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All-Polymer Solar Cells Based on Wide-Band Gap Conjugated Polymers

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Abstract. Recently, there has been an increased utilization of wide bandgap polymer electron donors in non-fullerene organic polymer solar cells. Consequently, scientists and engineers worldwide have shown substantial interest and research focus on all-polymer solar cells utilizing wide bandgap conjugated polymers. These advanced materials provide distinct benefits in terms of adjustable electronic properties, superior effectiveness, and possibility for cost-effective manufacturing, making them a central focus for the advancement of future solar energy technologies. This article will begin by giving a detailed summary of the progression of all-polymer solar cell development in recent decades. We will track the major achievements and advancements that have influenced the field of organic photovoltaics, from its earliest discovery to the most recent progress in polymer chemistry and device engineering. This historical viewpoint will focus on the continuous initiatives and advancements that have propelled the enhancements in performance and expanded the range of applications for polymer solar cells. Afterwards, the article will outline the fundamental layout and functioning principles of polymer solar cells. We will investigate the basic elements such as the active layer, charge transport layers, and electrodes, and demonstrate how these components work together to convert sunlight into electrical energy. In conclusion, the paper will explore the studies on donor materials of conjugated polymers with wide bandgaps. These materials are now seen as crucial elements needed to improve power conversion efficiencies and enhance stability in polymer solar cells.

Keywords: All polymer organic solar cell; Wide-band gap conjugated polymer.

1. Introduction

In today's society, energy problems and environmental pollution have become significant issues due to technological progress and modern advancements. Several non-renewable natural resources are in crisis due to their diminishing quantities and are frequently associated with pollutant emissions, causing environmental pollution. In order to preserve the environment that is crucial for human survival, it is necessary to decrease the consumption of harmful fossil fuels and to advance the utilization of renewable energy sources.

Solar energy technology, wind energy technology, tidal energy technology, hydroelectric power technology, and nuclear energy technology are all examples of renewable energy sources. Solar energy has attracted considerable interest from researchers because of its continuous availability and lack of environmental harm, as it is a renewable resource. The sun emits around 1.2×10^5 TW of energy to Earth, equaling 99% of the planet's total energy and offering a vast renewable energy opportunity. Different kinds of solar cells include silicon solar cells, multijunction thin-film solar cells, and organic polymer solar cells. Of these options, organic polymer solar cells are being heavily researched because of their affordable price, light weight, and bendability. Specifically, the combination of wide bandgap conjugated polymer donors and small molecule acceptors in films can capture a notable amount of sunlight, thus greatly enhancing the efficiency of solar cell conversion and drawing interest from researchers.

With ongoing technological advancements, organic polymer solar cells have seen significant progress in material synthesis, device structure design, and performance optimization. These developments have not just improved the effectiveness and durability of solar panels, but also expanded their range

of use, establishing them as an essential element in the upcoming energy industry. Scientists are always seeking out fresh materials and technologies to improve the efficiency of organic polymer solar cells, with the goal of making solar energy usage more effective and eco-friendly. By working on these initiatives, the aim is for humanity to accomplish sustainable energy advancement soon, lessening the harm to the environment and safeguarding our common residence.

2. Development of all-polymer solar cells

In the 1950s, the phenomenon of organic photovoltaic was first observed by scientists, and organic photovoltaic devices are based on anthracene single crystal materials. However, not only is the conversion efficiency of the device extremely low, but it can only generate 200mV photogenerated voltage under light [1]. This discovery has led to the exploration of organic solar cells, but it has not been able to improve the cell efficiency for almost two decades, and the cell efficiency has been less than 0.1%.

In 1986, Dr. C.W. Tang and other researchers of Kodak Company in the United States made new achievements in the photoelectric conversion efficiency which had been stalled for many years. Using N-type tetracarboxylperylene derivatives and P-type copper phthalocyanine in the active layer, the electron donor and electron acceptor were prepared into a double-layer device in the form of a sandwich by thermal evaporation method. The performance is greatly improved, and the photoelectric conversion efficiency is more than 1% under the simulated AM2 illuminance [2]. The success of this research lays a foundation for the development of all-polymer solar cells in the future.

In 1992, Sariciftci and other researchers used MEH-PPV as donor fullerenes (PCBM) as receptors to prepare double-layer battery devices while studying the active layer materials of devices, when they found that under light induction, charge transfer occurred on the order of femtoseconds. This discovery was monumental because it provided a new understanding of ultrafine charge separation processes, which are crucial for the development of high-efficiency solar cells. The ability to separate charges quickly and efficiently is essential for reducing energy losses and improving the overall performance of solar cells [3]. Sariciftci's work laid the foundation for future research in organic photovoltaics, encouraging scientists to explore and optimize other donor-acceptor combinations that could potentially offer even better performance.

