

End-chain effects of non-fullerene acceptors on polymer solar cells

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ABSTRACT

Four acceptor1-acceptor2-donor-acceptor2-acceptor1 (A1-A2-D-A2-A1) structural electron acceptors with different end-chains were designed and synthesized which all possessed indacenodithiophene (IDT) core, benzothiadiazole (BT) bridge as acceptor2, and rhodanine (R) end groups as acceptor1. The non-fullerene acceptor attached with ethyl group is called IDT-BT-R2 and used as control compound. And the other three of them are attached with methoxymethyl, trifluoroethyl and 1-piperidino groups generating IDT-BT-RO, IDT-BT-RF3 and IDT-BT-RN, respectively. The influence of end-chains on their optoelectronic properties were compared between four non-fullerene acceptors. Compared with IDT-BT-R2, the molecule IDT-BT-RF3 show red-shifted light absorption and lower LUMO level because of the electron withdrawing property of fluorine atoms. OSCs based on IDT-BT-RF3 display more efficient charge separation and lower degree of monomolecular recombination, allowing OSCs to show higher short-circuit current (J_{sc}) than the system of IDT-BT-R2. OSCs based on IDT-BT-RO also show more efficient charge separation and less monomolecular recombination. Due to the elevated LUMO level of the acceptor IDT-BT-RN, organic solar cells (OSCs) utilizing this material as acceptor display high open-circuit voltage (V_{oc}) of 1.10 eV and low energy loss of 0.49 eV when maintaining a relatively high power conversion efficiency (PCE) of 7.09%. We demonstrated that the end-chain engineering could finely tune the light absorption properties and energy levels of novel non-fullerene acceptors and eventually improved OSCs performance can be harvested.

1. Introduction

Organic solar cells (OSCs) are considered to be one of the most prominent renewable energy technologies which enables low-cost and low-environmental impact production and yields light-weight and flexible devices [1,2]. For a long time, the investigation of OSCs utilized fullerene derivatives as acceptor mostly [3–7]. Recently, the rapid development of non-fullerene OSCs (NF-OSCs) [8–14] have drawn extensive attention. Owing to advantages such as broad light absorption, easily tuned energy levels and self-assembling behaviours, lots of NF-OSCs displayed PCE exceeding 12% [15–28].

To improve the performance of NF-OSCs, many efforts have been devoted to adjust the molecule structure of acceptor-donor-acceptor (A-D-A) or A1-A2-D-A2-A1 structural acceptors, achieving lots of progresses. Until now, most of these works concentrated on the modification of fused-ring core [29–32], side chains [33–36] and main chain

structures [37–41]. However, the effects of end-chains on these A-D-A structural acceptors based OSCs have not been discussed a lot [42]. As we know, different heteroatoms possess varying electron withdrawing ability and miscibility [43]. Thus, it could be very interesting to introduce heteroatoms into end-chains of A-D-A structural acceptors. On one hand, electron withdrawing heteroatoms such as oxygen [44] or fluorine [45] atoms could lower the molecular energy level, increase absorption range and dipole moments of electron acceptors by inductive effects. These modifications may help the OSCs to achieve more efficient light absorption and charge separation and thus higher J_{sc} and fill factor (FF). On the other hand, electron donating heteroatoms such as nitrogen atom could elevate energy levels [44]. OSCs based on these materials with higher LUMO level may yield higher V_{oc} and lower energy loss.

In this report, four A1-A2-D-A2-A1 structural acceptors with different end-chains were designed and synthesized based on IDT-BT-R2

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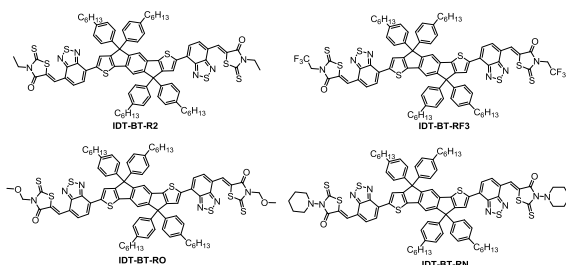


Fig. 1. Molecular structures of four A-D-A electron acceptors.

structure [46], which represents one kind of high efficient electron acceptors [47–49]. IDT-BT-R2 utilized indacenodithiophene (IDT) as core unit, benzothiadiazole as bridge unit (A2) and rhodanine as end group (A1). All other three molecules possess the same main structures as IDT-BT-R2, except for changing the end-chains of rhodanine from ethyl to methoxymethyl, trifluoroethyl and 1-piperidino groups, resulting in three novel acceptors named as IDT-BT-RO, IDT-BT-RF3 and IDT-BT-RN, respectively (Fig. 1). The energy levels and also their dipole moments of the latter three molecules was changed due to inductive effect of heteroatoms. The LUMO-LUMO offsets between polymer donor PTB7-Th and four acceptors are varying from 0.18 eV to 0.34 eV, and the HOMO-HOMO offsets are varying from 0.11 eV to 0.20 eV. Device performances fabricated from these four acceptors and PTB7-Th ranged from 7.09% to 8.96% with energy losses [50] changing from 0.49 eV to 0.57 eV (calculated in supporting information). Because of the deepening energy levels of IDT-BT-RF3 and IDT-BT-RO, the energy offsets in OSC systems based on these two materials are increased compared with IDT-BT-R2 system. Devices results indicated that more efficient charge separation and lower degree of geminate charge recombination were obtained in these two systems. IDT-BT-RF3 based OSCs achieved higher J_{sc} compared with IDT-BT-R2 system, owing to the redshifted absorption, higher electron mobility and more efficient charge separation. In contrast, nitrogen atom incorporated material IDT-BT-RN generated OSCs with high V_{oc} of 1.10 eV and low energy loss of 0.49 eV when maintaining a relatively high PCE of 7.09% due to elevated energy levels. Our results demonstrated that it is a valid way to adjust the properties of A1-A2-D-A2-A1 structural acceptors by attaching different heteroatoms incorporated end-chains.

