

Two-dimensional regioregular polythiophenes with conjugated side chains for use in organic solar cells

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ABSTRACT

We have prepared two two-dimensional polythiophenes (2D-PTs; **P1** and **P2**) possessing alkyl-thiophene side chains by Stille coupling reactions. Optical measurements indicate that the bandgaps of **P1** and **P2** being 1.98 and 1.77 eV, respectively. **P2** displayed a red-shift in its absorption spectrum because of the longer length of its conjugated side chains. Desirable highest occupied molecular orbital (HUMO) and lowest unoccupied molecular orbital (LUMO) energy levels were obtained from electrochemical studies, which suggested that these systems would exhibit high open-circuit voltages when blended with fullerene as electron acceptors. The hole mobility (thin film transistor (TFT) measurement) of **P1** and **P2** are 3.5×10^{-4} and $4.6 \times 10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, respectively. A power conversion efficiency of 2.5% is obtained under simulated solar illumination (AM 1.5G, 100 mW cm^{-2}) from a polymer solar cell comprising an active layer containing 25 wt% **P1** and 75 wt% [6,6]-phenyl-C₇₁ butyric acid methyl ester (PC₇₁BM).

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1. Introduction

The emerging field of polymer solar cells (PSCs) is receiving a great deal of attention because third-generation solar cell technology offers the prospect of low costs, light weights, short energy payback times, and solution-based processing [1–4]. The power conversion efficiency (PCE) of PSCs has been improved to 5% under AM 1.5G when using a blend film composed of poly(3-hexylthiophene) (P3HT) as the donor and [6,6]-phenyl-C₆₁-butyric acid methyl ester (PC₆₁BM) as the acceptor [5,6]. This encouraging solution fabrication method can advance this technology toward commercial application, where it may take a different form, i.e. inorganic photovoltaics (PVs).

In the active layer of a PSC, the conjugated polymer plays the key role of absorbing light, creating excitons for subsequent charge separation, and transporting holes to the anode. To further improve the device performance, one approach is to adopt materials that harvest more light from the solar spectrum. The solar emission spectrum ranges from 350 to 1500 nm, with a maximum flux at ca. 700 nm [7]. Nevertheless, the best PSC material developed to date, P3HT, absorbs only a part of the visible light spectrum (in the range from 350 to 650 nm). To enhance the absorption of semiconducting polymers, several effective approaches have been reported, including the preparation of low

bandgap (LBG) polymers [8,9] and side chain-conjugated polymers [10,11]. Using donor–acceptor strategies [9], several new polymers have been developed to better harvest the solar spectrum in the region 1.4–1.9 eV. Unfortunately, LBG polymers often absorb better in the long wavelength range [e.g., the near-infrared (NIR)], i.e., some part of the visible region absorption is sacrificed. Nevertheless, poly(2,7-carbazole) [12], poly(cyclopentadithiophene) [8], poly(thiophene–phenylene–thiophene) (TPT) [13], and poly(diketopyrrolo-pyrrole) [14] derivatives have been developed for PSCs that exhibit very promising PCE values (3.2–5.5%). Unfortunately relatively lower hole mobility and poor solubility are often associated with these LBG polymers. Thus, the main challenge of conjugated polymer engineering is to prepare materials that simultaneously exhibit high mobility and better utilization of the solar spectrum. Recently, Li and co-workers reported a solar cell having an efficiency of 3.2% that incorporated side-chain-conjugated polymers [10]. In this system, broad absorption and high mobility were achieved because the conjugated side chains also improved the degree of electronic communication between the polymer chains.

In an attempt to obtain broad absorption and desirable hole mobility, we here report a novel approach toward a regioregular conjugated polymer presenting alkyl-thiophene side chains (two-dimensional polythiophenes (2D-PTs)) (Scheme 1). Unlike the bi(thienylene–vinylene) system [10], the alkyl-thiophenes in this study were directly attached onto the polythiophene backbones without vinylene linkers. X-ray crystallography reveals a nearly planar conformation of 2-D monomer. The coplanar conjugated

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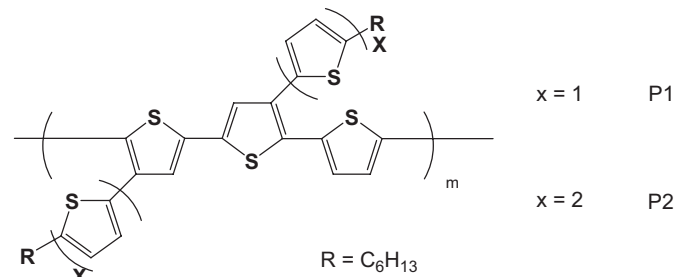
structures render strong intermolecular π - π interaction, which would extend the degree of π -conjugation and thus are expected to have remarkable hole mobility [13]. We expect (i) the regioregularity would result in good π stacking in film packing and would show red-shift in film absorption so as to improve harvesting of sunlight and (ii) the alkyl-thiophene side chains

should benefit charge transportation among the different polymer main chains because of the electronic communication between branched chains [15]. After optimization of the device fabrication parameters, we obtained a PCE of 2.5% with an active layer containing 25 wt% **P2** and 75 wt% [6,6]-phenyl-C₇₁-butyric acid methyl ester (PC₇₁BM) under the conditions of AM 1.5G illumination.

