Electronic Supplementary Information for:

Pairing 1D/2D-conjugation donors/acceptors towards high-performance organic solar cells

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Materials

FTAZ,[S1] ITIC1,[S2] and ITIC2[S2] were synthesized according to our reported procedures. J71 was purchased from Solarmer Inc.

Characterization

Solution (chloroform) and thin film (on quartz substrate) UV-vis absorption spectra were recorded on a JΛSCO V-570 spectrophotometer. Electrochemical measurements were carried out under nitrogen on a deoxygenated solution of tetra-*n*-butylammonium hexafluorophosphate (0.1 M) in CH_3CN using a computer-controlled CHI660C electrochemical workstation, a glassy-carbon working electrode coated with samples, a platinum-wire auxiliary electrode, and an Ag/AgCl as a reference electrode. Potentials were referenced to ferrocenium/ferrocene ($FeCp_2^{+/0}$) couple by using ferrocene as an external standard. The thickness of active layer was measured on a Bruker DektakXT profilometer. Steady-state photoluminescence (PL) were measured on FLS980 (Edinburgh Instruments Ltd). Transmission electron microscopy (TEM) measurements were performed on a JEM-2100 transmission electron microscope operated at 200 kV.

GIWAXS measurements were carried out with a Xeuss 2.0 SAXS/WAXS laboratory beamline using a Cu X-ray source (8.05 keV, 1.54 Å) and a Pilatus3R 300K detector. The incidence angle is 0.2°. GISAXS was conducted at 19U2 SAXS beamline at Shanghai Synchrotron Radiation Facility, Shanghai, China, using the 0.15° incident angle with 10 keV primary beam.

Fabrication and characterization of organic solar cells

Organic solar cells were fabricated with the structure: ITO/ZnO/active layer/MoO_x/Ag. The indium tin oxide (ITO) glass (sheet resistance = 10 Ω $\square^{-1}$) was pre-cleaned in an ultrasonic bath of acetone and isopropanol. A ZnO layer (*ca.* 30 nm) was spin-coated onto the ITO glass from ZnO precursor solution (100 mg $Zn(CH_3COO)_2 \cdot 2H_2O$ and 0.02 mL ethanolamine dissolved in 1 mL 2-methoxyethanol), and baked at 200 °C for 30 min. A chloroform solution of donor:acceptor (11.5 mg mL^{-1} in total) was spin-coated on ZnO layer to form a photoactive layer (*ca.* 100 nm). The devices were optimized according to our previous work.[S2, S3] The MoO_3 layer (*ca.* 5 nm) and Ag (*ca.* 70 nm) were successively evaporated onto the surface of the photoactive layer under vacuum (*ca.* 10^{-5} Pa). The active area of the device was 4 mm^2. The *J-V* curve was measured using a computer-controlled B2912A Precision Source/Measure Unit (Agilent Technologies). An XES-70S1 (SAN-EI Electric Co., Ltd.) solar simulator (AAA grade, 70 × 70 mm^2 photobeam size) coupled with AM 1.5G solar spectrum filters was used as the light source, and the optical power at the sample was 100 mW cm^{-2}. A 2 × 2 cm^2 monocrystalline silicon reference cell (SRC-1000-TC-QZ) was purchased from VLSI Standards Inc. The EQE spectra were measured using a Solar Cell Spectral Response Measurement System QE-R3011 (Enlitech Co., Ltd.). The light intensity at each wavelength was calibrated using a standard single crystal Si photovoltaic cell.

Mobility measurements

Hole-only and electron-only diodes were fabricated using the architectures: ITO/PEDOT:

PSS/active layer/Au for holes and Al/active layer/Al for electrons. Mobilities were extracted by fitting the current density-voltage (*J*-*V*) curves using space-charge-limited current (SCLC) method. The *J*-*V* curves of the devices were plotted as $\ln(Jd^3/V^2)$ versus $(V/d)^{0.5}$ using the equation $\ln(Jd^3/V^2) \cong 0.89(1/E_0)^{0.5}(V/d)^{0.5} + \ln(9\varepsilon_0\varepsilon_r\mu/8)$, where J is the current density, d is the film thickness of active layer, μ is the hole or electron mobility, ε_r is the relative dielectric constant of the transport medium, ε_0 is the permittivity of free space (8.85×10^{-12} F m^{-1}), $V = V_{appl} - V_{bi}$, 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 (for hole-only diodes, V_{bi} is 0.2 V; for electron-only diodes, V_{bi} is 0 V).

