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# Enhancement of organic solar cell performance through architectural innovations and incorporation of nanomaterials: A review

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## Abstract

*The global rise in energy demand driven by population growth has spurred scientists to explore novel, cost-effective, and sustainable renewable energy alternatives to replace fossil fuels. Among the most promising photovoltaic technologies addressing the energy crisis are organic solar cells (OSCs). These cells boast remarkable features, including flexibility, partial transparency, eco-friendliness, solution-based processing, and low manufacturing costs. Despite rapid advancements in OSC technology, challenges such as low power conversion efficiency, poor durability, and degradation have hindered large-scale production and implementation. Numerous effective strategies have been developed to enhance light absorption, charge transfer, and exciton recombination in OSCs. This review article discusses the core concept of OSCs, offering a comprehensive examination of their architecture, fundamental operating mechanisms, and classification. Additionally, it addresses common defects observed in OSCs. The study further elucidates how interfacial engineering, innovative materials, and plasmonic nanomaterials can be utilized to improve light absorption, charge transfer, and exciton recombination, thereby boosting the efficiency and stability of OSCs.*

## Nomenclature and units

## 1.0 Introduction

The global population surge around the world has led to increased energy consumption, prompting researchers to explore new renewable, sustainable, and cost-effective alternatives to fossil fuels. The development of solar energy technology is essential in the energy industry, as it can reduce dependence on fossil fuels, whose extraction and emissions are harmful to both humans and the environment. Solar energy is abundant and can be harnessed using various technologies, such as solar evaporation, photovoltaic (PV) cells, photoelectrochemical and photocatalytic splitting of water, and solar heating (Zhao, et al., 2020). Over the years, photovoltaic solar cells have undergone substantial advancements and have played a crucial role in addressing modern energy and environmental challenges. These cells are made from semiconductor materials that capture sunlight and release electrons, which are then used to produce electricity. The major hinderances restricting the generation of power using the photovoltaic technology are the high cost of materials and low power conversion efficiency (PCE). New technologies aimed at reducing the cost of PV cells, improving stability, enhancing PV cells performance, and efficacy in terms of commercial production have emerged over the years. Some of the PV technology developed for electricity generation are the silicon, copper-indium-gallium-selenide (CIGS), perovskite, tandem and organic solar cells. The silicon (Si) solar cells are most efficient, and their durability is over 25 years, but they are more expensive, possess poor recycling facilities and their PCE decreases as temperature increases (Bhattacharya, & John, 2019). The CIGS are thin film that are flexible and their PCE recorded in the laboratory have been shown to be above 20%. The perovskite SCs are cheaper to produce, flexible and have the highest laboratory efficiency up to 34.6 %, but they are less durable, contain some quantity of lead and have shorter life span (2 – 3 years) compared to silicon (Wang, et al., 2025). The tandem SCs are complex to manufacture and assemble, require specific current and voltage for optimal performance of about 34.8% in the laboratory. The OSCS are lightweight, flexible and can be printed on a variety of surfaces, but their PCE is low when compared to other PV cells (Oni et al.,2024). Figure 1 shows the PCE of silicon, copper-indium-gallium-selenide (CIGS), perovskite, tandem and organic solar cells at laboratory scale.

Organic solar cells (OSCs) offer a cost-effective option for harnessing solar energy, owing to their recent advancements in efficiency, and the ease of their solution-based manufacturing process (Kalowekamo, et al., 2009). Silicon semiconductors, which are employed in the majority of first- and second-generation solar cells, have excellent absorption in the blue spectrum but lose absorbance in the red and near-infrared regions (NIR) due to their low absorption coefficients (Baytemir, et al., 2019) but OSCs are highly proficient in absorbing solar radiation in the infrared spectrum because of the presence of electronic components associated with low-modulus organic materials and

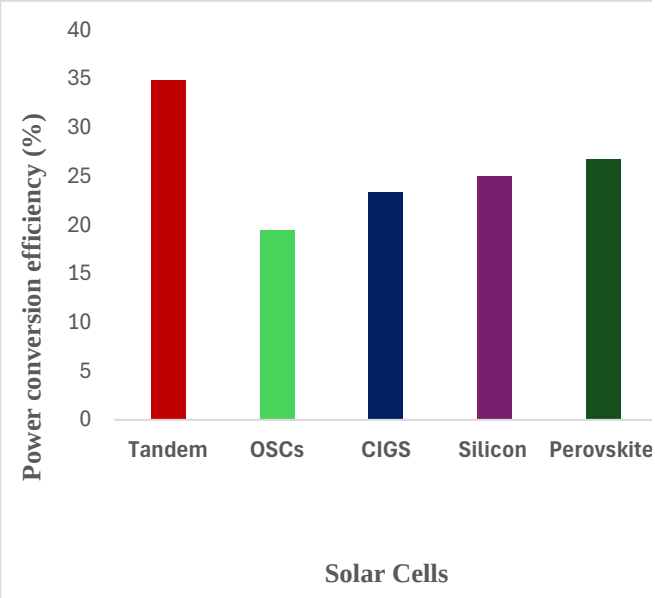



**Figure 1** Power conversion efficiency (PCE) of photovoltaic cells

conductive organic polymers, which facilitate charge transmission and light absorption. OSCs are made from sustainable natural materials that are inexpensive, nontoxic, recyclable, and easier to dispose of. Their lower production cost, lightweight, semi-transparency, and flexible characteristics facilitate their easy integration into Internet of Things (IoT) platforms and architectural designs (Liu, et al., 2020; Uddin, 2022; Cheng, & Zhan, 2016).

The OSCs global market is still emerging but has shown steady growth over the past years. The market is valued at USD 92.7 million in 2024 and projected to reach over USD 216.3 million by 2034 (GIS, 2025). Organic solar cells (OSCs) are currently not in direct competition with other types of solar cells, such as silicon, perovskite, and tandem cells, due to their relatively low efficiency and shorter operational lifespan. However, OSCs are predominant in applications such as building-integrated photovoltaics (BIPV), indoor energy harvesting for Internet of Things (IoT) sensors, and portable electronics, where the essential requirements for photovoltaic cells include flexibility, lightweight, and transparency. One of the driving forces behind the global market trend of OSCs, which present an alternative to traditional silicon-based solar cells, is the emphasis on using green materials that are less harmful to the environment. Despite significant advancements in OSC technology, these devices continue to face challenges in terms of their low power conversion efficiency (PCE) and limited longevity which stem from the short exciton diffusion length and poor charge mobility within the active layer of OSCs (Cheng, & Zhan, 2016). Nonetheless, additional

obstacles related to their stability, and scalability continue to impede their path to commercialization.

Recent technological progress in OSCs has focused on improving light absorption, reducing optical losses, preventing exciton recombination, facilitating charge transfer, enhancing stability, and boosting power conversion efficiency. To enhance the performance of OSCs, some of the latest strategies used include modifying the interface layers and incorporating additives such as powdered metals or nanoparticles (NPs) into the active and interface layers (Liu, et al., 2022). Localized surface plasmon resonance (LSPR) and anti-reflection effects of metallic NPs significantly enhance light absorption (Maake et al., 2020). In a two-phase active layer system, despite the limited range of interface materials suitable for solution processing over the active layer, the morphology that emerges from the crystallization and phase separation of materials is as important to the performance of the organic solar cell (OSC) device as the electrical configuration of the conjugated active materials (Wang, 2020). Consequently, their widespread commercialization requires enhanced research and development across various aspects, including device physics, optimization of device designs, stability, large-scale manufacturing, and the integration of novel concepts and technologies (Sampaio, & González, 2022). This review examines research conducted on optimizing materials, device structures, and processing parameters to improve the performance of OSCs, while discussing the fundamental concept of OSCs with the aim of providing a comprehensive overview of their architecture, basic operating principles, and common defects observed in OSCSs and how they influence the stability and performance of OSCs. Finally, we surveyed and analyzed strategies to increase performance and stability, such as interfacial engineering (modification of the interfacial and active layers) through doping, double HTL systems, and the use of novel materials.

