Improved Interface Engineering of Organic Photovoltaic Cells: Strategies for Enhancing Charge Separation and Transport Efficiency

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Abstract. This article investigates various strategies aimed at enhancing the efficiency of charge separation and transportation in organic photovoltaic (OPV) cells, with a specific emphasis on interface engineering. One of the primary challenges faced by OPVs is the restricted carrier mobility and high exciton binding energy, which can hinder effective charge separation and transportation. To tackle these challenges, this article highlights several optimization techniques including adjusting energy levels at electrode-organic material interfaces, employing surface passivation to minimize defects, and incorporating nanostructures to increase interfacial area for more efficient charge transport. Furthermore, it discusses the selection of materials for electron and hole transport layers, emphasizing novel materials and doping methods that enhance both energy conversion efficiency and device stability. The integration of nanomaterials is also examined as a means to manipulate interfacial morphology, leading to significant enhancements in charge separation, transportation, and overall photovoltaic performance - all contributing towards advancing OPV technologies.

Keywords: Organic Photovoltaic Cells (OPV), Interface Engineering, Charge Transport Efficiency.

1. Introduction

With the increasing global demand for energy and growing awareness of environmental conservation, there is a strong focus on developing efficient and sustainable energy technologies. In this regard, solar energy technologies, particularly organic photovoltaic (OPV) cells that rely on renewable resources, have demonstrated immense potential for development and societal value. OPVs are emerging as viable alternatives to traditional inorganic photovoltaic (PV) technologies due to their low energy consumption during production, wide availability of materials, and versatility in various applications. However, the current efficiency and lifespan of OPVs fall short of meeting the requirements for large-scale commercial use. Consequently, addressing this common challenge has become a shared goal for both academia and industry: enhancing OPV performance through scientific innovation and technological breakthroughs. Interfacial engineering stands out as a key technology expected to significantly enhance battery charge separation and transport efficiency by optimizing interface structure and properties. This advancement will facilitate the transition of OPVs from laboratory research to practical applications. Introduction to interface engineering in organic photovoltaic cells: Strategies for enhancing the efficiency of charge separation and transport. In recent years, there has been a growing interest in organic photovoltaic cells (OPVs) due to their potential for cost-effective production, ability to cover large areas, and lightweight flexibility. However, despite advancements in materials science and device engineering, OPVs still lag behind conventional inorganic solar cells in terms of energy conversion efficiency and stability. These performance deficiencies primarily arise from the intrinsic characteristics of organic materials, such as the elevated binding energy of photogenerated excitons and the non-uniformity and limited mobility of charge transport. To tackle these challenges, interfacial engineering serves as a pivotal strategy aiming to significantly enhance the overall performance of organic photovoltaics (OPVs) by optimizing the interface between organic materials and electrodes to ameliorate charge separation and transport efficiency.

2. Interface Mechanism of OPV Battery

The working principle of organic photovoltaic (OPV) cells is based on the absorption of light, the creation of photogenerated excitons, the separation of excitons, and the movement and collection of charge in organic semiconductor materials. When sunlight shines on the active layer of an OPV cell, photons are absorbed by the organic material leading to the formation of electron-hole pairs (excitons). However, due to high exciton binding energies typically ranging from 0.3 to 1 eV in organic materials, it becomes difficult to naturally separate electrons and holes. To achieve effective separation, photogenerated excitons need to diffuse into a specific interface called donor-acceptor interface (DAI), where electrons move from donor material into acceptor material while holes stay in donor material. This process relies on matching energy levels at the interface as well as chemical and physical properties of interface materials (as shown in figure 1). Afterwards, separated electrons and holes migrate through their respective transport layers towards cathode and anode respectively until they are eventually collected to generate electric current. The efficiency of charge transport is influenced by factors such as charge mobility, interfacial resistance, and complexity of materials involved; therefore interfacial engineering plays a crucial role in enhancing charge separation and transport efficiency.

