Photovoltaic Materials Hot Paper

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Design, Synthesis, and Photovoltaic Characterization of a Small Molecular Acceptor with an Ultra-Narrow Band Gap

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Abstract: The design of narrow band gap (NBG) donors or acceptors and their application in organic solar cells (OSCs) are of great importance in the conversion of solar photons to electrons. Limited by the inevitable energy loss from the optical band gap of the photovoltaic material to the open-circuit voltage of the OSC device, the improvement of the power conversion efficiency (PCE) of NBG-based OSCs faces great challenges. A novel acceptor-donor-acceptor structured nonfullerene acceptor is reported with an ultra-narrow band gap of 1.24 eV, which was achieved by an enhanced intramolecular charge transfer (ICT) effect. In the OSC device, despite a low energy loss of 0.509 eV, an impressive short-circuit current density of 25.3 mA cm⁻² is still recorded, which is the highest value for all OSC devices. The high 10.9% PCE of the NBGbased OSC demonstrates that the design and application of ultra-narrow materials have the potential to further improve the PCE of OSC devices.

Bulk-heterojunction (BHJ) organic solar cells (OSCs)^[1,2] have attracted considerable attention for their great potential in making large area flexible solar panels through low-cost coating methods, and the power conversion efficiencies (PCEs) of OSC devices have been boosted to over 11 %.^[3-6] As a type of device that converts sunlight into electricity, the application of photoactive materials with broad optical absorption spectra is deemed one of the key methods to promote PCE of solar cells.^[7-11] Successful single-crystal silicon solar cells, which possess a broad optical absorption band covering the entire region below 1100 nm, have demonstrated a high PCE over 25%.^[12] In the field of OSCs, therefore, it is very important to design and apply narrow band gap (NBG) photovoltaic materials for further improvement of photovoltaic performance.

Over the past decade, many polymers and small molecules with absorption spectra extending to the near infrared region have been designed and applied to OSCs.^[13–15] Significant progress has been achieved in OSC devices with photoresponse ranges within 800 nm, corresponding to an optical

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band gap (E_g^{opt}) over 1.55 eV, and PCEs over 11% have been demonstrated.^[3] However, further extending the photoresponse range to the infrared region often causes significant energy losses^[16-19] $(E_{loss} = E_g^{opt} - eV_{OC})$ from the E_g^{opt} to the open-circuit voltage (V_{OC}) of the device. To date, the most efficient OSC devices with $E_g^{opt} = 1.2 \pm 0.1$ eV only showed a low PCE of 5–6% with a high short-circuit current density (J_{SC}) over 20 mA cm⁻² but very low V_{OC} (0.4–0.5 V), corresponding to an E_{loss} of approximately 0.6–0.8 eV.^[20–21] Therefore, designing novel photovoltaic materials to significantly promote the PCE of NBG-based OSC devices is still a great challenge in the field.

Many efficient molecular design strategies have been developed to broaden the absorption spectra of conjugated polymers, such as the introduction of strong electron-donating groups,^[21-23] the formation of quinoid structures and donoracceptor (D-A) alternating copolymerization.^[10,24-25] Facile manipulation of the intramolecular charge transfer (ICT) from an electron-rich unit to an electron-deficient unit confers D-A structured conjugated polymer donors with absorption spectra that can be easily tuned to over 1000 nm.^[19-21] Recently, acceptor-donor-acceptor (A-D-A) structured small molecules, such as IEIC and ITIC, have emerged as highly efficient non-fullerene acceptors^[4,16,26-29] with absorption spectra limited at about 800 nm. Furthermore, researchers have reported non-fullerene-based OSC devices that show very small energy losses.^[16,30-31] Therefore, it is of great interest and importance to further extend the absorption spectra of non-fullerene small molecular acceptors; this can be easily realized by enhancing the ICT effect.

To broaden the absorption spectrum of the A-D-A structured small molecule IEIC,^[26] we introduced alkoxyl groups and fluorine atoms onto its D and A moieties, respectively, to enhance the ICT effect. In comparison to IEIC, the absorption spectrum of the newly designed nonfullerene acceptor IEICO-4F (see Supporting Information) was redshifted approximately 200 nm with an ultra-narrow E_{a}^{opt} of 1.24 eV.^[31] Use of six different polymer donors in the OSC devices all yielded impressive J_{SC} values over 20 mA cm⁻² despite low energy losses of approximately 0.5 eV. Furthermore, two of the donors were selected to fabricate the ternary OSC device for a complementary absorption, and a further improvement of J_{SC} to 25.3 mA cm⁻² was achieved, which is among the top values of all OSC devices. The optimal ternary OSC device gave a high PCE of 10.9%, demonstrating the great potential application of ultra NBG small molecular acceptors in the field of OSCs.

