



Solution-processed interlayer of discotic-based small molecules for organic photovoltaic devices: Enhancement of both the open-circuit voltage and the fill factor



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ABSTRACT

A novel alcohol/water-soluble, discotic type derivative of pyrene was obtained using a simple synthesis process. The pyrene derivative was dissolved in organic solvents and highly polar solvents. The absorption spectrum of the pyrene derivative in a thin film was almost identical with that observed in solution compared with a fluorene derived co-polymer, the extensive planarity of the pyrene unit is invoked to rationalize this observation. According to an XRD measurement, a huge portion of the pyrene derivatives are arranged face-on in regard of the substrate due to their discotic structure. A photovoltaic device containing the pyrene derivative exhibited an open-circuit voltage of 0.73 V, current density of 14.6 mA/cm², fill factor of 65.1% and a power conversion efficiency of 7.0%. The photovoltaic device with the pyrene derivative exhibited an improved fill factor compared with that of the fluorene co-polymer (60.7%) due to the discotic structure. An inverted photovoltaic device containing pyrene derivative showed a power conversion efficiency of 8.3%.

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1. Introduction

Conjugated polymers have been widely used in organic light emitting diodes (OLEDs) [1–4], organic photovoltaic cells (OPVs) [5–11] and organic thin film transistors (OTFTs) [12,13] for several decades. For some times, OPVs have drawn crucial concern for these applications due to the universal technology tendency toward economic potential and continuative growth coupled with efforts to preserve the environment. However, the poor power conversion efficiency (PCE) of these materials has been the greatest barrier in organic photovoltaic development [6].

The next ideal conditions must be achieved in OPV materials and devices to improve the PCE [8]: 1) increase of the short-circuit current (J_{SC}) through a wide absorption spectrum, 2) rise of the open-circuit voltage (V_{OC}) through optimization of the highest occupied molecular orbital (HOMO) and lowest unoccupied

molecular orbital (LUMO) energy levels, and 3) improve the fill factor (FF) by controlling resistance at the interfaces. To achieve these ideal conditions, various efforts continue to be applied to control the materials of the active layer and the device structure: various donor–acceptor (D–A) type polymers, additives, thermal treatments, and film thicknesses. However, there is still an inevitable loss at the interfaces because of the charge transport barriers between the active layer and the metal cathode [14].

To improve the charge transport between the interfaces, a number of investigations to study the effects of introducing an interlayer have been reported recently. In particular, most research efforts have focused on alcohol/water soluble conjugated polymer electrolytes (CPEs) for the interlayer. The Maes group recently reported that the PCE improved from 3.8% to 6.6% with imidazolium-substituted polythiophene used as the CPE [15]. In the Cao group, a PCE of 8.3% was reported with a device structure that introduced poly[(9,9-bis(30-(*N,N*-dimethylamino)propyl)-2,7-fluorene)-alt-2,7-(9,9-dioctylfluorene)] (PFN) between the active layer and the cathode, and an inverted device configuration with PFN improved the PCE to 9.2%, with increases of the J_{SC} , V_{OC} , and FF [16,17]. It has

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been suggested that these interlayers introduce an enhanced built-in potential across the device because of the presence of an interface dipole, which is conducive to a refinement in the charge-transport, an elimination of the built-up space charge, and a diminution in the recombination losses of the charge carriers [14,16].

Small molecules have various advantages compared with polymers, such as straightforward synthesis and purification, monodispersity and precise structures, residual end functionality and good reproducibility [18,19]. A number of research studies on active materials by small molecules have been reported [20–22], but only a few investigations of interlayers about small molecules by solution-process have been reported in the field of OLEDs and OPVs [4,23].

In this study, we synthesized novel alcohol/water-soluble discotic type small molecules. The discotic derivatives exhibit unique material properties, such as effective charge-carrier mobilities by one-dimensional structure and anisotropic mechanical and optical properties [13,24,25]. Discotic liquid crystal (DLC) materials with effective charge carrier mobility along columnar phases have the possibility to be used as the active constituent in electronic applications. Moreover the adjustment of their molecular packing and large fraction orientation exhibits a principal factor for the performance of devices due to the design of the molecular structure [26].

