Supporting Information for *Acta Phys. -Chim. Sin.* doi: 10.3866/PKU.WHXB201805161

通过非共价构象锁定和端基工程策略设计高效率的 A-D-A 型稠环电子受体

冯诗语，路皓，刘泽坤，刘亚辉，李翠红*，薄志山*
北京师范大学化学学院，能量转换与存储材料北京市重点实验室，北京 100875

Designing a High-performance A-D-A Fused-ring Electron Acceptor *via* Noncovalently Conformational Locking and Tailoring Its End Groups

FENG Shiyu, LU Hao, LIU Zekun, LIU Yahui, LI Cuihong *, BO Zhishan *
Beijing Key Laboratory of Energy Conversion and Storage Materials, College of Chemistry, Beijing Normal University, Beijing 100875, P. R. China.

*Corresponding authors. Email: licuihong@bnu.edu.cn (L.C.); zsbo@bnu.edu.cn (B.Z.).

1.1 Material and Instruments

Unless otherwise noted, all chemicals were commercially available and used without further purification. All reactions were monitored by thin layer chromatography (TLC) on silica gel 60 F254 (Merck, 0.2 mm). Column chromatography was carried out on silica gel (200–300 mesh). ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AV 600. UV-visible absorption spectra were obtained on a PerkinElmer UV-Vis spectrometer model Lambda 750. Elemental analyses were performed on a Flash EA 1112 analyzer. Atomic force microscopy (AFM) measurements were performed under ambient conditions using a Digital Instrument Multimode Nanoscope IIIA in the tapping mode. Transmission electron microscopy (TEM) images were obtained with a FEI Technai TF20 (Philip) transmission electron microscopy. Cyclic voltammogram (CV) measurements were carried out on Modulab XM Electrochemical Analyzer (Solartron Analytical Ltd., UK) with a standard three-electrode electrochemical cell in a 0.1 M Bu_4NPF_6 solution in CH_3CN at room temperature under an atmosphere of nitrogen with a scanning rate of 0.1 $V{\cdot}s^{-1}$. A Pt plate working electrode, a Pt wire counter electrode, and an Ag/$AgNO_3$ (0.01 M in CH_3CN) reference electrode were used. The experiments were calibrated with the standard ferrocene/ferrocenium (Fc/Fc^+) redox system, given that the energy level of Fc is 4.8 eV below vacuum.

1.2 Polymer Solar Cell Fabrication and Characterization

PSCs were fabricated with the device architecture of ITO/ZnO/active layer/MoO_3/Ag. The sheet resistance of ITO is 15 Ω per square. Pre-cleaned ITO substrates were treated by UV-ozone for 20 min. A thin layer of ZnO was spin-coated on top of a cleaned ITO substrate at 3500 rpm for 40 s and annealed subsequently at 200 °C for 20 min on a hotplate. The thickness of the ZnO layer was about 30 nm. A mixture of PBDB-T and IDT-IC/IDT-IC-B/IDT-IC-T in 1,2-dichlorobenzene (DCB) (with an 8 $mg{\cdot}mL^{-1}$ concentration) was stirred at 110 °C for an hour to ensure sufficient dissolution and then spin-coated on the ZnO layer at 1600 rpm. The thickness of the active layer was about 100 nm. The top electrode was thermally evaporated, with an 8.5 nm MoO_3 layer, then followed by a 100 nm Ag layer at a base pressure below 10^{-7} Torr. Six cells were fabricated on one substrate with an effective area of 0.04 cm^2. The measurement of the device was conducted in a glove box without encapsulation. The temperature while measuring the J–V curves was approximately 25 °C. Current-voltage characteristics were recorded under AM1.5G AAA class solar simulator (SS-F53A, Enli Technology Co., Ltd) with an intensity of 100 $mW{\cdot}cm^{-2}$ calibrated with a standard photovoltaic cell equipped with a KG5 filter (certificated by the National Institute of Metrology) and a Keithley 2400 source-measure unit. The EQE data were obtained using a solar cell spectral response measurement system (QER3011, Enli Technology Co. Ltd). A calibrated silicon detector was used to determine the absolute photo sensitivity at different wavelengths. The thickness of the blend films was determined by a Dektak 6 M surface profilometer.