On this basis, Yu et al. blended the donor wide-band gap material MEH-PPV with receptor fullerene (PCBM) derivatives in 1995, and made a photoactive layer with interpenetrating and interconnecting network structure using the spinning coating method. They considered this photoactive layer to be a bulk heterojunction structure system (BHJ). Then a new device structure model of bulk heterojunction is proposed. This structure can greatly increase the effective contact area of the two materials. Excitons can be fully dissociated and diffused, so that the amount of free charge obtained increases, which greatly improves the photoelectric conversion efficiency of the device, reaching nearly 2.9%. Soon after, wide-band gap copolymer PFB composed of fluorene and triarylamine structural units was also applied to fully polymerized organic solar cells [4]. Under the continuous research of researchers around the world, it has been found that the polymer solar cell with the bulk heterojunction blending system is the most excellent in the field of organic polymer solar cells in the past two decades.

Today, scientists and scholars continue to explore and innovate all-polymer solar cells. They study the working principle, optimize the device engineering process, and design new materials, which has improved the photoelectric conversion efficiency of photovoltaic devices based on fullerenes as accepter materials to nearly 13% [5]. Its material structure is shown in Figure 1. At this time, non-fullerene organic solar cells have entered the field of view of researchers, which absorb more powerful in the visible light region than fullerene-based organic solar cells, and have the most significant cost advantages in industrialization. With the continuous exploration of non-fullerenes by researchers, the single-junction photoelectric conversion efficiency of organic photovoltaic cells based on non-

fullerenes (ITIC and its derivatives) has broken through 19%, and the double-junction photoelectric conversion efficiency has broken through 20%.

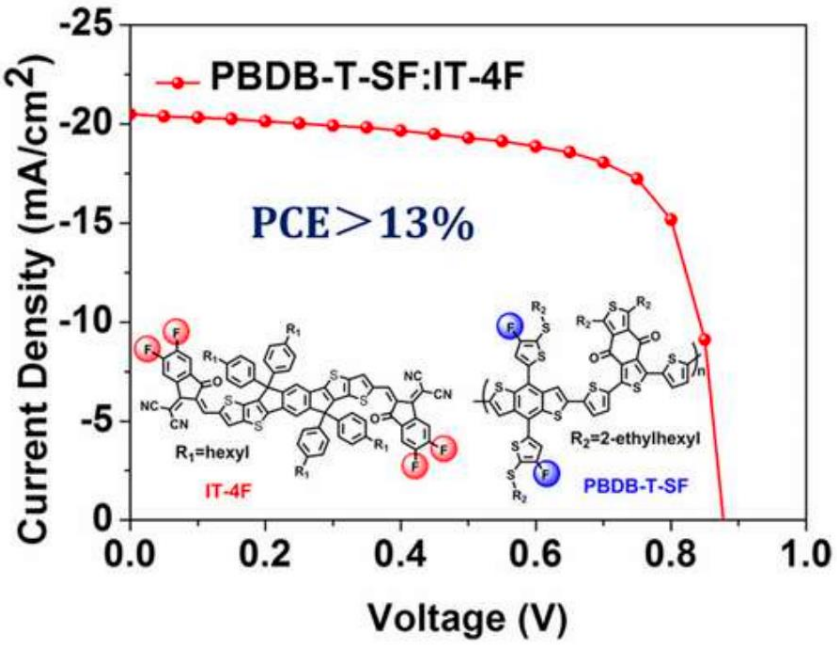

Figure 1. Single-layer organic solar cells with device efficiency of more than 13% [6].

All-polymer solar cells after such a long time of development, the development of all-polymer solar cells with narrow band gap non-fullerene receptors and wide-band gap conjugated polymer donors is very rapid. In order to achieve the commercialization of solar cells, solar cells based on wide-band gap conjugated polymers need to continue to develop. And I believe it will reach a new stage under the leadership of researchers around the world.

3. The basic structure and principle of polymer solar cells

3.1. Basic structure of polymer solar cells

The device structure of polymer solar cells is mainly bulk heterojunction, which can increase the contact area between the donor material and the acceptor material, promote the dissociation and diffusion of excitons, and improve the photoelectric conversion efficiency of the device [7]. Polymer organic solar cells provide numerous important benefits. Their uncomplicated manufacturing process has minimal energy usage, allowing for production at ambient temperature and facilitating solution processing and effective roll-to-roll (R2R) manufacturing. Furthermore, these solar panels are lightweight and can be mass-produced using printing techniques. Their adaptability enables them to be used in various applications, as their consistency in performance is maintained in various conditions of use. The advantages make polymer organic solar cells a promising technology for sustainable and flexible energy solutions.

