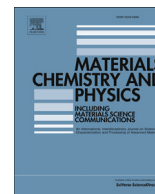




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Density functional study on the effect of aromatic rings flanked by bithiophene of novel electron donors in small-molecule organic solar cells

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HIGHLIGHTS

- A series of novel donors were designed based on a previously reported molecule.
- A study on the effects of aromatic rings flanked by bithiophene was performed.
- HOMO energy level goes up while E_g goes down along with the cycle extension.
- The charge transfer/transport characteristics of the molecules were investigated.
- The final designed compounds show more favorable photoelectronic properties.

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ABSTRACT

In order to further improve the short-circuit current (J_{SC}) and the overall performance of the already synthesized donor molecule (1s) used in organic heterojunction solar cells, six new A-A-D-A-A type small molecules composed of different donor (D, electron rich) and same acceptor (A, electron poor) moieties were designed and characterized by using density functional theory (DFT), time-dependent density functional theory (TD-DFT) and Marcus theory. Through calculating frontier molecular orbital energy levels and spectra properties, we found that HOMO level goes up while E_g goes down along with the cycle extension of the center part flanked by bithiophene. Next, character of excited state, ionization potentials (IPs) and charge transport properties were also investigated to provide an in-depth insight into the charge transfer/transport characteristics and the J_{SC} of organic solar cells. The results reveal that compounds 3c, 3n and 3^o exhibit favorable J_{SC} and comparable performance to original molecule (1s) and show promising potential in organic solar cells.

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1. Introduction

Organic solar cells (OSCs) have attracted much attention because of their advantages of light weight, mechanical flexibility, low energy consumption in fabrication, and low-cost manufacturing [1,2]. Among various OSC devices, bulk heterojunction solar cells comprising bi-continuous interpenetrating networks of organic donor molecules and fullerene derivatives acceptor have demonstrated remarkable achievements, these networks greatly increased D/A interface area and effectively achieved the separation of exciton to free charge [3]. Currently, polymer

donor solar cells have made great progress and the highest power conversion efficiency (PCE) reported has been over 10% [4]. In spite of the high PCE , there are disadvantages for polymer donors: (1) the high molecular weight dispersity; (2) the batch to batch reproducibility. In contrast with polymer donors, conjugated small molecules can offer several advantages including high purity, well-defined molecular structures, definite molecular weights and high charge carrier mobility [5,6]. The power conversion efficiencies of small-molecule based OSCs have reached 10% for single layer bulk heterojunction solar cells, which are approaching to those of their polymer counterparts [7,8]. Currently, compared with polymer solar cells, the optimized open-circuit voltage (V_{OC}) as well as the fill factor (FF) for small-molecule organic solar cells (SMOSCs) is usually higher. However, the short-circuit current (J_{SC}) for SMOSCs are still far behind those for polymer-based solar cells. It implied

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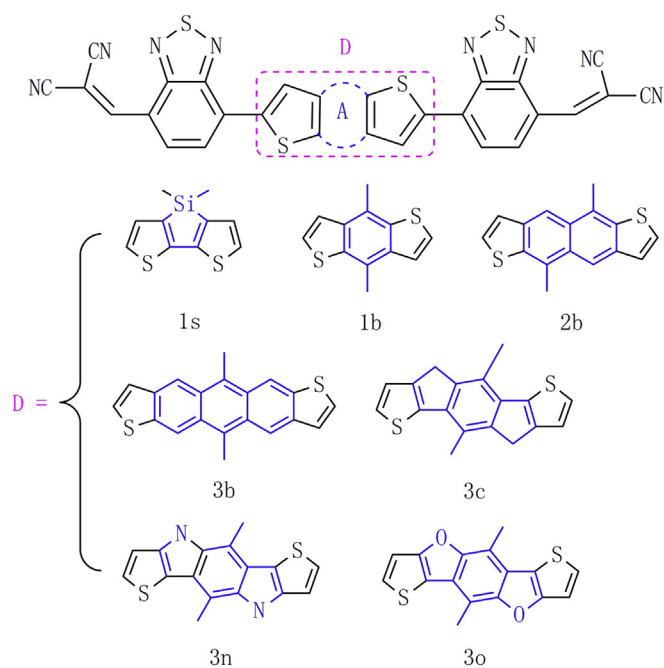
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that among three important performance parameters (V_{OC} , J_{SC} and FF), the property requiring the most improvement is J_{SC} . Hence, the question now is how to improve J_{SC} while retaining the best performance of V_{OC} and FF for small-molecule donors.

