Full paper

14%-efficiency fullerene-free ternary solar cell enabled by designing a short side-chain substituted small-molecule acceptor

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Abstract

A new fused-ring electron acceptor (FREA) IEICF-DMOT was designed and synthesized with 3,4-dimethoxythiophene (DMOT) as the π− bridges to link the IDT core and the end IC-2F units. Compared to IEICO-4F which uses 3,4-dialkylthiophene as the bridge, IEICF-DMOT with two much shorter side chains (methoxy) on the π− bridge exhibits a higher level of the lowest unoccupied molecular orbital (LUMO) (−3.85 vs. −3.93 eV), broadening absorption band, larger absorptivity, and a larger bandgap (1.38 vs. 1.27 eV), but reduced crystallinity in both the in-plane (100) and out-of-plane (010) directions, which makes a 0.13 V-larger open-circuit voltage (Voc) with a 10%-higher external quantum efficiency (EQE) and 9%-higher fill factor (FF), and thereby, a power conversion efficiency (PCE) of 13% in comparison with the IEICO-4F 10% efficiency. Adding the crystalline and narrower bandgap IEICO-4F as the near infrared absorber, the PBDB-T:IEICO-4F:IEICF-DMOT ternary blend shows increased crystallinity for both donor and acceptor phases with increased hole and electron mobilities, achieving increased short-circuit current-density (Jsc) and FF, and therefore, a promising PCE of 14%. These results indicate that DMOT with short side-chains on the thiophene-3,4-positions is a promise bridge unit to design nonfullerene small-molecule acceptors with tunable energy levels, optical bandgap, and crystallinity to simultaneously increase Voc, EQE, and FF, and ultimately, efficiency.

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1. Introduction

Polymer solar cell (PSC) that employs a blend of an electron donor polymer and an electron acceptor small-molecule has received a great attention in the past decades due to their potentials to convert the green sustainable solar light into electric power in ways that are low-cost, lightweight, semi-transparency, and mechanical-flexibility. Breakthroughs have been recently achieved with the ITIC (3,9-bis(2,2'-methylene-(3-(1,1-dicyanomethylene)indanone))-5,5,11,11-tetrakis(4-n-hexylphenyl)-dithieno[2,3-d:2,3′d′]-s-indaceno[1,2b:5,6b′]dithio- phene) [1] like fused-ring nonfullerene small molecules [2–15] and the dithionothiophen[3,2,b]-pyrrolobenzothiadiazole based acceptors [16,17] such as Y6 [18], which leads to over 14% power conversion efficiencies (PCEs) reported from binary devices recently [19,20]. These molecules are constructed in either A−D−A or A−π−D−π−A type, in which the fused-ring electron-donating (D) unit is linked with the fused-ring electron-accepting (A) units through a single carbon-carbon bond or a π−bridge. A distinct feature of the ITIC like acceptors is the perpendicular side-chains attached on the fused sp3-carbon of the electron-rich core [21], such as on the 4,4,9,9-positions of IDTT (4,4,9,9-tetrasubstitutedp-hexylphenyl)-4,9-dihydros-s-indaceno[1,2-b:5,6-b′]dithiophene) core, which act as steric effects to direct the acceptor molecules packing into a three-dimensional (3-D) J−π type architecture in which the perpendicular side-chains orient in the out-of-plane (OOP)

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Keywords:
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**A B S T R A C T**

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considered to pair with a donor polymer having a higher-HOMO-level with PBDTT-E-T, though the device $V_{oc}$, Bo et al. had reported that compared to the usage of the 3-(2-ethylhexoxy)thiophene for IEICO-4F, using 3,4-di(2-ethylhexoxy)thiophene led to the upshifting of the LUMO level of that acceptor, therefore, obtained a much larger $V_{oc}$ (0.897 vs. 0.771 V) when pairing with the donor polymer of PBDB-T [45]. Nevertheless, the device FF was yet low, only 64%. The relatively low FF might be associated with its great crystallinity originated from the long side-chains of the π–bridge. Taken considerations of these, we turn to choose DMOT, which contains the much short methoxyl, rather than the relatively long 2-ethylhexyl, as the side chains so as to not only raise the LUMO level but also reduce the crystallinity.

