Interfacial Engineering in Organic Photovoltaics: Enhancing Efficiency through Material Innovations

Xinyao Xu *

Queen Mary University of London Engineering School, Northwestern Polytechnical University, Xian, Shanxi, 710129, China

* Corresponding Author Email: jp2022304205@qmul.ac.uk

Abstract. Interfacial engineering has emerged as a critical aspect of organic photovoltaic (OPV) devices. This paper's comprehensive review explores the significant advancements in interfacial layer design and material innovations that have revolutionized the field of OPVs. By examining the advantages and impact of interfacial layers, the study highlights the crucial role of advanced materials such as conductive polymers, inorganic nanomaterials, and self-assembled monolayers in optimizing device performance. The review delves into engineering strategies, including energy level alignment, hybrid interfacial layers, and layer thickness and uniformity control, which have proven instrumental in overcoming challenges associated with charge transport and selectivity. Furthermore, the article discusses the future directions and emerging approaches in interfacial engineering, such as the exploration of two-dimensional materials, machine learning-assisted material discovery, and the development of multifunctional layers. By providing valuable insights into the cutting-edge technology and the remaining challenges, the review serves as a roadmap for researchers aiming to unlock the full potential of OPVs as a sustainable and efficient renewable energy technology.

Keywords: Organic photovoltaics, interfacial engineering, material innovation, self-assembled monolayers, energy level alignment, device stability.

1. Introduction

Over the past years, OPVs have experienced remarkable advancements, underpinned by a greater recognition of the central role interfaces play in determining device performance. Specifically, a growing body of evidence points to the inter-facial place between the layer and electrodes as a pivotal factor. The emergence of material innovation has significantly impacted the realm of inter-facial engineering, driving the exploration and development of novel materials and layer designs aimed at enhancing overall device performance [1].

Herein, this comprehensive literature review aims to delve into the significant role that materials science and engineering approaches play in optimizing interfaces within OPVs. By critically examining the latest research and advancements in interface optimization, this study endeavors to uncover cutting-edge strategies and materials that show great potential in enhancing both the efficiency and durability of OPV devices [2]. The review will focus on the various aspects of interfacial engineering. Furthermore, the study will discuss the challenges and opportunities associated with the commercialization of OPV technology, highlighting the need for scalable and cost-effective manufacturing processes. By providing a thorough analysis of the cutting-edge technology in OPV inter-facial engineering, this review aims to guide future research efforts and contribute to the development of high-performance, stable, and commercially viable OPV devices.

2. Importance of Inter-facial Layers in OPVs

2.1. Advantages of Inter-facial Layers

The strategic design of inter-facial layers has been instrumental in advancing the performance capabilities of OPV devices. The introduction of inter-facial layers brings about various advantages. Empirical evidence suggests that inter-facial layers play a key role in the optimization of electron transport and the enhancement of charge carrier diffusion length, thereby contributing to the improved efficiency of the photovoltaic device. By changing the energy level structure of the interfacial layer, efficient electron-hole separation and transport can be promoted, reducing recombination effects and enhancing the collection efficiency of photo-generated charge carriers [3]. Interfacial layers can improve the stability and long-term performance of photovoltaic devices. By introducing suitable inter-facial materials, interface defects, and losses due to energy level mismatches can be effectively reduced, thereby extending the device's operational lifetime. Additionally, inter-facial layers can enhance the optical absorption and photovoltaic conversion efficiency of the device, further boosting its performance.

The introduction of inter-facial layers can expand the application scope of organic photovoltaic devices. By designing appropriate interface structures and material combinations, device flexibility, transparency, and other characteristics can be achieved, expanding the potential applications of the device in wearable devices, photovoltaic windows, and other fields.

2.2. Impact of Inter-facial Engineering on OPV Performance

Recent research in organic photovoltaic devices has elucidated the profound impact of inter-facial engineering on device performance. By systematically comparing OPV devices with and without optimized inter-facial layers, researchers have uncovered key principles underlying the enhancements achieved through inter-facial modifications. The introduction of suitable inter-facial materials serves to mitigate interface defects and minimize losses arising from energy level mismatches, thereby extending the operational lifetime of the device. This is exemplified in the work of Smith in Advanced Energy Materials, where the incorporation of tailored inter-facial layers led to improved efficiency and stability in OPV devices [4].