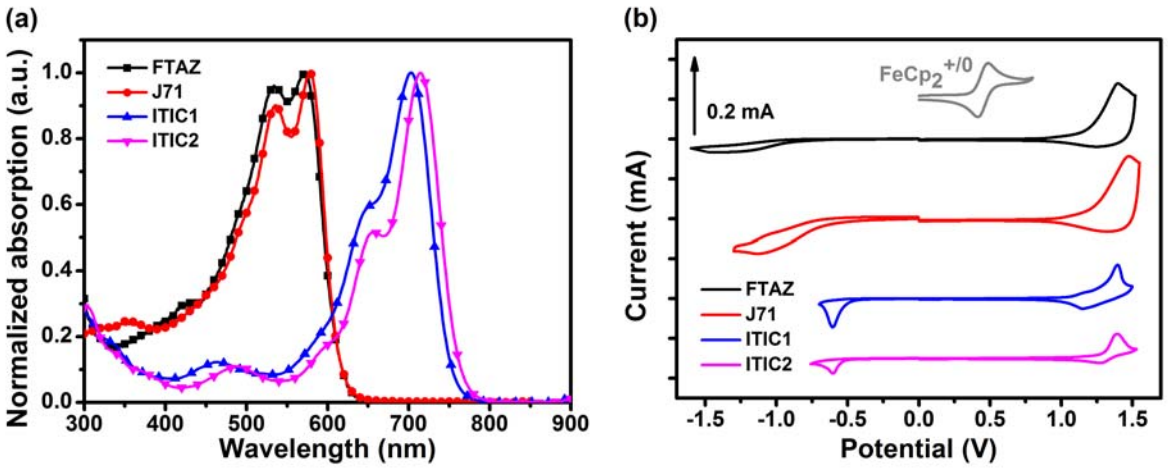

Fig. S1 (a) UV-vis absorption spectra of FTAZ, J71, ITIC1, and ITIC2 in chloroform solution. (b) Cyclic voltammograms for FTAZ, J71, ITIC1, and ITIC2 in CH_3CN/0.1 M $[^nBu_4N]^+[PF_6]^-$ at 100 mV s^{-1}, and the horizontal scale refers to an Ag/AgCl electrode.

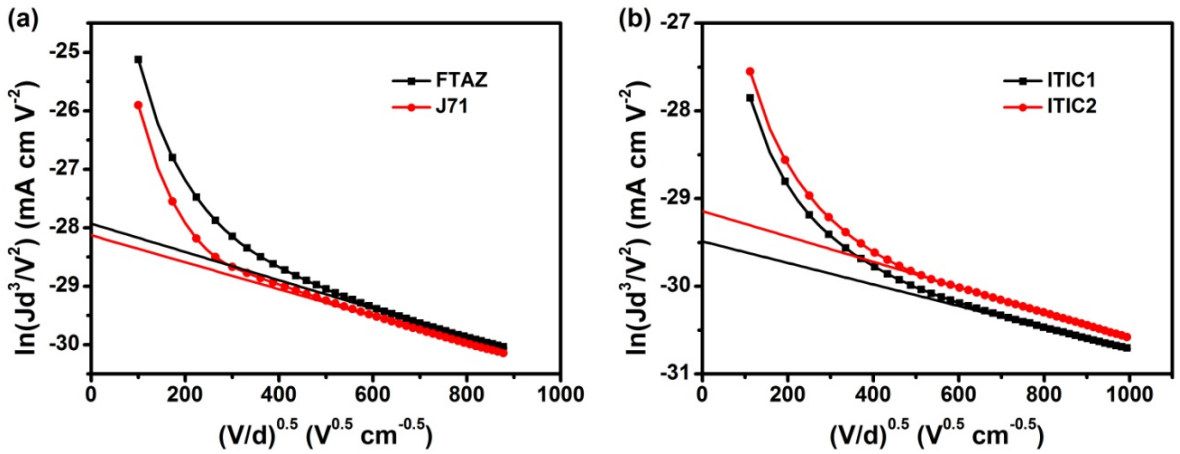

Fig. S2 *J-V* characteristics in dark for (a) hole-only devices based on FTAZ and J71; (b) electron-only devices based on ITIC1 and ITIC2.