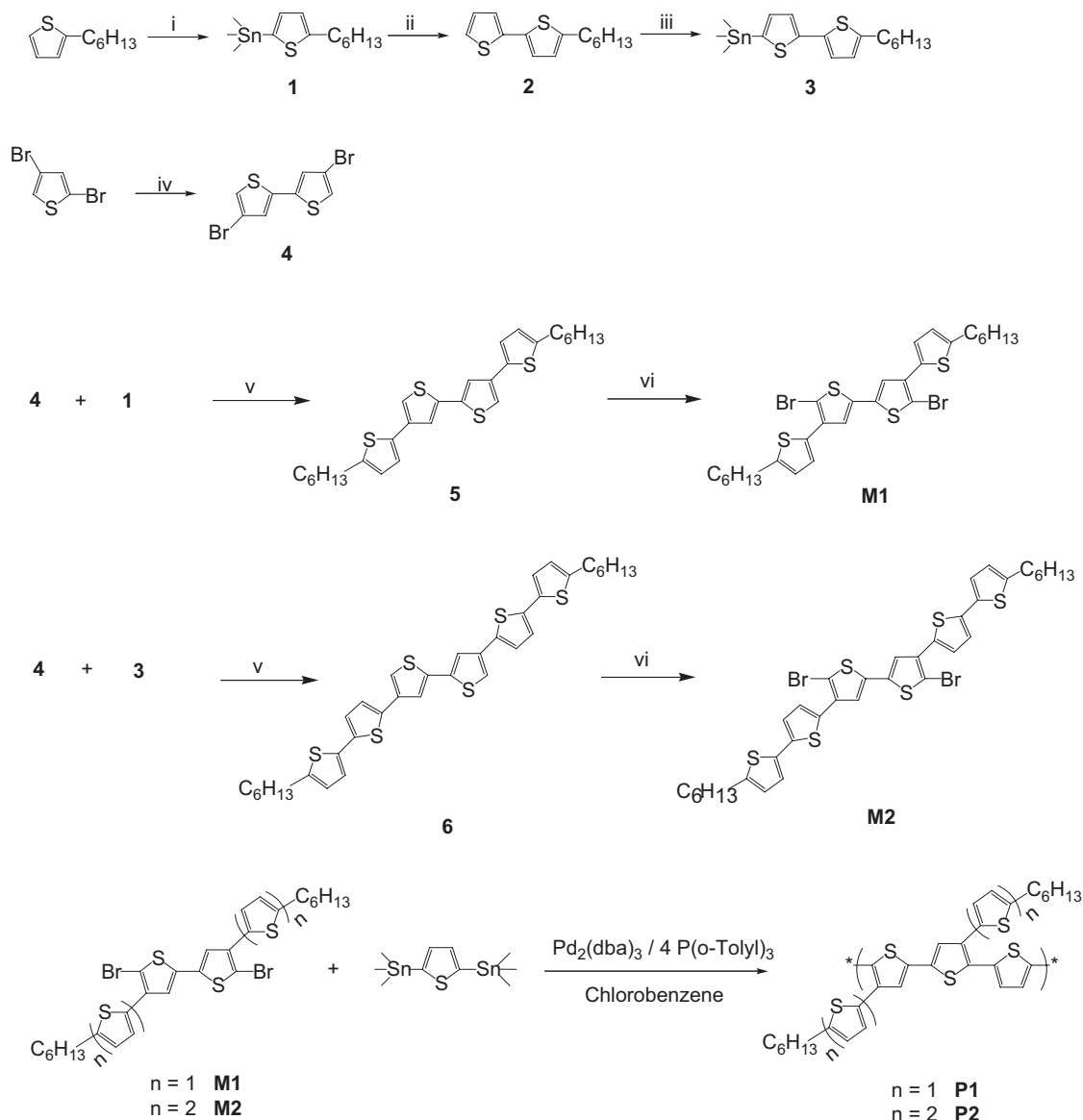
2. Result and discussion

2.1. Monomer synthesis

To further extend the absorption spectrum, polymers containing alkyl-thiophene side chains (**P1** and **P2**) were designed and synthesized. Scheme 2 presents the synthetic routes followed toward the starting monomers **M1** and **M2** and the 2D-PTs. Lithiation of 2-hexylthiophene and subsequent stannylation (1.2 equivalent of Me₃SnCl) gave the 2-trimethylstannyl derivative **1** in 65% yield. Compound **2** was synthesized via palladium-catalyzed



Scheme 1. Molecular structures of polythiophenes presenting conjugated thiophenes in their side chains.



Scheme 2. Synthesis routes toward polythiophenes presenting conjugated thiophenes in their side chains: (i) n-BuLi, -78 °C, Me₃SnCl; (ii) 2-Bromothiophene, Pd(PPh₃)₄, DMF/Toluene, 110 °C; (iii) n-BuLi, -40 °C, Me₃SnCl; (iv) n-BuLi, -78 °C, CuCl₂; (v) Pd(PPh₃)₄, DMF/Toluene, 110 °C; (vi) NBS, AcOH/CHCl₃.

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