## 2.0 Materials Architecture, Fundamental Working Principles, and Performance Characteristics of OSCS

### 2.1 Architecture of OSCs

Organic solar cells (OSCs) are third-generation photovoltaic cells that transform light energy into electrical energy using the photovoltaic effect. The structure of OSCs differs from that of inorganic photovoltaic cells in terms of the structure and efficiency. Organic solar cells are fabricated on plastic foils using organic polymers as a replacement for the silicon used in inorganic solar cells. As shown in Figure 2, an OSC typically consists of cathode and anode electrodes, an active layer that includes donor and acceptor materials, an electron transport layer (ETL), and a hole transport layer (HTL). A semi-transparent oxide layer, the anode is produced using indium tin oxide (ITO), which acts as the positive electrode to permit light transmission and hole collection from the device. HTL is a conductive polymer that is directly below the anode surface, and it transfers holes to the anode. It is composed of poly (34-ethylenedioxy-thiophene)-poly(styrenesulfonate) (PEDOT:PSS). They prevent electrons from entering the anode and prevent the anode material from diffusing into the photoactive layer (Arbouch, et al., 2014). The ETL transports electrons to the cathode, which is usually made of metal. The cathode and anode are responsible for collecting the charge carriers and passing the generated current to an external electrical circuit.

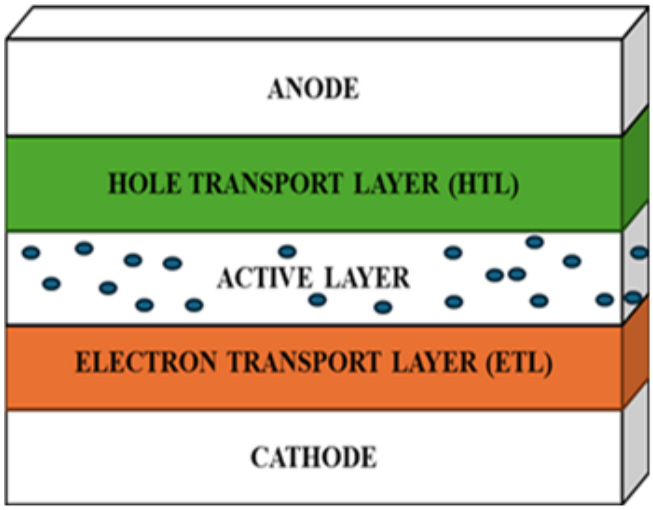



**Figure 2** Typical structure of organic solar cell

Organic semiconductor materials serve as an active layer in OSCs. To function as semiconductors in these devices, the organic materials must be capable of charge conduction through a molecular network or within highly conjugated molecules, characterized by alternating single and double bonds, and they must also be able to absorb light effectively. Figure 3 shows examples of conjugated materials used as active layers in OSCs. The active layer is placed between two electrodes (cathode and anode) and two transport layers (HTL and ETL) that permit electron or hole conduction using conjugated polymers as electron donors and fullerene derivatives as electron acceptors. The active layer is composed of tiny molecules, organic polymers, and their composites, which have recently shown the greatest increase in PCE compared to other solar systems at a lower cost (Benanti, & Venkataraman, 2006). OSCs' molecules are inexpensive and solution-processable at a high throughput, which lowers the cost of fabrication. The sections below discuss the different innovations of OSCs over the years with the aim of improving the performance and stability.

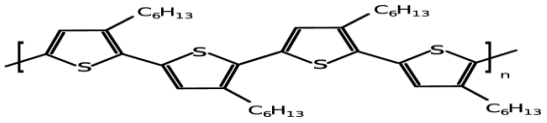
#### 2.1.1 Single layer

The earliest OSCs were single-layer devices that consisted of a thermally evaporated organic semiconductor photoactive material

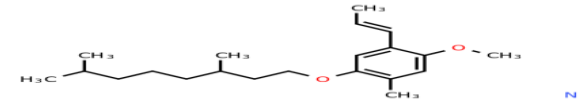
placed between two electrodes with differing work functions, as depicted in Figure 4. Conductive transparent oxides (CTO) and metal cathodes are typically used as single-layer organic semiconductors. Single-layer OSC have the most simplified architecture and low cost of production; however, their PCE is low, and the charge carrier mobility and diffusion length are limited. Owing to the increased energy required for exciton dissociation and the lack of a distinct hole-transporting layer, single-layer OSCs exhibit large recombination losses (Spanggaard, & Krebs, 2004; Bagher, 2014). They are commonly used in low-power devices, flexible electronics, and building-integrated photovoltaics.

### 2.1.2 Multiple layer (heterojunction) OSCs

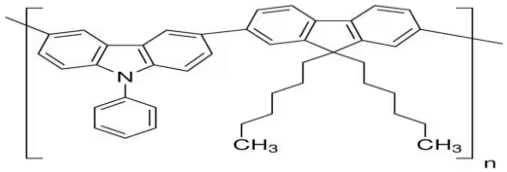
In multi-layer organic solar cells (OSCs), a donor and an acceptor are combined within a single cell. Electron acceptors are characterized by their high electron affinity and ability to easily



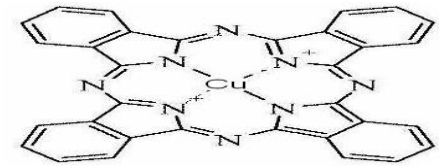
Poly-3-hexyl thiophene (P3HT)



Poly[2-methoxy-5-3(30,70-dimethyloctyloxy)-1-4-phenylene vinylene] (MDMO-PPV);



Poly[N-90-hepta-decanyl- 2,7-carbazole-alt-5,5-(40,70-di-2-thienyl-20,10,30-benzothiadiazole)] (PCDTBT);



Copper phthalocyanine (CuPc); (f) phenyl-C61-buytric acid methyl ester (PCBM)

**Figure 3** Selected organic photovoltaic materials.

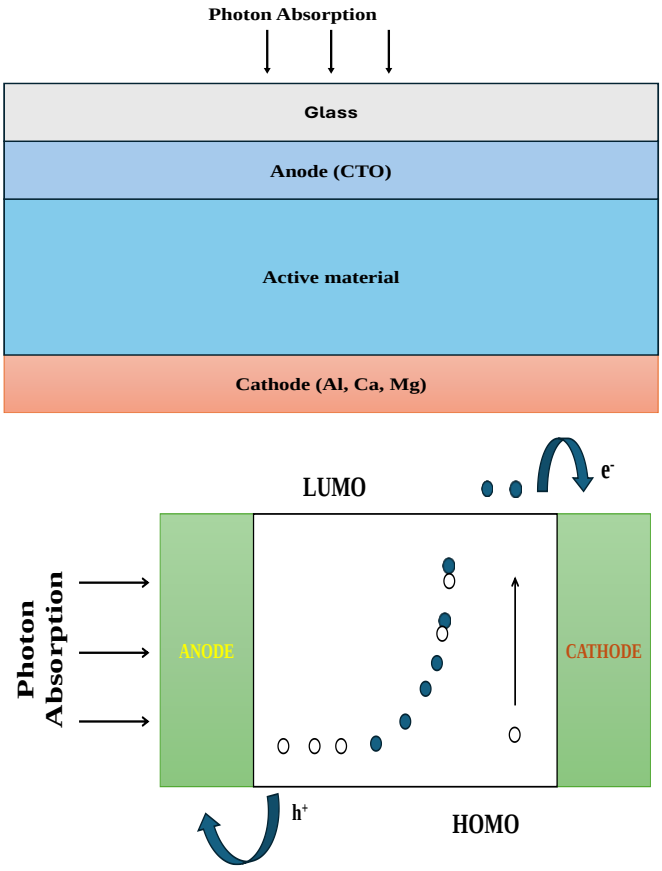



**Figure 4** Architecture of single OSCs and its energy diagram

accept electrons, while electron donors have a low ionization potential and readily donate electrons (Wöhrle, et al., 1991). These cells are engineered to enhance charge transfer and minimize recombination, thereby potentially boosting the power conversion efficiency (PCE). Solution-based coating methods at lower temperatures were employed to create multiple-heterojunction OSCs. Heterojunction cells are divided into bilayer, bulk, and tandem heterojunction OSCs.

