

# Composite Materials in Organic Solar Cells - Enhancing Efficiency, Stability, and Versatility

Xinyu Zhao \*

Department of Composites and Engineering, Nanchang Hangkong University, Nanchang, Jiangxi Province, Zip Code 330000, China

\* Corresponding Author Email: 21014229@stu.nchu.edu.cn

**Abstract.** The prominence of energy and environmental pollution issues has spurred cleaner alternative energy conversion technologies, among which organic solar cells (OSCs) attain extensive attention for their lightweight and flexible properties. However, the stability and photoelectric conversion efficiency (PCE) of OSCs still lag the traditional inorganic solar cells. Notably, the active layers in OSCs predominantly consist of composite materials. This paper analyzes the principles underlying performance enhancement through composites in OSCs, assesses the impact of different composite categories on PCE and stability, and explores their unique role in enhancing the multifunctionality of OSCs. The findings confirm the importance of composites in improving OSC stability and PCE by leveraging the properties of multi-component materials and achieving a synergetic effect. Moreover, employing a ternary strategy in composite applications emerges as a promising method to simultaneously enhance PCE and stability, offering a valuable research direction for OSC development in the future.

**Keywords:** Organic solar cells; stability; photovoltaic conversion efficiency; versatility; Composites.

## 1. Introduction

Due to the increasing energy demand, the energy crisis and environmental pollution have become a non-negligible problem. Solar energy, a renewable and clean energy source, is widely recognized for addressing power generation issues. OSCs, representing an emerging sector of solar cell industries, garnered extensive research interest due to their light weight, flexibility, and straightforward manufacturing process. However, compared with traditional silicon-based solar cells, the OSCs exhibit lower PCE. Moreover, the stability of OSCs is limited, typically functioning only under indoor laboratory conditions or mild environments, and can hardly meet the conditions of stable outdoor use. Ultimately, these limitations hinder their practical application for reliable and long-term usage in practical settings. The application of materials in OSCs is dominated by composites, as composites take advantage of the unique strengths of different components to enhance charge transport at the interface to achieve optimal performance. A range of excellent composites, mainly polymer-fullerene and all-polymer materials, are currently being extensively studied.

Herein, this paper investigates how composites affect the efficiency, operational stability, and application range of OSCs. It discusses the synergistic effects of composites, detailing the principles, advantages, and significant impacts of composite applications on OSCs enhancement.

## 2. Structure and Fundamentals of Organic Solar Cells

OSCs are semiconductor devices that convert light energy into electricity, with polymer-based active layers. Taking one of the current designs with better conversion efficiency enhancement as an example, Figure 2.1 demonstrates its basic structure, and the serial numbers in the figure show its power generation principle. The cell is mainly composed of a six-layer structure, with the third layer composed of donor and acceptor materials called the active layer. Its working principle, summarized in Figure 1, involves five steps:

1. Photon absorption: When sunlight irradiates the active layer, photons with wavelengths within the absorbing wavelength range of the donor/acceptor material are absorbed by the active layer.

2. Exciton generation: excitation of the base state of the electron to the excited state, at the same time in the original position of the electron to leave a positively charged vacancy (hole), at this time due to the Coulomb force binding, composed of electron-hole pairs, called excitons.

3. Exciton diffusion: Dissociation of excitons occurs after they diffuse to the receptor interface due to concentration difference.

4. Charge separation: the exciton dissociates into free electrons and holes.

5. Charge transport and collection: The trajectories of holes and electrons can be observed from the figure, they pass through the transport layer to reach the anode and cathode, respectively, owing to the built-in electric field and charge concentration gradient inside the device. The anode and cathode collect positive and negative charges, creating a current loop, which is manifested in the PCE.

