

Supporting information for

Chemical reaction between ITIC electron acceptor and amine- containing interfacial layer in non-fullerene solar cells

Lin Hu, Yun Liu, Lin Mao, Sixing Xiong, Lulu Sun, Nan Zhao, Fei Qin, Youyu Jiang,
and Yinhua Zhou*

Wuhan National Laboratory for Optoelectronics, School of Optical and Electronic
Information, Huazhong University of Science and Technology, Wuhan 430074, China

*Corresponding author: yh_zhou@hust.edu.cn

Experimental Section:

1.1 Materials

The polymer donor poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)-benzo[1,2-b:4,5-b']dithiophene))-alt-(5,5-(1',3'-di-2-thienyl-5',7'-bis(2-ethylhexyl)benzo[1',2'-c:4',5'-c']dithiophene-4,8-dione))] (PBDB-T) and the non-fullerene acceptor 3,9-bis(2-methylene-(3-(1,1-dicyanomethylene)-indanone))-5,5,11,11-tetrakis(4-hexylphenyl)-dithieno[2,3-d:2',3'-d']-s-indaceno[1,2-b:5,6-b']dithiophene (ITIC) were purchased from Solarmer Materials Inc. The zinc acetate dihydrate, monoethanolamine and methoxyethanol for ZnO precursor solutions were purchased from Sigma-Aldrich. Chlorobenzene (99.5%), branched polyethyleniminepoly (PEI) and polyethylenimine ethoxylated (PEIE) was also from Sigma-Aldrich. The monomers indacenodithieno[3,2-b]thiophene (IDTT) and 2-(3-oxo-2,3-dihydroinden-1-ylidene)malononitrile (INCN) were purchased from Derthon Optoelectronic Materials Science Technology Co LTD. The acetone and isopropanol were obtained from Sinopharm Chemical Reagent Co., Ltd.

1.2 Materials and film characterization

For the materials and film characterization, the ITIC and PBDB-T were first dissolved in chlorobenzene (99.5%) with a concentration of 10 mg/ml, respectively. The solution was stirred vigorously overnight for use. For the UV-vis-NIR measurement, the films were fabricated by spin coating the solution onto a quartz substrate at a speed of 1000 rpm. The PEI or PEIE treated films were processed by exposing the films in a covered Petri dish. Subsequently, two drops PEI or PEIE solution were dropped in the Petri dish at 160 °C hot plate for different time. As for the solution, the ITIC and the PEI was mixed directly in chlorobenzene with various mass ratios. The absorption spectra were recorded on a UV-vis-NIR spectrophotometer (UV-3600, Shimadzu Scientific Instruments). For the ESR measurements, films were prepared by drop casting onto quartz substrates. After dry in a N₂-filled glovebox, the resulted films were put into a quartz tube for test. The instrument model is Bruker ESR A300 and the frequency of the electromagnetic radiation was 9.425 GHZ. Fourier transform infrared (FT-IR) spectra were collected on a Bruker VERTEX 70 using potassium bromide (KBr) disks. The nuclear magnetic resonance (NMR) spectra were

collected on a Bruker Ascend™ 600 MHz NMR spectrometer with deuterated dichloromethane as the solvent and with tetramethylsilane ($\delta=0$) as the internal standard.

1.3 Solar cells fabrication and characterization

The pre-patterned ITO was first sonicated in baths using detergent in deionized water, deionized water, acetone, and isopropanol in sequence. Then the prepared ZnO precursor solutions were spin-coated onto ITO at 4000 rpm for 40 s. The substrate was annealed at 200 °C for 30 min to form a dense metal oxide film. The ZnO precursor solutions were prepared by adding 0.5 g zinc acetate dihydrate and 0.14 g monoethanolamine in 5 ml methoxyethanol, and stirring overnight. The PEI and PEIE interlayer was spin-coated on top at 5000 rpm for 1 min from isopropanol solution (0.1 wt.%), respectively. Subsequently, PBDB-T:ITIC (1:1 weight ratio) in a 20 mg/mL chlorobenzene:DIO (99.5:0.5 volume ratio) solution was spin-coated at 2500 rpm for 60 s. Then, the samples were then transferred into the vacuum evaporation system. 7 nm MoO₃ and 100 nm Ag was evaporated with a metal aperture mask to complete the device fabrication. Device area is 10.58 mm². The fabricated devices were measured under a simulated 100 mW cm⁻² AM 1.5G irradiation in a N₂-filled glovebox. A Keithley 2400 was applied to measure the current-voltage characteristics.

