Original Research Article

Research progress on strategies and mechanisms of interface engineering to enhance the stability of organic solar cells

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Abstract: Organic solar cells (OSCs) have broad application prospects in fields such as photovoltaic building integration and wearable electronics due to their advantages of flexibility, lightweight, solution processability, and low cost. In recent years, their photoelectric conversion efficiency has exceeded 20%, laying the foundation for commercial development. However, insufficient stability remains the core bottleneck that restricts its practical application. Environmental factors such as light, heat, and humidity can easily lead to rapid efficiency degradation of the device, with interface defects causing charge recombination, interlayer delamination, and water oxygen permeation being the main causes. As a key hub for charge separation, transmission, and collection in OSCs, the performance of the interface directly determines the stability and long-term service capability of the device. Therefore, interface engineering has become a key path to break through the bottleneck of OSCs stability. This article systematically reviews the mainstream strategies for improving the stability of OSCs through interface engineering through literature research, analyzes the mechanisms of each strategy, summarizes current research progress and existing problems, and proposes future prospects that fit the perspective of undergraduate research. It provides a basic reference for the preparation of high stability OSCs and promotes their commercialization process.

Keywords: interface engineering; organic solar cells; stability; mechanism

1. Introduction

With the intensification of the global energy crisis and the increasing demand for environmental protection, new clean energy technologies have become a research hotspot. Organic solar cells (OSCs) have shown broad application prospects in fields such as photovoltaic building integration, wearable electronics, and portable energy devices, thanks to their unique advantages of flexibility, flexibility, lightweight portability, solution processability, and low-cost preparation. In recent years, their photoelectric conversion efficiency has exceeded 20%, gradually approaching the threshold for commercial application[1].

However, insufficient stability remains the core bottleneck that hinders the commercialization of OSCs on a large scale. Compared to traditional inorganic solar cells, OSCs are prone to rapid efficiency degradation in practical service environments such as light, temperature, and humidity, mainly manifested as organic material degradation, hindered charge transfer, and interface failure. Therefore, regulating interface characteristics through interface engineering has become a key research direction to break through the stability bottleneck of OSCs and promote their transition from laboratory to practical applications. Relevant research has important theoretical and practical value.

2. The mainstream strategy for improving the stability of organic solar cells through interface engineering

2.1. Interface decoration strategy

Interface modification strategy is the core means to improve the stability of organic solar cells (OSCs). By introducing various modifiers at the critical interfaces of the device (active layer charge transport layer, charge transport layer electrode), targeted interface defects can be solved, interface characteristics can be optimized, and the device service life can be significantly extended. It is currently the most mature and widely used strategy in interface engineering research[2]. This strategy is mainly divided into three categories based on the type of modifier. Each type of modifier achieves precise control of the interface based on its own characteristics, adapting to different preparation needs and application scenarios. Small molecule interface modification is the most convenient type of application, and commonly used modifiers include NBE photosensitive molecules, BP2 UV absorbers, phosphate derivatives, etc. These modifiers have low molecular weight and good solubility, and can quickly cover the interface through solution spin coating. They can passivate interface defect states, reduce charge recombination, block water and oxygen permeation, and inhibit material degradation. For example, NBE photosensitive molecules can achieve hydrophilic hydrophobic conversion, greatly improving the wet heat stability of flexible OSCs. Polymer interface modification uses polymer materials as modifiers, which have the advantages of excellent film-forming properties, good compatibility with interface materials, and the ability to form a dense and uniform modification layer at the interface. This not only optimizes energy level matching, but also enhances interlayer adhesion, improves the mechanical stability of the device, and effectively avoids interlayer delamination problems. The interface modification of inorganic nanomaterials uses inorganic materials such as AgNWs and metal oxides. These materials have good conductivity and strong barrier properties, which can optimize charge transfer efficiency, reduce charge transfer losses, form a water oxygen barrier, and improve the heat resistance of the device. They are especially suitable for rigid OSCs that require high stability. The three types of modification strategies can be used alone or in combination to enhance the light, heat, humidity, and mechanical stability of OSCs by targeted regulation of interface characteristics, providing basic support for the preparation of high stability devices.