Theoretical calculations were conducted using density functional theory (DFT) to understand the influence of

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alkoxyl groups and fluorine atoms on the properties of A-D-A structured small molecules.^[32] IEIC and IEICO-4F did not show great differences in their optimized molecular conformations and the electron distributions of the frontier molecular orbitals (Supporting Information, Figure S1a). When compared with IEIC, IEICO-4F shows an up-shifted highest occupied molecular orbital (HOMO) level, a down-shifted lowest unoccupied molecular orbital (LUMO) level, and thus a decreased calculated band gap of approximately 0.22 eV. Additionally, we evaluated the strength of the intramolecular interaction between the electron-rich and the electrondeficient moieties by calculating the dipole moment of the molecules. Since both of the molecules have symmetrical structures (Supporting Information, Figure S1b),



Figure 1. a) Theoretical simulation of the intramolecular dipole moments of half molecule models using a DFT method. b) Synthetic procedure of IEICO-4F; mPEG = poly(ethylene glycol) methyl ether.

their overall dipole moments are very small. Therefore, we incorporated the half molecular models (Figure 1 a) into the calculation, and the results show that the dipole moment increases from 8.65 to 9.19 Debye for IEIC and IEICO-4F, respectively, suggesting the ICT effect from the electron-rich core unit to the electron-deficient unit is enhanced after modification.

Figure 1 b shows the synthetic procedure for IEICO-4F. The key intermediate, compound **5** (2-(5,6-difluoro-3-oxo-2,3-dihydro-1*H*-inden-1-ylidene)malononitrile), was obtained from 4,5-dichlorophthalic acid (compound **1**) in four steps. Firstly, compound **1** was converted to its anhydride by an intramolecular dehydration reaction, after which a halogen exchange reaction was performed in the aprotic polar solvent sulfolane at high temperature. Subsequently, compound **4** was obtained by reduction from compound **3**, and a dicyanovinylene moiety was added to afford compound **5**. Finally, the Knoevenagel Condensation reaction was conducted between compound **5** and compound **6** to produce IEICO-4F in high yield. Theoretically, IEICO-4F may have some regioisomers

because of differing double bond linkages. However, the possible regioisomers were not found on analysis of the nuclear magnetic resonance (NMR) spectra (include ¹H, ¹³C, ¹⁹F, and their decoupled spectra; see Supporting Information). Therefore, the configuration at the lowest energy is adopted to represent the chemical structure of IEICO-4F (Supporting Information, Figure S2).

As shown in Figure 2a, in chloroform solution, IEICO-4F shows a main absorption band from 600–900 nm, and the film has a red-shift of approximately 100 nm with an absorption onset of approximately 1000 nm, corresponding to an E_g^{opt} of 1.24 eV. There is a 0.26 eV decrease of E_g^{opt}

when compared with IEIC $(E_g^{opt} = 1.50 \text{ eV})$.^[31] Since the absorption band of IEICO-4F is located in the near-infrared region, suitable polymer donors with complementary absorption spectra should be carefully selected to absorb more solar photons when applying IEICO-4F in OSC devices. From the cyclic voltammetry (CV) plots (Figure 2b), we can determine that the HOMO level (-5.44 eV) is up-shifted and the LUMO (-4.19 eV) is down-shifted for IEICO-4F compared with the values for IEIC (HOMO = -5.47 eV, LUMO = -3.90 eV),^[31] which is consistent with the theoretical calculation and the absorption spectrum measurements. Furthermore, the electron mobility of IEICO-4F was evaluated by the space-charge-limited current method, as shown in Figure S3 (Supporting Information), and an electron mobility of $1.14 \times 10^{-4} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ was recorded.

To investigate the photovoltaic performance of the novel ultra NBG electron acceptor, we first blended PBDTTT-EFT^[33] (also known as PTB7-Th^[34]) and J52^[16] (Figure 3 a,b) as polymer donors in the OSC devices. The two polymers show different absorption bands covering 300–800 nm, and



Figure 2. a) Normalized absorption spectra of IEICO-4F in chloroform solution and as a thin solid film. b) CV plot of IEICO-4F film measured in Bu_4NPF_6 acetonitrile solution at a scan rate of 50 mVs⁻¹.

