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A Universal Nonfullerene Electron Acceptor Matching with Different Bandgap Polymer Donors for High-Performance Polymer Solar Cells

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Materials and Measurements

All solvents and reagents were used as received from commercial sources and used without further purification unless otherwise specified. m-ITCHO (Scheme S1) was purchased from Solarmer Materials Inc. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were measured on a MERCURYVX300 spectrometers. Elemental analyses of carbon, hydrogen, and nitrogen were performed on a Vario EL III microanalyzer. UV-vis-NIR absorption spectra were recorded on a Shimadzu UV-2700 recording spectrophotometer. Cyclic voltammetry (CV) measurements were carried out on a CHI voltammetric analyzer at room temperature. Tetrabutylammonium hexafluorophosphate (n-Bu_4NPF_6, 0.1 M) was used as the supporting electrolyte. The conventional three-electrode configuration consists of a platinum working electrode with a 2 mm diameter, a platinum wire counter electrode, and a Ag/AgCl wire reference electrode. Cyclic voltammograms were obtained at a scan rate of 100 mV/s. PL spectra were measured with a Shimadzu RF-5301PC fluorescence spectrophotometer. The film morphology was measured using an atomic force microscope (AFM, Bruker-ICON2-

SYS) using the tapping mode. The RMS values of the surface AFM images are averaged based on five times testing on different areas for each sample. DFT calculations were performed by using Gaussian at the B3LYP/6-31G* level, and the long alkyl chain was simplified as methyl. TEM images were performed on a JEOL JEM-1400 transmission electron microscope.

Mobility Measurements

Hole and electron mobility were measured using the space charge limited current (SCLC) method. The SCLC mobilities were calculated by MOTT-Gurney equation: $J = 9\varepsilon_0\varepsilon_r\mu V^2/8L^3$. Where J is the current density, ε_r is the relative dieletiric constant of active layer material usually 2-4 for organic semiconductor, herein we use a relative dielectric constant of 3, ε_0 is the permittivity of empty space, μ is the mobility of hole or electron and L is the thickness of the active layer, V is the internal voltage in the device, and $V = V_{Applied} - V_{Built\text{-}in}$ (in the hole-only and the electron-only devices, the V_{bi} values are 0.2 V and 0 V respectively), where $V_{Applied}$ is the voltage applied to the device, and $V_{Built\text{-}in}$ is the built-in voltage resulting from the relative work function difference between the two electrodes.

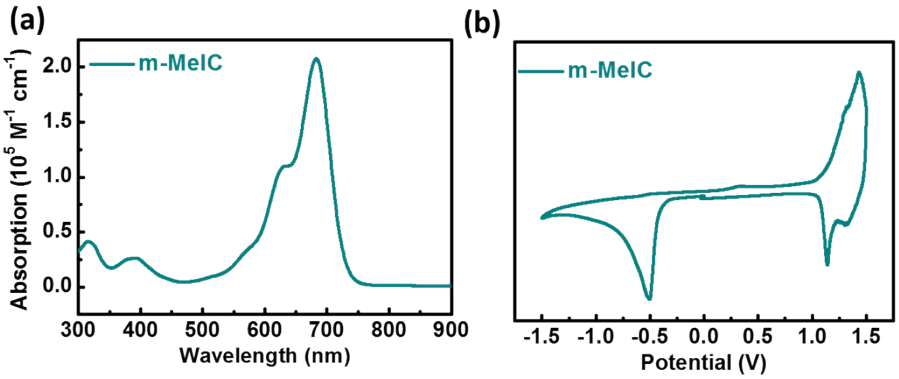


Figure 1. (a) UV-vis absorption spectra of m-MeIC in chloroform solution; (b) cyclic voltammograms of m-MeIC.

