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Organic Photovoltaics

Materials, Device Physics, and Manufacturing Technologies

Second Edition

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Part One
Materials for Thin Film Organic Photovoltaics

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1
Overview of Polymer and Copolymer Materials for Organic Photovoltaics

Solon P. Economopoulos, Grigorios Itskos, Panayiotis A. Koutentis, and Stelios A. Choulis

1.1
Introduction

Predictions of limited fossil fuels and issues associated with their environmental impact have led to a rapid growth of research on photovoltaics (PVs). Until recently, the majority of PVs were silicon-based conventional p–n junction devices; however, the dominance of these solar cells is being challenged by the emergence of third-generation PV technologies based on new materials and device approaches. Among these, are PV technologies based on solution processing methods that enable the low-cost fabrication of solar cell devices. These processes allow the incorporation of different semiconductor materials into single devices that are not necessarily lattice matched. Organic semiconductors are of particular interest as PV materials owing to their unique combination of properties: ease of fabrication, flexibility, tunability, lightweight, and the possibility of large surface coverage [1]. Organic photovoltaics (OPVs) refer to solar cells that contain at least one organic semiconductor in the cell active region [1]; as such, the term includes both all-organic and hybrid PV material approaches. Various OPV approaches that include combinations of organics such as conjugated polymers, fullerenes, small molecules, dyes and inorganics such as porous semiconductors, oxides, and colloidal nanocrystals have been successfully used [1]. In light of the above, OPVs based on light absorbers deposited by solution-processed techniques, in contrast to more involved processing of materials requiring vacuum- or vapor-phase deposition, are of particular interest.

Of the various OPVs, polymer–fullerene solar cells represent a unique category that has seen remarkable progress during the last 15 years, overcoming several key obstacles toward the anticipated OPV milestone efficiency of 10% (Figure 1.1). This chapter will focus on conjugated polymers used for polymer–fullerene bulk heterojunction OPVs with occasional references to all-polymer OPVs. In the first part, key developments over the past 15 years on the characteristics and understanding of such devices will be presented. This will be followed by a review of the effort to improve the performance of such solar cells via optimization of the

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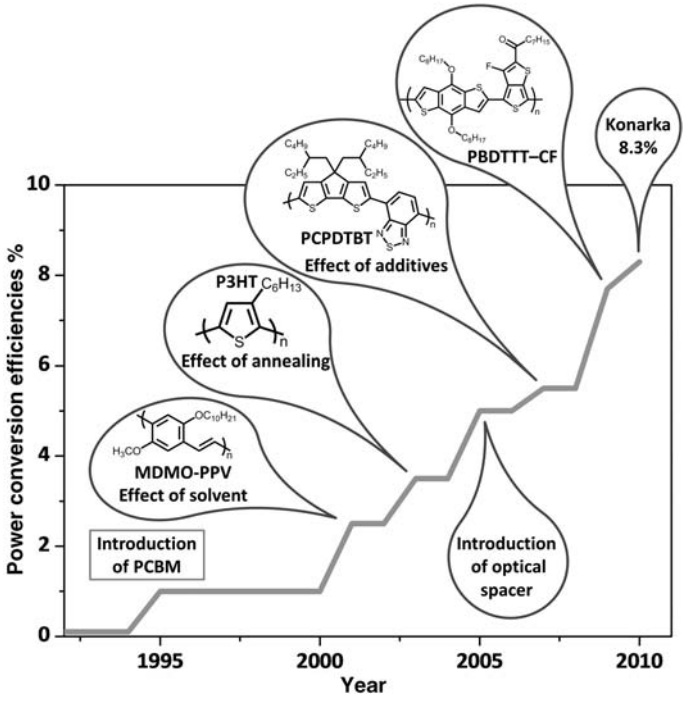

Figure 1.1 Timeline of power conversion efficiencies in OPVs since 1992 to the current best efficiency demonstrated by Konarka Technologies.

material donor (polymer) part of the device, guided by progress in the material design, and improvements on the physical and chemical properties of the conjugated polymers used. The most prominent state-of-the-art conjugated polymer families used in solar cells will be summarized, and their future potential will be discussed. Breakthrough ideas that contributed to the understanding of polymer physical chemistry in devices will be highlighted along with insights that can guide future efforts.