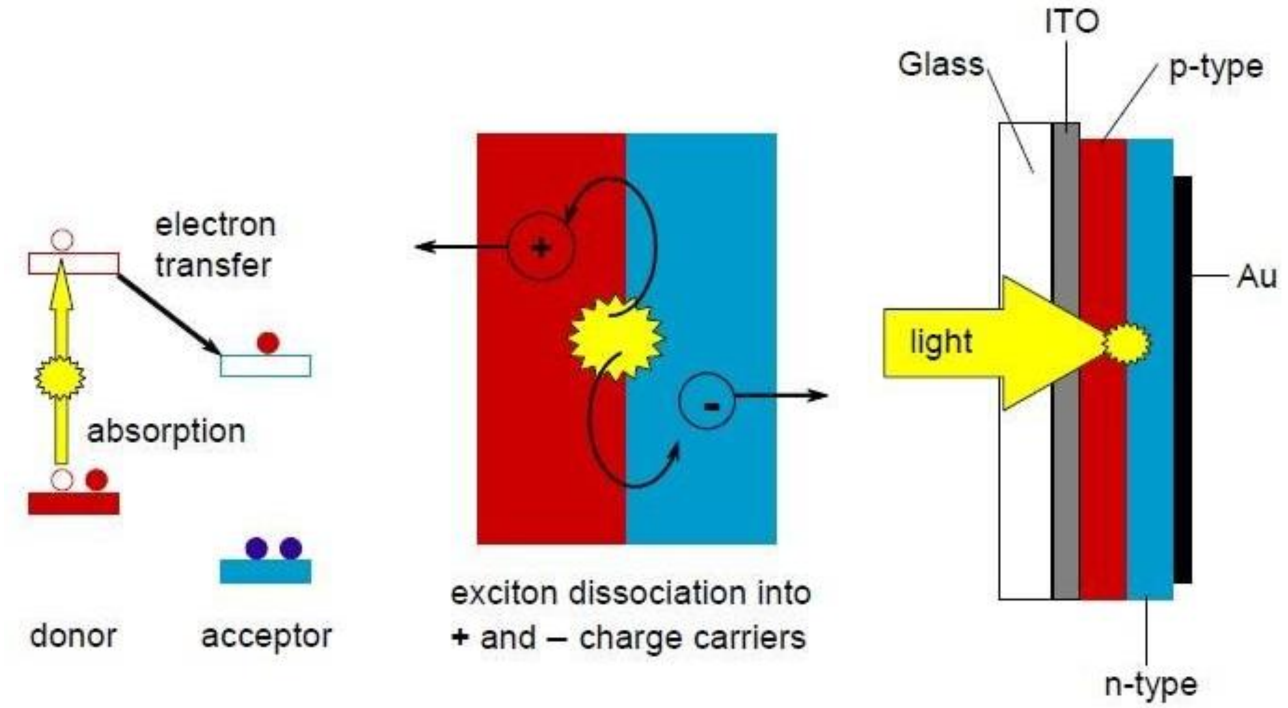

Fig. 1 Working principle of organic solar cell

The charge separation and transport processes at the interface are crucial in the working mechanism of OPVs, which rely on the generation, diffusion and effective separation of photogenerated excitons at the donor-acceptor interface, as shown in figure 2. However, since the binding energy of photogenerated excitons in organic materials is usually high, it is difficult to achieve the conversion of excitons to free charge by relying on thermal excitation alone, resulting in low charge separation efficiency at the interface. In addition, organic materials have relatively low carrier mobility and are prone to charge complexation at the interface, further limiting the effective charge extraction and transport.