Based on the polarity of the anode and cathode, the battery device structure can be categorized as either conventional structure or inverted structure. The structure is shown in Figure 2. The majority of formal device structures utilize ITO-coated glass substrates as the device anode. A layer of PEDOT: PSS (The structural formula is shown in Figure 3.) in its acidic aqueous solution is spin coated on ITO, then layered on the active layer with the donor and acceptor, and ultimately the cathode metal electrode is evaporated [8]. Nevertheless, the environment will impact the metal negative electrode in the formal device layout, leading to decreased stability, and the flip device structure can compensate for this issue [9]. The cathode of the flip device structure is made of indium tin oxide (ITO) which gathers holes, while the anode is typically composed of Ca, Ba, and Ag metals and is located at the top of the structure.

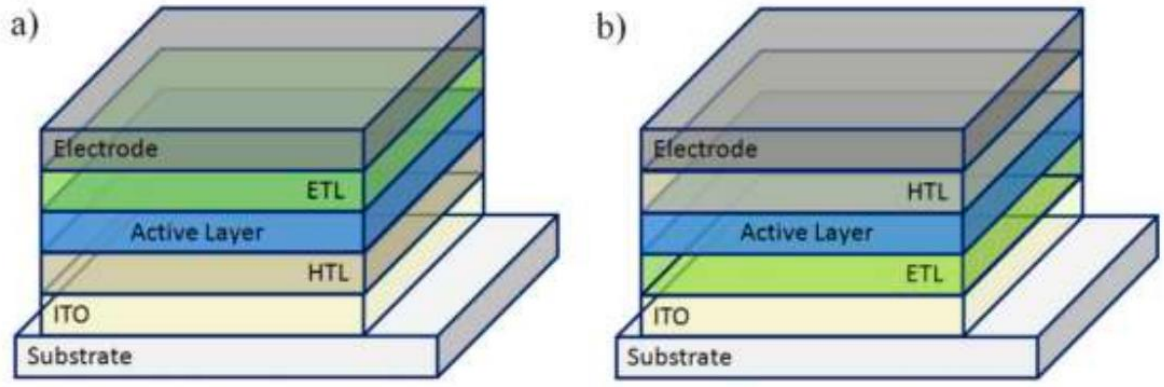

Figure 2. Different body heterojunction device structures: a. Standard devices; b. Flip device [6].

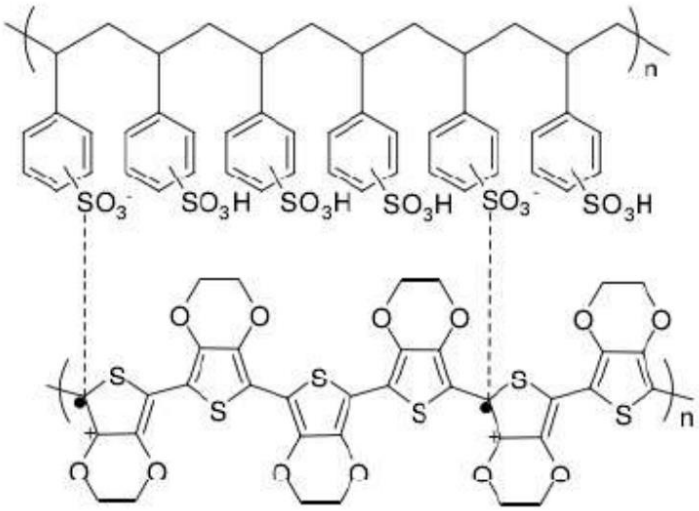

Figure 3. Structure of PEDOT: PSS [6].

3.2. Working principle of polymer solar cells

Polymer semiconductors typically have a low dielectric constant, and the photovolt-effect occurs when excitons, comprised of holes and electrons, are formed upon exposure to light. The efficiency of this exciton dissociation process is critical for the overall performance of polymer-based photovoltaic devices. Enhancing the dielectric constant of the material or engineering interfaces that facilitate exciton dissociation can significantly improve the efficiency of these devices.