1.2 Early Efforts

The first major development in the field came from the experimental observation that conjugated polymer photoexcited excitons efficiently dissociate from the conjugated polymer to the fullerene interfaces via ultrafast electron transfer processes [2]. This was directly exploited in organic solar cell devices using blends of the two material families (electron donor and electron acceptor) with length scale of heterojunctions within the blend approximately equal to the exciton diffusion length. The proposed structure resulted in the invention of the bulk heterojunction (BHJ)

architecture in 1995 [3]. Prior to this, the low conversion yield of photoexcited Frenkel excitons into mobile carriers heavily limited the efficiencies of polymer–fullerene bilayer OPVs structures; this was attributable to the large binding energies of the former. Yu *et al*. [3] introduced the notion of a bulk mixture of the polymer donor and the fullerene acceptor with phase-separated domain regions of the order of the exciton diffusion length to allow efficient interfacial polymer exciton dissociation. Bulk heterojunction device structures allowed the implementation of thick active layers for efficient light harvesting without compromising the efficiency of the charge separation process and are still the basis for today's best performing organic solar cells. Our review focuses on conjugated polymers used in this type of PV geometry. The success of BHJs was partly attributable to the early use of the highly soluble fullerene phenyl-C_{61}-butyric acid methyl ester ([60]PCBM) [4], which has good electron transport properties and is still the acceptor material of choice in OPVs. Recently, C_{70} [5] and C_{84} [6] fullerene adducts have been introduced and may offer additional advantages. In the same publication introducing the BHJ architecture, Yu *et al*. also investigated the effect of blend morphology on device performance by exploring parameters such as fullerene content, solvent type, and electrode material. Six years later in 2001, Shaheen *et al*. [7] convincingly demonstrated that the nanostructure morphology of the polymer–fullerene blend profoundly affected the PV device performance: The careful selection of solvent gave a better polymer–fullerene blend with smaller phase-separated fullerene domains. In addition, it was later shown that the addition of PCBM to the blend improved the hole mobility in the polymer due to enhanced intermolecular interactions of the polymer chains induced by the fullerene molecules [8]. The heterojunction morphology and its effect on exciton dissociation, charge recombination, and transport in polymer–fullerene BHJ solar cells is still an intense topic of research in polymer–fullerene OPVs [9,10].

1.3
Toward Devices with 5% Efficiencies

Polymer solar cells [2] and polymer light-emitting diodes (PLEDs) [11] were invented in the early 1990s alongside the precursor to polymer field-effect transistors (PFETs) [12]. As such, these branches of polymer electronics shared common grounds and materials that when found to work well in one area would be tried and tested in another. For example, the PPV analog poly[2-methoxy-5-(2′-ethylhexyloxy)-*p*-phenylenevinylene] (MEH-PPV), which was used as a proprietary material in the first PLEDs, was also used in early polymer PVs. MEH-PPV and the similar poly[2-methoxy-5-(3,7-dimethyloctyl-oxy)-*p*-phenylenevinylene] (MDMO-PPV) (Figure 1.1) dominated polymer-based solar cells for most of the 1990s. A large part of the aforementioned progress in understanding the basic physics underlying polymer fullerene solar cells was made using MDMO-PPV (Figure 1.2). Power conversion efficiencies at the start of the century were

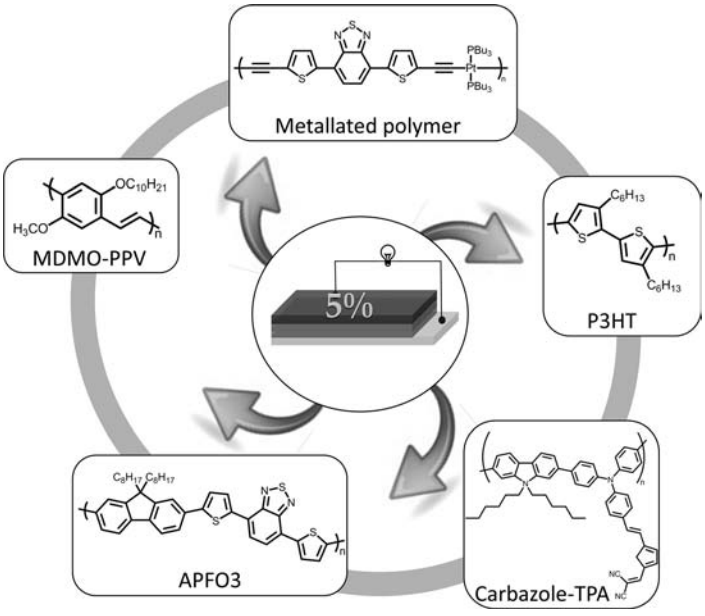

Figure 1.2 Illustration of prominent polymers used in solar cell devices with power conversion efficiencies up to 5%.

standing at the level of ~1%. Optimization of the blend morphology introduced by Shaheen *et al*. [7] led to a threefold increase. By that time, polymer groups worldwide were able to synthesize polymers more efficiently, and the factor of purity came into play in device performance. A research team at Linz Institute for Organic Solar Cells (LIOS) showed that high-purity samples were needed to reach higher efficiencies, pushing PPV-based devices to 3% efficiencies [13]. It is worth noting that another PPV analog synthesized in Cambridge [14] was targeted as a fullerene substitute in creating all-polymer solar cells, but efficiencies failed to compete with the fullerene counterparts.

