n low bandgap polymers for nt organic solar cells

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Organic photovoltaic cells are promising in terms of their light weight, mechanically flexibility, ease of processing and low cost. Establishing a predictive understanding between the chemical structures and physical properties of polymers is still challenging, and continuous effort is needed to progress toward full commercialization. In this review, recent progress in polymer/fullerene systems is highlighted and four synthetic principles are summarized to engineer the bandgap and tune the energy levels and the solubility of the targeted polymers.

Introduction

Traditionally, the direct conversion of solar energy into electricity has been achieved via inorganic solar cells, based on the photovoltaic effect associated with *p*–*n* junctions (PVs). These devices can deliver high power conversion efficiency (PCE), but come with a high manufacturing cost. More recently, a new form of solar cell based on organic semiconductors has emerged, which offer the potential for light weight, mechanically flexible, easy to process and low cost solar cells. Two forms of active material in organic solar cells are being investigated. The first one involves multilayers of donor–acceptor materials [1] and the second is based on composite materials containing both donor and acceptor molecules, so-called bulk heterojunction (BHJ) materials, which is a more effective approach for organic photovoltaic (OPV) devices. The most promising OPV solar cells, toward commercial viability, are based on composites of an electron-donating conjugated polymer and electron-accepting fullerene [2]. Significant progress has been made in this field. Power conversion efficiency (PCE) values above 9% have been reported for cells based on conjugated polymer/fullerene blends [3–5] and over 10% for tandem architectures in small area devices [6], which are approaching the performance of amorphous inorganic semiconductors. This progress has been made by various groups working on material development, physical understanding, device development and optimization. Among all of these, the material development plays a key role. This article reviews recent developments on the most prominent material systems. Device modification toward high performance is briefly introduced.

What is an OPV solar cell?

Solution-processed bulk-heterojunction (BHJ) solar cells were first reported by Friend et al. with all polymer active thin films [7] and followed by Heeger et al. in 1995 with a polymer/fullerene composite [2]. The general device architecture is fabricated in sandwich geometry (Fig. 1). Transparent, conducting electrodes such as ITO are used as the substrate which can be structured by chemical etching. Poly(ethylene-dioxythiophene) doped with polystyrene-sulfonic acid (PEDOT:PSS) is coated as the interfacial layer to facilitate the hole injection/extraction. Vacuum evaporation and solution processing techniques are two of the most commonly used thin film preparation methods to coat the blended active layers.

Low bandgap polymers are usually used as the donor materials and fullerene derivatives such as $PC_{71}BM$ have been widely adopted as the acceptor component given their relatively high electron affinity and charge carrier mobility [8–11]. The performance of polymer solar cells is evaluated by three parameters (see Fig. 2): open-circuit voltage (V_{oc}), short circuit current density (J_{sc}) and fill factor (FF). Numerous variables can influence the device performance, including the physical properties of polymers and the morphology of the active layer.

The general mechanistic picture of an organic solar cell comprises the following four steps: (1) light absorption and exciton formation, (2) exciton migration, (3) charge separation and (4) charge transport and charge collection. Because of the high

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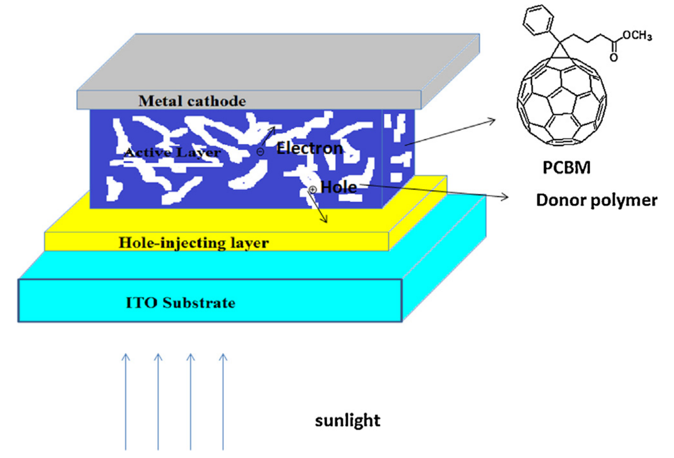

FIGURE 1

Graphic representation of the device architecture of BHJ solar cells.