The operational mechanism of polymer solar cells can be categorized into the subsequent four steps. To start, the active layer takes in solar energy, causing the incoming light energy to be higher than the polymer's optical band gap, leading to the creation of excitons [10]. Furthermore, the separation of excitons created by the absorption of photons by both the donor and acceptor molecules can only occur efficiently once they migrate to the boundary between the donor and acceptor. The active layer of interconnected network assists in the exciton dissociation process, enhancing the battery's photoelectric conversion efficiency. Next, at the exciton diffusion interface, the donor and acceptor divide into holes and electrons, creating free charges. The LUMO energy level and HOMO energy level of the donor material are higher than those of the acceptor material, with the energy level difference being greater than the exciton binding energy. This results in electrons moving from the LUMO energy level of the donor to the LUMO energy level of the acceptor, creating a charge transfer complex called the CT state. After the exciton separates into electrons and holes, the holes travel towards the positive electrode through the P-type semiconductor, while the electrons travel towards the negative electrode through the N-type semiconductor due to the built-in electric field [11]. The working principle of an organic polymer solar cell is shown in Figure 4.

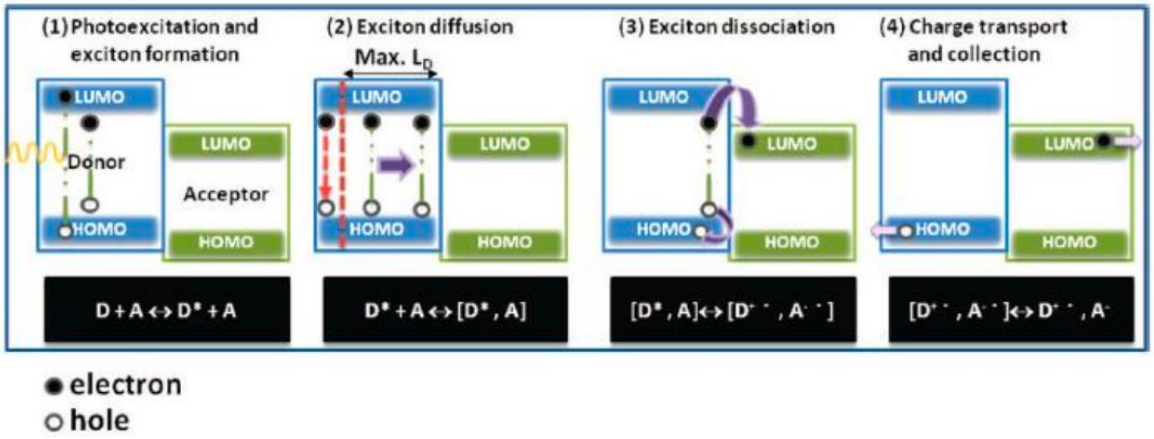

Figure 4. Organic polymer solar cell working principle schematic diagram [12].

The crucial aspect of the organic solar cell is the active layer material. Light shines on the active layer, causing it to absorb photons and create excitons that then move towards the interface between the donor and acceptor. Under the action of internal electric field, the holes and electrons transmit to the positive and negative electrodes to generate photocurrent and photovoltage. Therefore, to improve the photoelectric conversion efficiency, it is necessary to further optimize and improve the active layer material. The active layer is composed of donor material and acceptor material. The researchers found that the non-covalent interaction caused by the rotaxane structure can make the active layer form a fiber network structure. This phase separation scale can enhance the charge extraction efficiency of the device, thereby improving the charge transfer and collection rate. Rotaxane is a kind of main and objective compound which is composed of cyclic crown ether and dumbbell linear molecular polymer by non-covalent bond. When the rotaxane structure is applied to the polymer, the original properties of the polymer can be retained, but the ring molecules affect the intramolecular and intermolecular interactions through rotation and sliding, resulting in the influence of the complex properties.

4. Research and prospect of wide-band gap conjugated polymer donor materials

Researchers have focused a lot on wide-band gap polymer donors in the past few decades. As organic solar cells progress, improvements are consistently made to photovoltaic materials, boosting their overall efficiency and performance. This continuous progress demonstrates how the field is constantly changing and the consistent attempts to enhance the characteristics and functionalities of these materials for improved energy conversion and wider usage. The blend film of wide-band gap conjugated polymer donors and small molecule receptors can absorb most sunlight, and early research was based on the fullerene receptor material system. Researchers have used conjugated polymer donor materials such as benzodithiophene (BDT), difluorobenzothiadiazole (ffBT), naphthalene dithiadiazole (NT), and pyrrole pyrrodione (DPP). The researchers defined the wideband gap polymer donor as a conjugated polymer with an optical band gap greater than 1.80eV, and the wideband gap polymer donor material with complementary absorption spectrum has excellent photoelectric properties, which provides the possibility for realizing solubilizable processing, and is the most suitable donor material for solar cells [13]. In order to improve the performance of the donor material, the polymer donor material needs to form a complementary absorption spectrum with the acceptor material, so that the photovoltaic device can maximize the absorption of solar photons. It also needs to form a molecular energy level match with the acceptor material, have good solubility and film formation, and form a good nanoscale phase separation morphology with the acceptor material.