2.2. Interface structure optimization strategy

The interface structure optimization strategy improves the stability of OSCs by designing a reasonable interface layer structure, regulating the microstructure of the interface, optimizing the interface contact state and charge transfer path. Its core is to compensate for the inherent defects of the interface through structural design and achieve synergistic improvement of interface performance[3]. This strategy mainly includes three specific ways to adapt to different device structures and preparation processes. The design of double-layer/multi-layer interface structure is the most commonly used method, which involves preparing two or more interface materials in layers to leverage the advantages of each material. For example, the BP2 and PEDOT: PSS double-layer anode interface layer can achieve UV shielding, while the PEDOT: PSS layer optimizes hole transport, and the two work together to improve device photostability and charge transfer efficiency. Interface roughness control is achieved by optimizing the preparation process, adjusting the microstructure of the interface, reducing interface defects and voids, increasing the interface contact area, thereby reducing charge recombination, enhancing interlayer adhesion, and avoiding interlayer delamination. Common control methods include vacuum annealing, solution annealing, etc. Vertical phase distribution regulation guides the vertical distribution of active layer donor and acceptor materials through interface engineering, optimizing charge separation and extraction efficiency. For example, phosphate modified additives can guide acceptor materials to aggregate towards the electron transport layer interface through surface energy differences, reducing interface charge recombination and improving interface compatibility, further enhancing device stability.

2.3. Interface material functionalization strategy

The core of the interface material functionalization strategy is to modify or select functional materials for the interface layer, so that the interface layer has multiple functions such as charge transfer, defect passivation, water oxygen barrier, etc., to enhance the stability of OSCs from multiple dimensions, break the functional limitations of a single interface layer, and achieve synergistic optimization of stability and efficiency. This strategy mainly focuses on three core functions to address the main interface issues of OSCs. The functionalization of water oxygen barrier is a key direction. By selecting or modifying interface materials to form a dense barrier layer, it can block the penetration of water oxygen molecules, prevent organic material oxidation and electrode corrosion. For example, the interface layer after NBE photosensitive modification can greatly improve the water oxygen barrier performance, and the water vapor transmission rate is close to that of glass materials. UV shielding functionalization addresses the issue of device degradation caused by light exposure by selecting interface materials with UV absorption capabilities, such as BP2, which can effectively absorb UV radiation, reduce the damage of UV radiation to the active layer material, and do not affect the transmission of visible light, thereby improving the device's optical stability. Functionalization of charge transfer involves adjusting the energy levels of interface materials, optimizing interface energy level matching, improving charge transfer efficiency, reducing charge recombination losses, and enhancing interface stability to avoid interface failure during charge transfer, providing a guarantee for long-term stable operation of devices[4].

3. The mechanism of interface engineering to enhance the stability of organic solar cells

3.1. Interface energy level matching control mechanism

Interface energy level matching is a core prerequisite for achieving efficient charge separation and transfer in organic solar cells (OSCs), thereby improving stability. Interface engineering precisely regulates the arrangement of various interface energy levels to solve problems such as charge recombination and transmission obstruction caused by energy level mismatch, fundamentally enhancing device stability. This is also one of the core mechanisms of interface regulation. If the key interfaces of OSCs (active layer charge transport layer, charge transport layer electrode) have excessive energy level shift and poor energy level alignment, it will lead to insufficient driving force for charge separation. Free electrons and holes are prone to recombine at the interface, which not only reduces the photoelectric conversion efficiency, but also accelerates the generation of interface defects and material degradation, shortening the device life. Interface engineering mainly achieves energy level matching control through two methods: one is to select interface modifiers or functional layer materials that are compatible with the energy levels of adjacent layer materials, optimize the arrangement of interface energy levels, reduce energy level shifts, and provide sufficient driving force for charge separation and transmission; The second is to modify the interface material and regulate its work function to achieve precise alignment of interface energy levels. For example, phosphate ester modified additives can regulate the interface energy level between the active layer and the electron transport layer through intermolecular interactions, reduce the energy level difference, decrease charge recombination losses, and suppress the generation of interface defects, so as to maintain stable charge transport efficiency of the device in long-term service, effectively delay efficiency decay, and comprehensively improve the optical and thermal stability of the device. This mechanism has been verified in multiple cutting-edge studies and is one of the core paths for interface regulation to enhance the stability of OSCs[5].

3.2. Interface defect passivation mechanism

Interface defects are one of the main causes of decreased stability of OSCs. During the device fabrication process, various defects such as dangling bonds and defect states are easily generated at each interface due to material properties and processing techniques. These defects capture free charges, intensify charge recombination, and induce organic material oxidation degradation, accelerating interface failure. One of the core mechanisms of interface engineering is to achieve interface defect passivation and suppress the negative effects caused by defects. The core of the interface defect passivation mechanism is to use methods such as interface modification and material modification to fill interface defects and eliminate defect states by utilizing the interaction between modifier molecules and interface defect sites, thereby reducing charge capture and recombination and delaying interface degradation. Common defect passivation methods include chemical bonding passivation and physical adsorption passivation. Chemical bonding passivation refers to the formation of stable chemical bonds between modifier molecules and interface defect sites, completely eliminating defect states. For example, NBE photosensitive molecules can bind to defect sites at the electrode interface through thiol groups, filling interface gaps and passivating defects; Physical adsorption passivation refers to the adsorption of modifier molecules onto the surface of interface defects through intermolecular forces, blocking the contact between charges and defect sites and reducing charge capture.