### *A. Bilayer heterojunction OSCs*

Two separate organic layers sandwiched between conducting electrodes have been developed to address the challenges identified in single-layer OSCs. The bilayer heterojunction of donor-acceptor materials resembles the p-n junctions in inorganic solar cells. Bilayer architectures with non-fullerene acceptors (NFAs) can achieve competitive PCEs owing to their reduced voltage losses and suppressed recombination (Lee, et al., 2020). Acceptors demonstrated superior ionization potential and electron affinity compared to donors. When the donor layer absorbs incident photons, electrons transition from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO), producing excitons (Zhang, et al., 2022), as shown in Figure 5. Although bilayer heterojunction devices outperform single-layer devices, their maximum efficiency is limited because most excitons cannot reach the donor/acceptor junction (Hong, & Ge, 2021). The short diffusion length and limited mobility of excitons contribute to the poor PCE of the planar heterojunction OSCs. Aligning the diffusion length with

the bilayer heterojunction dimensions to maximize the PCE produces ultrathin films with low optical absorption. The pseudo-bilayer approach has shown enhanced exciton diffusion lengths and improved crystallinity, leading to higher PCEs (Jiang, et al., 2021). Although bilayer designs may have reduced donor–acceptor interfaces, they provide better transport pathways for charge collection. NFAs' unique properties make bilayer heterojunctions a viable alternative to bulk heterojunctions, potentially opening new avenues for efficient OSC development (Lee, et al., 2020).

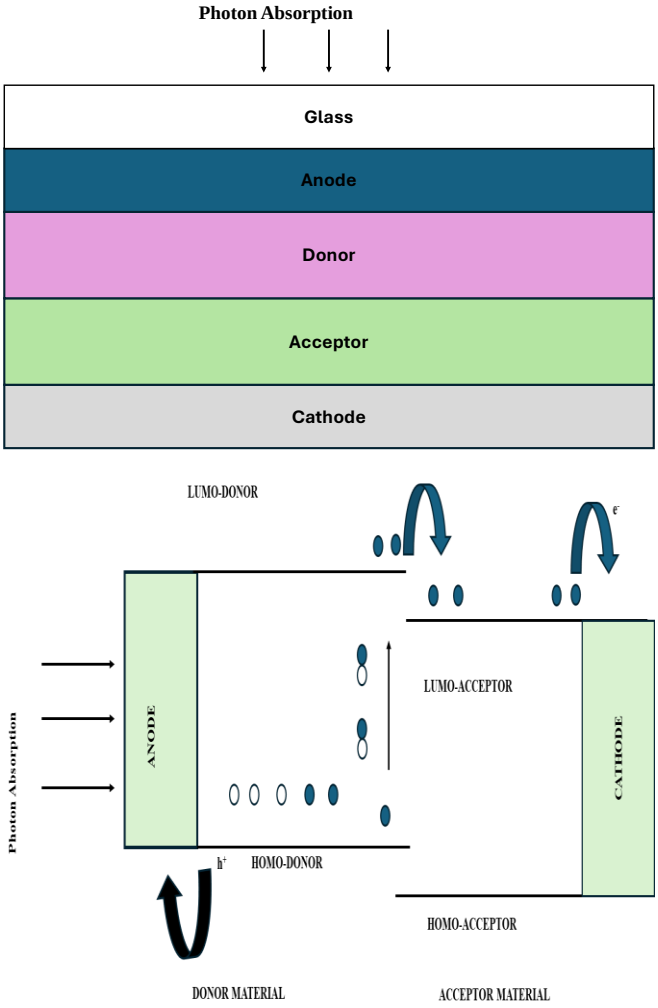



**Figure 5** Bilayer heterojunction OSCs and its energy diagram

### *B. Bulk heterojunction (BHJ)*

The active layer of a BHJ OSC comprises the donor and acceptor, which are made up of two different organic semiconductor materials combined, as shown in Figure 6 (Duan, & Uddin, 2020). To create this combination, electron acceptors and donor polymers were blended and placed between electrodes. Bulk heterojunctions (BHJ) use nanocomposites of π-conjugated organic semiconductors to create a large interfacial area for charge separation (Kang, et al., 2016). Compared to bilayer heterojunctions, bulk heterojunctions achieve a higher PCE by facilitating exciton migration to the interface and generating free electron and hole pairs upon dissociation. P3HT: PCBM is the most utilized donor and acceptor material combination for bulk heterojunctions (Ameri, et al., 2009; Abdulrazzaq, et al., 2013). The performance of bulk heterojunction OSCs has significantly increased with the development of inverted BHJ devices. Inverted devices exhibit superior environmental stability and function, like solar cells with standard construction (Abdulrazzaq, et al., 2017). The efficiency of charge transmission in bulk heterojunction organic solar cells (BHJ OSCs) with fullerene derivatives is hindered by the complex donor and acceptor networks. However, the limited exciton diffusion length of the BHJ active layer requires maintenance of an intricate donor/acceptor (D/A) network, altering the charge transport characteristics. To address the inefficient charge transfer and enhance the PCE of OSCs, researchers have developed advanced technologies. These innovations, including non-fullerene acceptors (NFAs) and novel donor materials in fullerene-free OSCs, have resulted in PCE values exceeding 17%, as reported by the National Renewable Energy Laboratory (NREL).

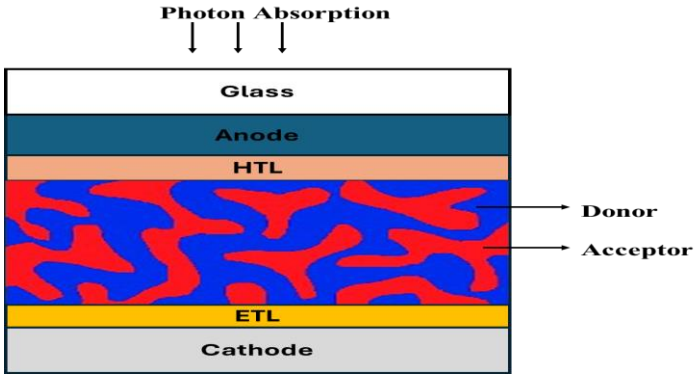



**Figure 6** Bulk heterojunction

### *C. Tandem heterojunction OSCs*

Light absorption in single-layer, bilayer, and bulk heterojunctions is confined to either the short or long wavelengths of the visible light spectrum. However, tandem solar cell configurations are utilized to capture a broader range of the spectrum (Soonmin, et al., 2023). The tandem heterojunction architecture can increase optical absorption, improve efficiency, and reduce thermalization losses (Ameri, et al., 2019; Yang, et al., 2022). The tandem heterojunction OSC utilizes two subcells with complementary absorption spectra and different bandgaps to capture a wider range of wavelengths, as shown in Figure 7. An interlayer separates the subcells to align the quasi-Fermi levels. A blend structure in which donor and acceptor materials lack a planar interface has been used to create tandem OSC devices with the highest PCEs (Choi, et al., 2024). Tandem heterojunction OSCs are classified

as inorganic-inorganic, organic-organic and hybrid. The inorganic–inorganic tandem cells combine two inorganic materials. Fara et al. (2023) investigated metal oxide heterojunction tandem solar cells using ZnO (bandgap of 3.3 eV) and $Cu_2O$ (bandgap of 2.07 eV). The device architecture consists of a ZnO/$Cu_2O$ top subcell and a c-Si bottom subcell in a four-terminal tandem configuration, which increases the PCE and current density. $Cu_2O$ and ZnO's characteristics make it viable for high-efficiency solar systems. Organic-organic tandem cells combine two organic materials such as polymers. The power efficiency of tandem OLEDs increased significantly when OHJs were used as the CGLs (Chen, & Ma, 2012). Hybrid tandem cells combine inorganic and organic components. Farooq et al. (2020) revealed that the hybrid tandem structure is more efficient and stable at high temperatures, making it suitable for practical applications. Common materials include conjugated polymers (P3HT and PTB7), small molecules (C60 and PTCDI), and

