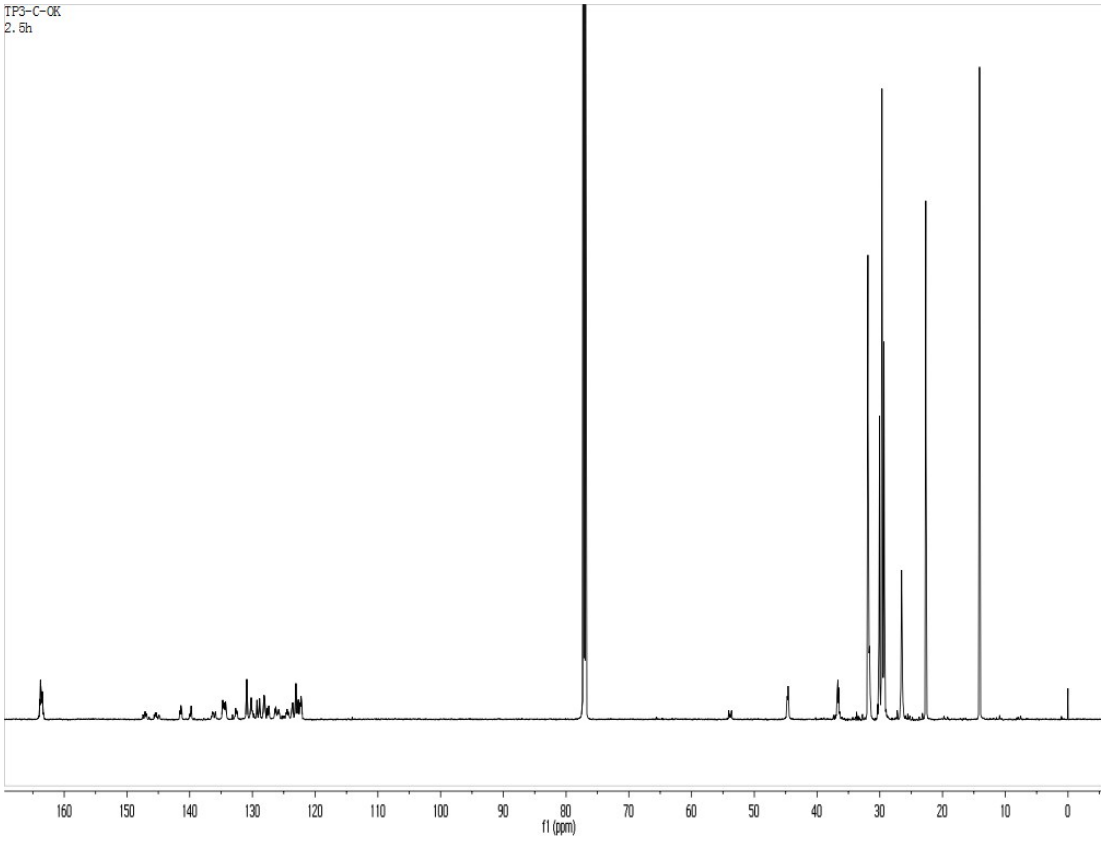
TPC-B3: Triiodotriptycene (0.6 g, 0.95 mmol) and bis(pinacolato)diboron (0.723 g, more than 3eq.) were dissolved in 10 mL anhydrous DMF (10 mL) in a two-neck round bottomed flask. Potassium acetate (0.28 g, 6eq.) and Pd(dppf)Cl_2 (0.026 g, 0.035 mmol) were then quickly added into the flask. Then, the reaction system was immediately performed successive creating of vacuum and filling with nitrogen more than three times. The resulting mixture was stirred vigorously and heated at 90 °C for 24 hours. After cooling down to room temperature, deionized water (120 mL) was added and the brownish black precipitate was collected by filtration, then washed with deionized water more than three times. After dried under vacuum, the precipitate was purified with a short column chromatography using DCM as eluent. At the last, the crude product was washed with methanol to give the TPC-B3 as a offwhite power.(320 mg, 53%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, 3H,triptycene aryl H), 7.45 (d, 3H, triptycene aryl H), 7.34 (dd, 3H, triptycene aryl H), 5.46 (d, 2H, triptycene bridge H), 1.27 (d, 36H, methyl H).