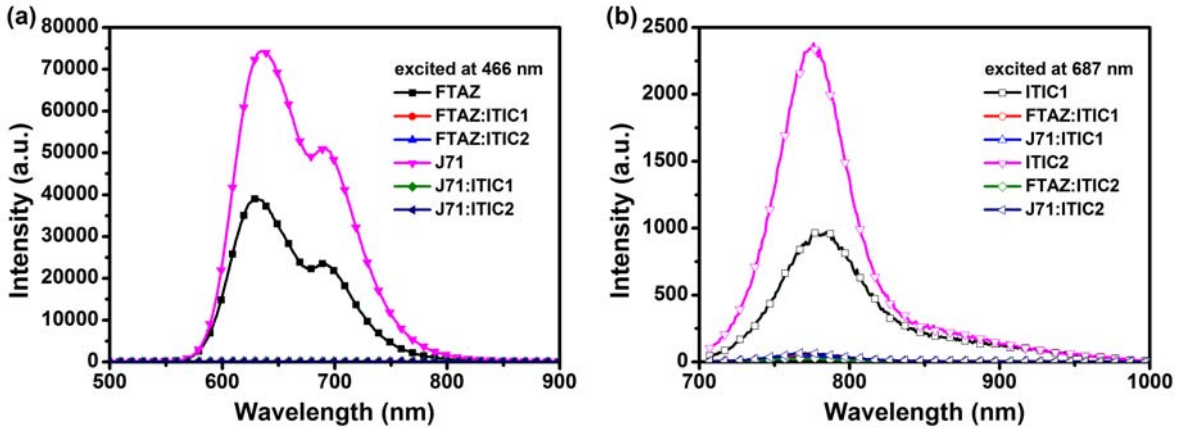

Fig. S3 PL spectra of (a) FTAZ, J71, and four blended films with same thickness (excited at 466 nm); (b) ITIC1, ITIC2, and four blended films with same thickness (excited at 687 nm).

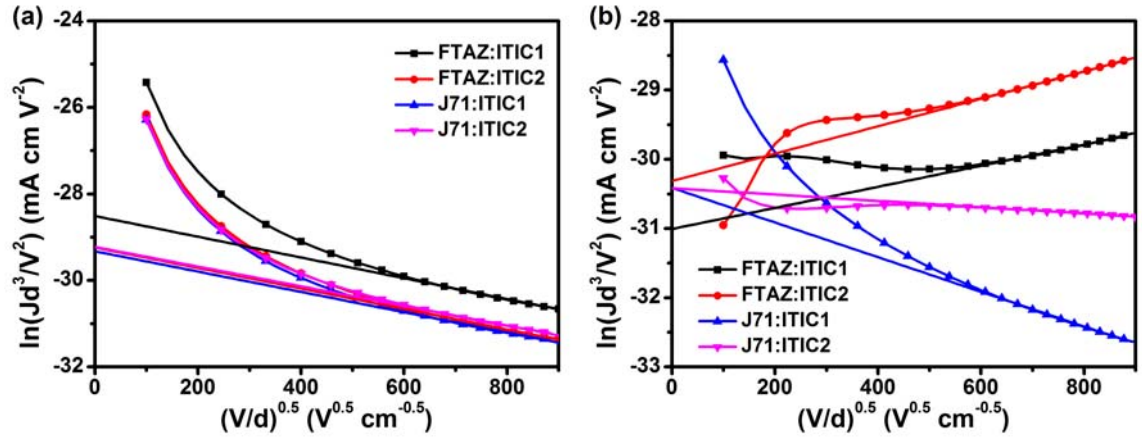

Fig. S4 *J-V* characteristics in dark for (a) hole-only and (b) electron-only devices.

