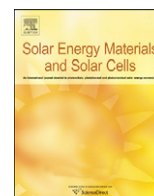




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Fused thiophene/quinoxaline low band gap polymers for photovoltaic's with increased photochemical stability

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ABSTRACT

We investigate a family of low band-gap polymers based on the common acceptor moiety 2,3-bis-(3-octyloxyphenyl)quinoxaline (Q) combined with thiophene (T) or the fused thiophene systems: benzo[2,1-b:3,4-b']-dithiophene (BDT) or dithieno[3,2-b,2',3'-d]-thiophene (DTT). The photochemical stability of the three polymers was examined and compared to P3HT. They were found to be substantially more robust than P3HT with a ranking of DTTQ > BDTQ > TQ1 ≫ P3HT, indicating that the fused ring systems of DTT and BDT impart a large degree of photochemical stability than thiophene. Furthermore devices with normal and inverted geometry were prepared and tested in air. The normal geometry devices showed the highest efficiencies compared to the inverted, in particular owing to a higher V_{oc} , with TQ1 being the most efficient with a power conversion efficiency (PCE) of 1.5% (1000 W m^{-2} , AM1.5 G). For the inverted devices TQ1 and DTTQ showed the best PCEs of 0.9%.

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1. Introduction

Much of the present research effort within the field of polymer photovoltaic's is directed towards increasing the power conversion efficiency (PCE) now in the range of 8% or higher [1]. A common trend is the development of the so-called low band-gap materials with alternating donor-acceptor motifs. Polymers of this type display additional optical absorption bands due to charge-transfer transitions at longer wavelengths [2]. The result is typically a better match with the solar spectrum, harvesting of more photons and the ability to offer higher current densities. Just as important, but somewhat less explored is the stability of the photovoltaic devices. Most of the high performance devices presented in the literature are prepared and studied under inert atmosphere conditions. The combination of high efficiency and good stability in the same device/materials are essential for the transfer to practical use and large scale production by roll-to-roll manufacture [3]. The stability of polymer photovoltaics depends on a complex interplay between many factors such as the photochemical reactivity of the polymer and on the physical/chemical stability of electrodes [4,5]. Enhanced stability has been observed for photovoltaic devices with the so-called "inverted" geometry [3,6] (see Fig. 1) with the front ITO electrode as the electron collector and the back metal electrode as the hole

collector. In the inverted geometry, the metal back electrode can be screen printed using a silver paste in contrast to the evaporated aluminum electrode used in the "normal" geometry device. The enhanced stability of these inverted devices is in part due to the lower reactivity of the silver electrode towards oxygen. Another attraction of the inverted geometry is the applicability in the fabrication of roll-to-roll coated devices [7–10].

In the present work, we investigate a family of low band-gap polymers based on the common acceptor moiety 2,3-bis-(3-octyloxyphenyl)quinoxaline (Q) combined with thiophene (T) or fused thiophene systems: benzo[2,1-b:3,4-b']-dithiophene (BDT) or dithieno[3,2-b,2',3'-d]-thiophene (DTT) as shown in Scheme 1. The simplest polymer in this series (TQ1) has already been investigated by Wang et al. [11] who obtained devices with efficiencies up to 6.0% with TQ1 in combination with [70] PCBM and 4.9% in combination with [60] PCBM. The synthesis and characterization of the polymers are presented together with photovoltaic devices in both the normal and inverted type geometry. Recently a fast method for assessing the photochemical stability of conjugated polymers was established by Manceau et al. and used in our group to rank the stability of more than 20 polymers used in OPV [12]. We have used this method to rank the stability of this series of polymers against standard P3HT. Part of the inspiration for this series of polymers also came from an OPV study by Bundgaard et al. [13] who investigated the low band-gap polymer formed from the DTT donor moiety and a dialkoxy-benzothiadiazole acceptor. They demonstrated power conversion efficiencies of 0.6% on 96 cm^2 roll-to-roll coated modules and also

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showed that this polymer had a superior photochemical stability compared to P3HT. Similarly the BDT donor has been copolymerized with a pyrrolo[3,4-c]pyrrole-1,4-dione acceptor by Hou et al. [14] to create a low band-gap polymer achieving a reported photovoltaic efficiency of 4.5% together with [70] PCBM.

2. Experimental

2.1. Synthesis

The monomers 5,8-dibromo-2,3-bis(3-(octyloxy)phenyl)quinoxaline [11], 2,5-bis(trimethylstannyl)-thiophene [15], ditrimethyltin dithieno[3,2-*b*:2',3'-*d*]thiophene [13] and benzo[2,1-*b*:3,4-*b'*]-dithiophene (BDT) were prepared according to literature.

2.1.1. Synthesis of 27-bis(trimethylstannyl)benzo[12-*b*:6,5-*b'*]dithiophene.

BDT (0.50 g, 2.63 mmol) was dissolved in dry THF (20 ml) under argon and cooled to -78°C . *n*-Butyllithium (6.75 ml, 1.6 M in hexanes, 10.8 mmol) was then added dropwise causing precipitation to occur. After stirring for 15 min at -78°C , it was allowed to reach

room temperature (RT) where it was left stirring for $\frac{1}{2}$ h. The solution was then cooled back to -78°C , after which chlorotrimethylstannane (3.50 g, 17.6 mmol) was added in one portion. The temperature was again allowed to reach RT at which the solution was stirred for an additional 2 h. Workup was performed by the addition of water followed by extraction with diethyl ether. The combined organic phases were washed with water and brine before drying over MgSO_4 and evaporation of the solvent. The crude product was purified by quickly passing the compound through a column of basic Al_2O_3 , using toluene with 2% NEt_3 as eluent. The resulting product was further purified by recrystallization from methanol yielding the pure product as fine white needles (0.92 g, 69%). ^1H NMR (500 MHz, CDCl_3) δ 7.73 (s, 2 H), 7.49 (s, 2 H), 0.64–0.23 (s, 18 H). ^{13}C NMR (126 MHz, CDCl_3) δ 138.28, 138.13, 138.06, 132.94, 119.66, -8.11 .

