

# Diketopyrrolopyrrole based highly crystalline conjugated molecules for application in small molecule donor-polymer acceptor nonfullerene organic solar cells



Jianyu Yuan\*, Wanli Ma\*\*

Institute of Functional Nano & Soft Materials (FUNSOM), Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Soochow University, 199 Ren-Ai Road, Suzhou Industrial Park, Suzhou, Jiangsu, 215123, PR China

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## ABSTRACT

In order to specifically investigate the low efficiency of small molecule donor-polymer acceptor (M-P) nonfullerene organic solar cells, we have successfully modify the synthesis of a series of D- $\pi$ -A- $\pi$ -D conjugated molecules containing diketopyrrolopyrrole (DPP) and different end groups. By incorporation of end group with different size of  $\pi$ -conjugation (benzene, naphthalene and pyrene), we further improved the fill factor (*FF*) and short current density ( $J_{sc}$ ) of the donors molecule. Our experimental results and theoretical calculations have proven that the size of the end groups can influence the molecule crystallinity, mobility and intermolecular packing by altering the molecular coplanarity. As the result of improved crystallinity, morphology and fine-tuned mobilities, we demonstrated an increased *FF*, a high  $J_{sc}$  of  $\sim 4.5$  mA/cm<sup>2</sup> and a power conversion efficiency of 2.05%, which is among the highest efficiency reported for M-P nonfullerene solar cells. Our results provide opportunities and possibilities of achieving higher performance M-P nonfullerene solar cells in the future.

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## 1. Introduction

Organic solar cells made of solution-processed bulk heterojunction (BHJ) organic materials are potential low-cost alternatives for renewable energy generation [1]. During the past decade, synergistic efforts in donor materials (small molecules, oligomers, polymers) design and device processing optimization have rapidly increased the power conversion efficiencies (PCEs) of organic photovoltaic (OPV) that approach 12% [2]. However, fullerenes are not ideal acceptor materials due to many intrinsic issues, such as weak light absorption, almost fixed chemical structure and energy levels [3], further limiting the open-circuit voltage ( $V_{oc}$ ) and short-circuit current density ( $J_{sc}$ ) of these solar cell devices. Furthermore, the inherent tendency of fullerene to aggregate under elevated temperatures has been considered a key factor for deteriorated morphology and consequently reduced lifetime of PSCs [4]. Therefore, despite the tremendous achievements to date, the research development of OPVs has reached the stage where the

scalability of the materials, stability and cost need to be further optimized before reaching the threshold for large-scale commercialization [5].

Functional photovoltaic materials applied into organic solar cells are usually synthesized via the *Suzuki*, *Stille* or *Negishi* cross-coupling reactions, which involve the preparation of organo-boron, organo-tin or organo-zinc reagents, respectively [6]. In recent years, attributing to the great progress of C-H activation reaction, thiophene has been regarded as an ideal moiety in synthetic organic chemistry for direct arylation with aryl halides due to the ease of palladation through a concerted metalation deprotonation pathway [7]. These reactions possess numerous advantages [8] over traditional cross-coupling reactions such as: (a) avoidance of the use of organometallic reagents in the starting materials leading to simpler by products and higher atom economy, (b) fewer synthetic steps, (c) higher yields, (d) better compatibility with chemically sensitive functional groups, and (e) the scalability preparation of the target conjugated materials.

Meanwhile, solution-processed organic solar cells (OSCs) using a nonfullerene electron acceptor has been rapidly improved relative to the fullerene counterparts, with PCE past 11% up to date [9]. Typically, the nonfullerene OSCs can be divided into four different

\* Corresponding author.

\*\* Corresponding author.

E-mail addresses: [jyuan@suda.edu.cn](mailto:jyuan@suda.edu.cn) (J. Yuan), [wлма@suda.edu.cn](mailto:wлма@suda.edu.cn) (W. Ma).

types: polymer donor-small molecule acceptor (P-M) [9], polymer donor-polymer acceptor (P-P) [3c,10], small molecule donor-small molecule acceptor (M-M) [11] and small molecule donor-polymer acceptor (M-P) [12]. However, among these nonfullerene OSCs, the development of small molecule donor-polymer acceptor system has lagged significantly behind in device performance. So far, only a few reported M-P OSCs exhibited power conversion efficiencies (PCEs) above 2% [12], with the very recent two ones reaching 4.5% [12b,13]. The lower PCEs of M-P OSCs are generally hypothesized to the large polymer phase separation, relatively low electron mobility of polymer acceptors and the inefficient charge dissociation at the donor/acceptor (D/A) interface [12a,14]. However, it is worth noting that few previous works have been focused on the effect of initial donor molecules properties on the relevant M-P OSCs performance. We should realize that the subtle changes in donor molecular structure may also have significant impact on the material optoelectronic properties, processing parameters, blend morphology, and the resulting solar cell characteristics selection. Especially, the morphology change is critical to the device performance.

