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Research progress in organic solar cells

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Abstract. In recent years, with the rapid development of human society, energy consumption has been increasing, and the use of traditional fossil fuels has also led to a certain amount of pollution. Solar energy, as a new type of energy, stands out due to its clean and large capacity, and solar cells have attracted hot attention. Although the overall development of solar cells started relatively late, the field of organic solar cells has benefited from breakthroughs in some materials and technologies, and has developed rapidly. This paper will introduce the basic principles of solar cells, summarize and analyze the development status of Schottky organic solar cells, donor acceptor materials, biomass based materials, and nanomaterials. It will summarize and analyze the efficiency improvement and performance optimization of these major categories of solar cells, draw prospects for future development in this field, and hope that organic solar cells will have more extensive applications in the future.

Keywords: Solar energy; Schottky organic cell; acceptor materials; biomass-based materials; nanomaterials.

1. Introduction

As the world entered the 21st century, global development necessitates the support of diverse energy sources. The world's conventional energy resources include coal, oil, and natural gas. However, the reserves of these resources are finite, and some are already nearing depletion, failing to meet current human development needs. The utilization of various traditional fossil fuels produces significant amounts of greenhouse and toxic gases, including carbon dioxide, nitrogen dioxide, and sulfur dioxide. These gases contribute to frequent natural disasters like global warming and acid rain, degrade the ecological environment, and pose serious threats to human life. In response to this situation, countries worldwide have prioritized sustainable development and are dedicated to advancing renewable energy sources such as solar, wind, hydro, and tidal energy. Among these various renewable energy sources, solar energy is arguably the most extensively utilized. Solar energy's inexhaustible supply distinguishes it from other energy sources, and importantly, it does not pollute the environment during its use. The vigorous development of the photovoltaic industry is more evident in the western provinces and regions of China Inner Mongolia Autonomous Region is one of the most suitable provinces for developing photovoltaic power stations, because the exploitable solar energy resources in Inner Mongolia exceed 9 billion kW, accounting for about 1/5 of China's total exploitable solar energy resources, and the annual sunshine time is about 3000 hours. [1] Solar cells can be classified into two types based on their production raw materials: inorganic solar cells and organic solar cells. The research on inorganic solar cells started earlier and was relatively extensive, but due to the high material cost and complicated production process of producing inorganic solar cells, it is not conducive to their further large-scale use. Organic solar cells, on the other hand, are pollution-free, lightweight, low-cost, have simple processes, a wide range of raw material sources, are easy to process, and form films on a large area, making their advantages even more prominent. Therefore, this paper will introduce the principles of organic solar cells, analyze and summarize the development and progress of different types and materials of solar cells, and provide evaluations. Roughly including Schottky organic solar cells, donor and acceptor materials, biomass based materials, and nanomaterials. These contents will be unfolded. This paper hopes to analyze and summarize different types of organic solar cells, so that they can be widely applied in the future.

2. Organic Solar Cells Working Principle:

Organic photovoltaic cell is a semiconductor device with optical and electrical conversion characteristics, which can directly convert solar radiation into direct current. Photovoltaic cell is the most basic unit of photovoltaic power generation. Throughout the development process of organic photovoltaic cells, the overall basic framework and structure have been relatively fixed. The main areas of improvement are the design of intermediate layers and the use of different materials to improve the overall efficiency of converting solar energy into electrical energy. For a relatively simple organic photovoltaic cell, the device itself mostly uses silicon as the material, with a positive electrode and a negative electrode set up, and a junction in the middle, which is also the core part of the entire principle.

For the operation of the entire battery like in fig.1, the first step is to receive sunlight in a place with sunlight, which means obtaining photons from it, which can provide energy for releasing electrons. For solar cells, reflection is usually a major way of energy loss. In order to preserve energy, an anti-reflection coating is applied on the upper layer of the solar cell to help photons enter the cell without being reflected off.

