

Two Novel Cyclopentadiene-Based Alternating Copolymers as Potential Donor Components for High-Efficiency Bulk-Heterojunction-Type Solar Cells

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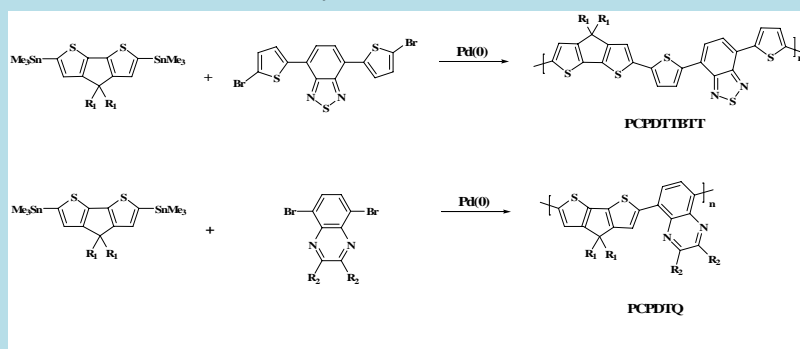
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Introduction:

Organic solar cells have received increasing attention from both academic and industrial laboratories due to their high charge-separation efficiency and ease of processing. Bulk-heterojunction-type solar cells use a phase-separated blend of an organic electron donor and an acceptor component. One of the most efficient donor components until now has been the semiconducting polymer poly(3-hexylthiophene) (P3HT) in combination with a soluble fullerene derivative (C₆₁-PCBM) as the nonpolymeric acceptor. In this contribution we detail the synthesis and characterization of two new low-band-gap polythiophenes, poly[4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene-2,6-diyl-*alt*-4,7-bis(2-thienyl)2,1,3-benzothiadiazole-5,5'-diyl] (PCPDTTBTT) and poly[4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene-2,6-diyl-*alt*-2,3-dioctylquinoxaline-5,8-diyl] (PCPDTTQ), for use in these applications. A high power efficiency of 2.1% under one sun was found for a PCPDTTBTT/fullerene mixture. The high efficiency was achieved by alteration of the morphology using a solvent additive. Analysis of atomic force microscopy phase images shows that material phases with distinct morphologies are formed and altered with the addition of the co-solvent.

Synthesis:



Scheme 1: Synthesis of the CPDT-based, alternating DA copolymers PCPDTTBTT and PCPDTQ (R₁ = 2-ethylhexyl, R₂ = n-octyl) in Stille-type cross coupling polycondensations

Optical Properties:

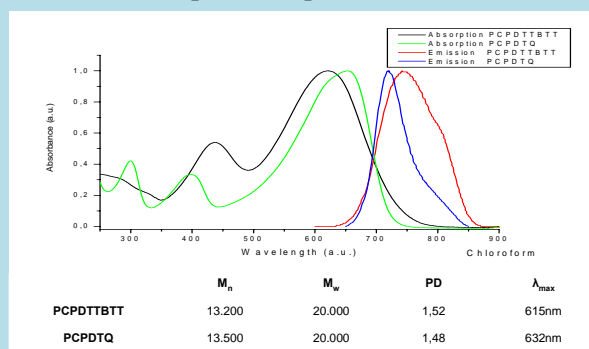


Figure 1: Optical properties of the copolymers PCPDTTBTT and PCPDTQ (R₁ = 2-ethylhexyl, R₂ = n-octyl) measured in CHCl₃ and GPC results using THF

Solar Cell Devices:

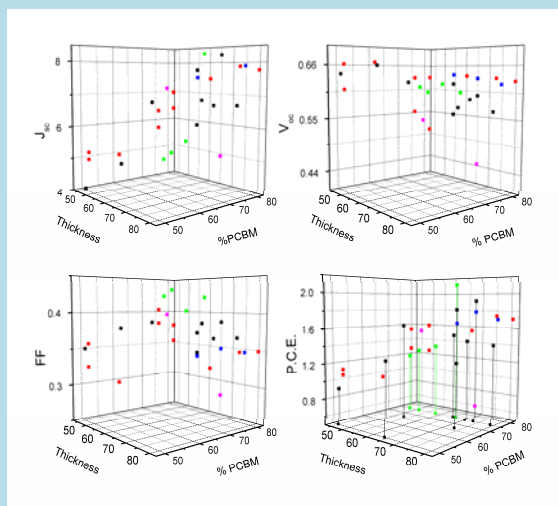


Figure 2: IV data including J_{sc} (upper left), V_{oc} (upper right), FF (lower left), and P.C.E. (lower right) for all of the PCPDTTBTT:PCBM PV as functions of wt% PCBM and active layer thickness. Casting Solvent: chlorobenzene (black), o-xylene (red), chlorobenzene + anisole (green), o-xylene + anisole (blue), and chlorobenzene + nitrobenzene (magenta)

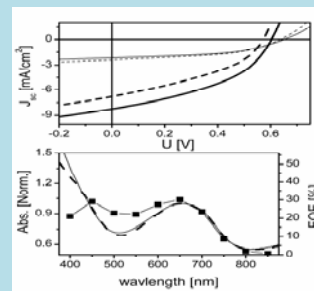


Figure 3. a) IV curves of bulk heterojunction type solar cell devices cast from 1:3 (w/w) PCPDTTBTT:PCBM mixtures in CB (dashed bold) and CB:Ani (solid bold); and a 1:3 (w/w) PCPDTQ:PCBM mixture in CB (dashed) and CB:Ani (solid). b) UV/vis spectra and EQE of the CB cast PCPDTTBTT-based device

AFM Images:

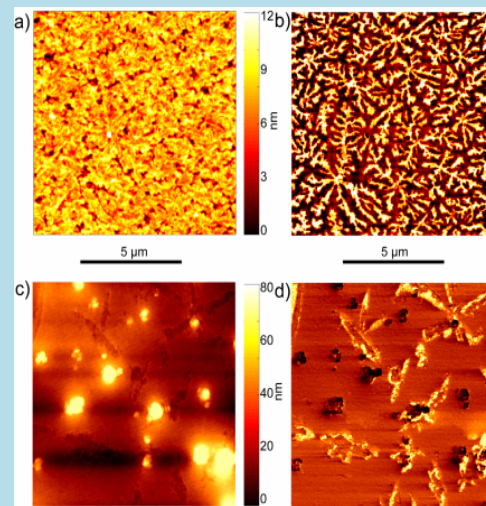


Figure 4. AFM topography and phase images of as-cast 1:3 (w/w) PCPDTTBTT:PCBM layers cast from CB (a,b) and CB:Ani (c,d)

Conclusions:

In conclusion, we report on the fabrication of two low band-gap copolymers that have been designed for use in “bulk heterojunction” solar cell devices. Devices fabricated from mixtures of PCPDTTBTT and PCBM show a promisingly high power efficiency of 2.1% and with EQE measured for wavelengths longer than 800 nm. The devices were fabricated from a number of casting solvents. The use of a 19:1 (v/v) mixture of chlorobenzene and anisole shows the best performance. Analysis of the morphology shows that all devices have a very large phase separation, which can be expected to reduce the efficiency of the devices. The addition of anisole to the chlorobenzene casting solvent resulted in the formation of larger PCPDTTBTT-rich and PCBM-rich domains, but also to the formation of an intermediate concentration domain that had superior electrical properties. This intermediate concentration domain led to improved FF and efficiency.

References:

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