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In-depth Exploration of the Electron Transport Layer in Perovskite Solar Cells: Fullerene Material Comparison and Performance Impact

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Abstract. In recent years, perovskite solar cells have developed rapidly, whose photoelectric conversion efficiency has exceeded 27%. As an important part of it, the electron transport layer affects the performance and stability of the battery. The film-forming quality, interface defect passivation, charge extraction and transport of perovskite solar cells are closely related to the electron transport layer, and are also the key to breaking through the performance bottleneck. Therefore, systematically analyzing and comparing the properties, optimization strategies, and influence mechanisms of different fullerene derivatives is of great significance for improving the stability of devices and facilitating industrial production. This review aims to analyze the impact of different electron transport layer materials on the performance of perovskite cells, explain the underlying mechanisms, and provide references for future, deeper mechanism studies and large-scale commercial production. This review not only provides theoretical guidance for the design and development of high-performance, low-cost electron transport materials, but also lays a foundation for advancing the commercialization process of perovskite solar cells.

Keywords: Perovskite solar cells; electron transport layer; fullerene materials; molecular design.

1. Introduction

Perovskite solar cells (PSCs) are a type of third-generation solar cells that utilize organic metal halide semiconductors with an ABX3 crystal structureas the light-absorbing material [1]. Since 2009, PSCs have attracted significant attention from both the academic and industrial communities due to their high photoelectric conversion efficiency, low material cost, and simple device fabrication process [2]. As a key component of the device, the electronic transport layer's performance affects the film formation quality, interface defect passivation, charge extraction and transmission of perovskite solar cells.

The representative achievements in the field of electronic transport layers currently include: by blending the synthesized alkyl fullerene derivative FC10 with PCBM as the electron transport layer, the self-aggregation was effectively inhibited and the interface morphology was improved, thereby increasing the efficiency of inverted perovskite cells from 17.97% to 19.65%. To address the surface defects of tin-based perovskite materials, a fullerene interface modifier F2N with pyridine dual functional groups was developed. This modifier effectively passivates Sn^{2+} defects through strong coordination interactions, achieving a conversion efficiency of 10.78% in tin-based perovskite cells.
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However, many current studies still have limitations such as insufficient research depth, inadequate surface defect passivation, and high costs of new materials, which severely restrict the further improvement of battery performance. Therefore, systematically analyzing and comparing the performance characteristics, optimization strategies and influencing mechanisms of various electronic transport layer materials, and deeply understanding the precise regulation rules, are of crucial significance for breaking through the existing technical bottlenecks, guiding the theoretical design of new electronic transport layer materials, and promoting the practical application of perovskite solar cells. This paper will specifically study the enhancement of perovskite performance by different new fullerene derivative molecule designs, as well as its impact on the future development of perovskite industries.

2. Traditional PCBM and New Fullerene Materials

Among various electronic transport layer materials, fullerenes (C60) and their derivatives [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) have been widely used in perovskite cells due to their excellent electron affinity, appropriate energy levels [3], and outstanding electron transport ability [4]. However, they still have many problems, such as poor solubility and insufficient ability to passivate defects in the perovskite layer [5]. In this part, we will compare the classic PCBM with the new fullerene derivatives and explore their performance-influencing mechanisms from multiple dimensions.

2.1. The performance Advantages and Drawbacks of the Traditional Material PCBM

PCBM (6,6-biphenyl-C61-butyric acid methyl ester) is the most classic and widely used fullerene derivative. Due to its excellent solubility and film-forming properties, it has become the standard ETL (Electron Transport Layer) for trans-structured PSCs (Perovskite Solar Cells). Compared to pure fullerene C_{60}, PCBM introduces a phenyl butyric acid methyl side chain, significantly improving its solubility in organic solvents (such as chlorobenzene), making it easier to process [3]. Additionally, the energy gap of PCBM is relatively small, which is conducive to the effective injection and transmission of electrons.

However, as an ETL, PCBM still has certain drawbacks, which restrict the further improvement of the device performance.

Because when multiple PCBM molecules are close to each other, they will form a strong π-π stacking effect, driving them to stack layer by layer in a "face-to-face" manner, thereby causing a serious self-aggregation phenomenon [6]. This leads to an increase in the film roughness, hindering the lateral transmission of electrons. Moreover, PCBM molecules lack polar functional groups that can interact with the uncoordinated lead ions (Pb2+) on the perovskite surface, and have limited ability to passivate the interface defects on the perovskite surface, making it difficult to increase the open-circuit voltage (Voc) of the device.

