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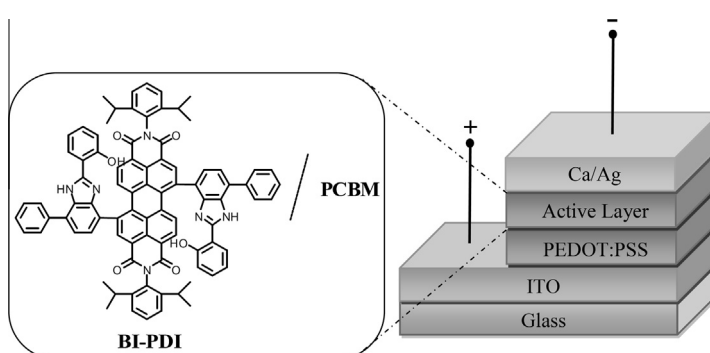
Synthesis, characterization and optoelectronic properties of a new perylene diimide–benzimidazole type solar light harvesting dye

Haluk Dinçalp^{a,*}, Oguzhan Çimen^a, Tayebah Ameri^b, Christoph J. Brabec^b, Siddik İçli^{c,*}^a Department of Chemistry, Faculty of Arts and Science, Celal Bayar University, Muradiye, 45030 Manisa, Turkey^b Institute of Materials for Electronics and Energy Technology (I-MEET), Friedrich-Alexander-University, Martensstraße 7, 91058 Erlangen, Germany^c Solar Energy Institute, Ege University, Bornova, 35100 Izmir, Turkey

HIGHLIGHTS

- Benzimidazole-substituted PDI dye for solution-processed BHJc was synthesized.
- Aggregation tendency of dye in the presence of P3HT polymer was observed.
- Electron mobility of PDI dye is calculated to be higher than the hole mobility.

GRAPHICAL ABSTRACT



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ABSTRACT

A perylene diimide type small molecule (**BI-PDI**) has been synthesized through Suzuki coupling reaction between *N,N'*-bis(2,6-diisopropylphenyl)-1,7-dibromoperylene-3,4,9,10-tetracarboxylic diimide and 2-(2-hydroxyphenyl)-7-phenyl-1H-benzimidazole-4-boronic acid. **BI-PDI** small molecule has showed an absorption band between 350 and 750 nm on thin films. HOMO and LUMO energy levels of **BI-PDI** dye have been calculated to be about -5.92 eV and -3.82 eV, respectively. Solution-processed bulk heterojunction (BHJ) solar cells have been constructed using **BI-PDI** as donor and [6,6]-phenyl-C₆₁-butyric acid methyl ester (PC₆₁BM) as acceptor or poly(3-hexylthiophene) (P3HT) as donor and **BI-PDI** as acceptor. The external quantum efficiencies (EQE) of the devices cover the most of the visible region between 400 and 700 nm for both configurations. Photovoltaic performances of **BI-PDI**-based organic solar cells are limited by the aggregation tendency of PDI structure and poor hole/electron mobilities of the active layer.

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Introduction

Small molecule semiconductors have been extensively used in BHJ solar cells for decades due to their exclusively properties such

as well-ordered molecular structures, simple synthetic pathways, well-defined molecular weights, easily changeable spectral tunings by variation of functional groups and advantageous on thin film morphology [1,2]. Nowadays most of the organic photovoltaic (OPV) materials have been configured by using well-known conjugated small molecules including phthalocyanines [3,4], boron-dipyrromethenes [5,6], fused acenes [7–9], thiazoles [10,11], triphenylamines [12,13], diketopyrrolopyrroles [14,15], isoindigos [16], tetraphenylphthalic-based diimides [17], and fullerenes

* Corresponding authors. Tel.: +90 236 2013158; fax: +90 236 2412158 (H. Dinçalp). Tel./fax: +90 232 3740118 (S. İçli).

E-mail addresses: haluk.dincalp@cbu.edu.tr (H. Dinçalp), siddik.icli@ege.edu.tr (S. İçli).

[18]. However, they have had still lower power conversion efficiencies (PCEs) with respect to their polymeric counterparts. It will be expected that higher efficiencies can be obtained by the development of suitable molecular designs for small molecule organic semiconductors in near future studies. Among the preferred small molecule-based BHJ configurations, donor–acceptor networks containing perylene diimides (PDIs) as acceptors and appropriate donor materials lead to efficient photoinduced charge separation in OPVs [19–21].

PDIs are suitable candidates as an acceptor in device structures due to their stronger visible absorptions within the range of 400–450 nm (B band) and 500–700 nm (Q band), better charge transporting properties [22], higher molar absorption coefficients [23], higher fluorescence quantum yields [24] and better photostabilities [25] under solar irradiation as compared to their conjugated counterparts. In the literature survey, PCE values given for OPV devices using PDI small molecules as acceptor are found within the wide range of 0.002–3.17 depending on both the nature of the active layer and the used techniques [26–33]. Sharma et al. have blended 1,7-substituted perylene-anthracene diimide with a donor molecule containing dithienyl-benzothiadiazole central unit and obtained PCE of 2.85% with short-circuit current density of 6.8 mA/cm² [27]. A diphenoxylated PDI small molecule in bay positions of perylene ring has been used as acceptor and *p*-phenylene-vinylene type small group has been used as donor group in OPV device with ZnO layer giving PCE of 3.17% by Sharma et al. in different study [33]. In that device, the PCE has been improved by both incorporating ZnO layer between the active layer and the Al electrode and also annealing to increase the crystalline of the active layer. Han et al. have manufactured the ternary structure for OPV device consisting of P3HT:PCBM with the addition of a butoxyphenoxy substituted PDI molecule and obtained a considerable improvement of over 70% in PCE with respect to reference cell without an additive [34].