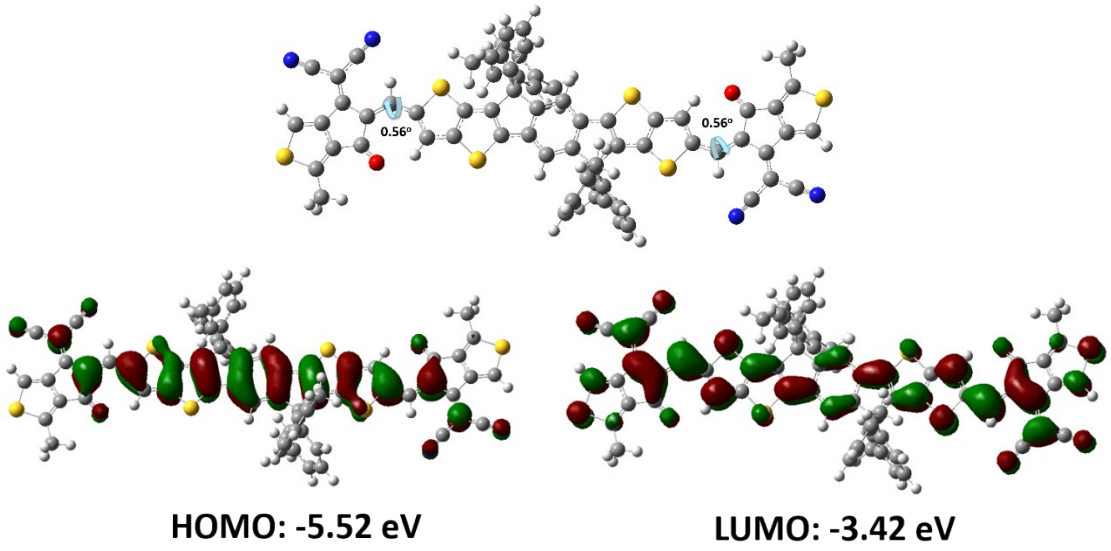


Figure S2. The optimized molecular structure and frontier molecular orbitals obtained by DFT calculations for m-MeIC.

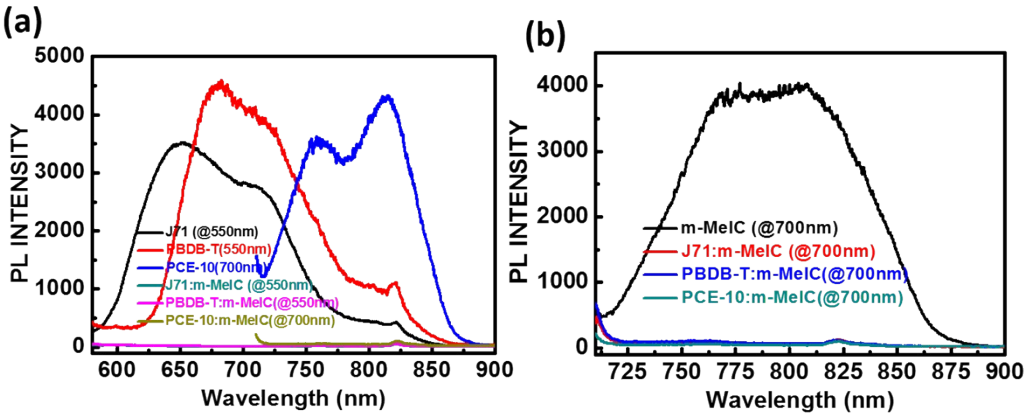


Figure S3. Photoluminescence spectra of the polymers J71, PBDB-T, PCE-10 and m-MeIC as well as the blend films of J71: m-MeIC, PBDB-T: m-MeIC and PCE-10:m-MeIC(excited at 550 and 700 nm, respectively).

Table S1. Photovoltaic performance parameters of the PSCs based on PTB7-Th/acceptors (the E_g of acceptor is close at 1.58 eV).

Donor	Acceptor	E_g (eV)	PCE (%)	*Reference*
PTB7-Th	**IDIC**	1.62	5.24	1
PTB7-Th	**ITIC-Th**	1.60	8.70	2
PTB7-Th	**IC-2IDT-IC**	1.57	4.38	3
PTB7-Th	**IC-3IDT-IC**	1.53	1.05	3
PTB7-Th	**DC-IDT2Tz**	1.60	5.81	4
PTB7-Th	**ITIC**	1.59	6.80	5
PTB7-Th	**m-MeIC**	1.54	8.34	This work

Table S2. The hole and electron mobility of Polymer donors:m-MeIC.