Section 2: NMR Spectra and High-Resolution Mass Spectra

^{1}H NMR Spectra of TP3:



^{13}C NMR Spectra of TP3:


TP3-C-OK
2.5h
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

High-Resolution MAlDI-TOF Mass Spectra of TP3:

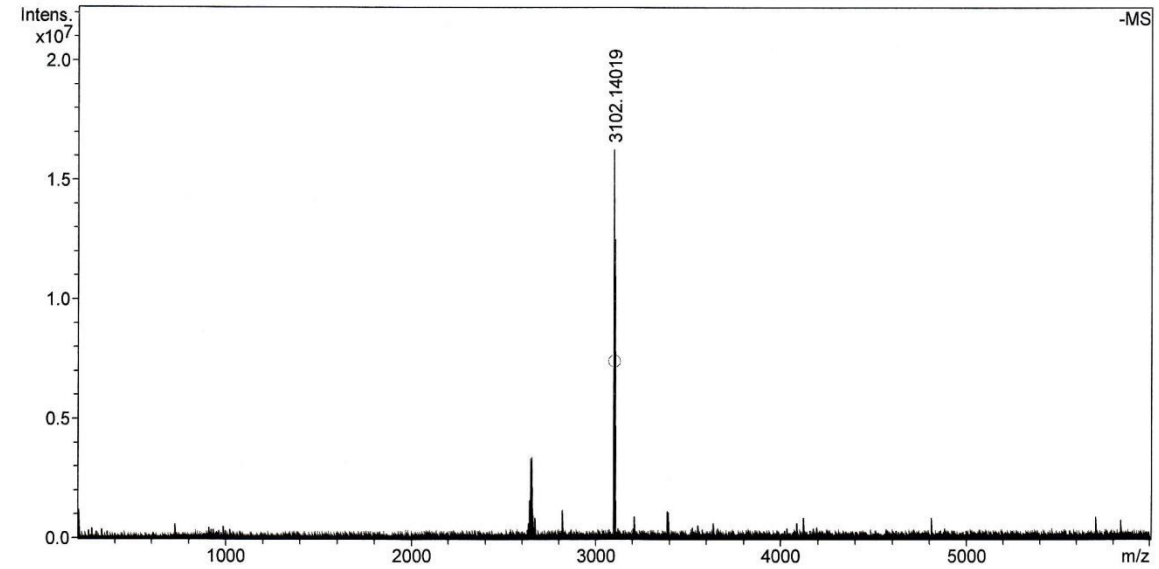
MALDI,TP3,20161116

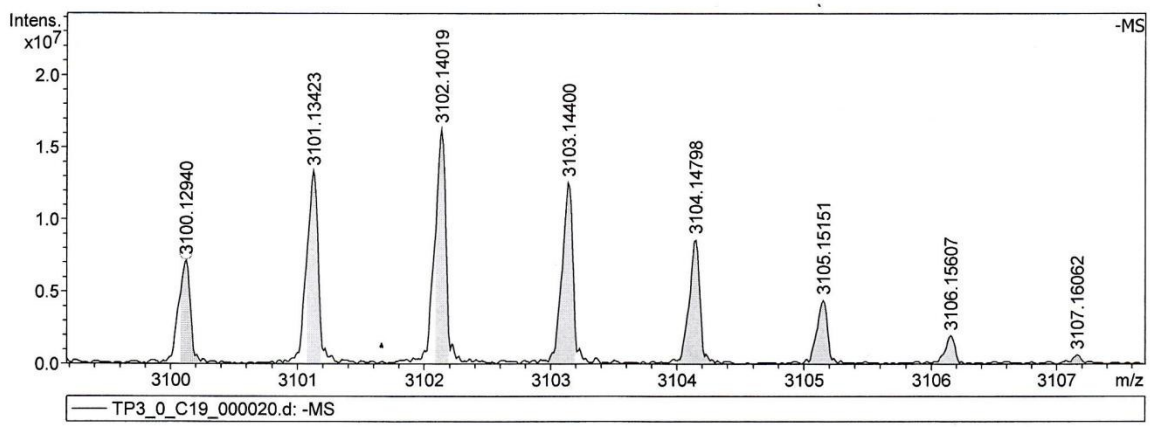
Analysis Info

Analysis Name	D:\Data\MALDI\2016\1116\TP3_0_C19_000020.d	Acquisition Date	11/16/2016 6:00:55 PM
Method	MALDI_P_100-3000	Operator	
Sample Name		Instrument	solariX