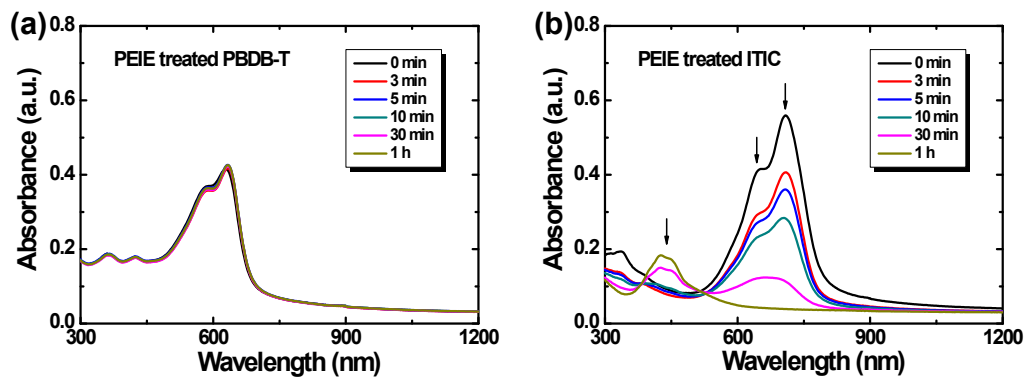


Figure S1. UV-vis-NIR absorption spectra of (a) PBDB-T and (b) ITIC films exposure for different time in amine vapor from PEIE.

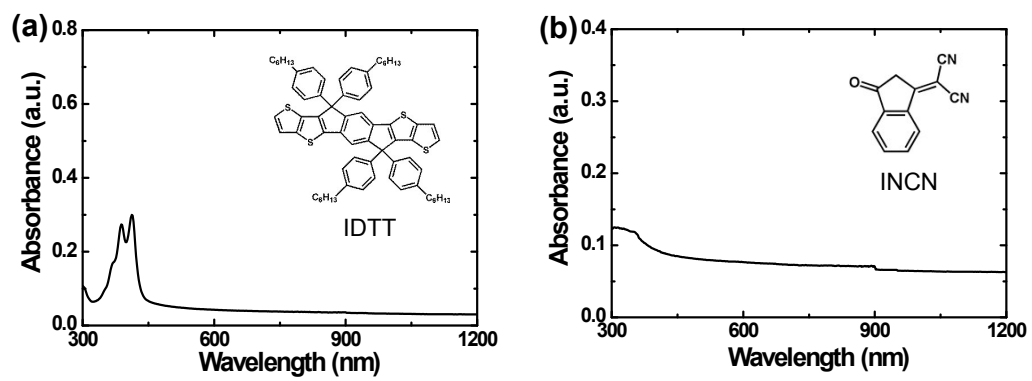


Figure S2. UV-vis-NIR absorption spectra of (a) the IDTT monomer and (b) the INCN monomer.

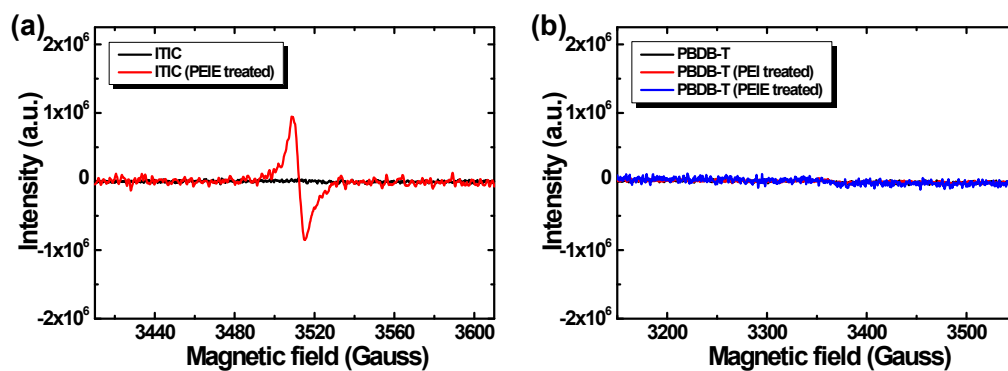


Figure S3. (a) The ESR spectra of pristine ITIC films and corresponding films treated with amine vapor from PEIE; (b) ESR spectra of pristine PBDB-T films and corresponding films treated with amine vapor from PEI and PEIE.