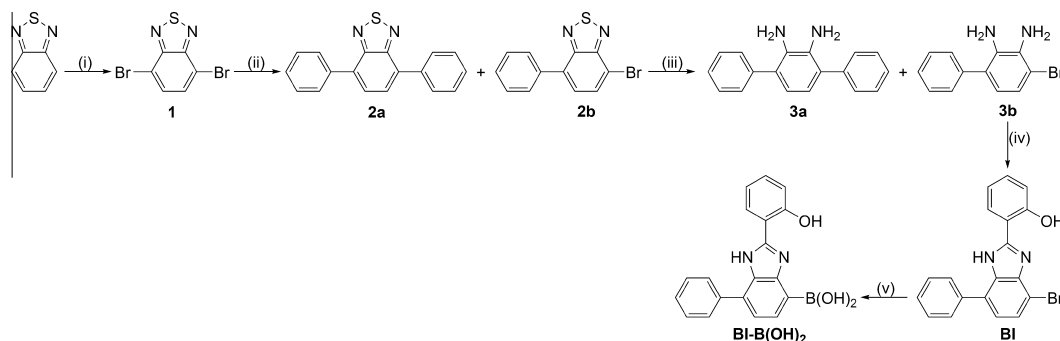
Generally, PDIs show two reduction waves with their planar structure responsible for high degree of π – π stacking [35–37]. The introduction of bulky substituents in bay positions of the ring disturbs the planarity of the perylene core. These deviations from planarity may decrease multi-dimensional electron transfer processes. Also, deformations from molecular planarity results the inhibition of aggregation which may be helpful to improve PCE of a desirable device. In such efforts, bay-functionalized groups on the perylene ring are the most important molecular building blocks for an effective OPV device [38]. The report herein is based to decrease the molecular planarity of perylene core by attaching with special benzimidazole derivative in 1- and 7-positions of the perylene ring. There are a limited number of studies about small organic molecules based on benzimidazole for OPV devices in the literature. A recent study is related to 2,2-dimethyl-2H-benzimidazole small molecule-based BHJ solar cell comprising benzimidazole derivative with PC₆₁BM giving FF of 27 with a low PCE of 0.37 [39].

In present work, we also targeted to synthesize a low band gap material by incorporating benzimidazole group to the perylene core. This kind of benzimidazole substituted PDI-type small molecule (**BI-PDI**) may ascribe the intramolecular charge generation. The absorption and emission properties of the dye in common solvents of different polarities and also on thin films have been investigated in detail. Also, hole and electron mobility performances of some selected devices have been tested. Synthetic routes and dye structures are shown in Schemes 1 and 2.

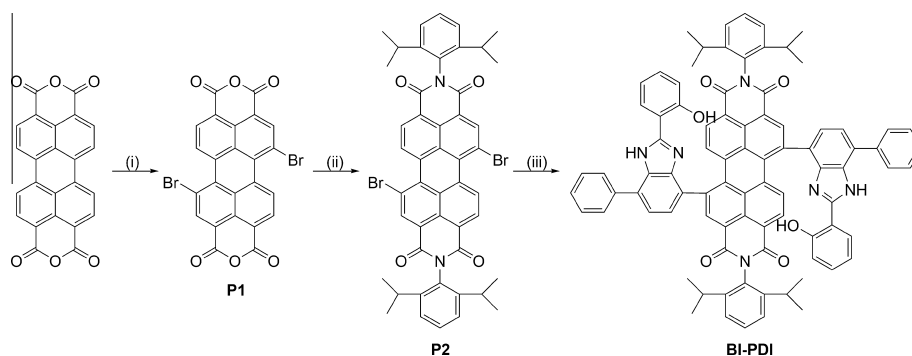
Experimental

General procedures

¹H NMR and ¹³C NMR spectra for characterization of the synthesized compounds were recorded on a Bruker 400 MHz



Scheme 1. Reaction pathway for the synthesis of **BI-B(OH)₂**. (i) Br₂/HBr, 120 °C, 93% [40]; (ii) phenylboronic acid, Na₂CO₃, benzene, Pd(PPh₃)₄, 80 °C, 10% (for **2b**) [41]; (iii) EtOH/THF, NaBH₄, CoCl₂·6H₂O, 80 °C [42]; (iv) Salicyl aldehyde, Me-CN, CoCl₂·6H₂O, room temp., 95% [43]; (v) *n*-BuLi, THF, –78 °C, B(OMe)₃, 75% [44].



Scheme 2. Reaction pathway for the synthesis of target **BI-PDI**. (i) H₂SO₄/Oleum, Br₂, 85 °C, 84% [45]; (ii) 2,6-diisopropylaniline, propionic acid, 130 °C, 72% [45]; (iii) 2-(2-hydroxyphenyl)-7-phenyl-1H-benzimidazole-4-boronic acid, **BI-B(OH)₂**, Na₂CO₃, Ar, Pd(OAc)₂, 80 °C, 80% [35].

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