

Research Status and Optimization of Small Molecule Organic Solar Cells

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Abstract. Organic solar cells, particularly those made from small molecule materials, have garnered significant attention in recent years due to their numerous advantages. One of the most notable benefits is their clear material molecular structures, which allow for precise regulation of energy levels. This clarity also extends to purification methods, which are simple and straightforward. Additionally, small molecule materials are highly adaptable and can be used in a variety of applications, ranging from building-integrated photovoltaics to wearable devices. This article delves deeper into the development status and application prospects of organic solar cell technology, with a particular emphasis on the benefits of small molecule materials and their manufacturing processes. By examining the potential applications of organic solar cells in different fields, this article provides valuable insights and guidance for those interested in studying and applying organic solar cell technology. Overall, this article highlights the exciting opportunities that exist for the advancement of clean energy technology through the use of organic solar cells.

Keywords: Organic solar cells, small molecule materials, manufacturing processes, performance optimization, application prospects.

1. Introduction

Small molecule organic solar cells (ASMSCs) have gained substantial interest recently as a viable alternative to traditional silicon-based solar cells, owing to their unique properties like flexibility, lightweight, and mass-printability. Their distinct advantages include a clear material molecular structure, a simple purification method, and ease of precise regulation of energy levels, making them more appealing for large-scale production and reducing production costs while enhancing efficiency.

This article aims to provide an overview of the development status and application prospects of organic solar cell technology, with a focus on the advantages of small molecule materials and their manufacturing processes. We will explore the unique properties of small molecule organic solar cells and how they compare to traditional silicon-based solar cells. Furthermore, we will examine the application prospects of organic solar cells in areas such as building-integrated photovoltaics and wearable devices.

Recent advances in the research of all-small-molecule organic solar cells (ASMSCs) have led to significant progress in the design and synthesis strategies of novel acceptor/donor materials. Researchers have focused on developing novel receptor materials with high absorption coefficients, good solubility, and suitable energy levels. Non-fullerene acceptors (NFAs) have been favored for their wide spectral absorption range and easy chemical tuning. Xiaowei Jim's group has developed an A-D-A type small molecule acceptor material, ITIC, with a thick ring unit as the central nucleus and a strong electron absorbing unit as the end group [1]. ITIC has a strong light absorption ability, suitable energy levels and excellent charge transfer ability, and has high performance when blended with polymer donors. The group has also carried out modular molecular design of A-D-A type thick ring electron acceptor materials and developed many SMAs with excellent performance, such as IDIC, IT-4F and COi8DFIC [2]. Polymer donor/small molecule acceptor OSCs based on these SMAs can achieve PCEs higher than 19%, and all-small molecule OSCs have also made great progress, with PCEs reaching 15% [2, 3]. OSCs based on such SMAs can achieve PCEs higher than 19%, and all-small-molecule OSCs have also made great progress, reaching PCEs of more than 15% [2-4].

Overall, the development of small molecule organic solar cells presents exciting opportunities for the advancement of clean energy technology. Through continued research and innovation, these solar cells have the potential to revolutionize the photovoltaic industry and play a crucial role in addressing the growing demand for renewable energy sources.

2. Fundamentals of photovoltaics and its optimisation

2.1. Basic Theory of Photovoltaic Energy

Solar energy refers to the thermal radiation energy of the sun. Although the power of the sun is as high as about 3.74×10^{26} watts, the only part that humans can currently use is the radiation that reaches the Earth [5]. However, if all of this energy can be utilized, it can still meet all of humanity's current energy needs.

Solar energy, as a renewable energy source, has unique advantages. For example, during the power generation process, there will be no pollution, no noise, no need for water or fossil resource maintenance, and fast regeneration speed. With the shortage of fossil resources and environmental pollution, more regions are choosing to use renewable resources instead of traditional energy sources. In 2023, due to the growth of renewable energy such as solar energy, the proportion of renewable energy generation in global electricity generation reached an unprecedented 30% [6].

Solar cells can collect solar energy with relatively high efficiency. Traditional solar cells are usually silicon-based semiconductors or macromolecular polymers. Small molecule solar cells refer to non-polymer solar cells that use organic compounds with small molecular weights as electron donors and acceptors.