Device	μ_h (10^{-4} cm^2 v^1 s^{-1})	μ_e (10^{-4} cm^2 V^{-1} s^{-1})	μ_e/μ_h
J71:m-MeIC	2.06	2.52	1.22
PBDB-T:m-MeIC	2.18	2.69	1.24
PCE-10:m-MeIC	1.36	1.85	1.36

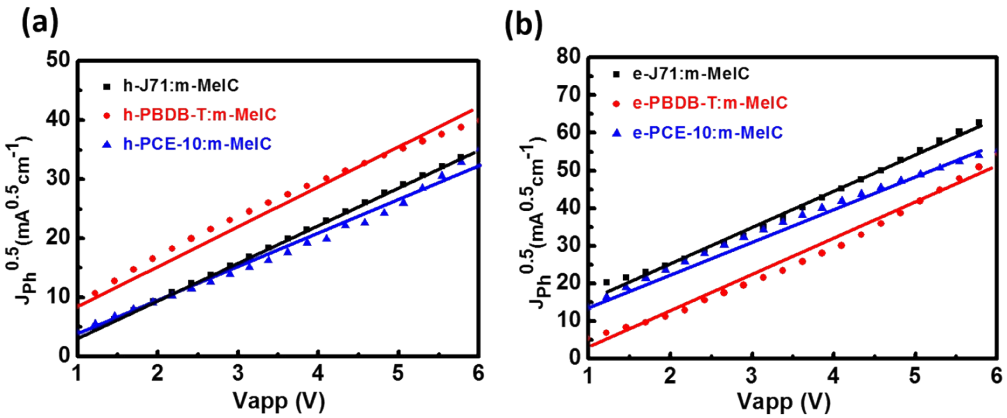
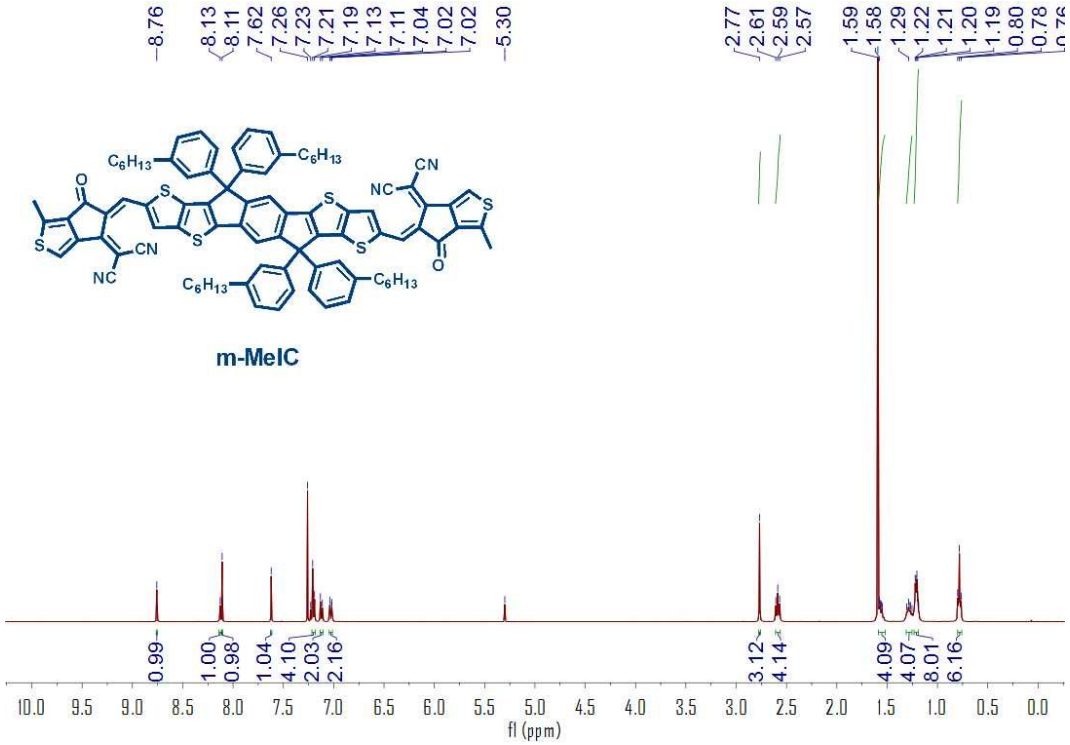


Figure S4. (a) J71:m-MeIC, PBDB-T:m-MeIC and PCE-10:m-MeIC blend films in hole-only devices; (b) J71:m-MeIC, PBDB-T:m-MeIC and PCE-10:m-MeIC blend films in electron-only devices.

Figure S5. 1H NMR of m-MeIC.



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