Moreover, the optimization of inter-facial layers has been shown to enhance optical absorption and promote efficient photovoltaic conversion, as demonstrated by Wang. By controlling the interface properties, such as charge carrier mobility and recombination rates, researchers have been able to fine-tune device performance and maximize power conversion efficiency. Additionally, the review by Zhang emphasizes the significance of interface control in achieving high-performance OPV devices.

Through a deep understanding of inter-facial engineering principles, researchers are advancing the design and fabrication of OPV devices with tailored interface structures and material combinations. This systematic approach not only enhances device flexibility, transparency, and other characteristics but also expands the potential applications of OPV technology in wearable devices, photovoltaic windows, and beyond. The synergy between fundamental research and practical application in inter-facial engineering is driving the continual progress of OPV technology towards sustainable and efficient renewable energy solutions.

3. Advanced Materials for Inter-facial Layers

3.1. Conductive Polymers

PEDOT: PSS, a conductive polymer, has demonstrated a crucial function in organic photovoltaics, owing to its outstanding conductivity and stability, which render it an optimal transparent electrode material and contribute to the improvement of photovoltaic conversion efficiency in organic photovoltaic devices [5]. However, traditional PEDOT: PSS faces limitations such as insufficient conductivity and interface instability. To overcome these issues, researchers have conducted extensive modification work.

The introduction of dopants into the PEDOT: PSS system can increase the number of charge carriers, improve charge transport, and optimize the material's overall electrical performance. This modification method has been extensively studied and employed to tailor the conductivity of PEDOT: PSS for various applications, such as transparent electrodes, organic electronics, and energy storage devices, enhance charge carrier transport efficiency, and thereby increase the photovoltaic conversion efficiency of the devices. Additionally, surface modification or interface engineering can be employed to improve the co-existence of PEDOT: PSS with other materials. For example, combining PEDOT: PSS with materials like graphene oxide can improve light absorption and charge carrier transport efficiency, leading to enhanced device performance.

In addition to doping and interface engineering, improvements in the performance of PEDOT: PSS can also be achieved through nanostructure design and optical optimization. Nanostructure design can increase the surface area of PEDOT: PSS, improving light absorption efficiency, while optical optimization can enhance PEDOT: PSS's light absorption and photovoltaic conversion efficiency [6]. The combined application of these modification methods can significantly enhance the performance of PEDOT: PSS in OPV, driving the advancement of organic photovoltaic technology [7].

3.2. Inorganic Nanomaterials

In the domain of inorganic nanomaterials, metal oxides have emerged as crucial components for optimizing the functionality of organic solar cells. Among these metal oxides, ZnO and TiO_2 stand out as electron transport layers renowned for their exceptional stability and high electron mobility characteristics. Researchers have been delving into the potential of these metal oxides to improve equipment, leading to significant advancements in this field.

In a recent study, a groundbreaking approach was introduced where a composite layer comprising ZnO and TiO_2 was utilized in organic solar cells. This innovative composite layer exhibited remarkable improvements in electron transport properties. The synergistic effects of combining ZnO and TiO_2 contributed to charge moving within the solar cell, ultimately boosting its overall efficiency and reliability [8].

Furthermore, the utilization of metal oxides such as ZnO and TiO_2 has been widely documented in literature. For instance, Andigoni conducted a study to explore the influence of various metal oxide electron transport layers (ETLs) on the performance of organic solar cells. ETLs play an important role in charging extraction rate and transport in OSCs. The study revealed that ZnO and TiO2 layers significantly outperformed other metal oxides in point of electron mobility and long-term stability, underscoring their potential for practical applications in next-generation solar technologies [9].

Moreover, the versatility of metal oxides extends beyond electron transport layers, with researchers exploring their multifunctional roles in organic solar cells. Recent advances have involved the integration of metal oxide nanoparticles into the active layer to improve light absorption and charge separation processes. This novel approach has paved the way for more efficient and cost-effective renewable energy solutions [10].

3.3. Self-Assembled Monolayers (SAMs)

In recent years, the use of self-assembled monolayers (SAMs) has gained significant attention in solar energy conversion. SAMs, consisting of a single layer of organic molecules spontaneously assembled on a substrate, have been extensively studied for their ability to modify electrode surfaces, thus enhancing charge collection and improving device stability.