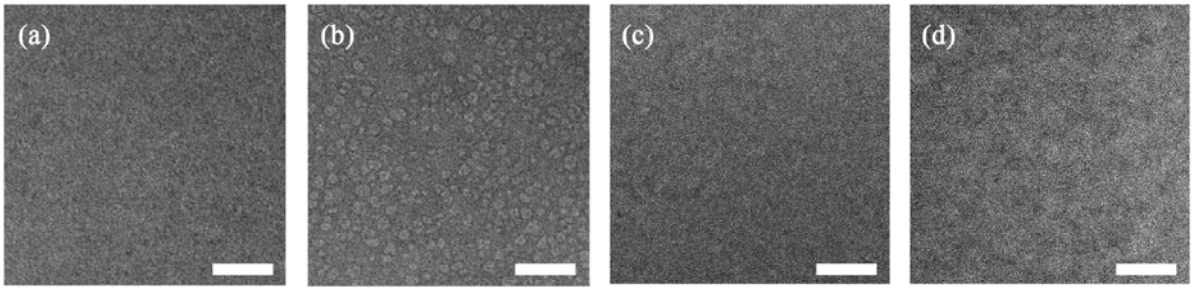

Fig. S5 TEM images of (a) FTAZ:ITIC1, (b) FTAZ:ITIC2, (c) J71:ITIC1, and (d) J71:ITIC2.

Scale bar: 200 nm.

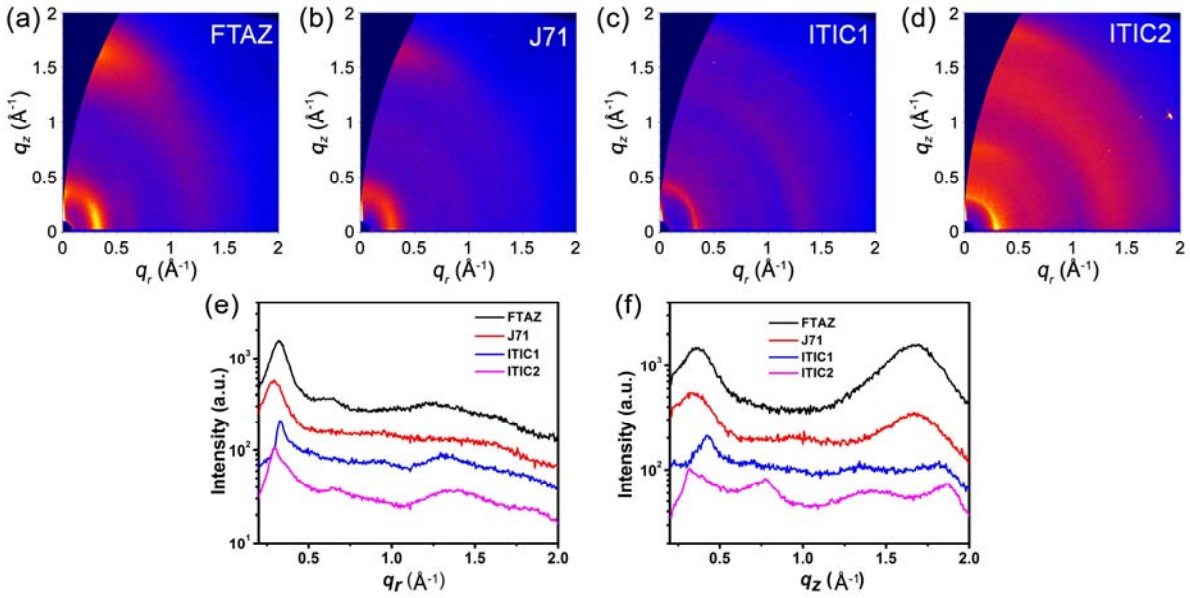

Fig. S6 (a-d) 2D GIWAXS patterns of FTAZ, J71, ITIC1, and ITIC2 neat films. The corresponding intensity profiles along the (e) in-plane and (f) out-of-plane directions.