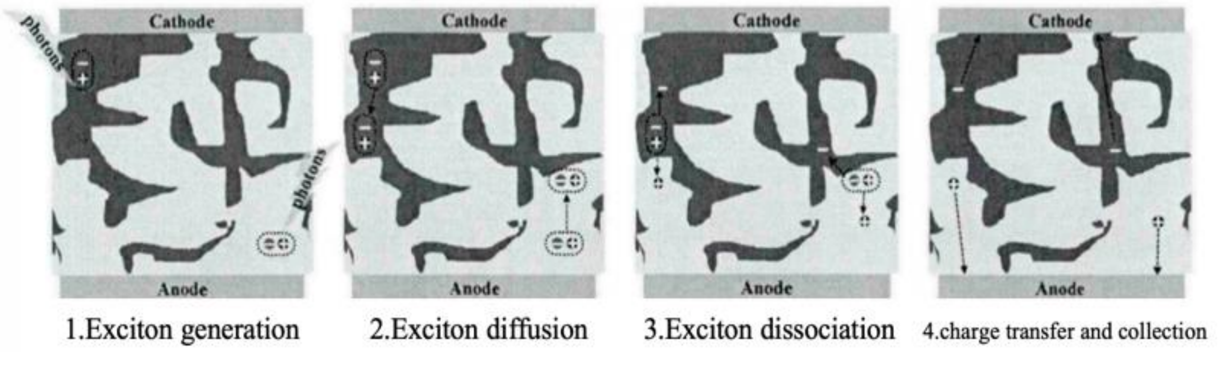
The second step is the formation of electrons and holes. As the energy of photons is absorbed by the semiconductor material in the battery, electrons are excited from their atomic orbitals to higher energy levels, resulting in the generation of free electrons and positive holes.

As the second step occurs, the third step forms an electric field in the battery. On either side of the junction are usually p-type semiconductors with positive holes as the majority of charge carriers, and on the other side are n-type semiconductors with electrons as the majority of charge carriers. Therefore, at the intermediate junction, an electric field will be generated.

In the fourth step, under the electric field of the p-n junction, free electrons are pushed towards one side of the n-type semiconductor, while positive holes are pushed towards one side of the p-type semiconductor. This separation forms a potential difference near the junction.

In the fifth step, potential difference will let electrons to flow from n-type semiconductors to p-type semiconductors through an external circuit, generating current. The entire current generating circuit is often set outside the positive and negative poles, and the electrons generated by its absorption of photons and internal reactions form a circuit, thereby converting solar energy into electricity.

After generating electricity, connect the circuit to a device that can load electricity, such as a light bulb or battery. When electrons flow through the load, they release energy and then return to the p-type semiconductor according to the circuit to complete the circuit. For the entire process, there is no damage to any components, and electrons return in their original path to form a cycle. Therefore, in theory, as long as a certain effective circuit is designed and a certain number of photons are absorbed, the power generation of organic solar cells can achieve a very ideal effect.



1.Exciton generation 2.Exciton diffusion 3.Exciton dissociation 4.charge transfer and collection

Fig 1. Organic Solar Cells Working Principle [2].

3. Improvement and Research Progress of Solar Cells of Different Types and materials

3.1. Schottky organic solar cells

Schottky cells are the earliest organic solar cells, that is, organic semiconductor dyes such as phthalocyanine are steamed on a substrate under vacuum conditions to form a sandwich single-layer structure. For the Schottky cell, excitons formed by light excitation achieve positive and negative charge separation in the diffusion layer of the Schottky junction driven by the electric field of the node region. Excitons formed at other locations in the device must first move into the diffusion layer to form a contribution to the photocurrent, and the migration distance of excitons in organic dyes is quite limited, usually < 10nm, so most excitons are recombined before separating into electrons and holes, resulting in low photoelectric conversion efficiency of such devices.