Our results indicate that compared to IEICO-4F, the newly synthesized IEICF-DMOT shows much broadening absorption with a larger full-width-at-the-half-maximum value (4073 vs. 2143 cm$^{-1}$), a larger absorption coefficient (2.9 vs. 2.2 × 10$^{-10}$ M$^{-1}$ cm$^{-1}$), a higher LUMO energy (−3.85 vs. −3.93 eV), a larger $E_{0.1}$ (1.39 vs. 1.29 eV), but reduced crystallinity in both the in-plane (IP) and out-of-plane (OOP) directions. When pairing with PBDB-T [55], a PCE of 13% with a $V_{oc}$ of 0.87 V, a $J_{sc}$ of 22.1 mA/cm$^2$, and an FF of 67.5% is obtained. In comparison, the IEICO-4F binary solar cell shows a PCE of 10% with a $V_{oc}$ of 0.74 V, a $J_{sc}$ of 23.1 mA/cm$^2$, and an FF of 58.4%. When using IEICO-4F as the near infrared (NIR) absorber, the resulting ternary device with a ratio of PBDB-T:IEICF-DMOT:IEICO-4F = 1:1:0.1 supplies a PCE of 14% with increased $J_{sc}$ and FF.

2. Results and discussion

2.1. Synthesis

The IEICF-DMOT was synthesized by following the procedures shown in Fig. 2. An aldehyde group was first introduced onto the commercial 3,4-dimethoxythiophene 5-position in a yield of 72% with $n$-ButLi and DMP as the solvent medium. The product of DMOT-CHO was then brominated on the 2-position, a yield of 72% with $n$-ButLi and DMP as the solvent medium. The product of DMOT-CHO was then brominated on the 2-position, a yield of 72% with $n$-ButLi and DMP as the solvent medium. The product of DMOT-CHO was then brominated on the 2-position, a yield of 72% with $n$-ButLi and DMP as the solvent medium. The product of DMOT-CHO was then brominated on the 2-position, a yield of 72% with $n$-ButLi and DMP as the solvent medium. The product of DMOT-CHO was then brominated on the 2-position, a yield of 72% with $n$-ButLi and DMP as the solvent medium. The product of DMOT-CHO was then brominated on the 2-position, a yield of 72% with $n$-ButLi and DMP as the solvent medium. The product of DMOT-CHO was then brominated on the 2-position, a yield of 72% with $n$-ButLi and DMP as the solvent medium. The product of DMOT-CHO was then brominated on the 2-position, a yield of 72% with $n$-ButLi and DMP as the solvent medium. The product of DMOT-CHO was then brominated on the 2-position, a yield of 72% with $n$-ButLi and DMP as the solvent medium. The product of DMOT-CHO was then brominated on the 2-position, a yield of 72% with $n$-ButLi and DMP as the solvent medium. The product of DMOT-CHO was then brominated on the 2-position, a yield of 72% with $n$-ButLi and DMP as the solvent medium.
2.2. Optical and electrochemical properties

In dilute chloroform solution, IEICF-DMOT exhibits an absorption band positioning at 733 nm, which is much blue-shifted compared to that of IEICO-4F (Fig. 3a). The absorption coefficients are of 2.9 and 2.2 × 10⁻⁵ M⁻¹ cm⁻¹, respectively, for IEICF-DMOT and IEICO-4F (Table 1). In thin film, IEICF-DMOT shows an absorption peak at 766 nm. The absorptivity is 1.64 and 0.85 × 10⁻⁵ cm⁻¹, respectively, for IEICF-DMOT and IEICO-4F (Table 1). The Eopt value is estimated to be 1.38 eV from the absorption onset of the film (892 nm), which is increased by 0.11 eV compared to that of IEICO-4F (1.27 eV, 964 nm). The full-width-at-the-half-maximum (FWHM) values are of 2417 and 1876 cm⁻¹ for IEICF-DMOT and IEICO-4F, respectively, for their dilute chloroform solutions, respectively, and in the thin films, they are 4073 and 2143 cm⁻¹, respectively.

From the cyclic voltammetry (CV) data (Fig. S1), the LUMO/HOMO energy levels were determined under the same conditions to be −5.24 and −5.11 eV, and their LUMO energies are of −3.38 and −3.31 eV, respectively. The experimental and DFT calculation data match well in the same trend. The HOMO and LUMO distributions are both similar for the two molecules. The 3-carbon of the bridged thiophene is a node of the acceptor LUMO, while the bridged thiophen-4-carbon is a node of the HOMO. Therefore, the oxygen on the bridged thiophen-3-carbon contributes to the HOMO, while no contributions to the LUMO. Oppositely, its 4-position oxygen contributes to the LUMO, but little to the acceptor HOMO.