Upon illumination, the organic material absorbs photons which excite electrons to form excitons. Subsequently, these excitons disassociate into free electrons and holes at the donor-acceptor interface. The electrons and holes then travel through the electron and hole transport layers, respectively, ultimately being collected at the cathode and anode to generate a current. This process can be succinctly described as follows: The process begins with light absorption, where photons are absorbed by the organic material, causing the formation of excitons. These excitons then undergo diffusion, moving through the donor-acceptor interface where they dissociate into free electrons and holes. The subsequent steps involve charge separation, where the electrons and holes are transported through the electron transport layer and the hole transport layer, respectively, and finally, charge collection occurs when the electrons and holes are collected at the cathode and anode, generating a current. The initial stage involves light absorption and exciton generation. The principles of photovoltaic cells is shown in Figure 1.

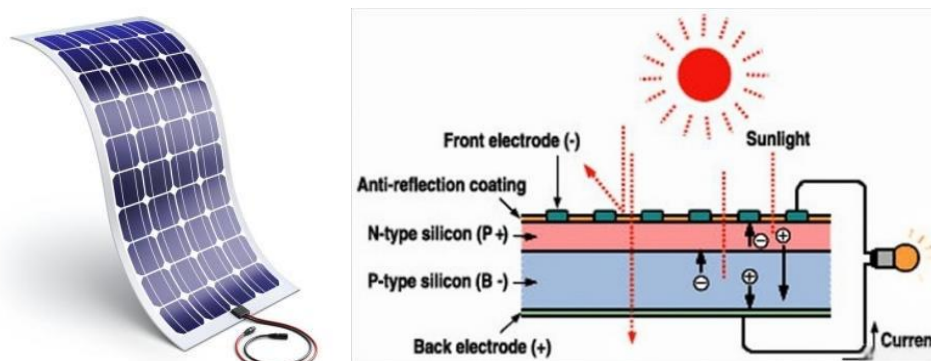


Figure 1. Principles of Photovoltaic Cells

2.2. Optimisation programmes - ASM OSCs

Compared with traditional solar cells, all small molecule solar cells (ASM OSCs) have the advantages of clear material molecular structure, simple purification method, and avoid the disadvantages of large batch differences in polymer solar cell devices [7].

The development of organic solar cells began in the 19th century with initial observations of the photovoltaic effect, but really took off in the late 20th century with the advent of conjugated polymers. In the 21st century, research on polymer-based organic solar cells has grown rapidly with increasing efficiencies. However, due to some inherent limitations of polymer materials, research has gradually shifted to all-small-molecule materials with better thermal stability and easier to precisely regulate the energy levels, which marks an important step towards higher performance and easier mass production of organic solar cell technology [8].

ASMSCs have demonstrated many usages for traditional silicon-based solar cells, especially their important properties in terms of flexibility, lightweight, mass printability, which have revolutionized the photovoltaic industry. Firstly, thanks to the use of flexible substrate materials, such as plastic film, ASMSCs have excellent flexibility and can easily adapt to a variety of curved or irregular surfaces, thus greatly expanding their scope of application, not only for building facades, and can even be embedded into everyday items such as clothing, backpacks, power supply for mobile power and portable electronic devices. Secondly, ASMSMS is significantly lighter than traditional silicon-based solar cells due to the use of lightweight organic materials, which not only simplifies the installation process and reduces installation costs, but also reduces the loading requirements on the mounting structure, making it particularly suitable for rooftops or other application scenarios with limited structural strength. What's more, the manufacturing process of ASMSCs can adopt roll-to-roll (R2R) technology similar to newspaper printing, and achieve continuous, high-speed mass production through solution processing. Compared to the complex manufacturing process of traditional solar cells, this solution-based processing method not only drastically reduces the production cost, but also improves the production efficiency, which makes ASMSCs able to respond to market demand faster. This enables ASMSCs to respond to market demand faster and accelerate the transformation from laboratory R&D to market application. In summary, all-small-molecule organic solar cells, with their flexible, lightweight and highly efficient mass production technology, are not only expected to promote the progress of solar cell technology, but also provide new perspectives for future energy solutions, foreshadowing their great potential in the future clean energy field. With the deepening of research and the increasing maturity of the technology, all-small-molecule organic solar cells are expected to become one of the mainstream clean energy technologies and make an important contribution to the realization of global sustainable development goals.

Organic small molecules have conjugated π -electron systems, and these systems absorb photons efficiently. The photons cause the electrons to jump from the ground to the excited state, lead to the production of excitons. Excitons are pairs of electrons and holes in bound states, and unlike free carriers in conventional semiconductors, excitons have a high binding energy. These high-energy excitons are transported within the material and are key to the operation of the battery. The two types of excitons shown in the figure are those with exciton radii larger and smaller than the lattice constant, respectively. In organic small molecule solar cells, the latter is often the Frenkel exciton. Due to the electroneutrality of the Frenkel exciton, the exciton migration in the organic photosensitive layer is not affected by the electric field and tends to be randomly diffused. However, the Frenkel exciton needs to migrate to the interface between the donor and the nnsn acceptor before returning to the ground state, under the energy level difference between.