In this contribution, a series of low band-gap donor molecules (DPP-B, DPP-N and DPP-P) sharing similar D- $\pi$ -A- $\pi$ -D backbone structure were synthesized via one-pot direct acylation reaction. We incorporated different end groups (benzene, naphthalene and pyrene) into the molecular backbone, in order to investigate how the subtle changes in molecular structure impact relevant optoelectronic properties and the resulting M-P nonfullerene OSCs characteristics. Finally, all these molecules were used together with a polymer acceptor P(NDI2OD-T2) (N2200) [15] in M-P nonfullerene solar cells. As shown in Scheme 1, to achieve higher intermolecular contacts, DPP-N and DPP-P were synthesized by substituting the benzene end-group with naphthalene and pyrene, aiming to enhance charge carrier mobility and light absorption of donor molecules. The properties of these molecules were systematically studied by UV–vis absorption, Density Functional Theory (DFT) simulation and 2D grazing incidence wide-angle X-ray scattering (GIWAXS). The corresponding M-P nonfullerene solar cells were also fabricated to investigate the effect of molecular structure on the device photovoltaic performance. We revealed that the structure change of small molecule donor acceptor can adjust the molecular ordering and crystallinity in solid film, resulting in

significantly different performance. The optimized M-P nonfullerene solar cells based on DPP-P/N2200 shows a relatively high  $J_{sc}$  of  $\sim 4.5$  mA/cm<sup>2</sup> (0.69 mA/cm<sup>2</sup> for DPP-B/N2200 and 1.14 mA/cm<sup>2</sup> for DPP-N/N2200), and a high PCE of 2.05% (0.20% for DPP-B/N2200 and 0.50% for DPP-N/N2200). More importantly, our results suggest that small molecule donor with higher crystallinity can be designed for creating better charge transport and blend morphology in M-P nonfullerene OSCs.

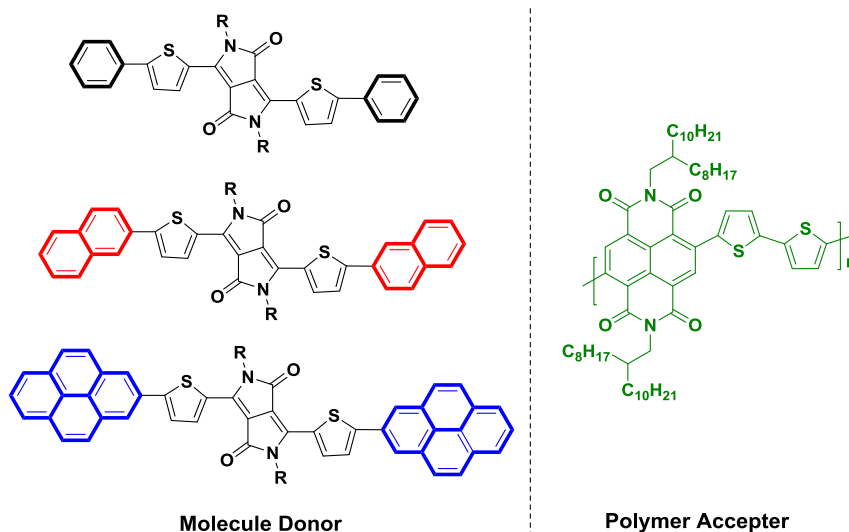
## 2. Results and discussion

### 2.1. Synthetic procedures

The structure and synthetic route of the donor molecules are illustrated in Scheme 2. The detailed procedure is described in the experimental part. All molecules were prepared via direct arylation reaction [16], using a phosphine-free catalytic system, and the reaction could be accelerated greatly with high yields (>90%) in the presence of pivalic acid (PivOH). Former reports demonstrated the preparation procedure of these DPP-based materials using Palladium(Pd)-assisted Suzuki cross-coupling reaction with multiple steps [17], however, the highly efficient one-pot synthesis of these functional materials in this contribution gives us a promising prospect for easier scale up production. These advantages make the direct arylation protocol an ideal and versatile strategy for the synthesis of structural complicated DPPs that may possess chemically sensitive functionalities. Herein, all the DPP molecules materials exhibit good solubility in common solvents at room temperature, like chloroform (CF), chlorobenzene (CB) and *o*-dichlorobenzene (ODCB).

### 2.2. Optical properties

UV–vis absorption spectra of DPP-based molecules and N2200 are shown in Fig. 1. The molecular solutions in chloroform display broad absorption from 450 to 680 nm. For DPP-N and DPP-P, both solutions show distinct shoulder peaks next to the absorption maximum in their solutions, which is typical for DPP based molecules. We noticed that the absorption in region of 400–600 nm of DPP-N and DPP-P are almost the same, indicating the similar intramolecular charge transfer (ICT) between the donor and



Scheme 1. Molecular structures of donor and acceptor.

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