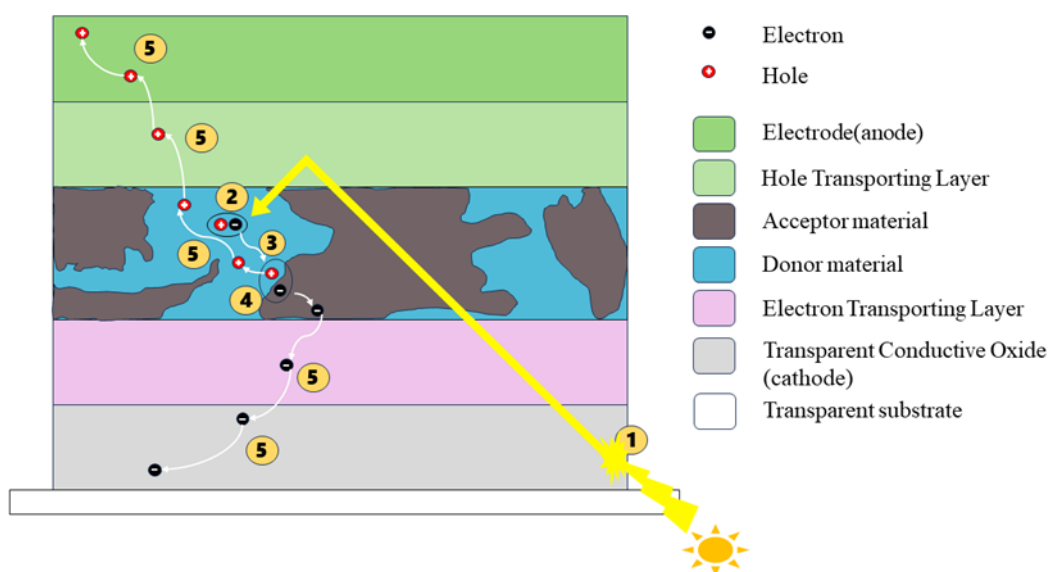


Fig 1. Working principle of bulk heterojunction solar cells (picture/image credit: original).

### 3. Performance Enhancement of Composite Organic Solar Cells

According to the analysis of the principles mentioned above, the improvement of the PCE in OSCs primarily hinges on several factors: a broad absorption spectrum in the photoactive layer for optimal light absorption; effective excitation to generate free charge; and efficient charge separation, transport, and recycling. Further, the stability of OSCs is influenced by external environmental conditions, morphological changes, diffusion of electrode and transport layer materials into the active layer, and mechanical stress from bending. Consequently, selecting suitable donor-acceptor materials is crucial for enhancing both the conversion efficiency and stability of OSCs. Efforts to boost OSC performance have included modifications to the material composition of the active layer, with five main types of composites currently employed.

Therefore, identifying appropriate donor-acceptor materials is key to enhancing both the conversion efficiency and stability of OSCs. Researchers have focused on improving OSC performance by modifying the materials in the active layer. Presently, five principal types of composite materials are applied as the active layer and will be discussed in this section.

#### 3.1. Organic-inorganic Hybrid Composites

Organic materials are widely researched due to their simplicity of fabrication and abundant source of raw materials, while these materials are typically accompanied by low charge mobility and low open-circuit voltage due to non-composite radiation. Friend et al. [1] have proposed a new idea to improve the PCE of the cell by identifying and suppressing non-radiative loss pathways to reduce the voltage loss, which has the potential to elevate the efficiency of organic solar cells beyond 20%.

While this strategy improves the PCE of pure polymer OSCs, their performance remains inferior to that of inorganic solar cells. Consequently, exploring the use of organic-inorganic hybrid composites as active layer materials is worthwhile. Incorporating inorganic materials such as fullerenes and metal oxides, etc. can improve the PCE of OSCs due to the higher electron mobility of these inorganic components. P-type conjugated polymers are a representative donor material for this typed composite, among which poly-3-hexylthiophene (P3HT) is a frequent choice. Acceptor materials typically include soluble fullerene derivatives, notably the phenyl ester-adducted C60 derivative, PCBM. The outstanding ability of fullerenes to accept and transport electrons depends heavily on the conjugated structure of their spherical shape. Since the initial development of this battery type in 1992, over two decades of continuous enhancements have recently led researchers to explore new methods to improve both the PCE and the stability of fullerene system OSCs.

Tang et al. [2] found that the devices after the addition of [9] cyclic p-phenylene ([9] CPP) increased up to 20% in PCE over the original devices. The study suggests that the [9] CPP  $\supset$  fullerene system boosts the electrical properties of OSCs by facilitating charge transfer between the component materials, impacting the  $\pi$ - $\pi$  stacking of acceptors. This finding could pave the way for the inclusion of fullerene rings as novel components in fullerene system studies.