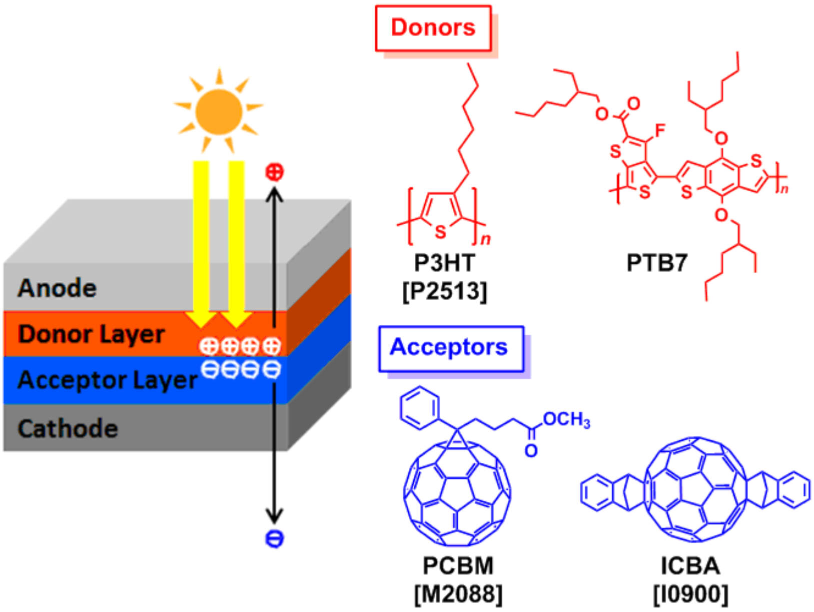

Fig. 2 Organic solar cell (OPV) materials

Interfacial engineering addresses the above challenges through a variety of strategies, mainly including adjusting interfacial energy level matching, introducing interfacial modification layers, optimising interfacial morphology and enhancing interfacial charge selectivity. The application of these methods can reduce charge complexation, improve charge separation efficiency and enhance charge transport. For example, the introduction of an intermediate layer or charge transport layer at the donor-acceptor interface can effectively regulate the interfacial energy level difference and promote selective charge transport and extraction. Meanwhile, interfacial modification of nanostructures can increase the interfacial area, improve the separation efficiency of excitons, and provide a more optimal charge transport path [1].

Through systematic interfacial engineering research, the energy conversion efficiency of OPVs has been improved from 3%-5% in the early stage to about 15% today in recent years, demonstrating the great potential of interfacial engineering in enhancing PV performance. With the further development and optimisation of interfacial engineering technology, it is expected to further promote the wide application of OPVs in the field of renewable energy.

3. Modification Method

Interfacial engineering of organic photovoltaic cells plays a crucial role in improving charge separation and transport efficiency. Strategies such as interfacial modification, material optimisation and control of interfacial morphology can significantly enhance the charge transport efficiency and reduce the carrier complexation problem at the interface. These modification methods not only help to enhance the photovoltaic conversion efficiency, but also improve the stability and lifetime of the devices, providing strong support for the further development of organic photovoltaic [2].

3.1. Interface Modification

Interfacial defects and trap states can be effectively reduced by chemically modifying the interfacial surface or adding a passivation layer to reduce charge complexation.

3.1.1. SAMs

Self-assembled monomolecular layers (SAMs) modification is a common approach to modulate the electrode's figure of merit by forming a highly ordered molecular layer on the electrode surface to achieve an optimal match with the energy levels of the active layer material. Surface passivation treatments, such as surface modification with fluoride or amine-based compounds, can passivate interfacial defects and enhance charge transfer efficiency.

For example, SAMs modification is an effective interfacial modification technique, which can regulate the electrode's figure of merit and improve the energy level matching with the active layer by forming a highly ordered molecular layer on the electrode surface. Chen et al. [3] showed that modifying ITO electrodes with self-assembled monomolecular layers of mercaptopropionic acid resulted in the electrode's figure of merit being closer to the HOMO energy level of the active layer, which significantly improved the charge separation efficiency and PCE.

3.1.2. Dipole molecularly modification

Professor Changzhi Li and his team from Zhejiang University have recently published a groundbreaking study on the manipulation of metal oxide nanoparticles. They have developed a unique technique to modify the interface of these nanoparticles through dipole molecular modification. This method not only improves the dispersibility and processability of ZnO nanoparticles in solutions, but also allows for the creation of highly conductive nanoparticle films using low-temperature solution processing methods. Moreover, this innovative approach effectively adjusts the energy bands at the interfaces, resulting in efficient charge transport across them. As a result, they were able to successfully fabricate high-performance organic solar cells by utilizing metal oxide electron transport layers. These solar cells achieved an impressive photovoltaic conversion efficiency of 18.14% and exhibited remarkable stability even when varying the thickness of the interfacial layer between 5-300 nm.