2.3. Crystallinity of IEICF-DMOT and IEICO-4F

The crystallinity of the pure IEICF-DMOT and IEICO-4F films have been tested with graze-incidence wide-angle X-ray scattering (GIWAXS). The data are shown in Fig. 4. The (100) peaks are observed at about 0.30 Å⁻¹ in the IP direction for IEICF-DMOT and IEICO-4F, respectively. The (010) scattering peaks are seen at about 1.79 and 1.81 Å⁻¹ in the OOP direction, corresponding to a ππ− stacking distance of 3.51 and 3.47 Å. Compacted ππ− stacks are formed for IEICO-4F. Another distinct difference is seen in the diffraction intensity. The (010) and (100) scattering are much more intense for IEICO-4F, suggesting greater crystallinity which is relative to the long side chains, 2-ethylhexyloxyl, on the bridged thiophene-3-positions. Nevertheless, similar crystalline coherent length (CCL) values are estimated for both IEICO-4F and IEICF-DMOT, either in the OOP (010) or the IP (100) directions as shown in Table 1, meaning that the replacement of the 3-(2-ethylhexylthiophene) with DMOT as the bridge does not reduce the crystalline coherent size of the aggregated domains.

2.4. Solar cell device property

The photovoltaic property of IEICF-DMOT was investigated using a normal device structure of ITO/PEDOT:PSS [57]/PBDB-T:IEICF-DMOT/PDINO/Al. Here, PBDB-T is poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b′]dithiophene-2-yl)-5,7-bis(2-ethylhexyl)benzo[1,2-c,4,5-c′]dithiophene-4,8-dione) [58] and PDINO is amino N-oxide perylene diimide [59]. The weight ratio of PBDB-T:IEICF-DMOT was 1:1 and a thermal annealing process at 100 °C for 10 min was applied to the active layer. 1% DIO (1,8-diiodooctane) was used for optimizing the IEICO-4F binary devices. No solvent additives were used for the optimizations of the IEICF-DMOT based binary and ternary solar cells. The optimizations were shown in Table S2.

Fig. 5a displays the current-density – voltage (J−V) curves from the optimal cells. The Voc and Jsc and FF of the PBDB-T:IEICF-DMOT device are of 0.870 V, 22.14 mA/cm² and 0.675, which ultimately afford a PCE of 13.01% (Table 2). The energy loss Eloss is estimated to be 0.51 eV by following Eq. Eloss = Eopt − Voc. Compared to the PBDB-T:IEICF-4F cell, the Voc from IEICF-DMOT based device is improved by 0.13 V, the FF is increased by 9%. The larger Voc provides a larger internal field, which contributes to the obtaining of the higher device FF. Due to the larger bandgap of IEICF-DMOT, the PBDB-T:IEICF-DMOT

Fig. 3. (a) The absorption spectra of the polymer PBDB-T in thin film (solid line) and acceptors IEICF-DMOT and IEICO-4F in solution (chloroform, dash lines) and in pure thin films (solid lines). (b) The diagram of energy levels of the polymer and acceptors.
Table 1
Optical and electrochemical properties of the acceptor IEICF-DMOT along with the CCL values.

<table>
<thead>
<tr>
<th></th>
<th>ɛ&lt;sub&gt;max&lt;/sub&gt; [10&lt;sup&gt;5&lt;/sup&gt;M&lt;sup&gt;-1&lt;/sup&gt;cm&lt;sup&gt;-1&lt;/sup&gt;]</th>
<th>λ&lt;sub&gt;max&lt;/sub&gt; &lt;sup&gt;film&lt;/sup&gt; [nm]</th>
<th>FWHM [cm&lt;sup&gt;-1&lt;/sup&gt;]</th>
<th>Absorptivity [10&lt;sup&gt;5&lt;/sup&gt; cm&lt;sup&gt;-1&lt;/sup&gt; cm&lt;sup&gt;2&lt;/sup&gt;1]</th>
<th>E&lt;sub&gt;g&lt;/sub&gt;&lt;sup&gt;opt&lt;/sup&gt; [eV]</th>
<th>LUMO [eV]</th>
<th>HOMO [eV]</th>
<th>CCL [nm]</th>
<th>OOP</th>
<th>IP</th>
</tr>
</thead>
<tbody>
<tr>
<td>IEICF-DMOT</td>
<td>2.9</td>
<td>733</td>
<td>2417</td>
<td>4073</td>
<td>1.48</td>
<td>-3.85</td>
<td>-5.49</td>
<td>4.9</td>
<td>24.6</td>
<td></td>
</tr>
<tr>
<td>IEICO-4F</td>
<td>2.2</td>
<td>806</td>
<td>832</td>
<td>1676</td>
<td>0.85</td>
<td>-3.93</td>
<td>-5.39</td>
<td>5.6</td>
<td>23.6</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 4. The GIWAXS data of the pure IEICO-4F (a) and IEICF-DMOT (b) films and the line-cut profiles in the out-of-plane (c) and in-plane (d) directions, respectively.