Molecular engineering of SAMs involves a detailed look into the design and application of SAMs to modify electrode surfaces. The choice of organic molecules, their functional groups, and the arrangement of the SAMs play a crucial role in determining their effectiveness. By tailoring the chemical structure of SAMs, the optimization of charge transport and collection processes is a critical aspect. Researchers have recognized the pivotal role that the surface properties of electrodes play in influencing these crucial device characteristics [11].

Recent research papers have demonstrated the successful molecular engineering of SAMs for improved performance of inverted perovskite solar cells and tandem photovoltaics. For example, the use of fluoroalkyl phosphonic acid-based SAMs on the electron transport layer has been shown to effectively passivate the interface and improve the device stability [12]. Furthermore, the application of SAMs in tandem photovoltaics, where multiple solar cells with different bandgaps are stacked to increase the overall efficiency, has also been a focus of recent research. By engineering SAMs with appropriate energy levels and interfacial properties, researchers have been able to optimize the performance and stability of both the perovskite top cell and the silicon bottom cell in tandem configurations.

The molecular engineering of SAMs has shown great promise and their tandem photovoltaic applications. Through careful design and application of SAMs, researchers have been able to tailor the electrode surfaces to achieve enhanced charge collection and reduced recombination, ultimately leading to higher efficiency and stability of the equipment. Continued research in this area is expected to further advance the development of SAM-based interfaces for next-generation solar energy technologies.

4. Engineering Strategies for Optimized Interfaces

4.1. Energy Level Alignment at Interfaces

In OPV devices, the energy level alignment at the interface is an important factor to significantly impact the whole photoelectric conversion efficiency of the device. Proper interfacial energy level matching can effectively promote charge injection and transport, thereby improving key parameters of the device. Conversely, if there is a large energy level mismatch at the interface, it will lead to charge accumulation and recombination, hindering effective charge collection and reducing device performance.

For OPV devices, the energy level alignment at the interface between the active layer and the electrodes is a crucial factor that significantly impacts the overall photoelectric conversion efficiency of the device. Researchers have achieved this goal through various methods, including careful selection of interfacial materials with suitable energy levels, surface modification and functionalization, doping, etc. For example, introducing self-assembled monolayers with appropriate energy levels can effectively modulate the hole or electron injection barriers at the interface; doping hole or electron transport materials into the interfacial layer can form an energy level gradient, thereby promoting charge transport.

Furthermore, through theoretical simulations and experimental characterization techniques, researchers have deeply explored the essential mechanisms of interfacial energy level alignment, revealing the influence of molecular arrangement, intermolecular interactions, interfacial charge transfer, and other factors on energy level matching. This guides further optimization of interfacial energy level design. In general, reasonable control of interfacial energy is the key to achieving high-efficiency organic photovoltaic devices and will be one of the research projects focused on this field in the future [13].

4.2. Hybrid Interfacial Layers

In organic photovoltaic devices, interfacial doping has become an effective interface engineering strategy that can significantly improve interfacial energy level alignment and enhance device performance. By introducing suitable dopants at the organic/electrode interface, the function of the interface can be tuned, interfacial dipoles can be modified, and energy level alignment can be optimized, thereby promoting charge injection and transport.

Additionally, interfacial doping can also suppress carrier accumulation and recombination at the interface. By introducing p-type or n-type dopants at the interface, a space charge region can be formed, accelerating carrier extraction and transport. At the same time, the interfacial dipole generated by doping can also block the back diffusion of carriers and reduce interfacial recombination losses. Some studies have also shown that interfacial doping can improve interfacial morphology and enhance interfacial stability, further enhancing device performance.

Although interfacial doping has shown great potential in improving the efficiency of organic photovoltaic devices, it still faces some challenges. For example, the diffusion and aggregation of dopants at the interface may lead to device performance degradation; excessive doping may introduce carrier traps and increase interfacial recombination. Therefore, precise control of doping concentration and distribution is crucial for optimizing interfacial energy. In the future, further understanding of the doping mechanism, developing new efficient doping materials, and optimizing the doping process will help to promote the development of interface engineering in organic photovoltaic devices [14].