3. Donor and the acceptor theoretical and optimistic analysis

Upon charge transfer, the electron is transferred from the LUMO energy level of the donor to the LUMO energy level of the acceptor, forming a charge transfer state of the exciton. The exciton may then either recombine back to the ground state or dissociate into free electrons and holes via the charge separation state. In the charge-separated state, there is minimal Coulomb interaction between electrons and holes. Free electrons are transported in the acceptor material, while holes are transported in the donor material. To minimize recombination losses, the material should possess a highly ordered structure. Ultimately, the electrons are collected at the cathode and the holes at the anode, generating

the desired photoelectric conversion output. The energy level difference between the HOMO of the donor and the LUMO of the acceptor dictates whether the exciton can dissociate. Ideally, the LUMO of the acceptor is lower than that of the donor to facilitate electron transfer, while the HOMO of the donor is higher than that of the acceptor to enable efficient hole return. In recent years, significant progress has been made in the research of all-small-molecule organic solar cells (ASMSCs), especially in the design and synthesis strategies of novel acceptor/donor materials. These breakthroughs have not only enhanced the photovoltaic conversion efficiency (PCE) of the materials, but also improved the stability and other key performance metrics of the devices. The following is an overview of this area, including breakthroughs in material design, improvements in synthesis strategies and techniques, and specific ways to improve PCE [9].

In recent years, researchers have worked on the development of novel receptor materials, especially those with high absorption coefficients, good solubility, and suitable energy levels. For example, non-fullerene acceptors (NFAs) are favoured for their wide spectral absorption range and easy chemical tuning. Several studies have reported NFAs based on ITIC (Indacenodithiophene-C70 imide) and its derivatives, which are structurally modified (e.g., side-chain engineering, end-group tuning, etc.) to optimize the molecule's absorption properties, crystallinity, and charge-transfer properties. To address the advantages and shortcomings of small molecules and polymers, researchers developed an 'N- π -N' dimer (i.e., highly efficient small-molecule N-type acceptor materials linked by conjugate groups) that is intermediate between small molecules and polymers [10]. The new dimer material combines the respective advantages of small molecules and polymers, achieving 18.2% device performance, which is higher than that of the corresponding small molecules (16.2%) and polymers (15.8%), and showing more excellent optical and thermal stability [11].

Organic solar cells have a wide range of application scenarios. For example, in terms of power generation on the external surface of buildings, it can be used for power generation on the external surface of buildings such as external walls, roofs, windows, etc.; in terms of power source for transport vehicles, it can be used as a source of power for transport vehicles such as automobiles, ships, and aircrafts; and in terms of power supply for outdoor equipment's, it can be applied to power supply for outdoor equipment's such as outdoor billboards, street lamps, and surveillance cameras. In addition, because of its lightweight, flexible, easy to process and other characteristics, so that it can be installed in a variety of complex shapes on the surface, and will not be affected by environmental factors, with a high degree of reliability and stability. Therefore, organic solar cells have a broad application prospect in the future.

4. Conclusion

In conclusion, the development of organic solar cells has shown significant progress in recent years, particularly in the design and synthesis strategies of novel acceptor/donor materials. The use of small molecule materials in organic solar cells offers several advantages, including clear material molecular structures, simple purification methods, and ease of precise regulation of energy levels. These advantages make small molecule solar cells more attractive for mass production, leading to a decrease in production costs and increased efficiency.

Small molecule solar cells demonstrate excellent flexibility and can easily adapt to various curved or irregular surfaces, expanding their scope of application beyond traditional silicon-based solar cells. They are also significantly lighter than traditional silicon-based solar cells, reducing installation costs and providing greater reliability and stability. The manufacturing process of small molecule solar cells can utilize roll-to-roll technology, allowing for continuous, high-speed mass production through solution processing.

Furthermore, small molecule organic solar cells offer promising applications in areas such as building-integrated photovoltaics and wearable devices. Their lightweight and flexible nature make them suitable for power supply in outdoor equipment, transportation vehicles, and power generation on the external surface of buildings. As research continues to advance, small molecule organic solar

cells are expected to become one of the mainstream clean energy technologies, contributing to the realization of global sustainable development goals.

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