The blend covers a narrower wavelength region of the solar spectrum, 300–890 nm, in comparison to the 300–960 nm coverage for the IEICO-4F blend. However, thanks to the higher external quantum efficiency (EQE) responded in the wavelength region of 450–800 nm (Fig. 5b), larger J<sub>sc</sub> value is still obtained: 21.5 mA/cm<sup>2</sup> for the IEICF-DMOT and 22.2 mA/cm<sup>2</sup> for the IEICO-4F device.

IEICF-DMOT and IEICO-4F are of structural similarity and IEICO-4F shows a narrower optical bandgap, which encourages us to use IEICO-4F as a second acceptor component. The photovoltaic properties of the ternary devices with the IEICO-4F contents varying from 0.05 to 0.3 are given in Table S3. The best device was obtained when using 0.1 IEICO-4F as the third component, which showed a PCE of 14% with 0.3 J<sub>sc</sub> and 0.3 FF values obtained from integrating the EQE spectra match well with those values from the J–V measurements (Table 2).

2.5. Charge mobilities

The hole and electron mobilities (μ<sub>h</sub> and μ<sub>e</sub>) of the binary and ternary solar cell blends were measured with space-charge-limited current (SCLC) method. The data were given in Fig. S3. Both the μ<sub>h</sub> and μ<sub>e</sub> values of the IEICO-4F based binary blend are higher than the IEICF-DMOT based (8.39 vs. 3.72 × 10<sup>-4</sup> cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup> for μ<sub>h</sub> and 4.32 vs. 1.93 × 10<sup>-4</sup> cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup> for μ<sub>e</sub>). Upon addition of 0.1 IEICO-4F resulting a ternary ratio of PBDB-T:IEICF-DMOT:IEICO-4F = 1:1:0.1, the μ<sub>h</sub> and μ<sub>e</sub> value are 5.33 vs. 3.18 × 10<sup>-4</sup> cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup>, respectively, which is increased either for the hole or the electron mobility in comparisons to that of the IEICF-DMOT based binary. The increase in both the electron and hole mobilities upon addition of 0.1 IEICO-4F into the 1:1 blended PBDB-T:IEICF-DMOT film a factor of the increased EQE of the ternary in comparison to that of the IEICF-DMOT binary device.

2.6. Recombination losses and collection of mobile charges

The recombination mechanisms of the mobile charges can be reflected by studying the light-dependent J–V characteristics of the solar cell [60]. By plotting the J<sub>sc</sub> and V<sub>oc</sub> as a function of light intensity (Figs. S4a and b) in a power law equation J<sub>sc</sub> ∝ P<sup>α</sup> and the Eq. V<sub>oc</sub> ∝ n<sup>α</sup>(kT/q) ln(P), where k, T, and q are the Boltzmann constant, temperature in Kelvin, and the elementary charge, respectively, α and n value are fitted. The α or n value approaches 1.0, indicating the recombination is dominated by the monomolecular or bimolecular mechanism at short-circuit or open-circuit, while if it deviates from 1.0, it means the involvement of bimolecular or monomolecular recombination. The fitting α/n values are 0.99/1.09KT/q, 0.99/1.11KT/q and 0.98/1.08KT/q for the IEICF-DMOT and IEICO-4F based binary and their ternary devices, respectively, demonstrating that the addition of 0.1 IEICO-4F does not enhance the charge recombination. The α value is close to 1, suggesting the monomolecular recombination is dominated at short-circuit with weak bimolecular loss involved. The n value is about 1.1, meaning the involvements of monomolecular mechanism at open-circuit.