Barcelona et al [3] carried out a comparative analysis of the UV effect on the OSCs stability. They discovered that OSCs, particularly those containing fullerene mixtures with 1, 8-di-2-octane (DIO) as an additive, exhibited improved photostability under UV irradiation. Although devices with residual DIO initially degraded in performance under prolonged UV exposure, they eventually demonstrated a self-healing effect. This study attributes the enhanced performance stability of OSC under simulated sunlight to the diffusion and crystallization of fullerenes induced by UV light. This finding provides theoretical insights that could aid in the development of efficient and stable OSCs for real-world solar applications.

Furthermore, fullerenes and their derivatives have several limitations. For example, they can only absorb photons of short wavelengths from the visible region as well as having hard-to-regulate LUMO and HOMO energy levels. Researchers have explored the use of other inorganic additives, including metal nanoparticles, to enhance OSC performance. Tao et al. [4] reported significant improvements in the stability of OSCs using self-assembled monomolecular layers (SAM) of conjugated molecules to passivate ZnO nanoparticles (ZnO NPs) in electron transport layers (ETLs), achieving a high PCE of 18.14%. The enhancement in electron transport and chemical properties due to interfacial modification with metal oxide nanoparticles (MO NPs) suggests better aggregation at the organic-inorganic interface, offering a promising method for improving OSC performance and inspiring further innovations in layer structure modifications.

### 3.2. All-Polymer Solar Cells

Compared to other composite OSCs, all-polymer solar cells (All-PSCs) have clear advantages with their broadly tunable light absorption and adjustable energy levels. Xu et al. [5] compared conventional fullerene devices with devices in which N2200 acts as a receptor, revealing that All-PSCs demonstrate enhanced stability against oxygen and moisture. These all-polymer films are morphologically stable, highly resistant to external environmental factors such as heat, water, and light, and are well-suited for large-scale production, a crucial aspect for the commercialization of future OSCs. The inherent material advantages, combined with innovative design approaches, have led to significant performance improvements in All-PSCs. For instance, Ma et al. [6] explored a tandem architecture that achieved an optimal PCE of 17.87% by utilizing a wider wavelength range to increase photon absorption and minimize heat loss, thereby enhancing device performance. Moreover, the PCE of All-PSCs has broken through 18% through a novel ternary strategy, which will be elaborated on later. Despite these advancements, the production of polymers on a large scale remains challenging, drawing attention to small molecule materials as a viable alternative.

### 3.3. Polymer/Non-Fullerene Small Molecule Hybrid Composites

Polymer/non-fullerene small molecule hybrid composite OSCs are characterized by two configurations: polymers as donors with small molecules as acceptors, and vice versa. Small molecules used as acceptors offer several advantages: they possess a strong and broad absorption spectrum in the visible to near-infrared light region, exhibit high charge mobility with lower energy losses due to rapid exciton separation and transfer, and are generally more accessible due to their defined molecular weight which facilitates higher purity and ease of chemical customization for energy level adjustments. These properties have significantly enhanced the performance of OSCs incorporating designed small molecules into the active layer.

Wei et al. [7] developed a new small-molecule donor (H31), based on a blend of H13 and Y6, achieving a 13% PCE by broadening the absorption spectrum. The study also assessed the stability of a PDINO-free device, noting that it retained 94% of its initial performance after approximately 140 days. The findings suggest that the absence of PDINO may avoid prolonged aggregation and morphological instability in the active layer, thereby enhancing device stability. Moreover, OSCs that integrate small molecules have demonstrated notable PCE improvements. Cheng et al. [8] crafted a PM6: BTP-eC9 organic solar cell that achieved a record binary efficiency of 19.31%, with a remarkably low non-radiative compound loss of 0.190 eV. These results bolster researchers' confidence in surpassing the 20% PCE threshold for OSCs.