2.2. Molecular Design and Performance Enhancement of New Fullerene Derivatives

2.2.1. Side Chain Engineering.

To address the inherent drawbacks of PCBM, Wu Cheng et al. designed and synthesized a new type of alkyl-rich fullerene derivative, FC10 (which introduces long alkyl chains onto the fullerene), and incorporated it into PCBM to form a FC10-PCBM blend as an electron transport layer material for perovskite solar cells [3]. This can enhance solubility and reduce the self-aggregation of PCBM molecules. Compared with PCBM coating, the surface of the perovskite film coated with FC10-PCBM has no obvious pinholes, which is more conducive to the transmission of electrons; and the surface of the film is smoother and flatter, which is beneficial to the improvement of the efficiency of the solar cell [7].

This research does not merely involve the simple addition of a "fluorine atom" to fullerene. Instead, it functionalizes the side chain, meaning that not only are groups with strong electron-donating ability such as triphenylamine (TPA) introduced to lower the LUMO energy level, but also the TPA group is fluorinated-modified. Furthermore, this research innovatively physically mixed F12 with the previously synthesized and proven-effective F6 (containing non-fluorinated TPA side chains) to construct a "F6/F12" binary electron transport layer. This synergistic side-chain engineering has led to a significant improvement in overall performance – the highest photoelectric conversion efficiency of tin-based perovskite solar cells reached 11.93%, significantly higher than that of the single F6 device (9.24%) and the traditional $PC_{61}BM$ device (approximately 8%), and the open-circuit voltage (Voc), short-circuit current density (Jsc), and fill factor (FF) of the device have also been optimized. This demonstrates that modern side-chain engineering has multiple advantages: a single side chain can accommodate multiple functions, and the optimal performance comes from the optimized combination of different functional molecules. Thus, through the design of multiple molecules, advanced materials with "multi-functional integration" can be created. This demonstrates that modern side-chain engineering has multiple advantages: a single side chain can carry multiple functions, and the optimal performance comes from the optimized combination of different functional molecules. Although this research has achieved success, it also reflects the fundamental challenges faced by side-chain engineering: the synthesis of F12 itself requires multiple steps, increasing costs and process complexity. Moreover, the efficiency of 11.93% still falls short of the current efficiency records of tin-based and lead-based perovskites. Optimizing fullerene ETL solely through side-chain engineering may have approached its "performance ceiling".

Furthermore, by regulating the peripheral conjugated groups, two new thienyl fullerene pyrrolidine derivatives, C60-TH (S1) and C60-TH3 (S3), can be designed and synthesized. These compounds can be used as electron transport layers in trans-silicon-based perovskite solar cells. This case ingeniously optimizes multiple properties of the material by precisely controlling the length of the side-chain conjugated groups - introducing thiophene groups and their quantity onto the fullerene framework - thereby increasing the number of thiophene units (from S1 to S3). As a result, the open-circuit voltage (Voc) reaches 0.73 V, significantly outperforming devices based on traditional PCBM; The sulfur atom of the thienyl group forms coordination with Sn2+ in the perovskite, effectively passivating interface defects. However, the synthesis route of S3 molecules is more complex, and the aforementioned coordination effect has limited universality for systems other than tin-based perovskites. Therefore, to achieve a breakthrough, more fundamental innovations in material structure might be required.

2.2.2. Energy level engineering.

The lower Voc will cause a significant energy level drop in the ETL interface, resulting in a greater loss of electrons and a lower transmission efficiency. Therefore, Wu Cheng et al. designed and synthesized two new fullerene derivatives, namely C60-MP (F5) and C60-ETPA (F6), as shown in Figure 2. The fullerene carbon cage in this molecule not only improves the electronic transmission characteristics but also can deepen the LUMO energy level by introducing electron donor groups [8], thereby promoting electron extraction and enhancing the Voc of the device.

The molecular design of this study is extremely ingenious. The two molecules, C60-MP (F5) and C60-ETPA (F6), do not achieve this through complex double or multiple additions, but rather, on the basis of maintaining the single-addition pyrrolidine structure, they adjust the LUMO by changing the electron-donating strength of the terminal side chains; and through the "electron-pushing" effect of the electron-donating groups, they inject electron density into the fullerene carbon cage, thereby "raising" or "sharpening" the LUMO energy level. The test results show that the LUMO energy level of F6 (-4.04 eV) is approximately 90 meV higher than that of $PC_{61}BM$ (-4.13 eV). The open-circuit voltage has significantly increased from 0.63 V to 0.76 V, and the device's photoelectric conversion efficiency (PCE) has also risen from 8.25% to 10.17%. Although this research was very successful, high-performance devices require ETL materials to possess multiple capabilities, such as excellent electron mobility, effective interface defect passivation ability, and good hydrophobicity, etc. However, purely energy-level engineering materials always have deficiencies in these aspects. Furthermore, if the "shallow LUMO" design optimized for tin-based perovskites is directly applied to lead-based perovskites, it may encounter a problem where the driving force for electron extraction is insufficient due to the excessively high LUMO level, thereby introducing new issues. This indicates that the energy level engineering strategy is not universally applicable and still has certain limitations.