From JinSongHuang research group [3], the structural design and simulation optimization of the Schottky structure perovskite solar cell are carried out by using wx-AMPS simulation software. The transparent conductive electrode with different work function and the influence of the opposite electrode on the performance of solar cell are studied. It is found that the transparent conductive electrode with appropriate work function is the key to determine the conversion efficiency of solar cell. The adjustment of electrode work function mainly changes the energy band structure at the interface of perovskite active layer and electrode, reduces the current carrier recombination significantly, and improves the device performance. When the work function of transparent conductive electrode is 3.8eV, the efficiency of solar cell is increased to 17.89%. When the work function of the electrode is 5.1 eV, the efficiency of the solar cell is increased to 18.75%. On the basis of optimizing the energy band, the defect state, thickness and p/n doping concentration of the active layer of perovskite are studied. The efficiency of Schottky perovskite solar cells increased to 20.01% when the main doped cells were lightly doped, the defect state density was low (2 × 1016-7 × 1016 cm-3) and the thickness was 300-600 nm, which was 63.4% of the planar heterojunction structure limit efficiency (30.1%). The performance optimization of energy band matching and absorption layer is the key to improve the performance of Schottky perovskite solar cells, and it also shows that Schottky perovskite solar cells can maintain high efficiency while further reducing the cost, and have application potential.

3.2. Donor material with organic solar cells

3.2.1. Oligopolythiophene small molecule donor materials

Oligopolythiophene has the advantages of both small molecules and polymers because of its excellent photoelectric properties, charge transport properties, good stability and easy regulation of energy levels. Such advantages have been widely concerned in the development.[4]

In 2006, Peter B ä uerle's team [5] designed and synthesized a small molecule donor DCV5T using oligothiophene as the core electron donating monomer and dicyanoethylene (DCV) as the terminal. The PCE of the device based on DCV5T: C60 is 3.47%. In 2011, the research team [6] synthesized three small molecule donors 1, 2, and 3 using selenophene as a substitute for thiophene at different positions and quantities based on DCV5T, and compared the device performance between the synthesized small molecule and DCV5T. Research has found that due to the increase of selenophene monomers, the absorption spectrum gradually shifts red and the molar absorption coefficient gradually increases. Based on 3:C60, the VOC of the two components is as high as 1 V, and the PCE is 3.09%. Research has shown that although reducing the optical band gap and HOMO/LUMO energy level of this type of material by changing the substitution mode of the conjugated main chain has not achieved excellent results, all three donors exhibit better thermal stability and wider absorption range than DCV5T. In 2013, Yang Yang's team [7] designed and synthesized a small molecule donor T3 by combining the selenophene strategy with octyl cyanoacetate end capping. The device performance was studied by binding to the fullerene receptor PC71BM. Study research has shown that the introduction of selenophene effectively regulates the optoelectronic properties of the material, and the performance of OSCs based on T3: PC71BM has been improved. With the addition of polydimethylsiloxane additive, the PCE reached 6.15%, and the JSC increased to 10.79 mA·cm^{-2}.

In 2009, Chen Yongsheng's team [8] synthesized a series of small molecule donors DCN3T, DCN5T, and DCN7T based on oligothiophene, and compared and studied them. The thermal, optical, and electrochemical properties. In 2010, the Yin Shougen team and Chen Yongsheng team [9] conducted a study on the device performance using DCN7T as the donor and PC61BM as the acceptor based on this. The results showed that the wide absorption range of DCN7T resulted in a high JSC of 12.4 mA·cm-2 and a high VOC of 0.88 V, with a PCE of 3.7%. The study pointed out the defect of low FF in the device and proposed research ideas to further improve device performance through molecular structure modification and other methods.

In 2018, based on extensive research on non-fullerene acceptors (NFAs), Chen Yongsheng's team [10] designed and synthesized small molecule acceptors F-0Cl, F-1Cl, and F-2Cl with different numbers of Cl atom substitutions for DRCN5T, and compared the effects of different degrees of chlorination on material and device performance. The results showed that end group chlorination led to absorption redshift, enhancing the crystallinity of the material and significantly improving electron mobility. The PCE of the device based on DRCN5T: F-2Cl reached 9.89%. Research has shown that molecular modification of receptors through strategies such as chlorination to obtain energy levels and active layer morphology that better match the donor material is an effective approach to further improve device performance. In 2020, the Lu Shirong team synthesized small molecules 2F7T and 2Cl7T based on DRCN7T by introducing halogen atoms F and Cl, respectively. Research has shown that the introduction of halogen atoms leads to a decrease in HOMO energy levels and an enhancement in charge transfer ability.