Comment			

Acquisition Parameter

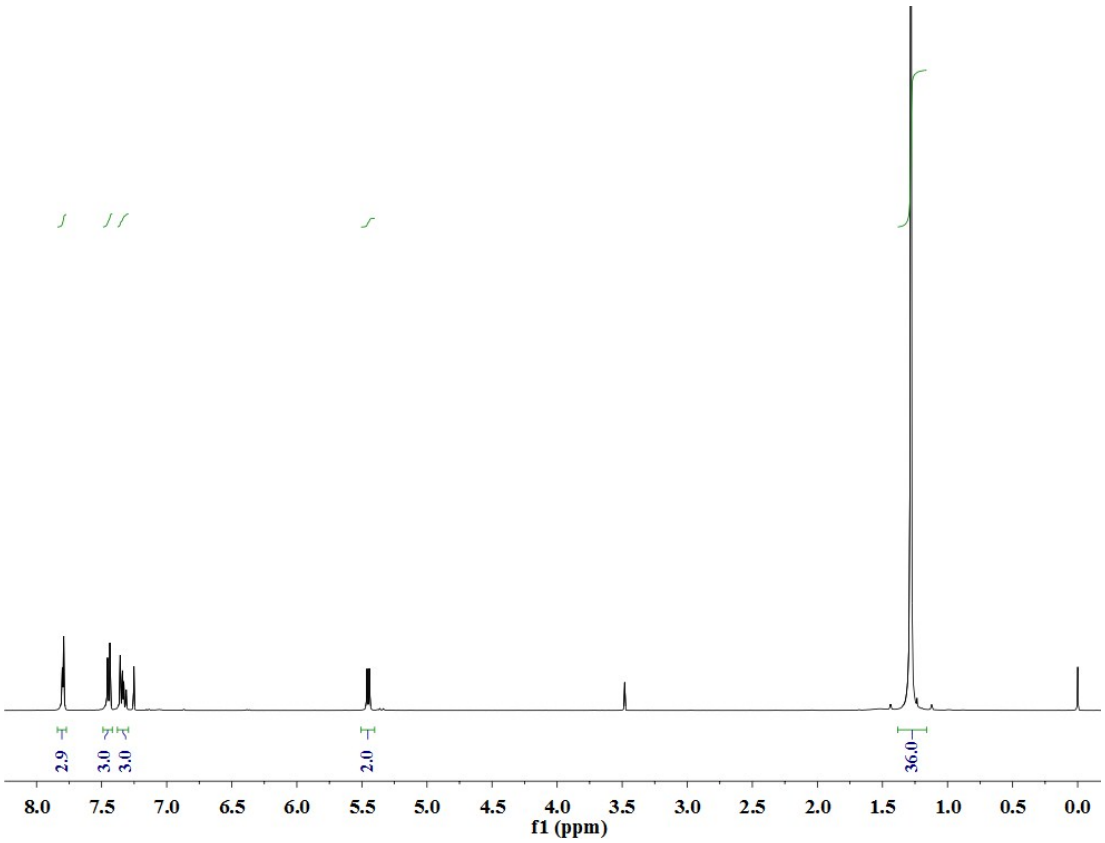
Acquisition Mode	Single MS	Acquired Scans	3	Calibration Date	Wed Nov 16 06:00:39
Polarity	Negative	No. of Cell Fills	1	Data Acquisition Size	2096152
Broadband Low Mass	202.1 m/z	No. of Laser Shots	200	Data Processing Size	4194304
Broadband High Mass	6000.0 m/z	Laser Power	90.0 lp	Apodization	Sine-Bell Multiplication
Source Accumulation	0.001 sec	Laser Shot Frequency	0.020 sec		
Ion Accumulation Time	0.300 sec				