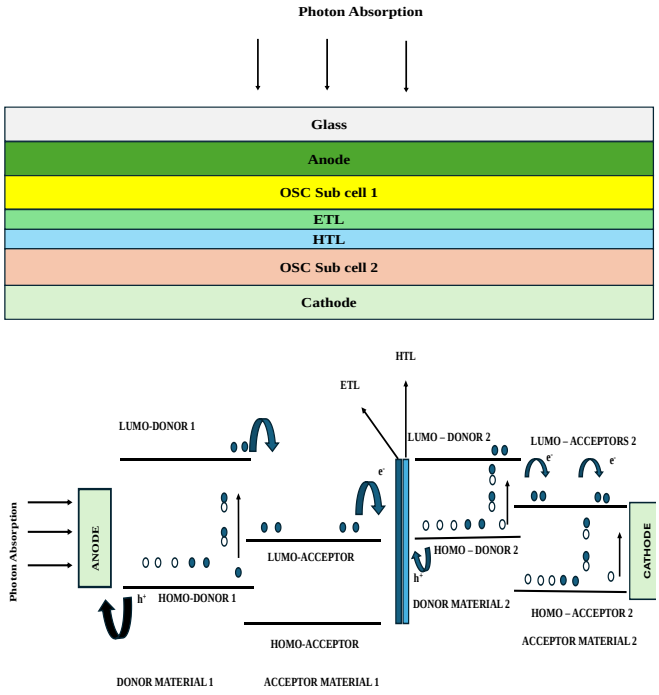



**Figure 7** Tandem heterojunction OSCs and its energy

inorganic materials such as Si, InP, and GaAs. Despite these advantages, Tandem OSCs require complex fabrication processes, additional material processing steps that increase production costs, and current matching of sub-cells to avoid losses.

## 2.2 Operating principles

Organic solar cells absorb photons and form excitons, unlike inorganic photovoltaic systems, which generate free charge carriers (Takahira, et al., 2017; Ratier, 2012). When OSCs absorb light with sufficient energy to excite electrons from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO), an excitonic bond forms between electrons and holes. To produce an electric current, excitons migrate across the active layer to the HTL or ETL interface, where they dissociate into holes and electrons, respectively. Energy is wasted when the absorbed light energy exceeds the bandgap energy. The electrons decay and ascend to a higher energy level than that of the LUMO. Excitons diffuse through the OSC component to the donor-acceptor interface, where dissociation is driven by the offset between LUMO levels. This must occur within a given timeframe; otherwise, the excited electrons undergo recombination. Exciton lifetime is typically defined as the distance that the exciton may diffuse by approximately 10 nm (Ossila, 2024). At the interface, the hole remains in the donor, while the electron travels to the acceptor material, causing exciton dissociation. These charge carriers create charge transfer conditions owing to their continued attraction. As the distance increased, attraction decreased. A charge-separated state was formed when the thermal energy exceeded the binding energy between them. Recombination may occur at the interface even in the charge-transfer state. During charge carrier transportation,

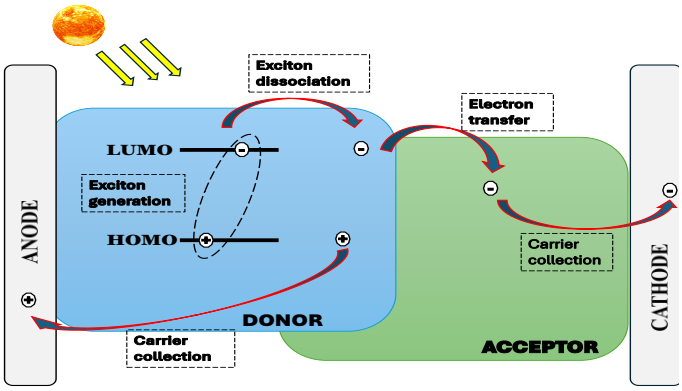



**Figure 8** Working principle of acceptor-donor organic solar cells

carriers diffuse to the appropriate electrode through the interfacial layers. Charge carriers can generate current if they exit the cell before recombination. In summary, electricity is produced in OSCs when light energy meets or exceeds the band gap, resulting in electron excitation from the HOMO to the LUMO. Figure 8 illustrates the working principle of OSCs.

## 2.3 Performance parameters

The OSC performance is assessed using the following parameters: power conversion efficiency (PCE), external quantum efficiency (EQE), short-circuit current density (Jsc), fill factor (FF), and open-circuit voltage ($V_{oc}$).

The fill factor (FF) is used to show the loss resulting from resistance over time. FF is given in Equation (1) as the cell's maximum output power (PM) divided by the product of Jsc and $V_{oc}$ **(**Sun, et al., 2023).

$$FF = \frac{P_M}{V_{oc} \times J_{sc}} = \frac{J_M \times V_M}{V_{oc} \times J_{SC}} \quad (1)$$

where Jsc is the short-circuit current density, which is the operating current of the OSCs under short-circuit conditions (zero output voltage), and $V_{oc}$ is the open-circuit voltage, which is the output voltage of the solar cell under open-circuit conditions (zero output current).

The maximum number of electrons that a photocurrent can extract when a photon is supplied is known as external quantum efficiency (EQE). This is determined using Equation 2, which gives the ratio of the number of electrons ($N_{electron}$) extracted to the number of photons ($N_{photons}$) injected.

$$EQE = \frac{N_{electron}}{N_{photon}} \times 100\% \quad (2)$$

Equation 3 gives the PCE, which is the ratio of the maximum output power (PM) of the OSCs to the incident light energy ($P_{in}$) per unit area. An OSC can generate more energy with a higher PCE under the same lighting conditions, resulting in higher cost performance and energy efficiency ratio (Granströ, et al., 1998).

$$PCE = \frac{P_M}{P_{in}} = \frac{J_{sc} \times V_{oc} \times FF}{P_{in}} \quad (3)$$

Molecular electronic forces (intra- and intermolecular interactions) within the active layers are important factors governing the performance of OSCs. However, these forces are both intricate and poorly understood. Excellent thermal and light stability must be established to commercialize the OSCs technology and ensure long-term functioning in both indoor and outdoor settings.

## 3.0 Defects and their Influence on the Stability and Performance of OSCs Semiconductors and Device

Despite the potential advantages and research interest in OSCs, their large-scale applicability remains limited owing to defects that cause charge trapping and recombination. These defects can lead to performance instability and device degradation. Defect creation can result from impurities, conformational changes, molecular defects from subpar synthesis, and atmospheric effects, which are sometimes accelerated by visible or UV radiation (Iqbal, et al., 2021; Huser, et al., 2000; Streiter, et al., 2019). Investigating defects, their causes, effect, and disordered states in OSCs is essential for understanding device deterioration and developing strategies to improve performance (Sutter-Fella, et al., 2017).