In 2024, Xiao Zeyun and Lu Shirong's team conducted a study on terminal side chain modification based on Tz6T, replacing the ethyl side chain on the original terminal with a propyl and isopropyl chain to synthesize oligothiophene based small molecule donors Tz6T-P and Tz6T-iP. The study showed that compared with the straight chain of Tz6T-P, the rigid branch chains in Tz6T-iP were almost planar in the ground state and had higher crystallinity. Therefore, Tz6T iP has lower bimolecular recombination and trap assisted recombination, higher exciton dissociation and charge collection abilities, and longer carrier lifetime, proving that oligothiophene donors still have considerable prospects in the large-scale production and application of OSCs.

3.2.2. Dithienopyrrole small molecule donor materials

The dithiophene pyrrole (DTP) monomer has advantages such as high carrier mobility and strong light absorption due to its planar structure and electron rich properties. Combined with its simple structure, easy modification, and simple synthesis process, it can be applied to SM-OSCs.

In 2014, Peter B ä uerle's team [11] connected DTP to the capped monomer DCV through alkylated thiophene π bridges with different substitution sites, designed and synthesized a small molecule donor 4-9, and conducted device research in combination with the fullerene receptor PC61BM, achieving a maximum PCE of 6.1%. In 2017, Peter B ä uerle's team and J ö rg Ackermann's team [12] improved the morphology of 9: PC71BM based devices through solvent vapor annealing (SVA), with PCE increasing from 7.1% to 7.74%. Subsequently, the team [13] performed subtle structural modifications on the side chains of DTP monomers based on small molecule 9, changing the branching points of alkyl side chains and synthesizing small molecule donor 11. The device performance based on 11: PC71BM was significantly improved, and combined with SVA post-treatment, the PCE reached 8.16%. Research has shown that the modification of side chains reduces the solubility and donor acceptor compatibility of the material, thereby slowing down the diffusion between donors and acceptors during the SVA process and improving the photovoltaic performance of the material.

In 2024, Ge Ziyi's team designed and synthesized small molecule donors G17 and G19 using PDT and DTS as fused ring π bridges, and conducted research on three components in combination with the D18-Cl: Y6 system. GIWAXS shows that the two-dimensional profile of G17 based on PDT exhibits circular scattering characteristics, indicating that the random orientation of the crystal towards the substrate is caused by the larger steric hindrance of G17. However, due to the introduction of Si atoms, G19 based on DTS exhibits higher molecular order and stronger edge on, resulting in more efficient charge transfer and good phase separation. The efficiency of the three components based on G19 has increased to 18.53% compared to G17 devices (17.13%).

3.2.3. Porphyrins small molecule donor materials

The highly conjugated system of porphyrin rings enables rapid electron transfer to receptors, combined with good light absorption ability, resulting in excellent photovoltaic performance of porphyrin materials, which has attracted widespread attention in the application of OSCs.

In 2012, Cao Yong's team designed and synthesized a novel small molecule donor DHTBTEZP with porphyrin as the core electron donating monomer. Subsequently, the team gradually improved the use of materials by replacing the 3,5-di (dodecyloxy) phenyl group of Por-2 with 4-octyloxyphenyl and 2-ethylhexyl-thiophene groups, and synthesized DPPEZnP-O and DPPEZnP-TEH. The PCE of the devices combined with PC61BM was significantly increased to 7.23% and 8.08%, respectively. The study found that by modifying the side chains on the porphyrin core, the intermolecular π - π stacking of the material in the thin film was significantly enhanced, and the JSC was significantly increased from 11.88 mA · cm-2 to 16 mA · cm-2 and 16.76 mA · cm-2 compared to Por-2 devices.

In 2016, Wai Kwok Wong et al. designed and synthesized small molecule donors 4a, 4b, and 4c, using 4-ethynyl-2,5-bis (hexoxy) benzaldehyde to connect the capped monomer 3-ethylrhodanine with the porphyrin core. A comparative study was conducted on the side chain modification on the porphyrin core. In 2020, Gao Ke's team et al. further modified the side chains of the porphyrin core with ZnP TBO to synthesize ZnP TSEH. They constructed ternary SM-OSCs using ZnP TBO and ZnP TSEH combined with 6TIC and 4TIC, respectively, with a maximum PCE of 15.88%.

