

## A novel thiazole based acceptor for fullerene-free organic solar cells



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### A B S T R A C T

In this work, an electron-withdrawing thiazole ring is used as a bridged unit in the design of the small molecular electron acceptor. The new electron acceptor, namely DC-IDT2Tz, was designed with indacenodithiophene as core and 1,1-dicyanomethylene-3-indanone as end-capped unit, and thiazole ring as spacers. Compared with the thiophene spacer, the thiazole bridge exhibited blue-shifted absorption and deep energy levels, which provides more complementary absorption and large driving-force for the exciton dissociation. Besides it has remained some advantages of the thiophene linked acceptors, such as strong and broad absorption in visible light region and planate backbone. The device based on PTB7-Th as the donor material and DC-IDT2Tz as the acceptor material exhibited a high PCE of 5.81%.

### 1. Introduction

Great improvement in field of bulk heterojunction (BHJ) organic solar cells (OSCs), make them promising sustainable power source. Over past decade, organic solar cells gain attention of scientific community due to their distinct advantages: (i) low-cost (ii) mechanical flexibility (iii) light weight (iv) possibility for large-area industrial (due to roll-to-roll method) (v) properties of donor and acceptor materials can be easily tuned (structural flexibility) [1–7]. In a long time, fullerene derivatives as electron acceptors played a major role in OSCs [8–11]. However, the drawbacks of fullerene derivatives like poor light absorption, limited chemical and energetic tunabilities, high-cost purification and morphology instability and film brittleness, are obstacle to further improve efficiency and practical applications [12–14]. Therefore, designing of alternative acceptors is ultimate need. Recently, many efforts have done [15–18] and efficiencies over 12% have been achieved for fullerene-free OSCs [19–22].

Among of them, indaceno[2,1-*b*:6,5-*b'*]dithiophene (IDT) and 1,1-dicyanomethylene-3-indanone (DC) based fullerene-free electron acceptors are regarded as a promising generation. The rigid and coplanar structure of IDT unit is beneficial for charge transport [23] and four hexylphenyl groups on peripheral position of coplanar backbones help control the solubility and intermolecular interactions of the target molecule [24]. While the strong electron-withdrawing ability of DC benefit give the low energy levels [25]. The combination of them

endow the according acceptor the deep energy level and high strong and broad absorption spectrum with a narrow bandgap, and good electron mobility. In 2014, Zhan et al. reported a small molecule non-fullerene acceptor, DC-IDT2T, based on IDT as a core and DC as end-capped units and thiophene as  $\pi$ -bridges. The according BHJ OSCs with PBDTTT-C-T as electron donor exhibited a modest power conversion efficiency (PCE) of 3.93% [26]. Further they introduced 3-(2-ethylhexyl) thiophene as a spacer, affording compound IEIC. When blended with PTB7-Th, the highest PCE of this device is 6.3% [27]. In addition, 4-((2-ethylhexyl)-oxy)thiophene as a linker was investigated by Hou et al., named as IEICO. PBDTTT-E-T:IEICO based OSCs give a high PCE of 8.4% [28]. In these work, the bridged units are all electron-donating unit. They play an important role on the absorption and energy levels, as well as the device performance. The electron-withdrawing bridged unit has been rarely reported so far in this system.

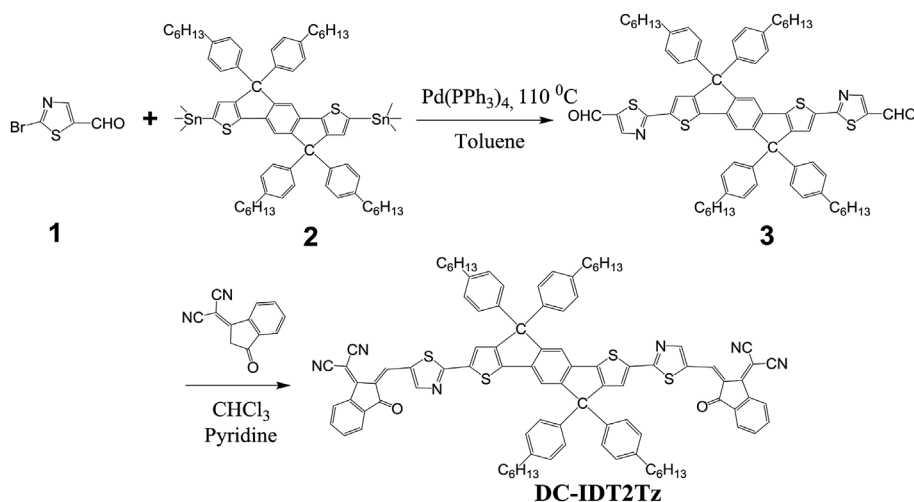
It is known that replacement of a CH group with a nitrogen atom within an aromatic unit increases the electron affinity [29]. So, thiazole is a typical electron-withdrawing heterocycling compound because of the electron-deficient nitrogen of imine (C=N). Thiazole and its close analogues containing thiazolothiazole [30], 5,5'-bithiazole [31] and bridged-bithiazole [32] based small molecules or conjugated polymers were used as electron donors in solution processed OSCs, and high PCEs were achieved in combination with fullerene acceptor. But their application in electron acceptors are still less. Here, to minimize the steric hindrance of the spacers, we have chosen thiazole to replace thiophene