### 3.1 Weak Intermolecular Interactions

#### 3.1.1 Causes of weak intermolecular interactions in OSCs

Intermolecular interactions, which include those occurring between both identical and distinct molecules, are commonly observed in OSCs and a thorough understanding and control of these subtle forces are crucial for the progress of OSC technology. In organic solar cells (OSCs), the interactions between molecules are relatively weak and are held together by weak, non-covalent forces while the inorganic materials such as silicon are held by strong covalent or ionic bonds (Li, et al., 2024). The relatively weak intermolecular forces in OSCs are due to the weak van der Waals forces that bind the molecules of organic materials together. When an OSC is applied as a thin film, the arrangement and organization of the molecules on the substrate are primarily influenced by van der Waals forces between them (Xu, et al., 2021). These forces are crucial in improving operational stability, miscibility, efficiency, the physical characteristics of materials, and their morphology. In the research conducted by Kim et al. (2023), two economical isomeric non-fused acceptors, TT-Naph2 and TT-Naph1, were created using 2-napthyl and 1-napthyl aromatic chains, respectively. The goal was to develop high-performing, cost-effective non-fused acceptors to improve molecular interactions and control miscibility in OSCs. The findings indicated that managing the intra- and inter-molecular interactions of acceptors can adjust their miscibility with donors, which is essential for determining OSC performance. This insight offers valuable guidance for the development of new low-cost non-fused acceptors. Zhao et al. (2024) conduct a comprehensive analysis of the stability of van der Waals heterostructures made from g-C3N4 and III-V materials, examining their electronic band structures and potential use in solar cells. The built-in electronic field, which results in a potential drop, significantly enhances the separation of photogenerated electrons and holes, while GaAs-D exhibits superior light absorption in the visible spectrum. Zhang et al. (2020) emphasized the importance of controlling molecular orientation and crystalline organic thin films for high-performance in OSC fabrication. The molecular structure of OSCs is mainly composed of large, flat molecules, which results in weak π–π stacking interactions and limited overlap of molecular orbitals.

The use of solvents during the fabrication of OSCs can disrupt these intermolecular interactions, thereby reducing the material's effectiveness. Zhang et al. (2024) illustrate that large-area OSCs exhibit high performance when processed using various solvents. The findings from this research indicate that the state of the solution significantly influences the morphology, and consequently, the performance of OSCs. Additionally, intermolecular interactions and the device's overall performance. are also affected by the morphology of OSC films, which is shaped by processing conditions and lack of strong electrostatic force in OSCs. Materials with small difference in surface electrostatic potential between the donor and acceptor

components exhibit weaker electrostatic interactions (Kim, Oh, et al., 2023).

### 3.1.2 Effect of weak intermolecular interactions on OSCs

The weak intermolecular interactions in OSCs generally have negative effect on the performance, resulting in limited charge transportation, increased charge recombination, poor molecular packing, phase separation, and crystallization in OSCs, leading to variations physicochemical and electrochemical characteristics (Wang, 2020; Mohammed et al., 2019). Weak intermolecular interaction makes the morphology of the OSCs' film to be highly sensitive to processing conditions such as solvent type and annealing temperature. This often results in non-uniform or suboptimal heterojunction structure and disordered domains (Ismaeel, et al., 2025). The weak intermolecular forces usually show lower glass transition temperature and are more prone to fluctuations in temperature or environmental degradation, impacting their long term operational stability (Jin, et al., 2019).

Due to weak interaction and low dielectric constant, absorbed photons create strong bound excitons. These excitons require additional driving force to separate into free charge carriers, a process that is less efficient in disordered materials resulting from weak interactions. The weak intermolecular interactions lower charge carrier mobility and create limited charge transport length, thereby increasing the possibility of holes and electrons recombining before they can be extracted as current. Ma et al., (2025), enhanced the charge transfer and exciton dissociation by tailoring two additives of 2,5-dibromo-3,4-ethylenedioxythiophene (DBEDOT) and 3,4-ethylenedioxythiophene (EDOT) into the structure of the donor and acceptors of OSCs. The stronger intermolecular interaction between DBEDOT and the non-fullerene acceptor BTP-eC9-4F leads to pre-aggregation and an extended crystallization period for BTP-eC9-4F. This process aids in creating films with tightly packed molecules and effective phase separation, thereby improving the PCE.

The weak intra-and intermolecular interactions of the active layer materials also influence their miscibility, controlling morphology formation, and domain purity (Ye, et al., 2018; Liang, et al., 2020; Zhang, et al., 2020). Unlike the crystalline inorganic semiconductors, most OSCs film possess significant morphology disorder and amorphous structure, causing poor molecular ordering, low material crystallinity and the formation of morphological defects and structural disorder in the active layer (Sawatzki-Park, et al., 2023). This causes non-ideal phase separation between the acceptor and donor materials and weakens the cumulative effect of intermolecular forces, resulting in less efficient transport pathways.

Han et al. (2022) studied the importance of multimodal intermolecular interactions in the photovoltaic performance of OSCs in addressing the effect of weak intermolecular force. The relationship between multidimensional intermolecular interactions and photovoltaic conversion in the active layer including the material itself, D/A interactions, and host/guest interactions in ternary matrices of OSCs was studied. The result showed that the OSC efficiency could be increased to over 19% by controlling multidimensional intermolecular interactions through end-cap engineering and side isomerization. The two main types of intermolecular interactions in these crystals are van der Waals contacts between the phenyl group and the endcap of neighboring molecules and dominant π–π stacking. Other methods have been proposed to improve intermolecular interactions, including the use of solid additives to enhance the interaction between polymer acceptors and donors. This aids in the formation of an optimal bulk heterojunction (BHJ) morphology and adds a fibrillar morphology for charge transport and exciton dissociation. Adding solid additives to the BHJ layer improves intermolecular π–π stacking among the non-fullerene electron acceptors. This enhances the PCE, device stability, and charge transfer within the BHJ (Liang, et al., 2022; Song, et al., 2022). Mei et al. (2024) evaluated the intermolecular binding energy (Eb) for different stacking conformations to understand interactions between photovoltaic materials and solid additives. This study explored the interaction between photovoltaic materials and solid additives in BHJ layers. Three solid additives with varying ESP distributions and dipole moments were added to the PM6:BTP-eC9 system, and their impact on BHJ morphology and performance was examined. These findings show that while these additives had a minimal impact on the π–π distance or lamellar spacing of the BHJ layer, they enhanced the crystal coherence length (CCL) in the π–π stacking direction.

## 3.2 Poor Charge transport and energy level in OSCs

### 3.2.1 Causes of poor charge transport and energy level

Poor charge transport and energy level defects in OSCs are majorly caused by material properties, morphology of the active layer, device interface problems and environmental degradation. Charge transport in OSCs is influenced by the energy alignment between materials. Optimizing the energy-level alignment and charge transport has been the focus of recent research to enhance device performance. Organic semiconductors consist of small low crystalline molecules or polymer chains that aggregate into a complex high-disorder state, unlike the periodic structures of inorganic semiconductors. Discrete energy levels are preserved in organic semiconductors, whereas energy bands are formed in inorganic semiconductors (Lo Sciuto, et al., 2019). Efficient three-dimensional charge transport is hindered by a high level of structural disorder or amorphous regions in the active layer, whereas transport occurs more rapidly in the crystalline areas. Van der Waals forces hold molecules together in organic conductors, preventing the molecular orbitals from perfectly overlapping. Intrinsic instability and incompatibility of materials frequently result in the formation of large, suboptimal donor-

acceptor domains over time. This phenomenon increases the distance that charges must traverse to reach the electrodes, which in turn leads to elevated recombination rates and inefficient transport (Krishna et al., 2023).

Chemical changes are observed to occur in the donor and acceptor materials due to external factors such as water, oxygen, heat and light, tuning the HOMO and LUMO levels and directly affecting the photogeneration of charge carriers and recombination processes (Sherafatipour, et al., 2019). Hernández-García et al. (2025) investigated the degradation processes of OSCs when subjected to various environmental conditions, such as air exposure, encapsulation, and nitrogen preservation. The study's results showed that air exposure predominantly affects the anode interface, leading to a decrease in interfacial dipole energy and a shift in the Fermi-level alignment of PEDOT:PSS. This shift causes a gradual decline in the hole transport properties, which in turn significantly hampers the performance of the device. On the other hand, the cathodic interface remains stable, indicating that the degradation is mainly driven by alterations in the hole transport layer. It is essential that the energy levels of the acceptor and donor materials are properly aligned with each other and the electrode for efficient charge separation and extraction. Voltage loss can be minimized by a large energy offset at the D/A interface but can also lead to poor charge generation and collection if the optimization process is not properly done.