Recently, Lin et al. synthesized a new A-A-D-A-A-type small-molecule donor (BCNDTS) [9], which possess a band gap of 2.17 eV. When it blended with [6,6]-phenyl C_{61} -butyric acid methyl ester (PC₆₁BM) using in OSCs, the PCE is up to 2.3%. To narrow the energy gap, they simultaneously obtained another molecule (BDCDTS, 1s) [9] which possess a band gap of 1.88 eV by using the stronger electron-withdrawing dicyanovinylene end groups. However, the 1s/PC₆₀BM cell shows lower PCE (0.07%) with a relatively lower V_{OC} (0.43 V) and a drastically reduced J_{SC} (0.73 mA/cm²). Therefore, we hope to find a suitable method to increase the J_{SC} of 1s-based organic solar cell. The photocurrent generation for J_{SC} is related with not only the absorption efficiency (η_A) but also the exciton diffusion efficiency (η_{ED}), charge separation efficiency (η_{CS}) and charge collection efficiency (η_{CC}) [10–12]. Hence, to obtain an rational small-molecule donor material, all the above factors should be taken into consideration, which are difficult problems in the experiment [13]. Fortunately, quantum chemical methods could rapidly screen out efficient donor materials, and provide a visual aid for understanding how molecular structure and properties affect device performance, saving synthesis efforts and economical cost [14,15].

The introduction of planar heteroarenes into π -conjugated organic small-molecule backbones as donor units has been proven to be able to bring several desirable characteristics into the corresponding materials, such as higher charge mobility, broader light absorption and larger J_{SC} owing to increasing effective conjugation length by facilitating π -electron delocalization [16–18]. Interestingly, He et al. had found that, upon increasing the number of fused rings as donor units, the packing structures as well as the J_{SC} of the relative molecules were obviously improved [19]. A series of three-ring-fused heterocycle-bridged bithiophenes planar donor units, such as cyclopenta[2,1-b:3,4-b'] dithiophene (CPT) [20] dithiophene (CPT) [21–23], dithieno-[3,2-b:2',3'-d]silole (DTS) [24], dithieno[3,2-b:2',3'-d]pyrrole (DTP) [25,26], and dithieno[3,2-b:2',3'-d]thiophene (DTT) [27,28] indicate the benefits of a bigger thienoacene, such as charge-mobility enhancement, band-gap reduction and the improvement of J_{SC} . A reduction of aromaticity in aromatic units in conjugated main chain is also an effective way to reduce the band gap and further optimize the overall performance of OSCs [29–33]. These works performed by predecessors provide some important information on how to design and judge a highly efficient donor of small-molecule organic solar cells.

Based on the studies above, we further optimized the electron-donating unit of the ever modified molecule to systematically discover better donors. As shown in Scheme 1, bithiophene flanking one or more aromatic rings was chosen as a template, since the flanking thiophenes would reduce steric hindrance and the novel donors containing benzodithiophene (BDT) unit or its analogs have high hole mobility and suitable electronic energy levels because the rigid, planar donor center is conducive to molecular conjugation and intermolecular π - π packing [34]. In this work, we modified the center part (A) by cycle extension and exchange of different five-membered rings (such as silole, cyclopentadiene, pyrrole, and furan) and six-membered phenyl aim to find the effects on the performance of donor materials, thereby obtaining six symmetric A-A-D-A-A-structured molecules. According to the number and variety of rings in part A, they were named 1b, 2b, 3b, 3c, 3n and 3o, respectively. This work presents an opportunity to understand many of the factors governing the J_{SC} for the fundamental semiconductor property and provides insightful strategy to the future rational design of conjugated donor materials. We expected to find



Scheme 1. Chemical structure of studied molecules.

more promising donor candidates than 1s for small molecule solar cells.

2. Theoretical method

Geometry optimization and simulation of optical absorption spectra were performed by DFT and TD-DFT in the Gaussian 09 package [35], respectively. The side chain alkyl of molecules merely aided in improving solubility without affecting electronic and optical properties [36]. Therefore, to simplify the calculation, all alkyl branched-chains were replaced by methyl groups. To evaluate the reliability of computational method used in the molecular system, we calculated highest occupied molecular orbital (HOMO) level, lowest unoccupied molecular orbital (LUMO) level and band gaps of 1s by using three different hybrid functionals including B3LYP [37], O3LYP [38] and PBE0 [39] and fixing basis set at 6-31G(d). As showing in Table S1, the calculated results of HOMO and LUMO energy levels as well as the energy gaps (E_g) at B3LYP/6-31G(d) level agree well with the experimental values [9]. Thus, the ground state geometries of all the molecules were optimized within B3LYP functional, using 6-31G(d) basis set. Based on the optimized geometries, the harmonic vibrational frequency calculations were performed at the same theoretical level to check the nature of the stationary point. In order to find an appropriate functional to simulate spectra properties, we choose B3LYP, O3LYP and PBE0 again to calculate the absorption spectra of 1s. As listed in Table S2, among those methods, the TD-PBE0/6-31G(d) approach reproduces the experimental results well. Therefore, we simulated the following absorption spectra using the same method. Partial density of states (PDOS) were visualized with GaussSum software [40]. Meanwhile, the electron-hole coherence of charge transfer upon electronic transitions were investigated by means of the transition density matrix (TDM) [41–43] and electron density difference (EDD) [44,45] implemented in Multiwfn 2.1 [46]. All calculations were carried out in gas phase.

J_{SC} is intimately related to charge transport property of donor materials, which is described by the incoherent hopping mode [46]

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