Meas. m/z	#	Ion Formula	Score	m/z	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
3100.129399	1	C212H278N6O12	100.00	3100.133327	0.3	179.3	77.0	odd	ok

[1]H NMR Spectra of TPC-B3:



Section 3: Supporting figures

DFT Calculation of TP3

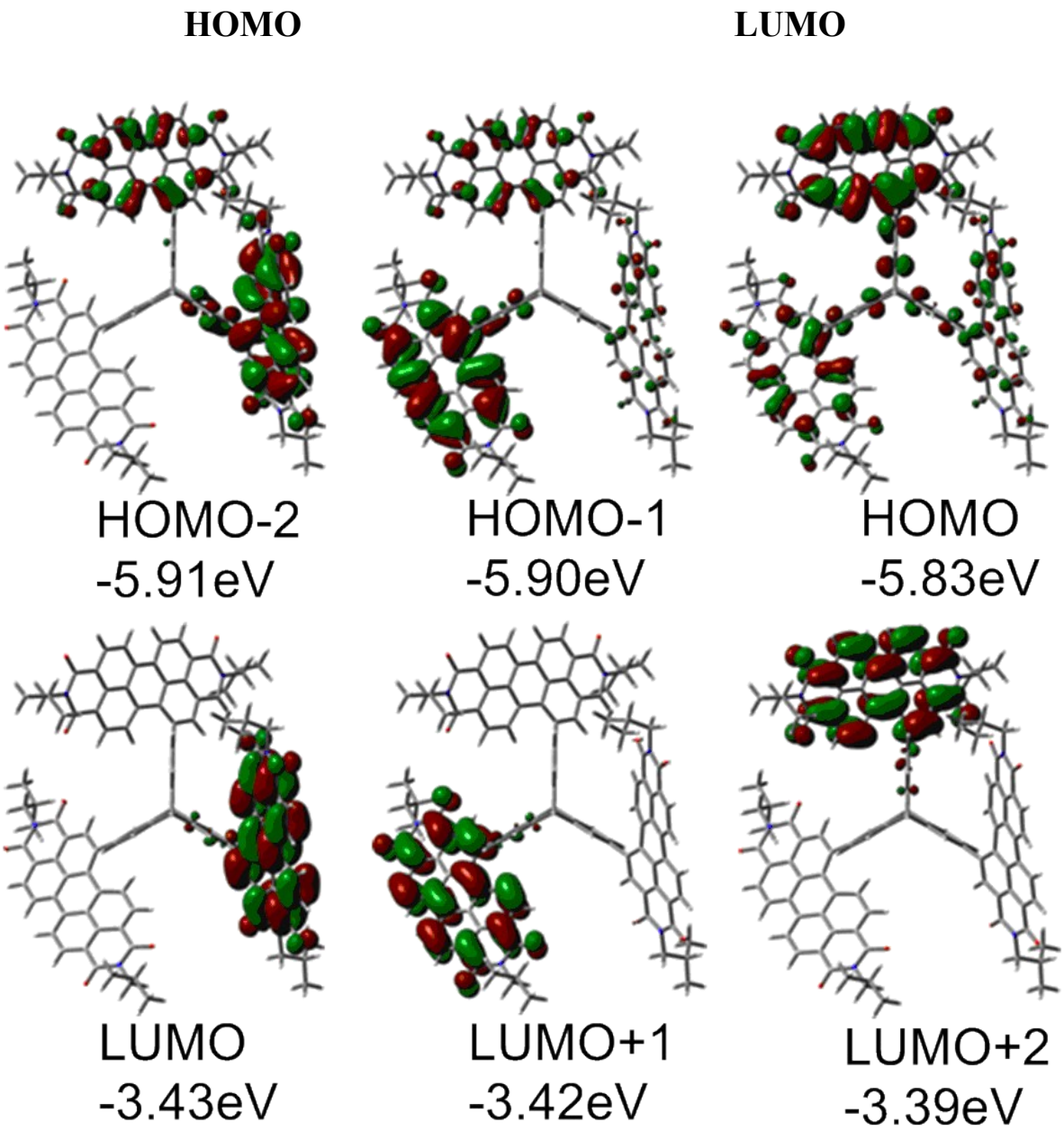


Fig. S1 Molecular frontier orbitals (HOMOs and LUMOs) and energies levels of **TP3** calculated with M06-2x/6-31 G(d) method.