3.3. Acceptor material on organic solar cells

Through the study of photoactive layer materials, receptor donor receptor A-D-A type (D and A are electron donating receptor units, respectively) and A-DA'D-A type small molecule receptor materials (SMAs, such as ITIC and Y6) were identified. It is one of the two most representative non fullerene receptor materials, thanks to its advantages of broadened absorption spectrum, adjustable molecular structure, and effective reduction of device voltage loss The photoelectric conversion efficiency (PCEs) of binary OSCs based on Y series non fullerene based SMAs has exceeded 19%, making them the most widely studied non fullerene based small molecule acceptor materials.

In 2015, Zhang et al. successfully synthesized the classic A-D-A type small molecule fused ring receptor ITIC, which has 7 fused rings in the core and an electron acceptor unit 2- (3-oxo-2,3-dihydroindene-1-yl) malononitrile (INCN) at the end group Each INCN group contains one carbonyl group and two cyanide groups, which are electron withdrawing groups. The cluster effectively reduces the LUMO energy level of the molecule, enhances the intramolecular charge transfer of the acceptor, and reduces the absorption band gap of the material In addition, the molecule also contains four 4-hexylbenzene side chains, which are used to regulate the molecular aggregation structure of the receptor molecule and the morphology of the blend film ITIC exhibits strong absorption in the near-infrared region of 500-800 nm and has appropriate frontier orbital (LUMO and HOMO) energy levels.

In 2019, A-DA'D A-type molecule Y6 was designed and synthesized by Zou and colleagues, with DA'D type fused cyclic dithiophene [3,2-b] pyrrolobenzothiadiazole as the central skeleton The coplanar structure of Y6 molecule reduces the distortion of the wave function in the system and promotes intramolecular charge transfer absorption. The nitrogen atoms of two pyrrole rings can selectively modify side chains with different structures, which not only improves the solubility of the molecule but also suppresses the excessive aggregation of rigid conjugated frameworks through steric hindrance effects This molecule has a wider absorption spectrum, with absorption occurring in the wavelength range of 600-1000 nm. Battery devices using PM6 as a polymer donor material provide 15.7% PCE From Fig.2, it can be clearly seen that the structures of ITIC and Y6 molecules mainly consist of three parts: end groups, central nuclei, and side chains Correspondingly, molecular structure modifications can be applied to these types of fused ring receptors from the perspectives of end groups, central nuclei, and side chains to obtain more high-performance fused ring receptor materials From the perspective of molecular structure, asymmetric modification strategies break the symmetric structure of fused ring acceptor molecules, resulting in larger dipole moments, higher binding energies, stronger intermolecular interactions, optimized active layer morphology, significantly improved filling factors, and lower non radiative energy losses than symmetric structures. Given the advantages and potential of asymmetric strategies, it is expected to obtain more efficient and stable asymmetric fused ring acceptor materials by optimizing molecular structure and regulating interface properties to improve the photoelectric conversion efficiency and stability of battery devices.

