

Small molecule semiconductors for organic photovoltaics: a truncation approach



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ABSTRACT

Solution-processable small molecule (SM) organic semiconductors for organic photovoltaics have been in the spotlight for several years. In particular, SM semiconductors have been developed in an attempt to control their film morphology, study their intermolecular interactions, and synthesize new electron donor and electron acceptor subunits. SMs have many advantages over polymers including well-defined molecular structures, monodispersity, and no batch-to-batch dependence. Although SM semiconductors can be designed by truncation from polymers, such examples have rarely been reported. Herein we designed SM semiconductors by truncating a representative polymer, Poly[4-(4,8-bis((2-hexyldecyl)oxy)benzo[1,2-*b*:4,5-*b'*])dithiophen-2-yl)-*alt*-benzo[*c*][1,2,5]thiadiazole] (PBDTBT). Based on density functional theory (DFT) calculations, 2,1,3-benzothiadiazole (BT) was chosen as an electron acceptor subunit instead of thieno[3,4-*c*]pyrrole-4,6-dione (TPD). The SM semiconductors were end-capped with pyridine derivatives. Thermal, optical and electrochemical properties of these materials were examined to confirm the degradation temperature, the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) energy levels, and the band gaps. In particular, the benzyloxy pyridine-capped semiconductor (SM1) exhibited power conversion efficiency (PCE) of 1.92% which is higher than those shown by the corresponding polymer PBDTBT (0.90% and 1.71%).

1. Introduction

Small molecule solar cells (SMSCs) have been developed extensively over several years as an alternative to conventional polymer solar cells due to numerous characteristics such as their well-defined molecular structures, monodispersity of small molecule (SM) semiconductors, and batch-to-batch independence [1–5]. Based on these characteristics, previous studies have achieved high efficiency in SMSCs by controlling film morphology, charge transport, and band gap [6]. Their power conversion efficiency (PCE) was recently reported to exceed 12% [7]. Despite the remarkable progress in SMSCs, new material design strategies still need to be developed to expedite the pace of improvement.

To achieve highly efficient solar cells, research has focused on improving the physical/chemical properties of semiconducting materials and ternary blend system with the aim of enhancing their mobility, fine-tuning their energy levels and broad light absorption [8–18]. Nevertheless, the structure–property relationships of these materials are

not yet fully understood. We envision that precise truncation of well-known polymeric semiconductors could be an effective approach to the design of SM semiconductors. Early in 2006, J.-M. Nunzi and coworkers reported sexithiophene truncated from polythiophene was used as a donor in organic solar cell for better understanding of polythiophene/fullerene blend system [19]. However, even though many kinds of SM semiconductors have been used for SMSCs, the approach that involves truncating a polymer semiconductor has rarely been studied [20–22].

Previously we reported that the molecular structure of truncated SM semiconductors could be optimized in terms of the performance of photovoltaic devices using density functional theory (DFT) calculations [23]. At the beginning, we tried to truncate poly[4-(4,8-bis((2-ethylhexyl)oxy)benzo[1,2-*b*:4,5-*b'*])dithiophene-5-octyl-4H-thieno[3,4-*c*]pyrrole-4,6-dione] (PBDTTPD) [24] to make the corresponding SM semiconductor, a pyridine-capped BDT–TPD–BDT core (Fig. 1). Functionalized pyridines have several advantages as an end-capping group. Various functionalities can be introduced into pyridine in order to