One significant advantage of this interfacial strategy is its ability to suppress the photocatalytic activity typically associated with ZnO nanoparticles. The details furnished within figure 3. By doing so, it enhances both the performance and durability of solar cells. Overall, this research offers a promising avenue for developing cost-effective photovoltaic devices that are highly efficient and stable by manipulating electronic energy bands, charge transport properties, and interfacial chemical stability at organic-inorganic interfaces [4].

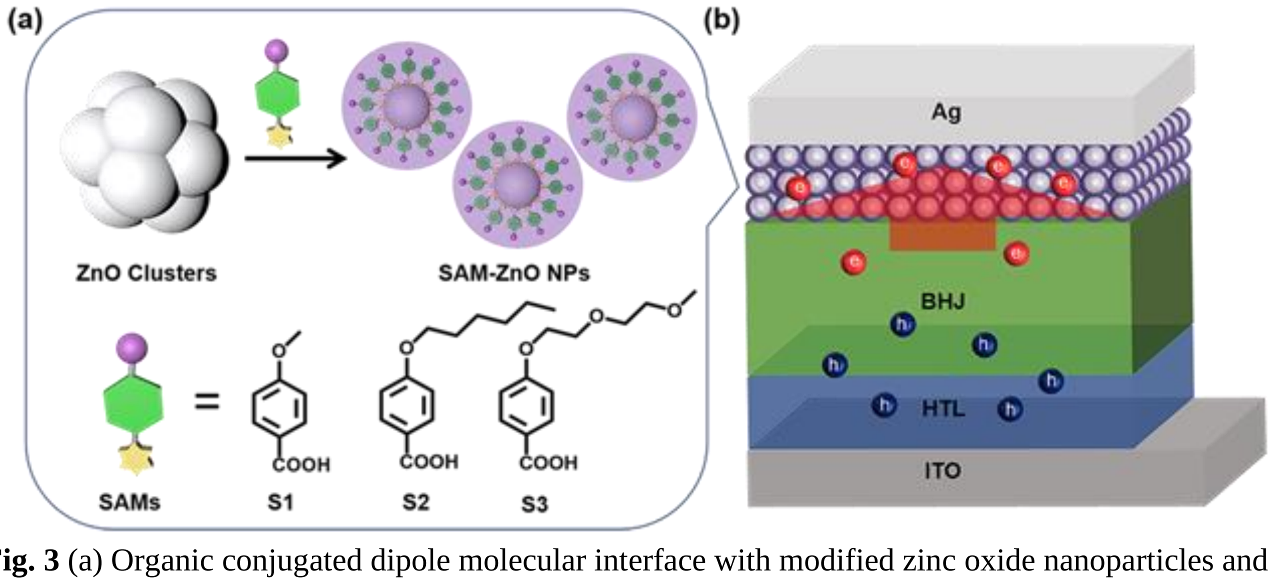

Fig. 3 (a) Organic conjugated dipole molecular interface with modified zinc oxide nanoparticles and (b) Schematic diagram of the corresponding organic solar cell

3.2. Material optimisation

The enhancement of organic photovoltaics (OPVs) performance heavily relies on the careful selection and optimization of suitable interfacial materials. Typically, PEDOT and MoO_3 are commonly employed as hole transport layer (HTL) materials, while ZnO and TiO_2 are frequently used as electron transport layer (ETL) materials. By fine-tuning the chemical composition and physical structure of these materials, it becomes feasible to adjust the energy level alignment at the interface in order to minimize charge transport resistance. Furthermore, by integrating intercalation materials such as chalcogenides, polymers or metal oxides between the active layer and electrodes, it is possible to further enhance charge extraction efficiency while simultaneously reducing composite formation at the interface [5].

