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Review

Polymer design for solar cell – Current trend and future scenario

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ABSTRACT

Polymer molecular design is a crucial aspect for fabricating a better polymer solar cell with enhanced efficiency. In this review, we discussed the various polymeric designs (**P1–172**) encompassed of electron rich donor and electron deficient acceptor moieties in the main chain as well as in the side chain to facilitate effective intra-molecular charge transfer. Further, the application of these polymeric materials influenced significantly on the PCE of polymeric solar cells. So far, PCE of 7–8% were reported for these polymeric materials along with the fullerene derivatives. Along with improved efficiency for the polymer solar cell (PSC), other desirable parameters were also considered like, easy processibility, broad absorption range, low band gap and improved thermal/device stability of the polymers. In this review, we have discussed the current trend in the polymer design to improve the power conversion efficiency and suggest a possible scenario for the future development in the polymer design.

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1. Introduction

From the past few decades, polymer materials have gained interests as a potential replacement for the conventional inorganic material as a solar cell. The conventional solar cell is unaffordable and unfriendly processing methods make the polymer material a better contender as photovoltaic material. To replace the traditional solar cell, the polymer solar cells (PSC) are expected to deliver a higher efficiency with improved processibility and amenable to be made in large scale. PSC with bulk heterojunction (BHJ) structures have been researched extensively in recent times [1,2]. BHJ consists of blend of polymer donor and acceptor fullerene. The efficiency of PSC has not been so encouraging when compared to the conventional solar cell materials. However, synthesis of new photoactive conducting polymer has witnessed a huge surge in recent years for the application of PSCs [3,4]. The designing of polymer for improved efficiency is very critical and it involves a lot of criterion to be taken care of during the designing of polymer for PSC application like the broad absorption range, narrow band gap and lower energy levels, charge carrier mobility and morphology of the polymer film. The power conversion efficiency (PCE) of photovoltaic (PV) device is a very important parameter that decides the candidature of the polymer. However, the efficiency of polymer depends on short circuit current (J_{sc}), open circuit voltage (V_{oc}), and fill factor (FF) of the PSC device.

The V_{oc} of the device depend on the frontier orbital of the photoactive layer, i.e., low laying highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energy levels [5]. The difference between the LUMO of the donor and the LUMO of the acceptor should be more than 0.3 eV to obtain higher efficiency [6]. Hence, the molecular designing is emphasised to lower the frontier orbitals. J_{sc} will improve with the donor capability of the polymer and hence, a very electron rich moiety is preferred as a donor material. The charge carrier mobility of the polymer can improve if the charge move along the polymer leading to intramolecular charge transfer (ICT) and across the polymer leading to intermolecular charge transfer. The ICT can be improved by the incorporation of an electron deficient, electron withdrawing moiety (A) as building block along with the donor (D) building block leading to D–A polymer [7–12]. The intermolecular charge transfer will depend on the proximity of the polymer chains to allow the charge to be transferred from one polymer to another molecule. The polymer when cast into film, assemble itself or stack itself to facilitate the intermolecular charge transfer. This stacking is called as π–π stacking of the polymer chains. Also, it depends on the steric hindrance along the chain which may hinder the stacking of the chains. Both inter and intramolecular charge transfer are very important in deciding the band gap of the polymer. The narrow the band gap, the broader will be the absorption range of the active layer in the solar spectrum which will increase the efficiency.

However, flanking the main chain with an alkyl side chain improves the solubility and processibility of the polymer and also enhances the hole mobility [13]. Side chain plays a vital role however the bulkiness of the side chain is very important. A less bulky side chain is more favourable for the better performance of the polymer and will improve the efficiency [14]. Ho et al. corroborated that presence of spacers like vinylene significantly improves that charge transfer with improves self-assembly of the polymer chain leading to higher PCE of the PSC [15]. This review focuses on the designing of the polymer, both the acceptor and the donor units of the polymer in the active layer to improve the performance of polymer as PSC and subsequent modification in the design to enhance the performance of the polymer. This review emphasis on the current trend in polymer solar cell with regard to the polymeric materials and to improve their performance by different techniques and invigorating concepts.

2. Thiophene based polymers

Polythiophene has been explored for its very good thermal and electrical properties. However, native polythiophene is insoluble and processibility is very poor [16]. Native polythiophene (**P1**) with up to ca. 350 thiophene units and low content of structural defects (3.46–3.64 mol%) and with a conductivity of $1.72 \times 10^{-5}\ \mathrm{S\ cm^{-1}}$ have been prepared by Jian et al. The synthetic strategy for this polymer is based on the combination of Stille-type polycondensation reactions, ultrasound-assisted dispersion technique, and microwave-assisted ring-closure reactions [17]. Unfortunately, native polythiophene is intractable for electronic and optoelectronic fields where, solution processable polymers are highly desired to obtain low cost and large area coverage [18]. poly-(3-hexylthiophene) (P3HT) is a substituted polythiophene with more regioregularity [19] and it is being extensively used as an active layer due to its carrier mobility [20], efficiency [21] and stability [22].

Jeng and co-workers synthesised polythiophene derivatives functionalized with conjugated side-chain pendants consisting of carbazole/triphenylamine moieties to obtain **P2** and **P3**. Flanking these moieties into the main chain improved the charge transfer property and increased the π–π stacking of the polymer chain in solid state. Compared to triphenylamine, carbazole pendent polymer blend with $PC_{61}BM$ showed better V_{oc}, J_{sc}, and PCE, due to better conjugation that exists with carbazole moiety on the polythiophene [23].

Introduction of strong electron withdrawing moieties into the main chain of pure thiophene drastically improved the performance of the PSC. A strong electron withdrawing group such as 1,3,4-oxadiazole (OXD) or 1,3,4-thiadiazole (TD) were used as building block with thiophene to afford D–A copolymers, **P4** and **P5**, respectively and compared with **P6** which has no acceptor in the main chain. Incorporation of acceptor reduces the HOMO of the polymer with increasing the open circuit voltage (V_{oc}). Consequently, **P6** has a poor charge mobility and low PCE when compared to **P4** and **P5** [24]. Another D–A polymer of thiophene with diketopyrrolopyrrole was synthesised to get **P7** having a lower band gap. The polymer has a very good solubility owing to the presence of alkyl side chains. The PSC of the polymer with fullerene delivered a better PCE