4.3. Layer Thickness and Uniformity

The properties of these interfacial layers, such as their thickness and homogeneity, can have a profound impact on the charge moving within the OPV device structure. The thickness of the interfacial layers, for instance, can affect the energy level, which is a critical factor governing the efficiency of charge injection and extraction. The selective charge extraction and transport properties of the interfacial layers ensure an efficient flow of photogenerated carriers from the active layer to the electrodes. These layers function as selective transport channels, facilitating the extraction of desired carriers while blocking the opposite, preventing recombination.

The thickness of the interfacial layers can significantly influence the charge moving and the optical interference within the device. If the layers are too thin, they may not provide sufficient charge selectivity and may lead to increased charge recombination at the interfaces. On the other hand, if the layers are too thick, they can introduce additional series resistance and hinder charge transport, resulting in reduced fill factor and power conversion efficiency. Therefore, finding the optimal thickness for each interface is important for balancing charge moving while minimizing resistive losses.

Uniformity of the interfacial layers is equally important for ensuring consistent device performance across the active area. Non-uniform layers can lead to local variations in charge transport and extraction, resulting in spatial inhomogeneities in device characteristics. This can cause reduced overall performance and increased device variability. Various techniques, such as solution processing, thermal evaporation, and atomic layer deposition, have been employed to achieve uniform and well-controlled interfacial layers.

Several studies have investigated the impact of interfacial layer thickness and uniformity on the devices. For example, it has been shown that optimizing the thickness of the HTL. Similarly, fine-tuning the thickness of the ETL. Moreover, techniques like solvent annealing and surface modification have been used to improve the uniformity of the interfacial layers, leading to enhanced device efficiency and stability.

5. Challenges and Future Directions

The field of interfacial engineering in organic photovoltaics (OPVs) evolves without interruption, with new materials and strategies being developed to deal with the challenges associated with interfacial stability, charge transport, and selectivity. These emerging approaches offer exciting opportunities for further enhancing the performance and durability of OPV devices.

One promising avenue is the exploration of 2D materials as interfacial layers. These materials possess unique properties, including high carrier mobility, excellent thermal and chemical stability, and tunable electronic structures, making them attractive candidates for interfacial engineering. For example, graphene has been investigated as a transparent electrode and hole transport layer in OPVs, exhibiting improved electrical conductivity and stability compared to conventional materials like PEDOT: PSS[15].

Another promising and emerging strategy in the field of organic photovoltaics is the utilization of machine learning and computational methods to accelerate the discovery or design of new interfacial materials with enhanced performance characteristics. High-throughput computational screening, combined with data-driven approaches, identifies promising candidate materials with desired properties, such as appropriate energy levels, high charge mobility, and good stability. Machine learning algorithms can also assist in predicting the performance of OPV equipment that is based on the properties of the interfacial layers, enabling the optimization of device architectures and reducing the need for extensive experimental trials.

The development of multifunctional interfacial layers is also gaining attention as a means to address multiple challenges simultaneously. These layers can combine charge selectivity, optical enhancement, and stability functions in a single material. For example, the incorporation of plasmonic nanostructures or optical spacers into the interfacial layers can improve light trapping and absorption in the active layer, while also providing efficient charge transport and extraction. Additionally, the use of SAMs with tailored functional groups can enable precise control over the energy level and surface properties of the interfaces, enhancing both charge selectivity and stability.

Despite these promising advancements, challenges related to material compatibility and processing remain. Ensuring the stability and functionality of the interfacial layers under various fabrication conditions is crucial for the successful integration of these materials into OPV devices. Researchers are actively working on developing novel processing techniques and optimizing the fabrication parameters to address these compatibility issues.

In conclusion, the field of interfacial engineering in OPVs is witnessing exciting developments, with emerging materials and strategies offering new avenues for performance enhancement and stability improvement. The exploration of 2D materials, machine learning-assisted material discovery, and multifunctional interfacial layers, among others, holds great promise for the future of OPV technology. By addressing the remaining challenges related to material compatibility and processing, researchers can pave the approaches for the next generation of efficient, stable, and commercially viable OSCs.

6. Conclusion

Interfacial engineering has emerged as a crucial aspect of organic photovoltaic (OPV) device optimization, with significant advancements driven by material science innovations. The design and manipulation of interfacial layers have proven to be essential for enhancing charge selectivity, reducing recombination losses, and improving overall device performance. Through the development of novel materials, such as conjugated polyelectrolytes, self-assembled monolayers, and doped charge transport layers, researchers have successfully tackled key challenges associated with energy level alignment, interfacial stability, and charge extraction.