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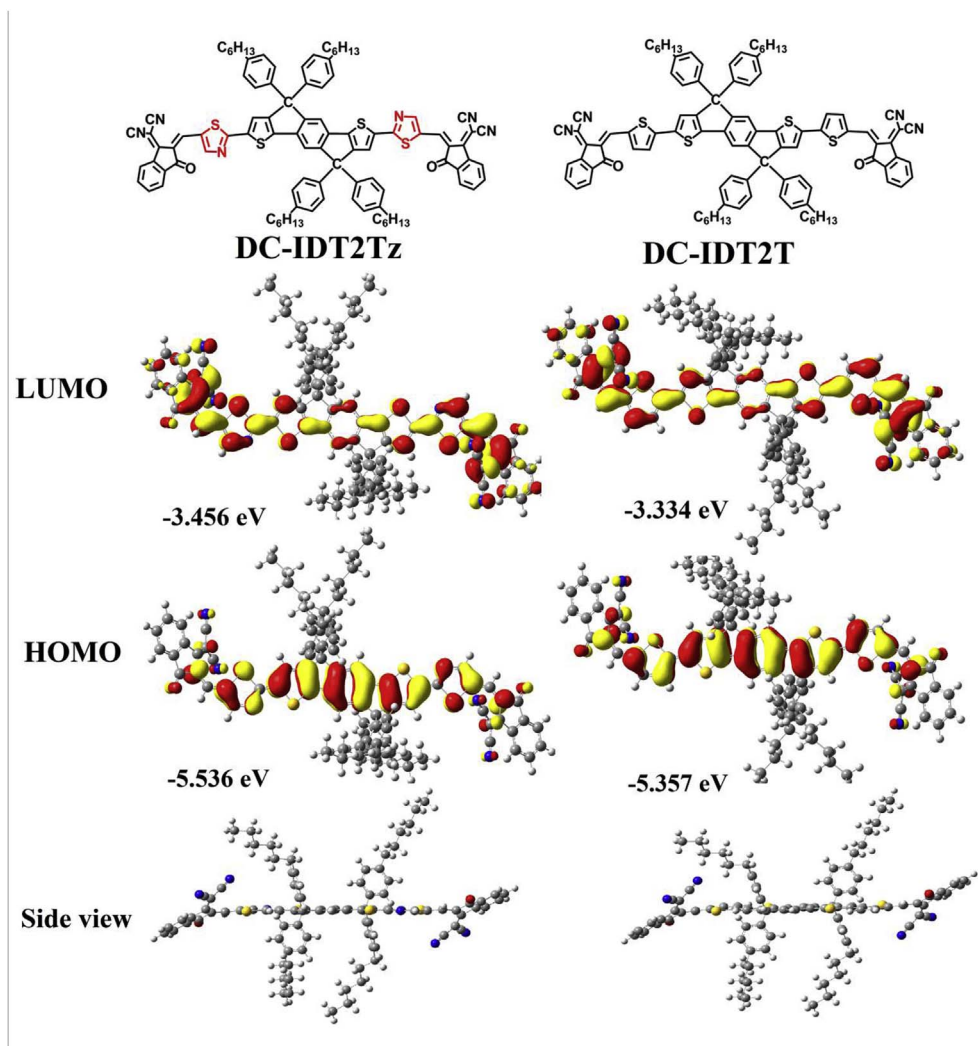
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as the  $\pi$ -bridge, as shown in [Scheme 1](#), affording a novel compound DC-IDT2Tz containing IDT as core and DC as end-capped unit. The solution processed BHJ OSCs based on PTB7-Th: DC-IDT2Tz showed a PCE as high as 5.81%. When we were revising this paper, Huang et al. also reported the same molecular design [33].

Firstly, we evaluated the molecular energy levels of the different spacers with density functional theory calculations at the B3LYP/6-31G

(d, p) level. As shown in [Fig. 1](#), from DC-IDT2T to DC-IDT2Tz, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) levels are gradually decreased by introducing a electron-withdrawing thiazole spacer. Relative to DC-IDT2T, the HOMO level of DC-IDT2Tz is 0.18 eV higher, and its LUMO level is 0.12 eV lower, making the bandgap of DC-IDT2Tz 0.06 eV larger. In addition, the change of the spacer has a little effect on the electron



**Fig. 1.** The optimized molecular geometries and frontier molecular orbitals of DC-IDT2Tz and DC-IDT2T.

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