4.1. Wide-band gap conjugated polymer based on benzodithiophene (BDT) as donor

Benzodithiophene (BDT) has a large planar and symmetrical structure, and is widely used as the donor of wide-band gap conjugated polymers because of its simple synthesis route [14]. By studying

the relationship between the molecular structure of BDT and the photovoltaic performance, the researchers found that the open circuit voltage of photovoltaic devices can be improved by improving the electron delocalization of the polymeric main chain and modifying the substituent groups of BDT units. Adjusting the separation of conjugated polymer electron donor and non-fullerene derivative electron acceptor blend films can help achieve an optimal morphology for exciton dissociation, greatly increasing the short-circuit current of the device.

Benzodithiophene 4, 8-dione (BDD) has the characteristics of weak electron absorption, which is beneficial in designing photovoltaic materials that require fine-tuning of their electronic properties. One of the standout features of BDD is its ease of chemical structure modification. This allows researchers to tailor the material's properties to better suit specific applications in solar cell technology. BDD also possesses a low HOMO (Highest Occupied Molecular Orbital) energy level, crucial for achieving high open-circuit voltage in solar cells. Additionally, BDD has a high absorption coefficient, even in the short-wave region of the spectrum, enhancing the material's ability to absorb solar energy efficiently, thereby improving the short-circuit current (Jsc) and fill factor (FF) of the solar cells. This characteristic is particularly important because it enhances the material's ability to absorb solar energy efficiently, thereby improving the short-circuit current (Jsc) and fill factor (FF) of the solar cells. These improvements directly translate to better overall efficiency of the photovoltaic devices. Another significant advantage of BDD polymers is their strong π-π (pi-pi) stacking, specifically M stacking and face-on stacking. These stacking arrangements facilitate efficient charge transport within the polymer matrix, further enhancing the performance of the solar cells.

4.2. Prospects of wide-band gap conjugated polymers

Solar cells made from wide-band gap conjugated polymers have made significant progress thanks to researchers' ongoing efforts globally for many years, but further development is still needed. For example, the efficiency and performance of organic solar cells need to be further improved, which requires efficient exciton dissociation and efficient carrier transport. In addition, under long-term light, wide-band gap conjugated polymer materials are prone to photooxidation and thermal degradation, which will have a certain impact on the performance and service life of solar cells. The synthesis of polymer donor materials for solar cells is often complicated by the production of by-products. It against the purity requirement of solar cells and hinders the commercialization and lifespan of organic solar cells. If these obstacles can be resolved, solar power has the potential to become a widely adopted sustainable energy source in human society.

5. Conclusion

Because of Earth's pollution and the depletion of energy resources, renewable energy sources are now considered an important solution to these issues. Recently, as environmental problems worsen and traditional energy sources diminish, new energy research and usage have become a focal point across society. Out of these, solar power has garnered broad interest and thorough exploration due to its limitless and eco-friendly nature.

This paper initially presents an in-depth examination of the evolution of solar cells made from organic all-polymer materials. From the 1950s onward, scientists have been researching methods to utilize solar energy and have consistently improved associated technologies. After many years of hard work, there have been notable advancements in solar cell technology, especially in the areas of materials and efficiency, paving the way for widespread use.

Following that, this paper provides an overview of the design and functioning principles of polymer solar cells. Polymer solar cells have become a popular area of research in the solar cell field due to their lightweight, flexibility, and low cost. This section aims to enhance readers' comprehension of the benefits and difficulties of these cells by explaining their fundamental structure, operation mechanisms, and charge transfer processes.

Lastly, the article examines the advancements in solar cells created using wide bandgap conjugated donor polymers. Wide bandgap conjugated donor polymers are extensively studied due to their remarkable optoelectronic properties and adjustable light absorption spectrum. This part offers an in-depth examination of the fabrication techniques, optical characteristics, and uses of these substances in solar panels, with the goal of providing useful guidance and perspectives for upcoming studies. Through the exploration of these subjects, this article aims to enhance readers' comprehension of polymer solar cell technology and encourage fresh ideas for utilizing alternative energy sources.

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