Optimization of PPV-based polymers brought OPVs based on this polymer family to their performance limits (~3%). Limitations included the relative large energy bandgap (2.5 eV) and low hole mobility of such polymers [15]. Efforts directed toward new polymer families quickly identified thiophene-based polymers [16] as promising materials owing to their good charge transport properties [17]. Alkyl-substituted polythiophenes, in addition to exhibiting good hole mobilities, had increased solubility as well as high regioregularity, a material property that was identified by the PV community at the time as being important. Regioregularity can be controlled during polymerization, and a breakthrough in obtaining high regioregular (>98%) head-to-tail poly(3-hexylthiophene) (P3HT) was first reported separately by Chen and Rieke [18] and McCullough *et al*. [19]. Brabec and coworkers used the optimized material in P3HT/[60]PCBM solar cells [20] and obtained a record high internal quantum efficiency approaching unity.

Further progress was achieved by Sariciftci's group that first introduced postproduction thermal annealing treatments (Figure 1.1) to demonstrate the best OPV efficiency of 3.5% at the time (Figure 1.2) [21]. Hosting a number of improvements over PPV analogs, P3HT took over as the workhorse of polymer–fullerene solar cell research for many years, pushing efficiencies forward [22–25], being a scaffold for interesting structures [26,27], and at the same time providing a prototype system enabling scientists to understand many aspects of the operation of BHJ polymer–fullerene solar cells.

Progress toward OPVs with a landmark of 5% efficiency was achieved by further optimization of PPV- and P3HT-based devices along with synthetic efforts to produce new polymer donors based on new building blocks such as fluorene (APFO3) and carbazole (carbazole–triphenylamine (TPA)) molecules or noble metal-based molecules (Figure 1.2).

The synthetic efforts to create new electron donor polymers were guided by the following desired attributes of the material:

1) Broad absorption covering most of the visible and extending to near-IR up to the predicted optimum gap for single-junction cells of 1.1 μm [28].
2) High hole mobilities for efficient charge transport with values within an optimum range matching electron mobilities in the fullerenes.
3) Optimum leveling of energy states of donor, acceptor, and electrode materials, allowing efficient charge separation with minimum losses to thermal energy while minimizing the energy barrier to the collecting electrodes.

A recently reported model [29] has shown that the maximum power conversion efficiency of a BHJ solar cell can be predicted by the aforementioned properties, namely, the energy bandgap and the lowest unoccupied molecular orbital (LUMO) level of the polymer donor, and by taking into consideration the need to optimize morphological properties controlling transport and recombination within the blend. Keeping this in mind, the LUMO level of an ideal donor polymer should be around 3.7–4.0 eV, considering that the LUMO level of the soluble fullerene (PCBM) is 4.3 eV, to provide the minimum energy difference of approximately 0.3 eV required for efficient Frenkel exciton dissociation. As the optimized bandgap of the ideal light harvesting material (polymer in this case) should be around 1.2–1.5 eV, the highest occupied molecular orbital (HOMO) level value should be adjusted between 5.2 and 5.5 eV. This range of values for the HOMO level of the donor polymer has the additional benefit to ensure a relatively high V_{oc} and air stability in the final devices. Electron and hole mobilities are also crucial parameters for OPV power conversion efficiencies. High mobilities for electrons and holes within the active region are necessary to favorably compete with losses due to geminate and nongeminate charge recombination. Recent theoretical prediction models [30] place desired mobility values, in BHJ cells, on the order of $10^{-2}\,cm^2\,V^{-1}\,s^{-1}$ for one and within a tolerance range of 10^{-1} to $10^{-3}\,cm^2\,V^{-1}\,s^{-1}$ for the other, irrespective of the type of carriers in each case. We note, however, that a balanced ambipolar transport within BHJs is the

ideal condition to eliminate space charge effects and recombination, both of which are essential parameters for optimized solar cell power conversion efficiency values.

Several synthetic strategies have been used [31] to engineer the desired optical absorption characteristics. Among these include increasing the quinoid character of the ground state of polyaromatic conjugated polymers [32,33] and introducing molecular rigidity to increase planarity between adjacent aromatic units, thus extending conjugation and facilitating delocalization [34–36]. An additional and widespread strategy includes the incorporation of electron-withdrawing and electron-accepting moieties, either in the aromatic unit [37] or, more effectively, in the same polymer backbone; this approach will be discussed in more detail later. Other efforts include the optimization of the charge transport properties such as that recently reported by Ying and coworkers who used pyridal[2,1,3]thiadiazole as a building block for conjugated polymers and reported on the increased regioregularity of the thiadiazole moiety, resulting in an increase in hole mobilities by two orders of magnitude compared with their regiorandom counterparts [38]. As more and better syntheses are being explored to tailor physical and chemical properties of donor materials to the desired functionalities mentioned, the current crop of polymers used in polymer–fullerene PVs exceeding 7% solar cell efficiencies (Figure 1.3) will be enriched. Such high-performance polymers are discussed in the following sections.