### 3.4. All-Small-Molecule Organic Solar Cells

In the active layer, the small molecule material enhances the PCE by increasing the light absorption through a wider light absorption band. Wang et al. [9] developed a wide-bandgap donor small molecule, BTTzR, which, when paired with the Y6 small molecule acceptor, achieved a PCE of 13.9%. The remarkable PCE is credited to BTTzR's strong absorption efficiency, ordered molecular orientation, and stacking within specific spectral wavelengths, which collectively minimize non-radiative energy loss.

Furthermore, the utilization of all-small-molecule system composites not only boosts PCE but also significantly improves the stability of OSCs. For instance, Xie et al. [10] observed that the M-PhS: BTP-eC9 cell maintained high stability, aging minimally over 1128 hours at 85 °C, demonstrating the intrinsic durability of all-small-molecule OSCs (ASM-OSCs). Additionally, Guo et al. [11] created a device using a new small-molecule donor, BDT with modified side-chain (TVT-SR) 2, and IDIC as the acceptor. This configuration exhibited only a 10% loss in PCE after 200 hours of light exposure and retained 87% of its initial efficiency following 96 hours of thermal annealing. The enhanced electrical properties were attributed to the increased effective  $\pi$ - $\pi$  conjugation length from the TVT-SR side chains, improving charge separation and transport, while the stability gains were linked to the extended conjugated side chains reducing thermally induced phase aggregation.

However, the primary challenge with small molecule systems lies in modulating the active layer morphology, which currently limits further efficiency improvements.

### 3.5. Polymer/Small molecule/Inorganic Ternary or Polymeric Hybrid Composites

Active layers composed of single electron donor or acceptor material pairs often absorb light incompletely or insufficiently across the solar spectrum. Researchers have developed a ternary strategy, using dual donors (D1:D2) or dual acceptors (A1:A2) in OSCs, to enhance light absorption across the solar spectrum and optimize interfacial morphology.

This strategy can mobilize the respective advantages of the dual acceptor/donor materials to optimize the interfacial morphology and reduce charge recombination, which effectively solves the problems of low exciton lifetime and hole mobility and ultimately enhances the PCE. For instance, Li et al. [12] achieved a PCE of 17.06% in ternary SM-OSCs by using a blend of SM-mB donors with dual acceptors, Y6 and L8-BO, which optimized the composite morphology for efficient charge generation.

Further, the ternary strategy offers extensive material design flexibility by allowing adjustments in the type, content, and ratio of component materials. Zhang et al. [13] used PBDB-TF and PBQx-TF dual donor systems to produce a terpolymer, PQB-x (where x stands for 1-3), with an optimal PCE of 18.1%. This study improved the performance by controlling the amount of receptor components and linearly modulating the spectral absorption range of the component materials. In addition, the integration of PBQx-TF increased the effective charge transfer efficiency, thereby improving the PCE. This also demonstrates one of the advantages of the ternary strategy: greater designability space, in other words, the possibility of modulating more OSC performance can be achieved by adjusting the content, ratio, or even type of the two-component materials in the dual donor or dual acceptor.

The ternary strategy has proven effective in enhancing the PCE while also boosting or maintaining the stability of OSCs, a feat not typically achievable with other designs. A good example is the MPhS-C2:L8-BO: L8-S9 ternary OSC developed by Gao et al. [14], which not only achieves a PCE of up to 18.1% but also loses only 20% of its efficiency after about 1,000 hours of sunlight exposure. This durability and efficiency are attributed to the improved compatibility and performance of hybrid components with the addition of L8-S9. This component not only enhances charge transport and exciton dissociation but also contributes to the device's resilience against environmental stressors, thereby extending its operational stability.

The study above revealed that ternary composites generally exhibit improved compatibility and stability at the interface compared to single-component materials. Ternary composites often feature materials that enhance charge transport, leading to significantly better overall performance of OSCs synthesized using this approach. The ternary strategy thus stands out as a highly promising method for boosting OSC performance. Further enhancing this approach, researchers, including Zhou et al. [15], have integrated computer simulations with the ternary strategy to study the relationships between component morphology, mechanical properties, and thermal stability. Zhou et al. developed a model for the prediction of the stability and mechanical properties, facilitating precise adjustments to the proportions of materials used in ternary composites. This innovation underscores the continued potential of the ternary strategy to advance OSC technology by optimizing the material composition for enhanced performance and durability.