3.3. Interface compatibility and interface bonding enhancement mechanism

Interface compatibility and bonding strength directly affect the mechanical stability and long-term service capability of OSCs. Interface engineering enhances the stability of flexible OSCs by regulating the physical and chemical properties of interface materials, improving interface compatibility and bonding strength, avoiding interlayer delamination, cracking, and other issues. This mechanism is the core support for improving the stability of flexible OSCs. The physical and chemical properties of OSCs interface layer materials vary greatly, which can easily lead to poor interface compatibility and insufficient bonding strength. Under external environmental stimuli or mechanical bending, interlayer separation and cracking are prone to occur, causing charge transfer obstruction, increased water and oxygen permeation, and ultimately leading to device failure. Interface engineering mainly achieves regulation through two methods: firstly, selecting interface modifiers or functional materials that are compatible with adjacent layer materials to reduce interfacial tension and enhance interlayer affinity; The second is to modify the surface of the interface material to form active functional groups, enhance interlayer chemical bonding, and improve adhesion.

3.4. Water oxygen barrier and interface protection mechanism

Water oxygen permeation is a key environmental factor that causes oxidation, electrode corrosion, and interface failure of OSCs organic materials. Interface engineering achieves interface protection by constructing an efficient water oxygen barrier interface to block the permeation of water oxygen molecules, thereby delaying device degradation and improving stability. This mechanism is the core of enhancing the wet heat stability of OSCs. Water and oxygen molecules can easily penetrate into the interior of the device through interface gaps and defect sites, undergo oxidation reactions with organic donor acceptor materials, leading to material degradation, reduced activity, corrosion of electrodes, destruction of interface structure, and rapid degradation of device efficiency. Interface engineering mainly constructs water oxygen barrier interfaces through two methods: one is to select interface materials with dense structure and hydrophobic properties to form a water oxygen barrier, which blocks the penetration of water oxygen molecules; The second is to modify the interface by changing the wettability of the interface surface, forming a hydrophobic interface, and reducing the adsorption and permeation of water and oxygen molecules. For example, the interface layer modified with NBE photosensitive molecules can achieve photosensitive hydrophobic conversion, forming a dense hydrophobic interface after illumination, significantly reducing water vapor transmission rate and approaching the barrier performance of glass materials. It can not only block water and oxygen permeation, but also protect the interface structure from damage, effectively delaying the degradation rate of devices in humid and hot environments, significantly improving the wet and hot stability of OSCs, fully reflecting the key role of this mechanism.

5. Conclusion

This article systematically reviews the mainstream strategies and mechanisms of interface engineering to enhance the stability of organic solar cells (OSCs) through literature research, and summarizes the current research progress and core achievements. Research has shown that interface defects are a key factor restricting the stability of OSCs, and four strategies including interface modification, structural optimization, material functionalization, and auxiliary regulation can be targeted to solve interface problems. The main mechanism of its action is reflected in energy level matching regulation, defect passivation, compatibility improvement, water oxygen barrier, and multi mechanism synergy, where each mechanism promotes each other and comprehensively delays device degradation. The conclusions drawn from the strategies and mechanisms outlined in this article provide a fundamental reference for the preparation of highly stable OSCs. At the same time, this article also has limitations such as insufficient depth of literature research. In the future, further research can be conducted on low-cost, multifunctional interface regulation strategies and multi mechanism collaborative mechanisms to promote the commercialization of OSCs.

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References

[1]Nath B ,Ramamurthy C P ,Hegde G . The role of interface engineering in boosting efficiency and stability of perovskite solar cells: a review [J]. ISSS Journal of Micro and Smart Systems, 2025, 14 (2): 1-31. DOI:10.1007/S41683-025-00141-1.

[2]Xi Q ,Hong J ,Qin J , et al. Self-Assembled Benzotriazole Interlayer Stabilizes ZnO/Polymer Interfaces Enables Thermally Robust Organic Solar Cells. [J]. ACS applied materials & interfaces, 2025, DOI:10.1021/ACSAMI.5C18226.

[3] Wang Xin, Wang Yu, Mu Fumao, etc Application and prospect of carbon dots in organic solar cell interface engineering [J]. Journal of Chemistry of Higher Education, 2025, 46 (06): 57-72.

[4] Zhang Xu, Jorge Pascual, Li Zhihao, wait Bottom hole selective interface engineering for enhancing the chemical stability of high-efficiency tin lead perovskite solar cells [J]. Science Bulletin, 2025, 70 (04): 556-562.

[5] Zhao Yong, Zhao Yuan, Huang Peng Research progress on cathode interface materials for organic solar cells [J]. Chemical Industry Progress, 2025, 44 (06): 3524-3540.