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Figure 3. a) Molecular structures and energy level diagram for PBDTTT-EFT and J52. b) Normalized absorption spectra for the donor films. c) *J-V* curves of the binary OSC devices fabricated by PBDTTT-EFT:IEICO-4F and J52:IEICO-4F. d) EQE curves of the corresponding binary OSC devices.

their HOMO levels are located at similar positions. As shown in the current density and voltage (*J-V*) curves (Figure 3 c) and the corresponding photovoltaic parameters in Table 1, the PBDTTT-EFT:IEICO-4F device yielded a PCE of 10.0% with an impressive $J_{\rm SC}$ of 22.8 mA cm⁻² and a $V_{\rm OC}$ of 0.739 V,

Table 1: Detailed photovoltaic parameters for the binary OSC devices.

Device	V _{oc} [V]	ر [mA cm ⁻²] ^[a]	FF	PCE [%] ^[b]
PBDTTT-EFT:IEICO-4F	0.739	22.8 (22.4)	0.594	10.0 (9.7)
J52:IEICO-4F	0.734	21.9 (21.4)	0.585	9.4 (9.3)

[a] Calculated integrated current density from EQE spectra. [b] Average PCE values obtained from ten devices are shown in parentheses.

and the corresponding energy loss is as low as 0.501 eV. Meanwhile, the J52:IEICO-4F-based OSC device demonstrated comparable $J_{\rm SC}$ and $V_{\rm OC}$ values with those of the PBDTTT-EFT:IEICO-4F-based device, and a PCE of 9.4% was recorded. Under the same device processing conditions, the two polymer donors yielded moderate PCEs when PC71BM or IEICO were used as acceptor materials (Supporting Information, Table S1). Furthermore, we selected another polymers, including PBDTTT-E-T,^[35] PBDTSfour DTBTO,^[36] PBQ-3,^[37] and PBDB-T^[38] (Supporting Information, Figure S4), as donor materials for the fabrication of IEICO-4F-based devices because of their good applicability in fullerene-free OSC devices. These polymers have varied optical absorption bands (E_{g}^{opt} ranging from 1.55 to 1.77 eV), and the four OSC devices show V_{OC} values ranging from 0.689 to 0.771 V. As presented in Table S2 (Supporting Information), the four devices all yielded $J_{\rm SC}$ values over 20 mA cm⁻² even though they have relatively low energy losses from 0.469 to 0.551 eV.

As shown in Figure 3d, the external quantum efficiency (EQE) curve of the PBDTTT-EFT:IEICO-4F-based device shows very high EQE values in the long wavelength region from 600–900 nm, and the edge of the photoelectron response reached near 1000 nm. Even though the calculated integrated current density from the EQE spectrum is as high as 22.4 mA cm⁻² for the PBDTTT-EFT:IEICO-4F-based device, its EQE values in the region 300–600 nm are relatively low for their limited absorption bands of donor and acceptor. For the EQE curve of the J52:IEICO-4F-based device, a similar phenomenon was observed. High EQE values in the regions of 300–600 nm and 800–900 nm were recorded. However, the EQE values in the region 600–800 nm are quite low because the main absorption band of J52 is located at 400–600 nm.

With the purpose of further improving the photocurrent by using more solar photons in the whole region of 300–1000 nm, we fabricated a ternary OSC device based on PBDTTT-EFT and J52 as donors and IEICO-4F as acceptor.^[39,40] As both of the binary OSC devices have similar $V_{\rm OC}$ and FF values, the resulting ternary OSC device is not expected to have many changes in comparison. Different blend ratios (J52:PBDTTT-EFT; 0.1:0.9, 0.3:0.7, and 0.5:0.5) for the two donors were scanned to obtain an optimal

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photovoltaic performance for the ternary OSC devices (Figure 4 and Table 2). In comparison with the binary devices, the J_{SC} values of the ternary OSC devices show big changes with an increase of J52 content, while $V_{\rm OC}$ (0.731–0.737 V) and FF values (0.580-0.603) display small variations. Impressively, by increasing the J52 content to 30%, the J_{SC} of the ternary OSC device reaches 25.3 mA cm⁻²; to the best of our knowledge this is among the top values for all types of OSCs. The optimal ternary OSC device was tested by the National Institute of Metrology, China, and a similar PCE of 10.6% was recorded (Supporting Information, Figure S5). From the EQE curves we can clearly find that the photoelectron response of the ternary OSC devices in the short wavelengths are enhanced with the addition of J52. The integrated current density first increase to 23.1 and 24.1 mA cm⁻² and then drops to 22.6 mA cm⁻² for the ternary OSC devices with donor ratios of 0.1:0.9, 0.3:0.7, and 0.5:0.5, respectively.