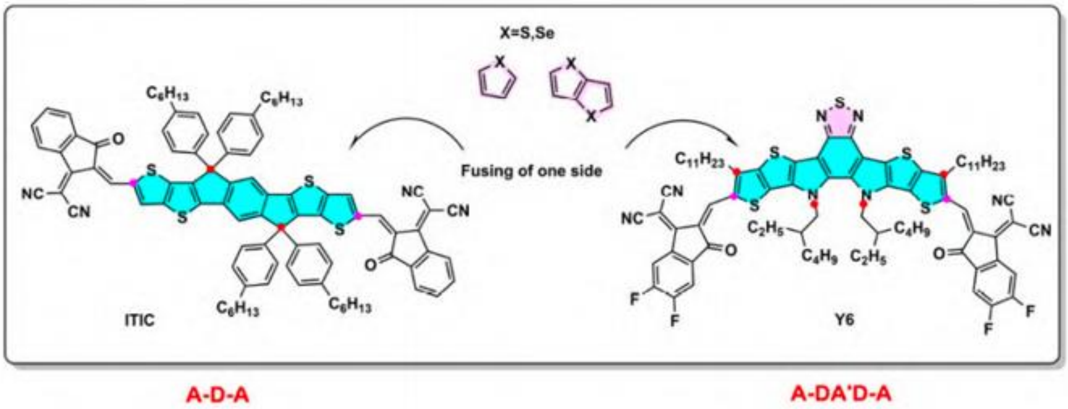


Fig 2. Structures of A-D-A (ITIC) and A-DA’D-A (Y6) type molecules and the structural modification positions (colored) on these two types of molecules (color online) [14].

3.4. Biomass based organic solar cell materials

Currently, the vast majority of OSC photosensitive active layer, electron transport layer, and hole transport layer materials. All preparations are based on derivatives of fossil materials, which not only consume various types of fossil materials, but also face problems such as cumbersome preparation processes, low yield of optoelectronic materials, and high costs. More importantly, optoelectronic materials derived from fossil materials are not easily degraded by nature after disposal, which can cause secondary pollution to the natural environment. This is clearly contrary to the original intention of OSCs to be clean and environmentally friendly, and does not conform to the theme of clean utilization of solar energy. Compared with fossil resources, biomass-based resources not only have advantages such as a wide range of raw material sources, strong sustainability, and easy degradation in the natural environment, but also have unique advantages in raw material costs. Therefore, researching and developing high-efficiency OSCs based on renewable materials not only broadens the utilization pathways of biomass-based resources, but also has important research value for promoting the sustainable development of OSCs. Starting from this, researchers have successfully utilized the crystal cross evolution structure of cellulose and the multi hydroxyl properties of cellulose derivatives to use cellulose based materials as OSCs substrates with excellent light regulation characteristics and cathode interface materials with energy level regulation characteristics ; At the same time, researchers also utilized the polyphenolic hydroxyl characteristics of lignin and the doping effect of lignin sulfonates with quinone like structures to prepare high-performance electron and hole transport materials . In addition to bulk biomass derivatives such as cellulose and lignin, researchers have also successfully extracted small amounts of biomass-based resources such as chlorophyll, amino acids, and betulin and applied them to the carrier transport layer and photosensitive active layer of OSCs [15]. These studies have demonstrated that biomass based OSCs materials have very broad application prospects.

3.5. Nano material organic solar cells

Due to the varying conversion efficiency of organic solar cells with different concentrations of nanomaterials, the energy conversion efficiency of organic solar cells with the addition of 16 pm concentration nanomaterials are high. Moreover, the nanomaterials are easy to manufacture, have uniform size distribution, and can be well combined with solar cell devices. They are important means to improve the conversion efficiency of organic solar cells and have certain practical application significance [16].

4. Conclusion

At present, in the commercial market of solar cells, inorganic crystalline silicon solar cells still dominate and occupy a significant market share. However, inorganic crystalline silicon solar cells have the following problems: the processing technology is very complex; Very strict requirements for raw materials; Not easy to carry out large-scale flexible processing; Some materials required during the production process are toxic. Therefore, it can be seen that cost and resource distribution limit its large-scale production, and further improving the performance of solar cells, reducing costs, and reducing environmental pollution are the main directions for the development of inorganic crystalline silicon solar cells in the future. The efficiency of organic solar cells composed of different materials and principles is gradually increasing, and the replacement and improvement of materials can also reduce overall pollution. For the two main types of solar cells, donor acceptor solar cells, the efficiency improvement is significant and have good development prospects in the future. For Schottky organic solar cells, efficiency has also been improved, but it is difficult to widely involve them in commercial applications. The efficiency improvement of solar cells by biomass based materials and nanomaterials cannot be ignored, both of which to some extent enhance the ultimate energy conversion capability. Therefore, in summary, solar energy, with its unique advantages of clean energy and large total capacity, as well as continuously improving utilization efficiency, will have great development prospects in the future.

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