1.3 pace-Charge Limited Current Measurement

Hole/electron devices with a structure of ITO/PEDOT:PSS (30 nm)/active layer (120 nm)/Au and FTO/active layer (105 nm)/Al were fabricated. Dark J–V curves of the hole/electron devices were measured by the space-charge limited current (SCLC) method. Hole and electron mobilities of devices were calculated according to the Mott-Gurney equation: $J = 9\varepsilon_o\varepsilon_r\mu V^2/8d^3$, where J is the space charge limited current, ε_o is the vacuum permittivity ($\varepsilon_o = 8.85 \times 10^{-12}$ $F{\cdot}m^{-1}$), ε_r is the relative permittivity of polymer ($\varepsilon_r = 3$), μ is mobility, and d is the thickness of active layer.

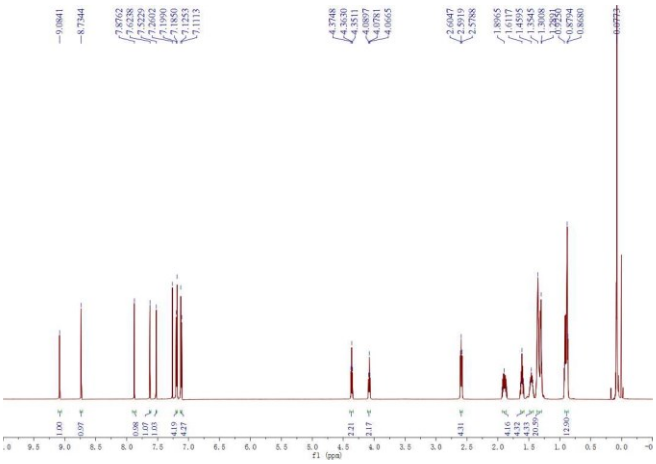

Fig. S1 ^{1}H NMR spectrum of ITOIC-2Cl.

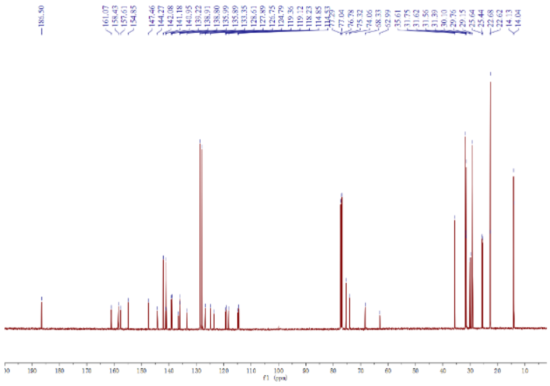

Fig. S2 ^{13}C NMR spectrum of ITOIC-2Cl.

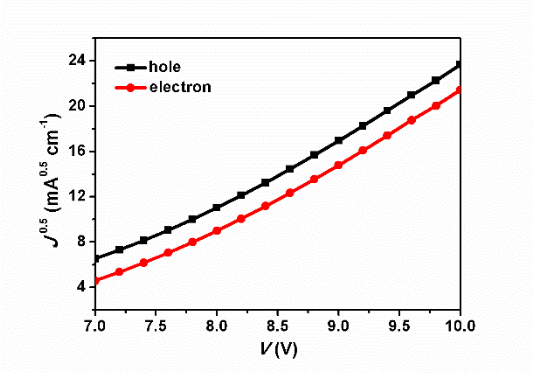

Fig. S3 The hole mobility and electron mobility of the optimized PBTB-T:ITOIC-2Cl based blend films.