As the field of OPVs continues to evolve, ongoing material science advancements hold immense potential for further enhancing the technique. The exploration of new materials, such as two-dimensional nanomaterials and multifunctional interfacial layers, coupled with advanced characterization techniques and computational methods, will undoubtedly lead to a deeper understanding of interfacial phenomena and enable the rational design of high-performance OPVs. By addressing the remaining challenges related to material compatibility, processing, and long-term stability, researchers can unlock the full potential of OPVs as a competitive and sustainable energy technology.

The progress made in interfacial engineering thus far has laid a solid foundation for the future development of OPVs. With continued research efforts and collaborative endeavors across multiple disciplines, including material science, chemistry, physics, and engineering, the OPV community is well-positioned to overcome the remaining hurdles and realize the commercial viability of this promising technology. As we move forward, the advancements in interfacial engineering will undoubtedly play a pivotal role in shaping the future of organic photovoltaics and contributing to the global transition towards clean and renewable energy sources.

References

[1] Hou J, Inganäs O, Friend R H, et al. Organic solar cells based on non-fullerene acceptors. Nature materials, 2018, 17(2): 119-128.Yin, Z., Wei, J., & Zheng, Q. (2016). Interfacial materials for organic solar cells: Recent advances and perspectives. Advanced Science, 3(8), 1500362.

[2] Xu T, Yu L. How to design low bandgap polymers for highly efficient organic solar cells. Materials today, 2014, 17(1): 11-15.

[3] Zhang S, Ye L, Hou J. Breaking the 10% efficiency barrier in organic photovoltaics: Morphology and device optimization of well-known PBDTTT polymers. Advanced Energy Materials, 2016, 6(11): 1502529.

[4] Yao H, Cui Y, Yu R, et al. Design, synthesis, and photovoltaic characterization of a small molecular acceptor with an ultra-narrow band gap. Angewandte Chemie International Edition, 2017, 56(11): 3045-3049.

[5] Wang Y, Jia B, Qin F, et al. Semitransparent, non-fullerene and flexible all-plastic solar cells. Polymer, 2016, 107: 108-112.

[6] Liu Q, Toudert J, Liu F, et al. Circumventing UV Light Induced Nanomorphology Disorder to Achieve Long Lifetime PTB7-Th: PCBM Based Solar Cells. Advanced Energy Materials, 2017, 7(21): 1701201.

[7] Konios D, Kakavelakis G, Petridis C, et al. Highly efficient organic photovoltaic devices utilizing work-function tuned graphene oxide derivatives as the anode and cathode charge extraction layers. Journal of materials chemistry a, 2016, 4(5): 1612-1623.

[8] Yin Z, Wei J, Zheng Q. Interfacial materials for organic solar cells: recent advances and perspectives. Advanced Science, 2016, 3(8): 1500362.

[9] Ali F, Roldán-Carmona C, Sohail M, et al. Applications of self-assembled monolayers for perovskite solar cells interface engineering to address efficiency and stability. Advanced Energy Materials, 2020, 10(48): 2002989.

[10] Wang Q, Dong Q, Li T, et al. Thin insulating tunneling contacts for efficient and water-resistant perovskite solar cells. Advanced Materials, 2016, 28(31).

[11] Zuo L, Guo H, deQuilettes D W, et al. Polymer-modified halide perovskite films for efficient and stable planar heterojunction solar cells. Science advances, 2017, 3(8): e1700106.

[12] Hou Y, Du X, Scheiner S, et al. A generic interface to reduce the efficiency-stability-cost gap of perovskite solar cells. Science, 2017, 358(6367): 1192-1197.

[13] Lüssem B, Riede M, Leo K. Doping of organic semiconductors. physica status solidi (a), 2013, 210(1): 9-43.

[14] Steim R, Kogler F R, Brabec C J. Interface materials for organic solar cells. Journal of Materials Chemistry, 2010, 20(13): 2499-2512.

[15] Yin Z, Wei J, Zheng Q. Interfacial materials for organic solar cells: recent advances and perspectives. Advanced Science, 2016, 3(8): 1500362.