

Isoindigo-based conjugated polymer for high-performance organic solar cell with a high V_{OC} of 1.06 V as processed from non-halogenated solvent

Eui Hyuk Jung^{a,b}, Hyungju Ahn^c, Won Ho Jo^a, Jea Woong Jo^{d,*}, Jae Woong Jung^{e,**}

^a Department of Materials Science and Engineering, Seoul National University, Gwanak-ro, Gwanak-gu, Seoul, 151-744, Republic of Korea

^b Division of Advanced Materials, Korea Research Institute of Chemical Technology (KRICT), Daejeon, Republic of Korea

^c Pohang Accelerator Laboratory, Kyungbuk, Pohang, 37673, Republic of Korea

^d Department of Energy and Materials Engineering, Dongguk University-Seoul, 04620, Seoul, Republic of Korea

^e Department of Advanced Materials Engineering for Information and Electronics, Kyung Hee University, Yongin-si, Gyeonggi-do, 26035, Republic of Korea

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ABSTRACT

The fabrication of organic solar cells using non-halogenated solvents have been recently explored in order to replace conventionally used halogenated solvents that cause environmental, health and safety problems. For achieving highly efficient organic solar cells using non-halogenated solvents, conjugated polymer should be designed and developed to afford high solubility in non-halogenated solvent and desirable photovoltaic properties in finally fabricated devices. Here, we demonstrated that an isoindigo-based copolymer, PiI2fT, composed of isoindigo with 2-decyltetradecane and bithiophene with fluorination is a promising polymer for organic solar cells using eco-friendly non-halogenated solvent. We found that the introduction of fluorine atom in conjugated polymer affords improved photophysical properties including intense light absorption, lowering of the highest occupied molecular orbital energy level and increase of dipole moment, while the introduction of bulk alkyl chain in the polymer may enhance the solubility in organic solvents. When solar cells were fabricated from using *o*-xylene and diphenyl ether as solvent and additive, PiI2fT polymer exhibited a high PCE of 8.80% with an open-circuit voltage of 1.06 V.

1. Introduction

High-efficiency organic solar cells (OSCs), fabricated from blends of conjugated polymers and fullerene derivatives in organic solvents, have intensively been developed for the last two decades owing to low specific weight, low cost, mechanical flexibility, and large area device fabrication [1–9]. To date, most of OSCs exhibiting high power conversion efficiency (PCE) have been fabricated by using halogenated solvents such as chloroform, chlorobenzene and dichlorobenzene along with halogenated additives such as 1,8-diiodooctane and 1-chloronaphthalene [10–16]. However, the use of non-halogenated solvents such as *o*-xylene for fabrication of high performance OSCs has recently attracted much attention, because the halogenated solvents and additives cause serious environmental, health and safety problems [17–21].

Recent efforts to replace halogenated solvents with non-halogenated ones have revealed that improving the solubility of conjugated polymer in non-halogenated solvent through rational molecular design is a key

factor [22–25]. Hence, side chain engineering is considered to be an effective and simple strategy to enhance the solubility in non-halogenated solvents [18,19,26,27]. However, although the incorporation of bulkier side chain enhances the solubility of conjugated polymer, it may affect adversely the photovoltaic performance of the resulting polymer because most of side chains introduced in conjugated polymers have insulating property.

Among several strategies to compensate for the negative effect of bulky side chains on photovoltaic properties and thus to achieve high-efficiency OSCs, the introduction of fluorine atom in conjugated polymer has been one of most effective methods, because the fluorine introduction in conjugated polymers affords deeper energy levels with unchanged optical bandgap, high absorption coefficient, molecular ordering by induced dipole along the C–F bond, and reduction of recombination loss in bulk heterojunction systems [28–31]. Recently, we reported the syntheses of fluorinated conjugated polymers based on 3,3'-difluoro-2,2'-bithiophene (2fT) as promising polymer for achieving high-efficiency OSCs [6,32–35].

* Corresponding author.

** Corresponding author.

E-mail addresses: whwp78@dongguk.edu (J.W. Jo), wodndwdj@khu.ac.kr (J.W. Jung).

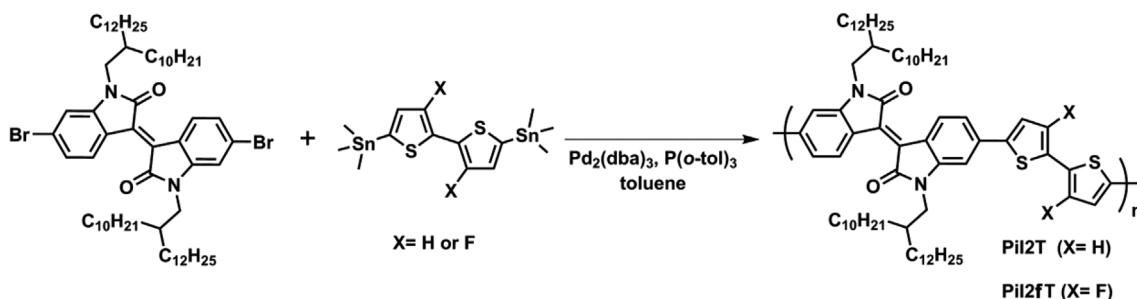


Fig. 1. Synthesis of PiI2T and PiI2fT.