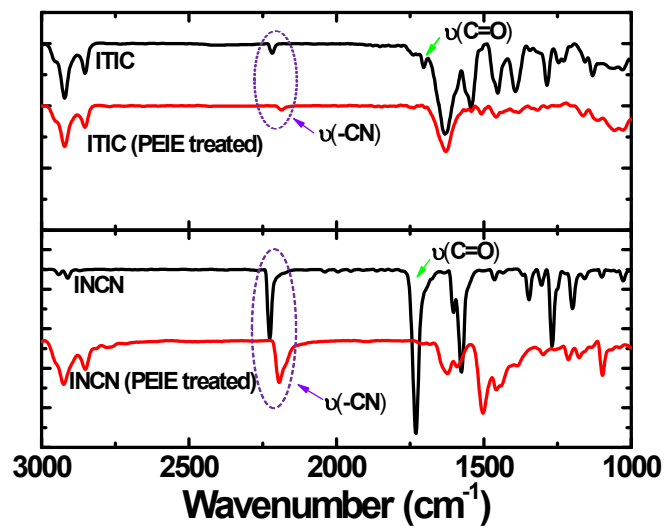


Figure S4. FT-IR spectra of ITIC and INCN monomer as well as the corresponding samples exposure in amine vapor from PEIE.

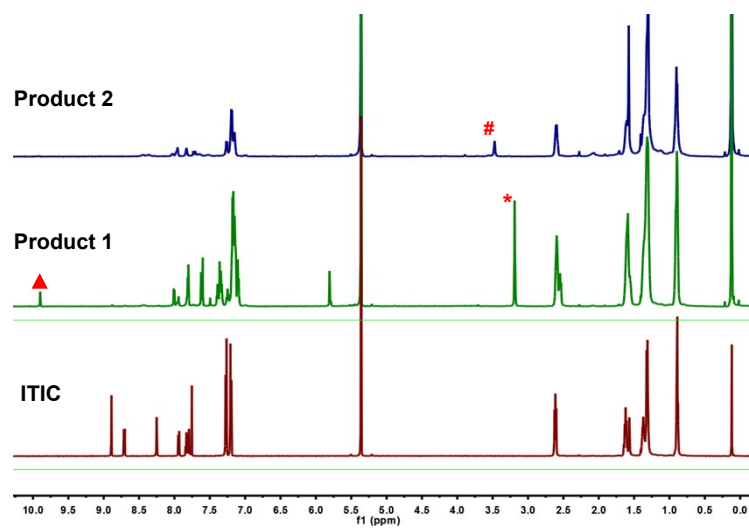


Figure S5. The ¹H NMR spectra of pristine ITIC and corresponding products. The reagent is CD₂Cl₂.

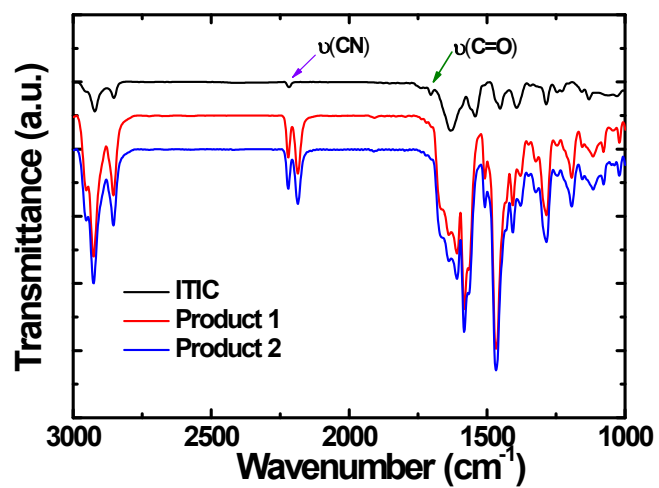


Figure S6. FT-IR spectra of ITIC and separated products from the reaction of ITIC and methylamine.