In addition, Li Chun et al. successfully prepared a cis isomer monomer fullerene material with an accurate chemical structure and an extremely high LUMO position, and used it as the electron transport layer of tin-based perovskite calcium minerals. The core of their innovation lies in directly obtaining a single compound that simultaneously possesses a high LUMO energy level and excellent molecular stacking order, thereby fundamentally overcoming the energy disorder problem caused by mixed isomers. The open-circuit voltage exceeds 0.86V, and the photoelectric conversion efficiency has also increased to 12.3%. However, this case also has limitations: To ensure the acquisition of a single pure isomer, the synthetic route is usually more complicated, with a low yield and high material cost, which is not conducive to large-scale application; and overly pursuing a shallow LUMO energy level may lead to a decrease in the driving force for electron extraction, thereby having a negative impact on the fill factor and short-circuit current density.

2.2.3. Construction of a multifunctional interface modification layer.

The intermediate layer or interface modification layer between the perovskite layer and the electron transport layer has interface defects. Therefore, the focus of the molecular design lies in introducing polar functional groups that can have strong chemical interactions with the surface of the perovskite, thereby eliminating the interface defects. By attaching Lewis base groups such as pyridine and poly-pyridine to the fullerene framework, and forming coordination bonds with the perovskite, the chemical binding force between the ETL material and the perovskite layer is strengthened. Firstly, the surface defects of the perovskite are passivated, then a good π-π stacking is formed with the upper ETL layer, and finally the charge extraction path of the entire interface is optimized[8].

This study introduced "complexation coordination chemistry" into the design of the interface modification layer. The nitrogen atoms of the pyridine group on the molecule can form strong coordination bonds with the unstable Sn^{2+} ions on the perovskite surface, thereby providing stronger chelation and a better molecular configuration. This enables more effective interface defect passivation and a smoother film morphology, resulting in an electron mobility increase of 10.78% for the device. However, the upper limit of performance improvement through this improvement method is constrained by the main ETL material, and it has a high requirement for the accuracy of the molecular structure. Therefore, the limitations are quite obvious.

Furthermore, in order to enhance the anchoring ability between the interface layer and the tin-based perovskite, Sun et al. designed and synthesized a series of polydentate fullerene molecules with diethyl malonate groups attached to their peripheries [8]. It ingeniously achieves this by gradually increasing the number of peripheral coordinating groups, thereby constructing an interface molecule library with "multi-dentate anchoring" properties. This enables it to provide stronger interface binding forces than single-point anchoring, and more effectively suppress various types of interface defects. When using FM5, a compound with five coordination groups, as the interface layer, the photoelectric conversion efficiency of the battery significantly increased from 11.2% of the reference device to 15.05%, and the interface charge transport path and environmental stability were both optimized. However, the synthesis of FM molecules requires controlling the quantity and position of the peripheral groups, which makes the synthesis process complex and the yield low. The cost for large-scale production is also high. The final effect of the interface layer is highly dependent on the performance of the host electron transport layer material, and it is difficult to achieve a breakthrough in performance alone. Therefore, this scheme also faces significant challenges.

2.3. Existing Challenges and Future Development

There are three major challenges in the molecular design of the electron transport layer in perovskite solar cells - the energy level mismatch between traditional materials and the new perovskite leads to excessive energy loss at the interface and a low open-circuit voltage [9]; the fullerene derivatives tend to self-aggregate during film formation, resulting in a rough and porous film with a high defect density[10], thereby affecting the interface quality. Interface defects and weak interactions also limit the performance ceiling; The weak chemical coupling between traditional materials and the perovskite layer makes it impossible to effectively passivate the large number of uncoordinated ions on the perovskite surface, resulting in an increase in non-radiative recombination and a low charge extraction efficiency. In future research, efforts should be made to break through the limitation of single electron-donating side chains and move towards "multifunctional monomers"; at the same time, progress should be made from "two-dimensional planar interfaces" to "three-dimensional interface integration", optimizing charge extraction, defect passivation and film morphology through binary/trinary blending. Moreover, simplifying the synthesis route, improving material yield and stability are the key to promoting its transition from the laboratory to industrial application [11].

3. Conclusion

This review systematically compiles and compares the performance impacts of various fullerene derivatives as electron transport layers in perovskite solar cells. The research shows that the classic PCBM has inherent defects such as self-aggregation. Through molecular design such as side-chain engineering and energy-level engineering, these defects can be weakened, such as improving the electron transport rate and energy-level matching degree, thereby expanding the commercial application prospects. The future exploration of ETL should focus on deeper mechanisms and practical applications. This includes not only further research on processes such as interface passivation and charge transfer, but also efforts to address key industrialization issues such as the synthesis cost for large-scale production. Only by considering all aspects comprehensively can the fullerene-based electron transport layer continue to play its significant role in the process of transitioning calcium phosphate solar cells to large-scale commercialization.

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