In organic semiconductors, electrons for conduction reside in the LUMO level, whereas holes are restricted to the HOMO level, ensuring charge carrier delocalization (Nelson, 2002). Introducing dopants and impurities like aluminum or indium into the active layer modifies the local energy levels, leading to the formation of trap states, altering transport properties, energy level alignment, and overall performance of the active layer (Wang, et al., 2023). Molecular design modifications affect charge carrier mobility and domain size (Zhan, et al., 2022). The use of annealing treatments and solvent additives during the fabrication of OSCs have the tendency to distort the molecular arrangement, thereby affecting the resulting energy level and the performance of the device. Proper energy-level alignment between layers is crucial for reducing energy loss and efficient charge transfer. Hole-transport layer materials such as HXMoO3 enhance device efficiency through better energy-level matching.

### 3.2.2 Effect of poor charge transport and energy level on performance of OSCs

The charge transport and energy level alignment both affect the performance of OSCs by influencing the charge generation, separation, transport and recombination processes and understanding the effect on these is essential for optimizing OSC efficiency (Zhan, et al., 2022). Charge transport is essential in the movement of photogenerated electrons and holes to their respective electrodes before the combination. The presence of low charge mobility leads to the accumulation of charge carrier, thereby increasing the possibility of charge recombination, which results in significant reduction in the short-circuit current density (Jsc) and fill factor (FF). It is anticipated that the mobilities of electrons and holes are balanced, as any disparity in their transport can result in space-charge effects, which may subsequently heighten recombination losses and diminish performance.

Regarding energy level alignment, the correct positioning of the energy levels, particularly the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) of the materials, determines the movement of charge carriers at the interface. To ensure that excitons can dissociate, there must be a sufficient energy difference between the donor's HOMO and the acceptor's LUMO, along with proper alignment at the electrode interface. This setup is crucial for the selective and efficient extraction of charges while preventing the flow of the opposite type of carrier. When the energy levels at the interfaces between the active layer and charge transport layers (CTLs) are well-aligned, energy barriers are minimized, surface recombination is reduced, and the device's performance and stability are enhanced. Lee et al. (2022) employed BTP-eC9 and PM6 to develop OSCs featuring a photoactive layer in conjunction with Ag nanowires. They replaced PEDOT:PSS with HXMoO3 as the HTL to improve the charge transport and energy-level regulation. The Ag nanowires enhanced conductivity while the HXMoO3 increased the open-circuit voltage and energy-level alignment, resulting in a PCE of 14.0%. Doping a poly(3-hexylthiophene) (P3HT): indene-C60 bisadduct (ICBA) active layer with F4-TCNQ enhances the charge carrier transfer of OSCs (Liu, et al., 2016). Evaluation of the charge carrier transport balance resulted in an optimal PCE of 5.83%. F4-TCNQ increased the charge carrier density, reduced electron/hole recombination, and improved the electron mobility. The donor polymer improved electron mobility by providing "bridges" or shortcuts, affecting OSC power conversion efficiency (Yin, et al., 2019).

These findings provide insights into the development of more stable and efficient OSCs through improved charge transportation and energy-level control.

## 3.3 Interfacial and active-layer defects in OSCs

### 3.3.1 Causes of interfacial and active layer defects in OSCs

Organic devices have lower efficiencies than inorganic semiconductors because of undesired internal defects that alter the material properties and degrade the solar cell efficiency. Defects in structures such as molecular vacancies and grain boundaries broaden the optical band edge and alter the energy-level alignment at organic/substrate interfaces, leading to device degradation (Yang, et al., 2017a; Yang, et al., 2017b). This type of defects in OSCs are caused by a combination of processing conditions, intrinsic material properties and environmental factors, which leads to reduction in stability and efficiency.

Interfacial defects occur at the boundary between that active layer and the charge transport layers (HTL and ETL) or electrodes. A physical mismatch between the crystal structures or surface energies of the adjacent layers can lead to defects and poor contact, impeding efficient charge transfer and causing energy losses (Njema et al., 2024). The use of incompatible materials such as some non-fullerene acceptors (NFAs) can lead to undesirable chemical reactions. This type of NFAs can react with certain interlayers such as PEI, thereby, changing their electronic structure and destroying the function of the interface layer.

The active layer defects occur within the active layer especially in the bulk heterojunction blend of donor and acceptor materials. They are primarily related to its nanoscale morphology and intrinsic materials stability. The desired nanoscale interpenetrating network (nanomorphology) of the active layer can be highly sensitive to processing conditions such as drying time, annealing temperature and solvent choices and can change over time due to thermal aging or light exposure. During fabrication, shiny spots, bubbles, gas, shrinkage porosity, cavities, and photooxidation can be detected on the active and metal layers at the interface introducing defects to the device.

Inhomogeneity or variations in the active layer thickness, particularly in large area device can lead to electrical losses, increased defect density and shunting paths. Boudia et al. (2024) enhanced the active layer blend in the TO/SnO2/PM6:D18:L8-BO/PEDOT:PSS/Ag structure of inverted ternary organic solar cells. They examined the device's efficiency parameters, such as EQE, Photo-CELIV, PCE, Jsc, Voc, and FF, by varying the active layer thickness from 50 to 200 nm. The active blend was fine-tuned to a thickness of 80 nm, achieving a PCE of 20% with a Jsc of 27.2 mA cm−2, a $V_{oc}$ of 0.89 V, and an FF of 82.3%. This optimized thickness decreased the distance charge carriers needed to travel to reach the charge transport layers. Using $SnO_2$ has been found to improve electron mobility, which is a vital factor in minimizing energy losses and boosting the Voc.

Researchers are studying the effect of environmentally induced mechanisms on OSCs performance degradation. The organic semiconductor molecules degrade when exposed to external factors such as heat, water, light and oxygen, leading to chemical decomposition and the formation of new defect states. Trace O3 can cause oxidation, leading to defects in organic semiconductor-based devices. Van Der Pol et al. (2023) studied charge photogeneration in OSC architecture using sensitive EQE measurements. They found that O3 interaction with the PM6:Y6 blend causes defects, and MoO3 work function changes affect band bending, leading to a higher defect density and response. O3 increases the defect signal around PM6's HOMO but doesn't affect Y6's DOS. Anjusree et al. (2020) developed traditional bulk-heterojunction (BHJ) ITO/PEDOT:PSS/P3HT:PC61BM/Al organic solar cells (OSCs) entirely under ambient conditions. They examined how aging time, light intensity, and the thickness of the hole transport layer (HTL) affected the performance parameters and degradation of the devices. Over time and with continuous exposure to light during testing in ambient air, the devices showed a noticeable decline in performance metrics. This observed deterioration was due to the infiltration of environmental oxygen and moisture into the photoactive layer through existing defects, which can be avoided by promptly applying encapsulation. Oxygen or water can trigger oxidation, altering material work function by increasing trap states and lowering mobility (Lo Sciuto, et al., 2019).

### 3.3.2 Effect of interfacial and active layer defects in OSCs

Defects at the interface and within the active layer of the OSCs play an important role in determining the performance of the device. Interfacial defects act as traps for charge carriers, which leads to increase recombination rates and reduce the extraction charge efficiency. Liu et al. (2024) studied the effect of interfacial defects on OSC device time stability by examining trap state density distribution during aging. The results show that aging OSCs have fewer nonradiative recombination losses and lower interfacial deep traps. Older devices with WS2 interlayers and HTL-free configurations have a higher deep trap density, increased carrier recombination, and decreased performance. Changes in ITO work function changes impact energy loss in aging cells. These findings show that interface engineering can enhance energy loss and device stability for long-term performance. Similarly, imperfection in the active layer such as molecular disorder and impurity can hinder exciton diffusion and limit the generation of free charges. Defects in the active layer introduce energy level within the bandgap, causing increased non-radiative recombination, and lowering the Voc and Fill factor (FF) of the device (Liu et al., 2024). Table 1 gives a summary of the defects found in OSCs, their location, cause and effect on the performance of OSCs.