3.2.1. Doping

For example, PEDOT is widely used as a hole transport layer (HTL), the information presented in figure 4, and its good conductivity and match with the organic active layer make it an important material to enhance the charge separation efficiency. However, Li et al. effectively enhanced the stability and PCE of the cell by introducing tungsten oxide (WO_3) modification to the PEDOT layer, suggesting that the charge transfer efficiency can be further improved by optimising the interfacial material [6].

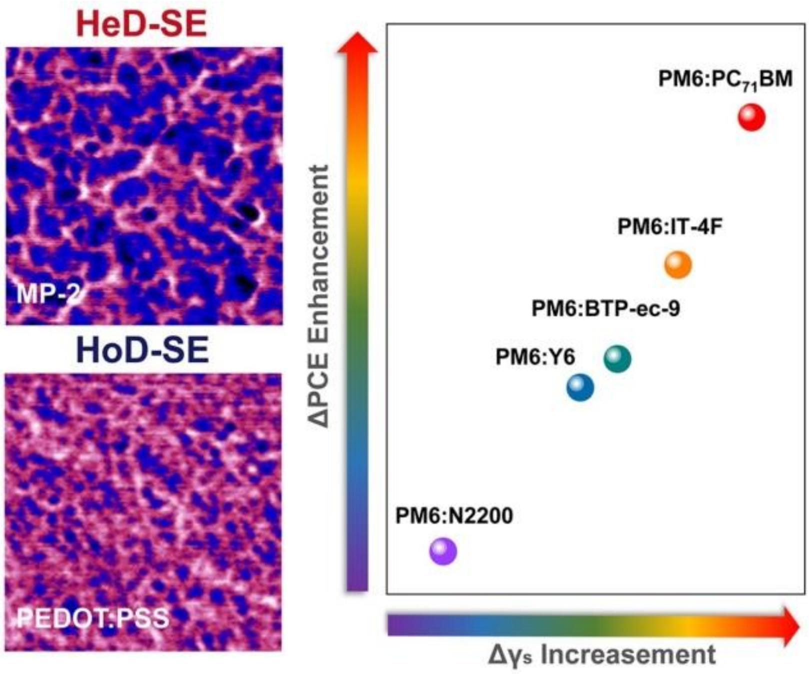

Fig. 4 PEDOT: nanoscale surface energy distribution of PSS film and MP-2 film; connection between inhomogeneous surface energy distribution and surface energy difference between donor acceptors and improved device efficiency

3.2.2. PAA

Professor Tao Wang's team at Wuhan University of Technology has successfully developed a cost-effective and eco-friendly biomolecule called potassium aspartate (PAA) for use as an interfacial modification layer in organic solar cells.[7] Through experimental findings and theoretical calculations, it has been determined that PAA effectively adjusts energy level alignment, passivates ZnO defects, and enhances the π-π stacking of the active layer. As a result, according to figure 5, the photovoltaic performance of the solar cells is significantly improved while demonstrating exceptional stability under continuous white light and ultraviolet light irradiation. This study presents a highly efficient and stable approach to fabricating inverted organic solar cells. By introducing PAA between the ZnO electron transport layer and the active layer, both efficiency and stability are enhanced in Y-series PM6:BTP-4F-C5-16-based organic solar cells as well as IT-series PM6:IT-4F-based ones. It is evident that PAA not only adjusts energy level alignment and passivates surface defects on ZnO but also improves contact with the active layer, thereby enhancing π-π stacking within it. Moreover, incorporating a ZnO/PAA electron transport layer greatly improves stability under continuous white light and UV irradiation. The presence of defects in metal oxides poses limitations to their widespread use as electron transport layers in solar cells; however, this paper proposes an innovative method using environmentally friendly materials to address these limitations by passivating the ZnO electron transport layer. These findings provide valuable insights into interfacial layers research for improving solar cell technology [8].