#### 4. Applications Beyond Conventional Solar Cells

OSCs are recognized for their flexibility, semitransparency, lightweight, and ease of fabrication, making them highly suitable for a range of applications across various fields. In building-integrated photovoltaics, OSCs can be integrated with large glass surfaces common in modern architecture, offering power generation while maintaining translucence. This integration optimizes unused space and enhances building aesthetics, with ongoing research into color adjustment of OSCs to further tailor their architectural integration. When the sun-power property of OSCs is mobilized together with the bendability, the two factors of self-powering and wearability can then be linked. As a result, wearable electronic devices that do not need to be recharged can be designed in conjunction with this idea. These electronic devices are currently more commonly used for life detection, such as detecting changes in the user's movement, pulse, or even blood pressure.

In terms of apparel, photovoltaic fabric can be designed and produced by taking advantage of the fact that OSCs can be printed and produced. If the fabric is combined with an electrical appliance, it can be used to create flexible and functional apparel, such as smart temperature-controlled clothing. ShadePlex has used this advantage to sell a sun-shading textile that generates electricity.

The overall thickness of the OSC functional layer is only a few hundred nanometres, making the mass much higher than the weight and power density of conventional silicon-based solar cells, making it an ideal material for aerospace vehicles. Through testing, Cardinaletti et al. [16] confirmed that flexible organic solar cells have high efficiency as well as stable performance in space, demonstrating their great potential for space applications.

## 5. Challenges and Future Directions

With evolving applications of composite materials in OSCs, their efficiency and stability have seen significant improvements, and the PCE of single-junction OSCs has now surpassed 19%. However, for OSCs to achieve widespread commercial use, further enhancements in both efficiency and stability are required. The main mechanism for the performance decay of OSCs is still explored from the interfacial stability of the composite material and the component compatibility of the composite material. The interfacial light stability and interfacial chemical stability can be enhanced by designing the matching of material properties. At present, the efficiency and stability of most types of OSCs are like the two ends of a buckboard, i.e., some OSCs tend to lose part of their stability for the improvement of efficiency. Addressing this challenge requires a balanced approach to simultaneously improve both attributes. The ternary strategy has emerged as a promising solution, having already led to devices with PCEs exceeding 18%. This approach may be pivotal in achieving OSCs with PCEs of 20% or higher. Moreover, while researchers continue to experiment with different materials, much of this work remains in the proof-of-concept stage. The accumulation of experimental data could soon benefit from integrating artificial intelligence, which would aid in simulating and optimizing the combinations of various materials, potentially accelerating the development of high-performing OSCs.

As the production of composite-based OSCs scales to industrial levels, researchers face critical challenges related to consistency, quality control, and cost management. Addressing these issues may necessitate the establishment of industry standards in the future. Additionally, environmental concerns, chemical safety, health implications, and economic viability are increasingly important. Consequently, the use of biologically derived natural materials as donor or acceptor components in OSCs may become a focal point of future research due to their potentially lower environmental impact. By optimizing the composition of OSCs and harnessing the synergistic effects of composites, where the combined impact is greater than the sum of individual parts ( $1+1>2$ ), and focusing on the interfacial effects introduced by composites, there is optimism that significant advancements in PCE and stability can be achieved soon. With these improvements, OSCs are expected to become an integral part of everyday life, offering a sustainable and efficient alternative for energy generation across various applications.

## 6. Conclusion

This paper begins with an introduction to the basic principles and structure of OSCs. Subsequently, the composites that constitute the active layer materials of OSCs are classified to discuss their transformative impact on the field of plastic solar cells, mainly outlining the advances in efficiency and stability. Finally, the diverse applications of OSCs and their future perspectives are presented. In conclusion, the ongoing development of OSCs, particularly through innovative composite strategies, has markedly improved the performance and operational stability of OSCs. The enhancements stem from the unique properties of composites that optimize charge transport and exploit the synergistic effects of different materials to overcome the inherent limitations of traditional solar cell components. Despite these technological strides, OSCs still face challenges, including the need for further enhancement in PCE and the overall stability of the cells under varying environmental conditions. Moreover, the integration of nanocomposites, while beneficial, introduces complexity in manufacturing processes that need to be addressed to scale production economically and sustainably. Future research in OSCs should focus on refining the composition through novel material advancements of composites and interface engineering to balance efficiency with stability better.