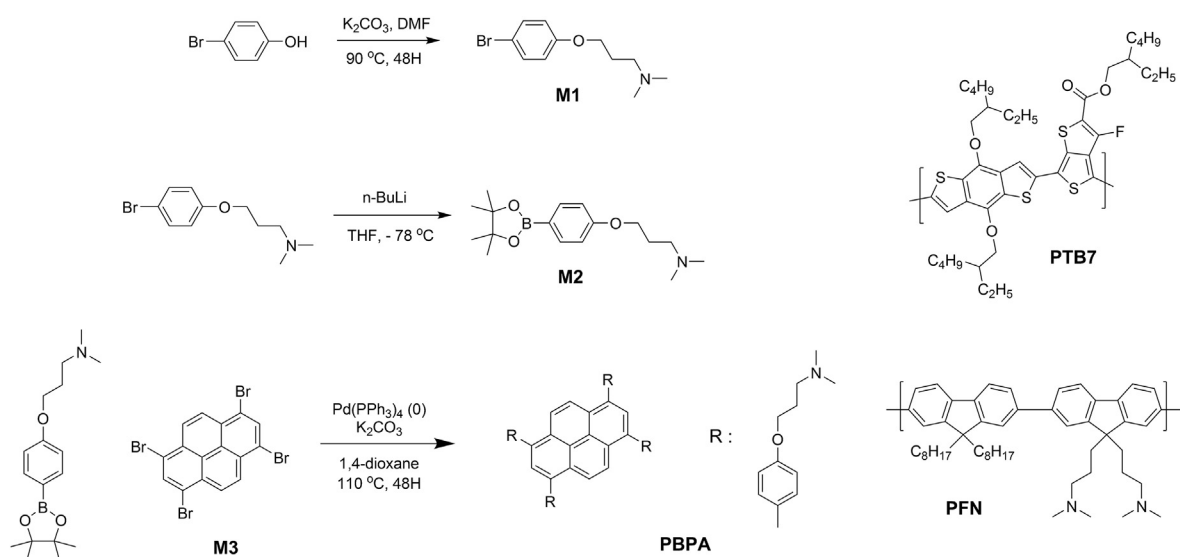
Thus, we synthesized 3,3',3'',3'''-((pyrene-1,3,6,8-tetrayltetrakis(benzene-4,1-diyl))tetrakis(oxy))tetrakis(*N,N*-dimethylpropan-1-amine) (PBPA) using a simple synthesis process, as shown in Scheme 1. The dimethyl-amine derivative was introduced as the end group of the pyrene derivative to provide good alcohol/water-solubility. Due to their molecular packing and long-range organization, improved FF and V_{OC} values are expected in OPVs using these discotic type pyrene derivatives.

2. Experimental section

2.1. Instruments and characterization

Unless otherwise specified, all reactions were performed under a nitrogen atmosphere. The solvents were dried using the standard procedures. All column chromatography was performed with silica gel (230–400 mesh, Merck) as the stationary phase. ^1H NMR

spectra were collected by a Bruker ARX 400 spectrometer using solutions in CDCl_3 with chemical concentrations recorded in ppm units using TMS as the internal standard. The elemental analyses were measured with an EA1112 apparatus using a CE Instrument. The electronic absorption spectra were measured in chloroform using an HP Agilent 8453 UV–Vis spectrophotometer. The cyclic voltammetric waves were obtained using a Zahner IM6eX electrochemical workstation with a 0.1 M acetonitrile (purged with nitrogen for 20 min) solution containing tetrabutyl ammonium hexafluorophosphate (Bu_4NPF_6) as the electrolyte at a constant scan rate of 50 mV/s. ITO, a Pt wire, and silver/silver chloride [Ag in 0.1 M KCl] were used as the working, counter, and reference electrodes, respectively. The electrochemical potential was calibrated against Fc/Fc^+ . The HOMO levels of the polymers were determined using the oxidation onset value. The onset potentials are the values obtained from the intersection of the two tangents drawn at the rising current and the baseline changing current of the CV curves. TGA measurements were performed on a NETZSCH TG 209 F3 thermogravimetric analyzer. Differential scanning calorimetry (DSC) was used to determine phase-transition temperatures on a Netzsch DSC 200 F3 maia differential scanning calorimeter with a constant heating/cooling rate of 10 °C/min. Texture observations by polarizing optical microscopy (POM) were made with a Leica DM2500M and DFC295. All GPC analyses were performed using THF as an eluent and a polystyrene standard as a reference. Grazing Incidence X-ray diffraction (GIXD) patterns were obtained using a SmartLab 3 kW (40 kV 30 mA, Cu target, wavelength: 1.541871 Å) instrument of Rigaku, Japan. Topographic images of the active layers were obtained through atomic force microscopy (AFM) in a tapping mode under ambient conditions using a XE-100 instrument. Scanning Kelvin probe microscopy (SKPM) measurements were carried out on AFM equipment, using the standard SKPM mode. Theoretical analyses were performed using density functional theory (DFT), as approximated by the B3 LYP functional and employing the 6-31G* basis set in Gaussian09. The contact angle measurements were performed using a Kruss DSA100. SEM microscopy was performed on a JEOL model JSM-6701F field-emission scanning electron microscope operating at 10 kV. The melting point was evaluated using a Carl Zeiss AXIO IMAGER MIM polarizing optical microscope (POM) equipped with a Linkam TH-600PM and L-600 heating and cooling stage with temperature control.



Scheme 1. Synthesis route of PBPA and chemical structure of PTB7, PFN.

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