2.1.2. General procedure for Stille cross coupling polymerization

One equivalent of the Q monomer and the appropriate donor monomer (T, BDT or DTT) were dissolved in degassed toluene of 0.04 M solution. Tri-*o*-tolylphosphine (0.1 mol%) and tris-(dibenzylidene acetone) dipalladium(0) (0.02 mol%) were added and the solution was brought to reflux where it was stirred for at least 24 h under nitrogen atmosphere. The polymer was precipitated to about 10 times the volumes of methanol. The suspension was filtered to give the polymer, which was purified by Soxhlet extraction, first with methanol, then with hexane and finally with chloroform or chlorobenzene. The polymer was then precipitated by slowly adding into 10 times the volume of methanol. The suspension was filtered and dried in vacuum oven to give the purified polymer.

2.1.3. Synthesis of poly[2,3-bis(3-(octyloxy)phenyl)quinoxaline-5,8-diyl-*alt*-thiophene-2,5-diyl] (TQ1)

2,3-bis(3-(octyloxy)phenyl)quinoxaline (Q) (403.8 mg, 0.580 mmol), thiophene (T) (238.0 mg, 0.580 mmol), tri-*o*-tolylphosphine (10.0 mg, 0.033 mmol) and tris(dibenzylideneacetone)dipalladium(0) (6.0 mg, 6.55 μmol), yield: (324 mg, 90%).

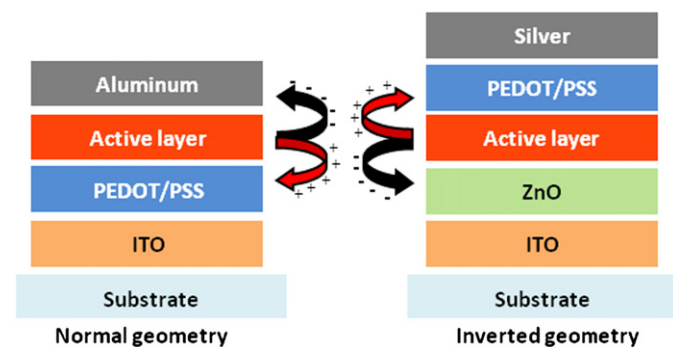
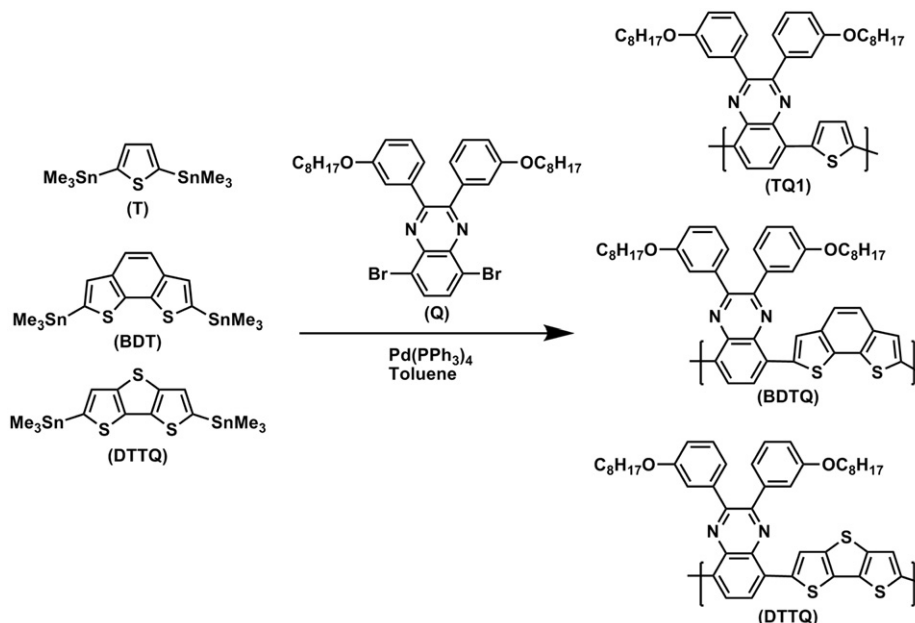


Fig. 1. Schematic representation of OPV devices with: (a) normal geometry where the electrons are collected at the back electrode (normally evaporated aluminum) and (b) inverted geometry where the electrons are collected at the front electrode (ITO).



Scheme 1. Polymerization of the three polymers through a Stille cross coupling polymerization. 2,3-Bis(3-(octyloxy)phenyl)quinoxaline (Q) is the acceptor moiety, which is coupled with a donor moiety, being either thiophene (T), benzo[21-*b*:3,4-*b'*]dithiophene (BDT) or dithieno[3,2-*b*:2',3'-*d*]thiophene (DTT), to give the polymers TQ1, BDTQ and DTTQ, respectively.

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