## 4.0 Architectural Innovations in Organic Solar Cells to Enhance their Performance

Several technological developments have been explored to modify the OSC architecture and increase its PCE. A typical OSC structure consists of a photoactive layer sandwiched between two electrodes (anode and cathode) and their corresponding interlayers. The interfacial layer between the photoactive layer and the anode/cathode electrodes is crucial for effective charge extraction and transport (Fahlman, et al. 2019; Sorrentino, et al., 2021). An optimal film morphology in the photoactive layer is essential for balancing exciton dissociation and charge transport to achieve high performance. Anode engineering through PEDOT:PSS hole transport layer modification, novel donor-acceptor material combinations, and optimized arrangements have increased the OSC's performance (Farooq, et al., 2020; Ma et al., 2021). Cathode modification improves charge extraction

and reduces recombination through mixed electron-transport materials to boost the efficiency (Jiang, et al., 2021). These architectural modifications collectively optimize OSC performance and enhance potential commercialization.

## 4.1 Modification of the interfacial layers

**Table 1** Causes and effects of defects on the performance of OSCs.

| Defects | Location | Causes | Effects |
|---|---|---|---|
| **Weak Intermolecular Interactions** | Between individual molecules | • Limited molecular polarity<br>• Inappropriate Donor/Acceptor Miscibility<br>• Surface defects and roughness<br>• Non-optimal processing solvent | • Morphological instability<br>• Inefficient exciton management<br>• Increased charge recombination |
| **Poor charge transport and** | Interface between different materials and at the electrode | • Low intrinsic mobility<br>• Structural disorder and defects<br>• Suboptimal morphology<br>• Unbalanced transport<br>• Interfacial issues<br>• Environment degradation | • Charge carrier accumulation<br>• Increased recombination<br>• Reduced fill factor (FF) and current density<br>• Performance degradation with thickness unbalanced |
| **Poor energy level alignment** | Interface between different materials and at the electrode | • Energy level misalignment<br>• Molecular structure and packing<br>• Degradation-induced changes<br>• Interfacial dipoles and defects | • Inefficient Charge extraction<br>• Voltage loss (Voc)<br>• Interface Recombination<br>• Suboptimal charge transfer<br>• Interface dipoles |
| **Interfacial and** | Boundaries between the active layer and the charge transport layers | • Lattice Mismatch and Poor Contact<br>• Chemical Reactions<br>• Surface Roughness and Defects<br>• Energy Level Misalignment<br>• Material Diffusion: | • Increased Charge Recombination<br>• Energy Level Misalignment<br>• Charge Accumulation<br>• Reduced Stability<br>• Leakage Current Pathways |
| **Active-layer defects** | active layer | • Morphological Instability<br>• Incorrect Phase Separation<br>• Material Intrinsic Degradation<br>• Film Inhomogeneity/Thickness Issues<br>• Trap States | • Increased Recombination rate<br>• Decreased Carrier Mobility<br>• Photocurrent and Voc Loss<br>• Enhanced leakage current<br>• Morphological and interface degradation<br>• Reduced power conversion efficiency |

Three types of interlayer materials–conductive conjugated polymers, metal oxides, and non-conjugated polymers (Figure 9)–have been used to enhance the efficiency, stability, and commercialization of OSCs. The properties of these materials make them unique for application as interfacial layers.

### 4.1.1 Anode interfacial layer

Improving the anode hole transport layer (HTL) is crucial for boosting the performance of organic solar cells (OSCs). Poly(3,4-ethylenedioxythiophene): poly(styrene-sulfonate) (PEDOT:PSS) is the most widely used HTL material because of its outstanding transparency across visible to near-infrared (NIR) wavelengths, eco-friendliness, thermal stability, flexibility, and durability. Nonetheless, it encounters issues such as low conductivity and vulnerability to moisture and acid (Ma et al., 2021; Tsang, et al., 2024; Lv et al., 2024). To address these challenges, various methods have been explored to modify the anode interfacial layer, including doping strategies, double-HTL systems, and the development of new materials.

**A. Modification using the doping strategy**

The performance of PEDOT:PSS anodes can be improved by incorporating tungsten oxide (WOx), vanadium oxide (Vox), and molybdenum trioxide (MoO3). This approach addresses the challenges posed by the high acidity and hydrophilicity of PSS, which can lead to the corrosion of the active layer and adjacent electrodes, ultimately affecting the efficiency and durability of OSCs. In their research, Tsang et al. (2025) discovered that introducing three alkyl amine derivatives as dopants into Al 4083 PEDOT:PSS significantly enhanced conductivity, charge carrier mobility, and work functions. The dopants also improved the surface morphology of the spin-coated HTL films, leading to better charge extraction efficiency. This study provides insights and potential strategies for optimizing and enhancing the efficiency of OSC anodes. In a similar study, modified HTLs (PEDOT:PSS-PA, PEDOT:PSS-TA, and PEDOT:PSS-DA) were developed by incorporating phenylethylamine derivatives into Al 4083. This modification enhanced both the work functions and conductivities. Devices utilizing PEDOT:PSS-TA achieved a peak PCE of 17.10% when paired with PM6:Y6 active layers. The

doping approach also boosted the efficiency of the PM6:PY-IT high-performance system from 14.78% to 15.62% (Lv, 2024). Cui et al. (2019) incorporated 4-heptyl-4'-cyanobiphenyl (7CB) into the anode (PEDOT:PSS) and cathode (ZnO, SnO2) interlayers, leading to enhanced performance of OSCs. The interlayers doped with 7CB improved the physical interface with the active layer, boosted light absorption, and minimized carrier recombination. OSC devices featuring a PM6:Y6 active layer and a ZnO:7CB cathode interlayer reached a power conversion efficiency (PCE) of up to 16.2% and a peak external quantum efficiency of 87%. All devices with 7CB-doped interlayers exhibited higher short-circuit current density (Jsc), fill factor (FF), and PCE compared to those with undoped interlayers, regardless of the interlayer type, marking a remarkable occurrence in interlayer modification.

Chen et al. (2020) investigated how doping the anode layer affects the efficiency of inverted organic solar cells. They utilized a combined p-doped layer of CBP:MoO3 and NPB:MoO3 as an anode-modifying layer (AML) to boost performance, comparing it to the use of single NPB:MoO3 and CBP:MoO3 layers. MoO3 is ideal for inverted organic solar cells due to its ability to achieve high PCE, ease of fabrication, high work function (6.9 eV), and transparency to visible and NIR light. The CBP:MoO3/NPB:MoO3 AML improved the fill factor by enhancing hole injection into the active layer. AMLs based on CBP:MoO3 increased Voc because of their higher work function compared to NPB:MoO3. The combined AML resulted in better PCE than using either component alone. Doping the anode alters the work function, aligns with the HOMO of organic materials, and improves hole injections, which increases current density, reduces series resistance, and enhances fill factor and PCE values.