The charge collection efficiency is reflected by the plot of photo-generated current-density (J<sub>ph</sub>) vs. the effective voltage (V<sub>eff</sub>) (Fig. S4c) [61] with V<sub>eff</sub> = V<sub>bi</sub> – V<sub>bi</sub>, where V<sub>bi</sub> is the voltage when J<sub>ph</sub> = 0 mA cm<sup>-2</sup>, and V<sub>bi</sub> is the applied voltage; J<sub>ph</sub> = J<sub>0</sub> – J<sub>B</sub>, where
Table 2
The photovoltaic data of the binary and ternary solar cells. All data were obtained under illumination of the AM 1.5G (100 mW/cm²) light source.

<table>
<thead>
<tr>
<th>Blend</th>
<th>( V_{oc} ) [V]</th>
<th>( J_{ph} ) [mA/cm²]</th>
<th>( FF ) [%]</th>
<th>( PCE ) [%]</th>
<th>CCL_{IP} [nm]</th>
<th>CCL_{OP} [nm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>PBDB-T:IEICF-DMOT:IEICO-4F</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1:1:0</td>
<td>0.87 (0.87 ± 0.01)</td>
<td>22.14 (21.98 ± 0.23)</td>
<td>21.47</td>
<td>67.83 (66.62 ± 1.17)</td>
<td>13.01 (12.79 ± 0.15)</td>
<td>3.6</td>
</tr>
<tr>
<td>1:1:0.1</td>
<td>0.86 (0.86 ± 0.01)</td>
<td>23.31 (23.10 ± 0.24)</td>
<td>22.39</td>
<td>69.75 (69.09 ± 1.38)</td>
<td>14.00 (13.73 ± 0.19)</td>
<td>4.0</td>
</tr>
<tr>
<td>1:0:1</td>
<td>0.74 (0.74 ± 0.01)</td>
<td>23.10 (22.87 ± 0.16)</td>
<td>22.18</td>
<td>58.36 (57.29 ± 1.81)</td>
<td>9.98 (9.81 ± 0.26)</td>
<td>6.7</td>
</tr>
</tbody>
</table>

* The average value of the device parameter are calculated from 20 devices.
* Calculated from the EQE spectra.
* Calculated form the (010) scattering peak around 0.29 Å⁻¹ at the OOP direction.
* Calculated form the (100) scattering peak around 0.29 Å⁻¹ at the OOP direction.

2.7. Film-morphologies

The GIWAXS data of the binary and ternary blends are given in Fig. 6 and Fig. 55. For the IEICO-4F binary blend, a set of strong diffractions seen at 0.0311, 0.476, 1.787 Å⁻¹ at the OOP direction and the strong peak at 0.332 Å⁻¹ at the IP direction both indicate formation of great crystallinity for IEICO-4F, which can be due to the use of 1% 1,8-diiodooctane (DIO) as the solvent additive. For the IEICO-4F pure film, no solvent additives are used. The crystallinity is greatly reduced and no detailed scattering rings or arcs observed between q ~0.4–1.4 Å⁻¹ region. Again, for the IEICO-4F ternary blend, no solvent additives are used and no scattering peaks are seen between the q ~0.4–1.4 Å⁻¹ region. For the IEICF-DMOT binary blend, no solvent additives were used.

We have observed that the IP (100) scattering peak can reflect the packing ordering and crystallinity of the acceptor molecules along the OOP direction, e.g. on the \( \pi\pi \) stacking direction [62]. In these cases, the crystallinity of the acceptor phases can be revealed by the coherent crystalline length (CCL) value calculated from the IP (100) scattering around 0.30 Å⁻¹, and again, by the OOP (010) scattering around 1.8 Å⁻¹, e.g. the \( \pi\pi \)-stacks. The CCL values shown in Table 2 demonstrate the increase of the crystallinity of the acceptor phases upon addition of 0.1 IEICO-4F into the PBDB-T:IEICF-DMOT (1:1) blend. Again, the PBDB-T phase crystallinity is indicated by the OOP (100) scattering around 0.29 Å⁻¹, which is increased upon the addition of IEICO-4F. The trend in the crystallinity going from the IEICF-DMOT binary to the ternary blend is in accordance with the increase of their electron and hole mobilities. Again, the increase in the acceptor phase crystallinity and no additional scattering peaks observed when IEICO-4F is added into the IEICF-DMOT binary blend suggest the mixing of the two acceptors, which is due to the similarity of the molecular structures of the two acceptors.