DFT Calculation of Potential Interface Models

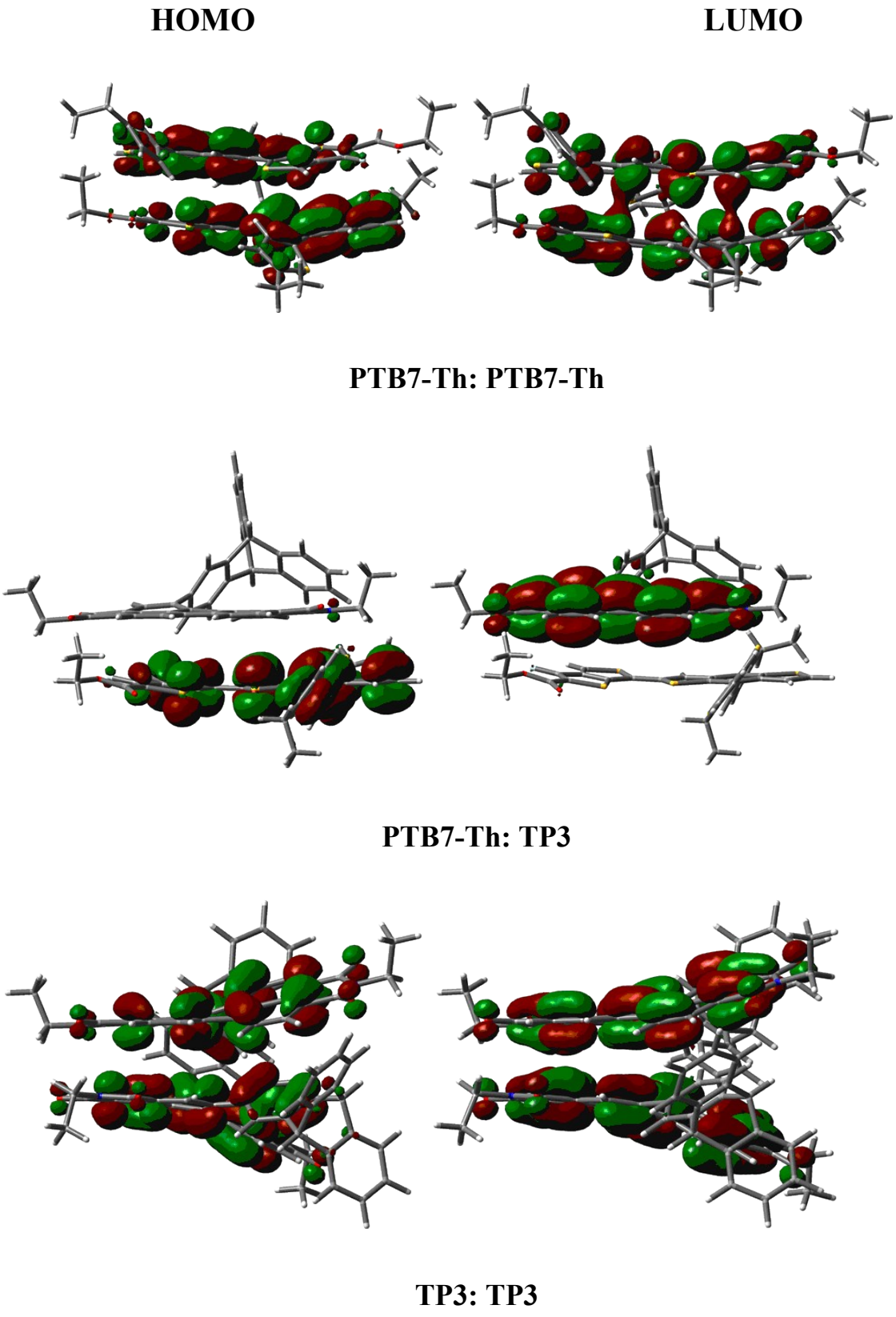


Fig. S2 Molecular frontier orbitals (HOMOs and LUMOs) of D-D, D-A and A-A interfaces.

