Synthesis, Characterization, and Photovoltaic Properties of a Low Band Gap Polymer Based on Silole-Containing Polythiophenes and 2,1,3-Benzothiadiazole

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Polymer solar cells have been attracting considerable attention due to their unique advantages of being low in cost and lightweight, as well as their potential application in flexible large-area devices. To realize high efficiencies, the active layer of polymer solar cells must have good absorption of sunlight. Since 54.3% of the sunlight energy is distributed in the visible region from 380 to 800 nm, an ideal active layer for a polymer solar cell should have a broad and strong absorption spectrum in this range. Fullerene and their derivatives, such as [6,6]-phenyl-C61-butyric acid methyl ester (PCBM), are widely used as electron acceptor materials in polymer solar cells, but they exhibit weak absorption in the visible range. As a result, the absorption of polymer:PCBM based solar cells is mainly from the electron donator material. Hence, to improve harvesting of sunlight, some low band gap conjugated polymers were designed, synthesized, and used in polymer solar cells. In several works, poly[(4,4'-bis(2-ethylhexyl)-cyclopenta-[2,1-b;3,4-b']dithiophene)-2,6-diyl-alt-2,1,3-benzothiadiazole-4,7-diyl], PCPDTBT, has been proven to be one of the most efficient low band gap photovoltaic materials. For the PCPDTBT/PC70BM based device fabrication process, the efficiency of the solar cell device was calculated to be 3.2%. As reported, the response of the solar cell based on PCPDTBT covers the range 380–900 nm; this wide response range is the main advantage of this material, and as a result, the short circuit voltage of the solar cell reaches 16 mA/cm².

To ensure good solubility, 2-ethylhexyl side chains were employed in the polymer. As shown in Scheme 2, dichlorobis(2-ethylhexyl)dithieno[3,2-d]silole-containing polymer as the active layer material reached 0.02 cm² V⁻¹ s⁻¹. another dithieno[3,2-b:2',3'-d]silole-containing polymer, poly[(4,4'-bis(2-ethylhexyl)dithieno[3,2-b:2',3'-d]silole)-2,6-diyl-alt-(4,7-bis(2-thienyl)-2,1,3-benzothiadiazole)-5,5'-diyl], was used in polymer solar cells and exhibited some interesting photovoltaic properties. Therefore, to incorporate the broad absorption spectrum and good hole transport property of both the low band gap and silole-containing polymers, a new dithieno[3,2-b:2',3'-d]silole polymer, poly[(4,4'-bis(2-ethylhexyl)dithieno[3,2-b:2',3'-d]silole)-2,6-diyl-alt-(2,1,3-benzothiadiazole)-4,7-diyl] (PSBTBT shown in Scheme 1), was designed and synthesized through a facile synthesis route.

To ensure good solubility, 2-ethylhexyl side chains were employed in the polymer. As shown in Scheme 2, dichlorobis(2-ethylhexyl)dithieno[3,2-d]silole-containing polymer reached a maximum efficiency of 0.02 cm² V⁻¹ s⁻¹, which is comparable to that of the PCPDTBT-based device. The band gap of the PSBTBT polymer is 1.45 eV, which is similar to that of the PCPDTBT polymer. As a result, the absorption of polymer:PCBM based solar cells is mainly from the electron donator material. Hence, to improve harvesting of sunlight, some low band gap conjugated polymers were designed, synthesized, and used in polymer solar cells. In several works, poly[(4,4'-bis(2-ethylhexyl)-cyclopenta-[2,1-b;3,4-b']dithiophene)-2,6-diyl-alt-2,1,3-benzothiadiazole-4,7-diyl], PCPDTBT, has been proven to be one of the most efficient low band gap photovoltaic materials. For the PCPDTBT/PC70BM based device fabrication process, the efficiency of the solar cell device was calculated to be 3.2%. As reported, the response of the solar cell based on PCPDTBT covers the range 380–900 nm; this wide response range is the main advantage of this material, and as a result, the short circuit voltage of the solar cell reaches 16 mA/cm².

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After measuring the metal electrodes with an area of 12 mm², which were defined by C for 5 min. The devices were completed by evaporating Ca/Al layer of poly(3,4-ethylene dioxythiophene):poly(styrenesulfonate) organic photovoltaic applications. These characteristics indicate that PSBTBT is an ideal polymer for organic photovoltaic applications.

We fabricated the photovoltaic device with a structure of ITO/PSBTBT/Ca, 10 min, then TMSCl, ambient temp 15 min; then compound 2, ambient temp 1 h; (iv) NBS, THF, ambient temp 2 h; (v) butyllithium, −78 °C, 10 min; then trimethyl chloride, 1 h; (vi) Pd(PPh₃)₄, toluene, reflux, 24 h.

In conclusion, a new low band gap silole-containing conjugated polymer, PSBTBT, was designed and prepared. Photovoltaic properties of the material were investigated, and a PCE of up to 5.1% was observed under AM 1.5G, 100 mW/cm² illumination, and the response range of the device covers the whole visible range from 380 to 800 nm. These results indicate that PSBTBT is a promising candidate for applications of translucent polymer solar cells.

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Supporting Information Available: Experimental details of the synthesis of the polymer, the fabrication and characterization of the polymer solar cells, measurements, and instruments. This material is available free of charge via the Internet at http://pubs.acs.org.

References