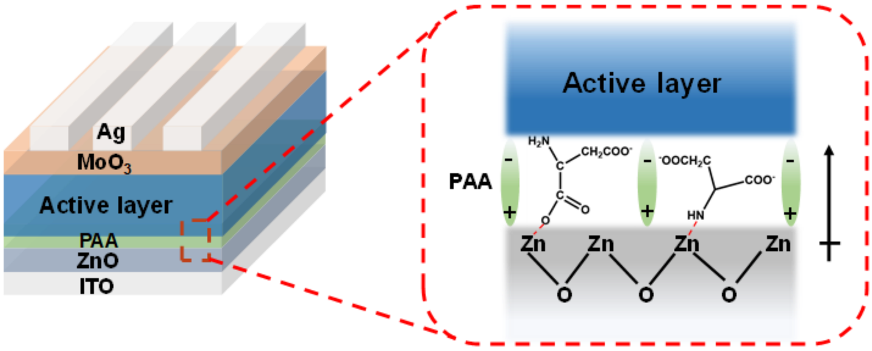

Fig. 5 Schematic diagram of the device structure and interface dipole formation of inverted organic

3.3. Control of interface morphology

The physical structure of the interface plays a critical role in separating and transporting charges. By incorporating nanostructures like nanopillars and nanopores, we can increase the specific surface area of the interface, thereby improving charge separation efficiency [9]. Additionally, roughening the surface helps with charge collection and transport by increasing the effective contact area of the electrode surface. Nanostructured interfaces not only aid in charge separation but also enhance light absorption and improve photoelectric conversion efficiency through localized enhancement of the light field. Metal oxides are commonly used as electron transport layers (ETLs) in organic solar cells; however, they have inherent surface defects and mismatched figure of merit that negatively impact charge transfer efficiency, ultimately limiting overall cell performance. Nevertheless, these surface defects can be effectively reduced through a surface modification strategy utilizing natural antioxidants (CA, FA, DMCA). This approach leads to improved charge transport performance while significantly enhancing both efficiency and environmental stability [10].

3.3.1. Natural antioxidants modify metal oxides

Song et al. [11] showed that zinc oxide (ZnO) as an electron transport layer (ETL) for organic solar cells (OSCs) limits the charge transfer efficiency and overall performance due to its surface defects and mismatched figure of merit. To address this issue, the research team modified ZnO thin films using three natural antioxidants (CA, FA, and DMCA) to passivate surface defects and reduce the figure of merit. The modified ZnO was used in inverted organic solar cells (IOSCs), which significantly improved the photovoltaic conversion efficiency up to 18.22% (PM6: L8-BO system).[2] The surface modification not only optimises the interfacial morphology, but also improves the environmental stability of the device, which provides a new idea for the development of highly efficient and stable photovoltaic devices .

3.3.2. Carbon nanomaterials

The research incorporated carbon nanotubes into the active layer of organic solar cells, creating a composite system that combines carbon nanotubes with organic semiconductors. Carbon nanotubes possess exceptional properties for transporting electrons, effectively improving the efficiency of charge transport within the active layer. Additionally, they function as a nano-scale conductive network to enhance the structural stability of the active layer. This study introduces an innovative approach to design and manufacture high-performance organic solar cells [12].

4. Conclusion

This paper reviews strategies to optimise the charge separation and transport efficiency of organic photovoltaic cells through interfacial engineering. The main optimisation methods include interface modification, material optimisation and interface morphology control. Interfacial modification (e.g., self-assembled monomolecular layer) can effectively passivate defects, reduce carrier complexation, and improve charge transport efficiency; material optimisation improves energy level matching and reduces transport resistance by selecting and modifying suitable interfacial layer materials (e.g., ZnO, PEDOT); and interfacial morphology control makes use of nano-structures (e.g., carbon nanotubes, ZnO nanoparticles) to increase the interfacial area, improve charge separation efficiency, and enhance crystallinity of active layer. and enhance the crystallinity of the active layer. In particular, by controlling the interfacial morphology, it not only facilitates the effective extraction and transmission of charge, but also significantly improves the photoelectric conversion efficiency and stability of the device. These methods can help to develop highly efficient, stable and low-cost organic photovoltaic devices and promote their commercialisation [13].

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