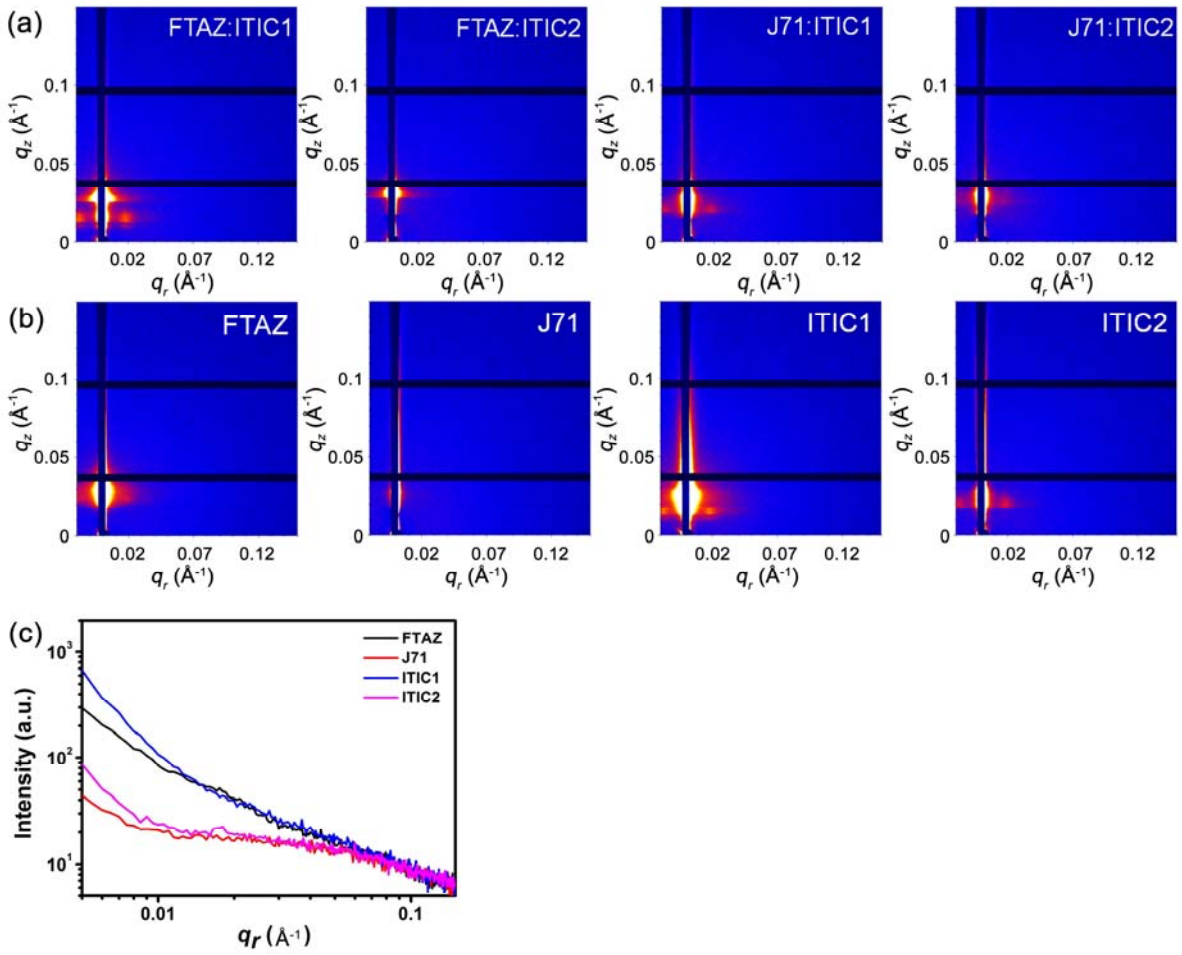

Fig. S7 2D GISAXS patterns of (a) the blend films and (b) the pure donors and acceptors. (c) the corresponding intensity profile of the pure donors and acceptors along the in-plane directions.

References

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