In this work, we synthesized two isoindigo-based conjugated polymers composed of isoindigo with 2-decyltetradecane (DT) and bithiophene with/without fluorination. The two polymers are soluble in both chlorinated solvents (chloroform, chlorobenzene and *o*-dichlorobenzene) and non-halogenated solvents (*o*-xylene and toluene) due to bulky solubilizing side chain (DT) in the polymers. Although both polymers are processable in non-halogenated solvents, the polymer (denoted as PiI2fT) with 2fT exhibits higher photovoltaic performance than the polymer (denoted as PiI2T) with 2,2'-bithiophene (2T). When we fabricated the OSCs using *o*-xylene and diphenyl ether (DPE) as solvent and additive, respectively, PiI2fT-based OSC exhibits a PCE of 8.80% with a high open-circuit voltage (V_{OC}) of 1.06 V, while PiI2T-based OSC shows a PCE of 4.92%.

2. Results and discussion

Two polymers (PiI2T and PiI2fT) were synthesized via microwave-assisted Stille coupling polycondensation in toluene with $Pd_2(dba)_3$ and $P(o-tol)_3$, as represented in Fig. 1. The number average molecular weights (M_n) of PiI2T and PiI2fT, as measured by gel permeation chromatography at 70 °C with chlorobenzene as eluent, are 79.2 and 91.6 $kg\ mol^{-1}$ with polydispersity index of 4.65 and 2.25, respectively. Although it is well-known that the fluorination of polymer decreases the solubility of polymer [6,32], PiI2fT with DT as side chain is soluble in *o*-xylene, while PiI2T with 2-octyldecane is not soluble, indicating that the introduction of bulky alkyl side chain affords the solubility in common solvents to the polymer.

When UV–visible absorption spectra of the two polymers in *o*-xylene solution and solid film state are compared, as shown in Fig. 2, an identical onset of absorption is observed for both polymers at 753 nm, corresponding to an optical bandgap ($E_{g,opt}$) of 1.65 eV. The maximum molar absorption coefficient of PiI2fT in *o*-xylene solution is $4.26 \times 10^4\ M^{-1}\ cm^{-1}$, which is much higher than that of PiI2T

($3.29 \times 10^4\ M^{-1}\ cm^{-1}$ at 702 nm), indicating that PiI2fT-based OSCs may exhibit higher photocurrent than PiI2T-based ones.

The highest occupied molecular orbital (HOMO) energy levels of PiI2T and PiI2fT were determined by cyclic voltammetry (CV) (Fig. 3a), ultraviolet photoelectron spectroscopy (UPS) measurement (Fig. 3b) and density functional theory (DFT) calculation (Fig. S1), and the data are summarized in Table 1 to clearly evaluate the relative HOMO energy level alignment of PiI2T and PiI2fT. The HOMO energy level of PiI2fT as determined from the oxidation potential of CV is $-5.48\ eV$, which is 0.1 eV lower than that of PiI2T ($-5.38\ eV$). UPS measurement and DFT calculation of HOMO energy levels also show the same trend although the absolute values are different from each other, indicating that the incorporation of fluorine atom in polymer chain can effectively lower the HOMO energy level. Consequently, PiI2fT-based OSCs are expected to exhibit higher V_{OC} than PiI2T-based OSCs, because V_{OC} is proportional to the difference between the HOMO energy level of donor material and the lowest unoccupied molecular orbital (LUMO) energy level of acceptor [36]. When the LUMO energy levels of polymers are determined by adding the optical bandgap to the HOMO energy level from CV measurement, the LUMO energy levels of PiI2T and PiI2fT are $-3.73\ eV$ and $-3.83\ eV$, respectively, indicating that the LUMO energy level offsets between donor polymer and acceptor for effective exciton dissociation are marginally small. To examine exciton dissociation at the interface between polymer donors and $PC_{71}BM$, we measured the steady-state photoluminescence (PL) in polymer: $PC_{71}BM$ blends (Fig. S2). Since both PiI2T: $PC_{71}BM$ and PiI2fT: $PC_{71}BM$ blend films show high PL quenching efficiencies, we conclude that the LUMO offsets between polymers and $PC_{71}BM$ are sufficient for exciton dissociation. When we also calculated the dipole moment changes from ground to excited state ($\Delta\mu_{ge}$) for repeating units of two polymers in order to evaluate the exciton dissociation and charge generation, as listed in Table 1, it reveals that PiI2fT has larger $\Delta\mu_{ge}$ than PiI2T, suggesting that PiI2fT exhibits higher photovoltaic performance, because it has been reported that

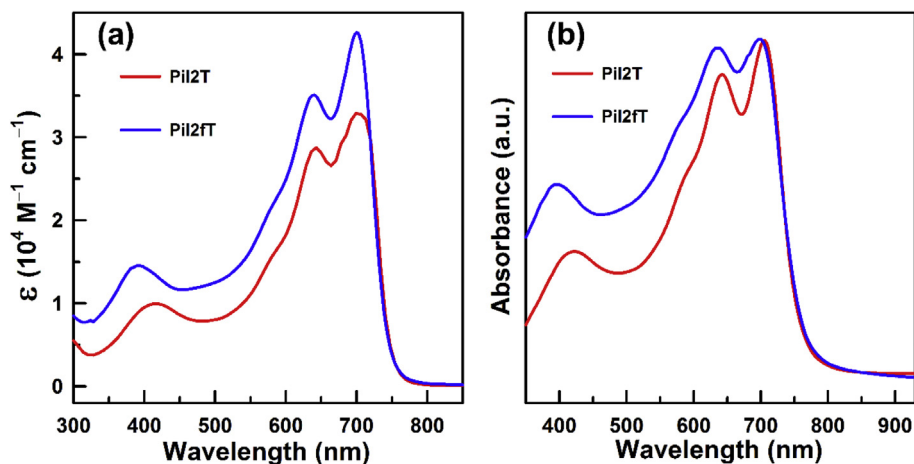


Fig. 2. UV–visible absorption spectra of polymers in (a) *o*-xylene solution and (b) solid film.

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