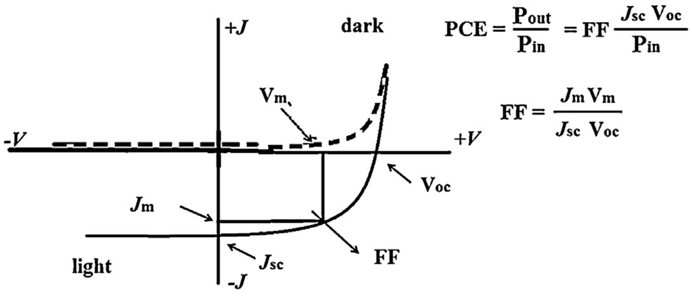

FIGURE 2

Typical current–voltage characteristics for dark and light current in a solar cell.

absorption coefficient and low carrier mobility, thin electroactive films with a thickness of around 100 nm are used. Upon photo-absorption, an exciton is formed due to the low dielectric constants of organic semiconductors. The exciton has to migrate to the interface between donor and acceptor domains, where charge separation occurs. Since the lifetime of an exciton is short, the migration distance of the exciton is therefore limited (~10 nm). Thus, controlling the morphology in BHJ solar cells is crucial. Further device studies have suggested that the utilization of an electron or hole blocking layer is beneficial to achieving high efficiency in the final solar cell. Due to the versatility in fine tuning the absorption windows of the resulting polymers, tandem solar cells become an attractive option to harvest more solar energy in the whole solar spectral range.

Synthetic principles toward high performance materials

A bandgap of 1.1 eV (1100 nm) is capable of absorbing 77% of the solar irradiation, but semiconducting polymers have bandgaps higher than 2 eV (620 nm) and can only harvest about 30% of the solar photons [12]. In order to harvest as much as solar spectrum, conjugated polyaromatic polymers, especially those with thiophene moieties, have been developed to provide polymers with tunable bandgaps, from 1.0 to 2.0 eV. In the meantime, the tuning of energy levels, as well as the solubility, is crucial to achieve high PCE values in OPV devices via the optimization of solar cell parameters. Two strategies are used for these polymers: to tune both solubility and energy levels, various substituents are attached to the polymer backbones so that morphology and performance of the electroactive layer can be optimized. Several structures of promising building blocks for potential high performance materials are presented in Fig. 3. Stille coupling polycondensation is widely used for thiophene-containing polymers, which can tolerate numerous functional groups. The Suzuki coupling reaction is applied for preparing polymers with phenyl repeating units [13,14].

Fused heterocycles

Fused heterocycles represent an important class of building blocks to achieve either low bandgap or high carrier mobility depending on the orientation of the fused ring to the polymer main chain. Polyisothianaphthlene (PITN) was the first well-known narrow bandgap polymer with the fused ring normal to the polymer backbone [15]. The main chain of PITN (P1) tends to favor the quinoidal mesomeric structure to maintain the benzene aromaticity, resulting in the band gap being as low as 1.0 eV. The most successful low bandgap polymers for solar cell application were based on the fused thienothiophene (TT) moiety. Bandgaps as low as 1.6 eV have been achieved and performances of over 5% have been reported with alternating TT and benzodithiophene (BDT) moieties called PTBs polymers (Fig. 4) [3,16,17]. Both benzothiadiazole and pyridalthiadiazole are widely used monomers to

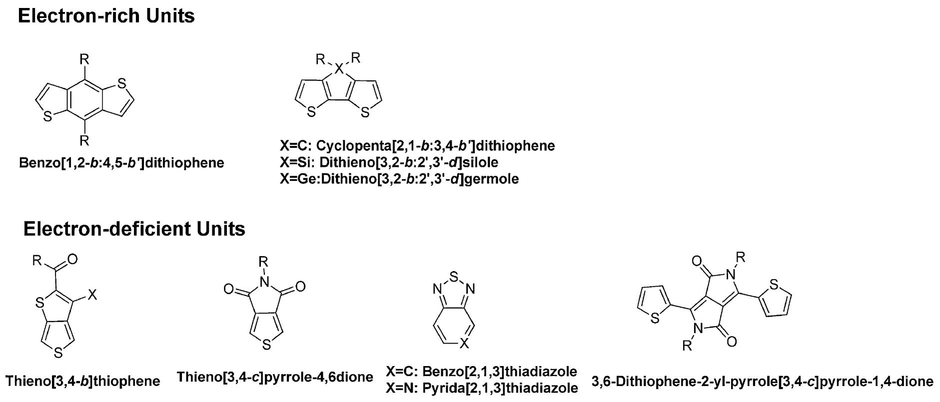

FIGURE 3

Several promising building blocks toward high performance materials.