2. Results and discussion

2.1. Material synthesis and characterization

Four small molecules were synthesized via two facile reactions as depicted in Scheme S1 (In Supporting information). The intermediate compound IDT-BT-CHO was synthesized by Stille coupling reaction between IDT-diTin and Br-BT-CHO using $\text{Pd}(\text{PPh}_3)_4$ as the catalyst. Subsequent Knoevenagel condensation between IDT-BT-CHO and rhodanine derivatives give the products of IDT-BT-R2, IDT-BT-RO, IDT-BT-RF3 and IDT-BT-RN. These molecules were characterized by matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS), ^1H NMR and ^{13}C NMR spectra. All of them are readily soluble in common organic solvents, such as dichloromethane, chloroform, or *o*-dichlorobenzene (*o*-DCB) at room temperature. The thermal properties were characterized by thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). These compounds exhibit decomposition temperatures (5% weight loss) above 300 °C in a nitrogen atmosphere (Figure S2 in supporting information). We note that, although the IDT-BT-RF3 shows 5% weight loss at temperature of 309 °C, this material shows a little weight loss around 200 °C. This indicates that IDT-BT-RF3 have poorer thermal stability than other three materials, but is stable enough to be used as OSC material. The DSC curves of the four materials except IDT-BT-R2 display no obvious peak, which indicates that these materials are low-crystalline (Figure S3 in

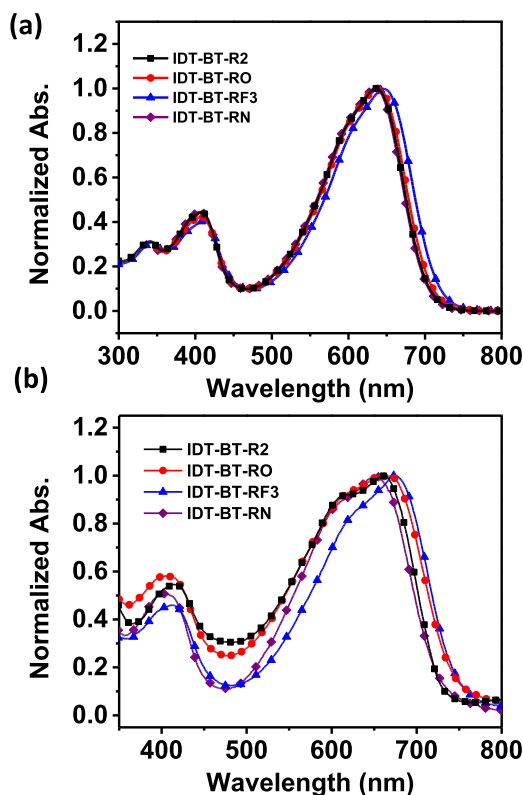


Fig. 2. UV-vis absorption spectra of four acceptors (a) in *o*-DCB solution; (b) as thin films.

supporting information).

The ultraviolet-visible (UV-vis) absorption spectra are depicted in Fig. 2. All acceptors show strong optical absorption from 500 to 700 nm either in the diluted *o*-DCB solution or as thin films. Their solution absorption peaks range from 657 nm to 674 nm, with the extinction coefficient around $1 \times 10^5 \text{ M}^{-1} \text{ cm}^{-1}$. And their thin film absorption peaks further red-shifted with 22–33 nm (Table S1 in supporting information). From solution to film, the IDT-BT-RO red-shifted most, which is probably because of the methoxymethyl chain. It is reported that alkoxy-functionalized molecule has lower steric hindrance than alkyl-functionalized molecule, resulting in higher ordered molecular packing [51–53]. In order to probe the aggregation behaviors of IDT-BT-RO and IDT-BT-R2, we acquired UV-Vis absorption spectra of these two materials in solution (0.02 mg ml⁻¹ in DCB) from 10 °C to 60 °C (Figure S4 in supporting information). The results displayed that both materials showed redshift absorption as the temperature decreasing. The two materials have nearly the same absorption peak at 60 °C which is 631 nm and 632 nm, respectively. After the temperature decrease to 10 °C, the absorption peaks of IDT-BT-R2 and IDT-BT-RO redshifted to 636 nm and 641 nm, respectively. The redshift of IDT-BT-RO is larger than that of IDT-BT-R2. This phenomenon demonstrates that IDT-BT-RO display higher aggregation tendency than IDT-BT-R2.

The energy levels of four acceptors were determined by cyclic voltammetry (CV) measurements with the films on ITO glass working electrode in an acetonitrile solution containing 0.1 mol L⁻¹ of Bu_4NPF_6 using a potential scan rate of 100 mV s⁻¹ (Table S1, Figure S5 in supporting information). The LUMO and HOMO values were evaluated from the onset reduction potential and the onset oxidation potential, respectively. It is found that the energy levels of four molecules are effectively affected by different end chains. Compared with IDT-BT-R2 (LUMO = -3.70 eV, HOMO = -5.31 eV), IDT-BT-RO and IDT-BT-RF3 have lower LUMO/HOMO levels of -3.74/-5.33 eV and -3.78/-5.35 eV, respectively. And IDT-BT-RN display elevated LUMO/HOMO level of -3.62/-5.26 eV. Considering the electron-withdrawing effect

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