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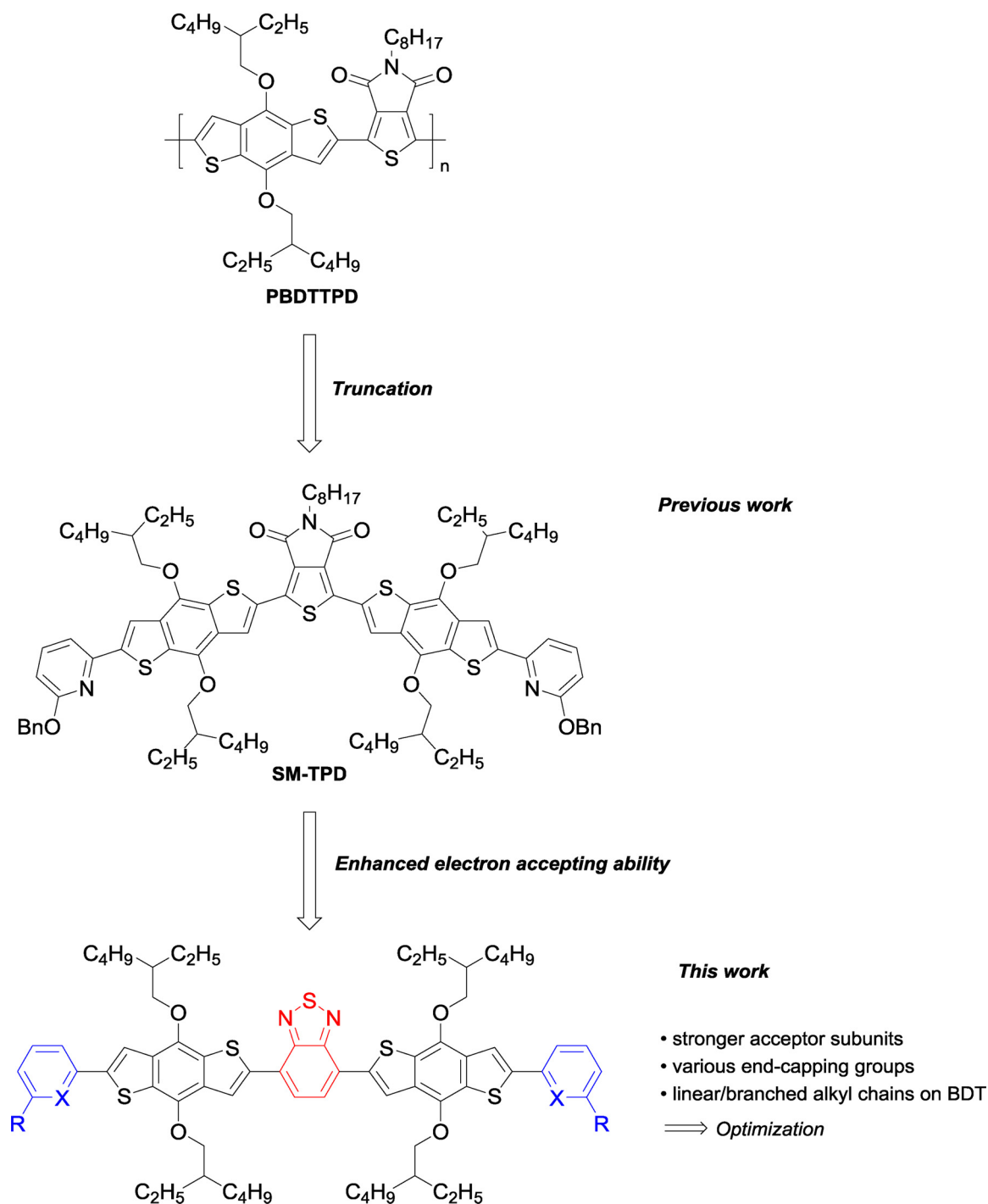


Fig. 1. The concept of development of new SM semiconductors.

control solubility, film morphology, and electronic property. In addition, benzyloxy pyridines as a weak electron-accepting subunit can be easily transformed into pyridones which are capable of complementary hydrogen-bonding to induce self-assembled structures. The calculation suggested that replacing TPD with more strongly electron-accepting subunits (e.g. 2,1,3-benzothiadiazole (BT) and 5,6-difluoro-BT (DFBT)) could lead to better PCE values. This modification seems reasonable because BT has a deeper LUMO energy level than TPD, which makes it easy to obtain a low band gap [25–27]. Furthermore, from the perspective of crystalline phase formation in the solid state, BT could be an appropriate candidate. Among representative BT-containing alternating

copolymers, Poly[4-(4,8-bis((2-hexyldecyl)oxy)benzo[1,2-*b*:4,5-*b'*]dithiophen-2-yl)-*alt*-benzo[*c*][1,2,5]thiadiazole] (PBDTBT) has good coplanarity in the backbone and is well-delocalized along the conjugated backbone due to a strong push-pull characteristic [28,29].

In this work, based on the previous computation results, we designed and synthesized new SM semiconductors composed of the representative BDT as a donor subunit and BT as an acceptor subunit. To extend the conjugation while maintaining the push-pull structures, these compounds were capped with various pyridine derivatives, which are weak electron-withdrawing groups [30,31]. Although the truncated SM semiconductors have relatively short conjugation length compared

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