SCLC Results of PTB7-Th: TP3 blend Film

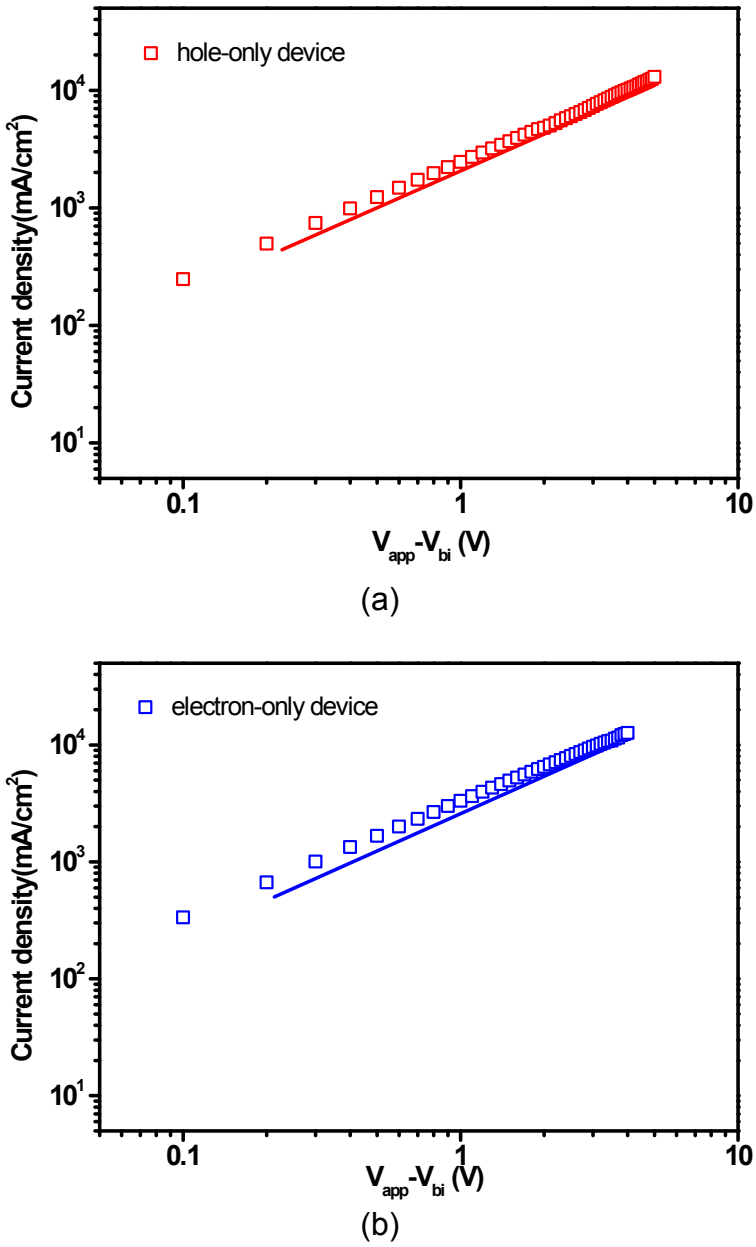


Fig. S3 *J-V* curves for hole-(a) and electron-(b) only devices of PTB7-Th: TP3 (w/w, 1:1.5) blend film with 0.5% DIO.