In summary, the application of composite materials plays a practical and positive role in promoting the stability and PCE of OSCs. We believe that with more and more in-depth research on the principles of OSC performance enhancement and continuous innovation of the composite method of materials, the industrialized and diversified applications of OSCs will eventually be realized soon.

## References

- [1] Gillett A J, Privitera A, Dilmurat R, et al. The role of charge recombination to triplet excitons in organic solar cells. *Nature*, 2021, 597(7878): 666-671.
- [2] Tang Y, Li J, Du P, et al. Fullerene's ring: A new strategy to improve the performance of fullerene organic solar cells. *Organic Electronics*, 2020, 83: 105747.
- [3] Barulina E, Khodr A, Dkhil S B, et al. Improved ultraviolet stability of fullerene-based organic solar cells through light-induced enlargement and crystallization of fullerene domains. *Thin Solid Films*, 2022, 757: 139394.
- [4] Tao Y, Liu H, Wang D, et al. Healing the degradable organic-inorganic heterointerface for highly efficient and stable organic solar cells. *InfoMat*, 2022, 4(2): e12276.
- [5] Xu Y, Yuan J, Zhou S, et al. Ambient Processable and Stable All-Polymer Organic Solar Cells. *Advanced Functional Materials*, 2019, 29(8): 1806747.
- [6] Ma Q, Jia Z, Meng L, et al. 17.87% Efficiency All-Polymer Tandem Solar Cell Enabled by Complementary Absorbing Polymer Acceptors. *Advanced Functional Materials*, 2023, 33(6): 2210733.
- [7] Bin H, Wang J, Li J, et al. Efficient Electron Transport Layer Free Small-Molecule Organic Solar Cells with Superior Device Stability. *Advanced Materials*, 2021, 33(14): 2008429.
- [8] Fu J, Fong P W K, Liu H, et al. 19.31% binary organic solar cell and low non-radiative recombination enabled by non-monotonic intermediate state transition. *Nature Communications*, 2023, 14(1): 1760.
- [9] Wang Y, Wang Y, Zhu L, et al. A novel wide-bandgap small molecule donor for high efficiency all-small-molecule organic solar cells with small non-radiative energy losses. *Energy & Environmental Science*, 2020, 13(5): 1309-1317.
- [10] Xie F, Fang J, Zhang L, et al. Correlating the Photovoltaic Performance and Stability of the All-Small-Molecule Organic Solar Cells to Their Intermixed Phases Determined by Concentration-Dependent Ultraviolet-Visible Absorption Spectroscopy. *ACS Applied Materials & Interfaces*, 2024.
- [11] Guo J, Bin H, Wang W, et al. All-small molecule solar cells based on donor molecule optimization with highly enhanced efficiency and stability. *Journal of Materials Chemistry A*, 2018, 6(32): 15675-15683.
- [12] Guo J, Qiu B, Xia X, et al. Miscibility Regulation and Thermal Annealing Induced Hierarchical Morphology Enables High-Efficiency All-Small-Molecule Organic Solar Cells Over 17%. *Advanced Energy Materials*, 2023, 13(25): 2300481.
- [13] Zhang T, Xu Y, Yao H, et al. suppressing the energetic disorder of all-polymer solar cells enables over 18% efficiency. *Energy & Environmental Science*, 2023, 16(4): 1581-1589.
- [14] Gao Y, Yang X, Sun R, et al. All-small-molecule organic solar cells with 18.1% efficiency and enhanced stability enabled by improving light harvesting and nanoscale microstructure. *Joule*, 2023, 7(12): 2845-2858.
- [15] Zhou K, Xian K, Ma R, et al. Correlating miscibility, mechanical parameters, and stability of ternary polymer blends for high-performance solar cells. *Energy & Environmental Science*, 2023, 16(11): 5052-5064.
- [16] Cardinaletti I, Vangerven T, Nagels S, et al. Organic and perovskite solar cells for space applications. *Solar Energy Materials and Solar Cells*, 2018, 182: 121-127.