1.4 Novel Thiophene-Containing Polymers

Moving away from P3HT homopolymers, the community realized that the chemical tailoring required to attain the variety of properties for this particular technology would necessarily involve copolymerization. This meant targeting the incorporation of various molecular units, each enriching the final material with specific properties. Thiophenes and their analogs are still encountered as basic building blocks in many copolymers in new polymer–fullerene solar cells with record high efficiencies. In part, this is because thiophenes are good electron donators in donor–acceptor copolymers, and their facile incorporation was attributable to the wide commercial availability of analogs suitable for copolymerization. In light of thiophenes' widespread use in low-bandgap copolymers, a reference to specific outstanding thiophene-based copolymers follows.

A copolymer specifically designed for solar cells was introduced based on the 4,4-dialkylcyclopentadithiophene-2,6-diyl (CPDT) [39,40]. Copolymerization of CPDT with benzothiazole afforded the copolymer PCPDTBT (Figure 1.2) [41] exhibiting desirable optical characteristics and charge transport mobilities, leading to initial device efficiencies of ~3%. PCPDTBT, however, seemed to underperform based on theoretical estimations (Figure 1.4) [29]. The main drawback was attributable to poor morphological characteristics of PCPDTBT–PCBM blends. A year later, Bazan and coworkers introduced additives to control the blend morphology,

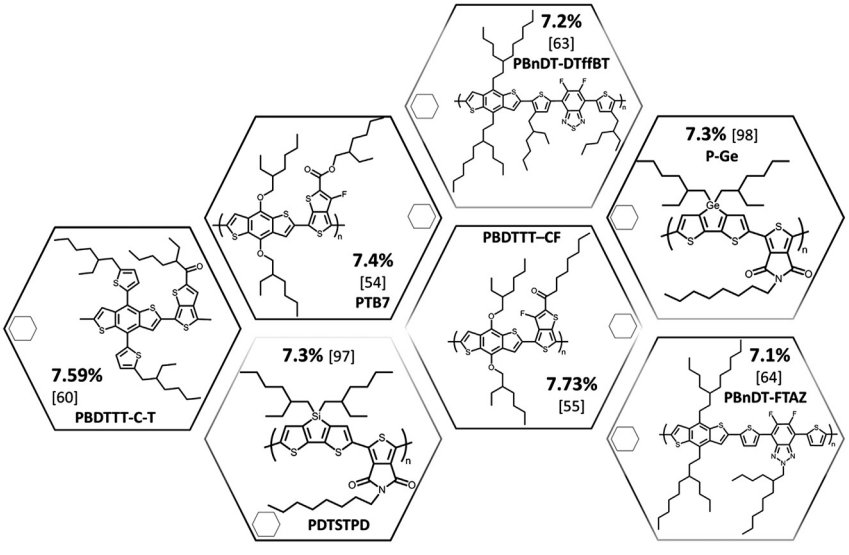

Figure 1.3 Various polymer electron donors with some of the highest device efficiencies reported to date.

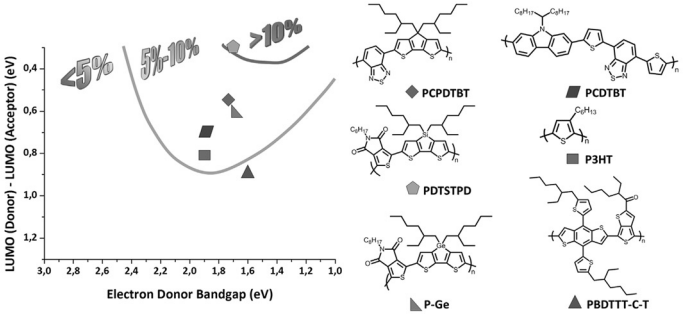

Figure 1.4 Schematic illustration of the theoretical prediction by Scharber *et al.* [29] of the efficiency of polymer–PCBM solar cells based on the polymer energy gap and the polymer–PCBM LUMO band offsets. Various high-performance polymer donors synthesized are placed on the prediction graph. In publications in which the exact LUMO of the acceptor is not mentioned, a value of 4.0 eV for [60]PCBM and 4.1 eV for [70]PCBM is assumed.