Figure 4. a) J-V curves of the ternary OSC devices at different blend ratios (J52:PBDTTT-EFT:IEICO-4F). b) EQE curves of the corresponding ternary OSC devices.

Table 2: Detailed photovoltaic parameters of the ternary OSC devices at different blend ratios.

Device	V _{oc} [V]	ر [mA cm ⁻²] ^[a]	FF	PCE [%] ^[b]
0.1:0.9:1.5	0.737	23.7 (23.1)	0.603	10.5 (10.2)
0.3:0.7:1.5	0.731	25.3 (24.1)	0.589	10.9 (10.5)
0.5:0.5:1.5	0.732	23.9 (22.6)	0.580	10.1 (9.9)

[a] Calculated integrated current density from EQE spectra. [b] Average PCE values obtained from ten devices are shown in parentheses.

Atomic force microscopy (AFM) and transmission electron microscopy (TEM) measurements (Figure 5) were performed to investigate the morphology of the blend films. Figure 5 a–c displays the AFM height images of blend films, from which we can find that J52:IEICO-4F presents a relatively rough surface with a mean-square roughness (R_q) of



Figure 5. a-c) AFM height images of the binary films and the ternary film at a donor ratio of 0.3:0.7. d-f) TEM patterns of the binary and ternary blend films.

1.53 nm compared to PBDTTT-EFT:IEICO-4F films ($R_q = 1.22$ nm), and that the addition of J52 (30%) does not cause a very significant change in the surface roughness of the PBDTTT-EFT:IEICO-4F host blend ($R_q = 1.25$ nm). Furthermore, the phase separation properties of the ternary blend (Supporting Information, Figure S6) are close to those of the PBDTTT-EFT:IEICO-4F film. Nanoscale phase separation morphologies with appropriate domain sizes are also observed in the TEM images (Figure 5d–f). The favorable nanoscale phase separation properties should benefit the charge generation and transport processes in the devices, and thus high J_{SC} values could be obtained.

To obtain more insight into the exciton dissociation, and the carrier transport and collection processes of the OSCs, we measured the photocurrent dependence (J_{ph}) on the light density (P_{light}) and the effective voltage (V_{eff}) of the devices.^[27,41,42] The J_{ph} versus V_{eff} plots (Supporting Information, Figure S7a) show that the devices obtained saturated photocurrents (J_{sat}) at relatively low voltages of approximately 2 V. The $J_{\rm ph}/J_{\rm sat}$ ratios under short-circuit conditions are calculated as 0.86, 0.88, and 0.89 for the devices fabricated with PBDTTT-EFT:IEICO-4F, J52:PBDTTT-EFT:IEICO-4F, and J52:IEICO-4F, respectively, suggesting the overall charge collection processes are quite efficient.^[43] Furthermore, the power-law exponents of the relationship $J_{\rm ph} \propto P_{light}^{S}$ (Supporting Information, Figure S7b) for the devices are all close to 1, indicating minor bimolecular recombination occurs in both binary and ternary devices.^[27]

In summary, by enhancement of the ICT effect for an A-D-A structured small molecule, we have successfully designed and synthesized an ultra NBG non-fullerene acceptor, IEICO-4F, with an ultra-narrow E_g^{opt} of 1.24 eV.

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IEICO-4F shows HOMO and LUMO levels of -4.19 and -5.44 eV, respectively. Using six different polymer donors, high J_{SC} values over 20 mA cm⁻² were all recorded in the corresponding OSC devices, despite low energy losses of approximately 0.5 eV. Moreover, we have demonstrated that J_{SC} can be further improved to 25.3 mA cm⁻² using a ternary OSC device; this is among the top values of all OSC devices. The optimal ternary OSC device yields a high PCE of 10.9%, suggesting the great potential of ultra NBG small molecular acceptors in the field of OSCs.

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Conflict of interest

The authors declare no conflict of interest.

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Communications

Photovoltaic Materials
H. Yao, Y. Cui, R. Yu, B. Gao, H. Zhang, J. Hou* ∎∎∎−∎∎∎

Design, Synthesis, and Photovoltaic Characterization of a Small Molecular Acceptor with an Ultra-Narrow Band Gap



Mind the gap: A non-fullerene electron acceptor with an ultra-narrow optical band gap of 1.24 eV was prepared. Despite a low energy loss of 0.509 eV, the organic solar cell (OSC) device demonstrated a high power conversion efficiency of 10.9% with an impressive short-circuit current density of 25.3 mA cm⁻².

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