The morphology of the binary and ternary blends is further characterized with the resonant soft X-ray scattering (RSoXS) at 285.2 eV photon energy. The data were plotted in Iq² versus q format and given in Fig. 7. A strong and broad scattering band peaking around 0.066 Å⁻¹ with a hump at ~0.02 Å⁻¹ is observed from the PBDB-T binary blend, suggesting the formation of multi-length scaled crystalline phase separation. The domain size is calculated to be 47.7 nm. Comparatively, a relatively weak but fine scattering band at 0.098 Å⁻¹ is seen in the IEICF-DMOT binary blend, which corresponds to a smaller domain size, 32.3 nm. The differences in the scattering from the RSoXS experiments further support the distinct changes in the film-morphology upon the replacement of side chains on the thiophene bridge, going from the long 2-ethylhexyl to the short methoxyl ones. For the ternary blend with the addition of 0.1 IEICO-4F into the 1:1 blended PBDB-T:IEICF-DMOT binary, a fine scattering band yet observed implies the formation of homogeneous phase separation. The small shift from the IEICF-DMOT binary 0.098 Å⁻¹ to the ternary 0.090 Å⁻¹ relates to a small increase in the domain size (32.2 vs. 35.0 nm) and the slight increase of the scattering intensity agrees with the small increase in the phase crystallinity, as revealed by the GIWAXS data. Again, the phase purity is slightly increased from 0.62 to 0.64 after the addition of 0.1 IEICO-4F, which is consistent with the maintaining of the device FF.

Fig. 5a–c collects the transmission electron microscopy (TEM) images of the binary and ternary blends. All these three blends show...
nanoscaled phase-separated bright and dark domains. The thinner morphology observed on the IEICF-DMOT in comparison to the crystalline fibril morphology seen on the IEICO-4F blend is consistent with the morphology revealed by the GIWAXS and RSoXS data and agrees with the higher FF of the IEICF-DMOT binary device. Upon addition of IEICO-4F into the PBDB-T:IEICF-DMOT blend, fine and homogenous morphology is observed, which again suggests the mixing of the two acceptors and agrees with the high FF of the ternary solar cell. Fig. 8d–f is the atomic force microscopy (AFM) height images. The AFM reflected surface morphology is very close to that observed from TEM. Fine morphology is seen in the IEICF-DMOT binary and the ternary blend, while fiber-like morphology is observed in the IEICO-4F blend. The room-mean-roughness (rms) value is 2.28 nm, 2.64 nm, and 3.53 nm for the IEICF-DMOT binary, the ternary, and the IEICO-4F binary blend, respectively.

From the TEM images, clear fibril morphology can be seen in the IEICF-DMOT and IEICO-4F binary and their ternary blends. The anisotropic orientation of the fibril structures will induce polarization scattering, which can be clearly seen on their 2D scattering images (Fig. 9a–c). The $I q^2$ versus $q$ plots (Fig. 9d–f) clearly indicate the different integrated sectors with orthogonal angles in the 2D scattering images. Compared to IEICO-4F binary blend, greater difference is seen on the IEICF-DMOT binary blend. The difference is slightly reduced with the addition of 0.1 IEICO-4F into the PBDB-T:IEICF-DMOT binary blend.

3. Conclusions

In summary, we have reported that 3,4-dimethoxythiophene (DMOT) substituted by the methoxyl short side-chains is a promising $\pi$-bridge with which the synthesized small-molecule acceptor like IEICF-DMOT shows reduced crystallinity in both the out-of-plane and in-plane directions and simultaneously has a higher LUMO energy level and improved absorption of solar photons. When pairing with the donor polymer of PBDB-T, simultaneous increased $V_{oc}$, FF, and EQE are readily obtained, in comparisons to the long-side-chain 3-(2-ethylhexyloxy)thiophene bridged acceptor such as the known IEICO-4F, and therefore a higher efficiency (13% vs. 10%) is readily obtained. The ternary device by adding 0.1 of the crystalline IEICO-4F into the PBDB-T:IEICF-DMOT binary blend displays an efficiency of 14% with increased crystallinity and higher electron and hole mobilities, compared to the host binary solar cell.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.nanoen.2019.103934.
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