**B. Modification using double HTL systems**

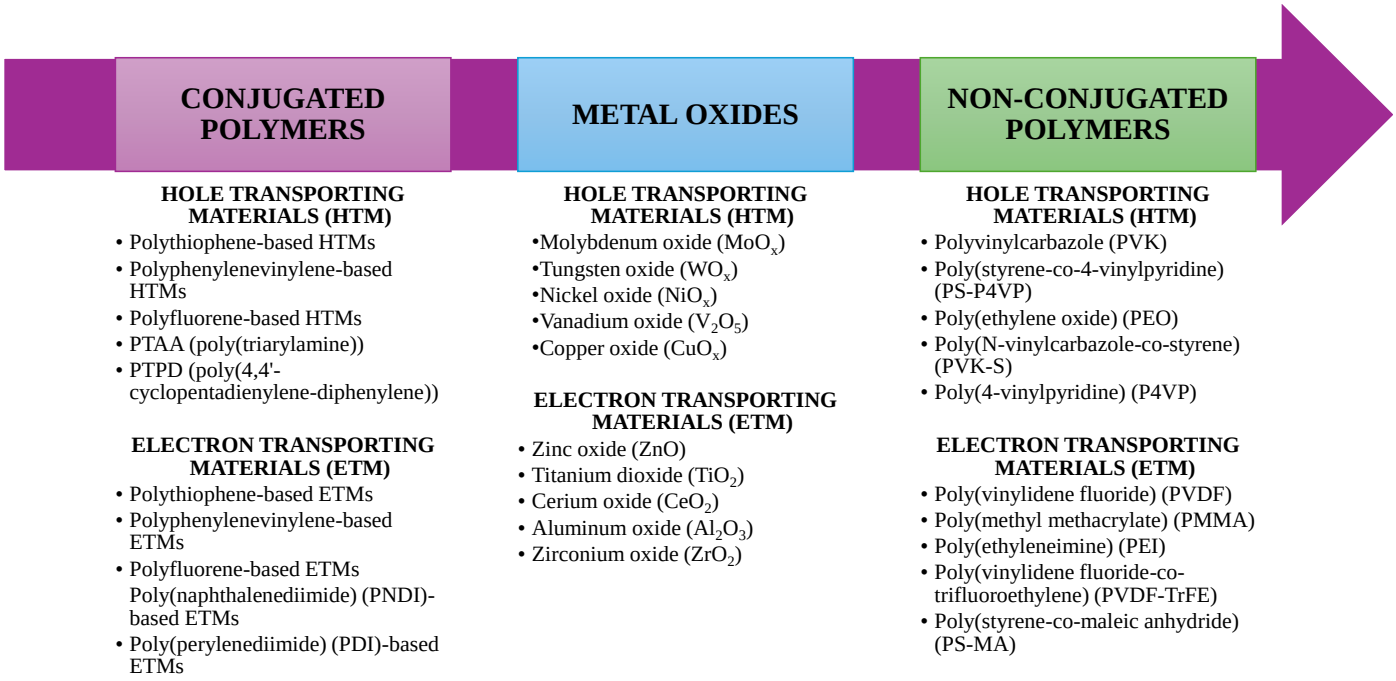



**Figure 9** Interfacial materials used in the OSCs

The presence of PSS ions in the PEDOT:PSS HTL negatively impacts device performance by causing unwanted local chemical reactions and by diffusing to the interface between the HTL and the active layer (Kim, et al., 2023b; Wijeyasinghe, et al., 2017). Chou et al. (2012) employed a dual-hole transport layer method to create OSCs utilizing copper phthalocyanine and bulk fullerene. To enhance the performance of the OSCs, they incorporated a double HTL consisting of PEDOT:PSS and a 4 nm layer of copper phthalocyanine between the anode and the active layer. The PEDOT:PSS layer modified the surface configuration of the ITO anode, while copper phthalocyanine facilitated improved hole transport. The findings indicated a Jsc of 8.8 mA/cm2, Voc of 0.46 V, and a PCE of 1.37%. Kim et al. (2023b) utilized a self-assembled monolayer of 2PACz along with a dual-component HTL made of PEDOT to boost the performance of OSCs. The PCE increase to 17.7% with the PEDOT:PSS/2PACz HTL, compared to 17.1% with just the PEDOT:PSS HTL. The 2PACz layer contributed to enhanced stability, minimized recombination losses, reduced electrical shunts, and improved performance in large-area devices. In cells measuring 1 cm2, the PCE increased from 12.3% to 13.3%. Zhu et al. (2021) [72]

integrated PEDOT:PSS hole transfer layers with TTF-PZ, a novel tetrathiafulvalene derivative, as anode interlayers in conventional non-fullerene PM6:Y6 based OSCs. The TTF-PZ/PEDOT:PSS bilayer used as the hole-transport layer achieved a high short-circuit current density (Jsc) of 26.19 mA/cm2 and a PCE of 15.84% for the PM6:Y6 organic solar cell. The bilayer structure's improved mobility, optimized morphology, and reduced carrier recombination led to a higher Jsc. These findings indicate that TTF-PZ is a promising material for hole transfer in photoelectric research.

In conclusion, the implementation of a dual-HTL system within the anode has significantly bolstered the stability of OSCs by facilitating better hole injection and minimizing the degradation of organic materials. However, to further elevate the performance of OSCs, it is imperative to refine the interface between the HTLs and the organic components. Fine-tuning the thickness of each HTL is crucial for maximizing device efficiency. Ongoing research is essential to develop innovative, high-quality HTL materials with enhanced properties to further improve the stability and performance of OSCs.

### C. Modification using novel materials and nanomaterials

To improve the flexibility and conductivity of anodes, a range of cutting-edge materials, including graphene, metal oxide conductive polymers, and carbon nanotubes, have been utilized, leading to enhanced performance (Yang, et al., 2020; Na et al., 2009; Lin et al., 2019). Nanomaterials, including nanoparticles, nanostructured metal oxides, graphene quantum dots, and metal-organic frameworks, have enhanced the conductivity and transparency of anodes (CSwart, et al, 2025; Samavati, et al., 2021). Gao et al. (2010) improved the anode interface in inverted bulk-heterojunction (BHJ) polymer solar cells by spin-coating a thin graphene oxide (GO) layer atop the organic active layer. The presence of GO led to a marked increase in power conversion efficiency (PCE) compared to devices without an interfacial layer, indicating that GO successfully modified the BHJ/metal anode interface to enhance hole collection. Optimal results were achieved with a GO layer thickness of 2-3 nm. Kavuri et al. (2020) introduced innovative anode interlayers (AILs) to boost the stability and efficiency of OSCs. They employed poly(vinyl pyrrolidone) (PVP) to alter molybdenum trioxide (MoO3) and vanadium pentoxide ($V_2O_5$) AILs in OSCs. The PVP-modified metal oxide AILs enhanced the adhesion between the anode and active layer, improved wetting properties, and elevated the overall quality of the device, including its morphology, optical properties, and chemical composition, when compared to unmodified metal oxide AILs.

The surface free energy (γS) of the underlying interfacial layer had an impact on both the overall performance of the OSC and the morphology of the BHJ films. It is crucial to modify the γS of these interfacial layers to align with the chemical structure of BHJ materials while ensuring their charge extraction capabilities remain intact (You et al., 2013). Nanoparticles of tungsten oxide (WOx) were incorporated into a PEDOT:PSS HTL to improve γS and the photovoltaic efficiency in fullerene-free OSCs that utilize PBDB-TF:IT-4F blends (Zheng, 2018). Devices utilizing a WOx:PEDOT:PSS HTL demonstrated superior performance, achieving an FF of 80.79% and a PCE of 14.57%. This enhancement was credited to the refined configuration of the active layer and the more efficient carrier extraction, which minimized nonradiative recombination. Hou and Yu (2020) integrated 2D Ti3C2TX nanosheets into PEDOT:PSS to create composite layers as HTLs in polymer solar cells (PSCs). The PCE increased by 13.5% compared to pure PEDOT:PSS HTL (9.72%). Using PM6:Y6 as the active layer, PCE increased from 13.10% for PEDOT:PSS to 14.55% for PEDOT:PSS/Ti3C2TX. This

**Table 2** Performance of organic solar cells with various anode and active layers

| Active layer | Anode | PCE (%) | FF (%) | Jsc (mAcm-2) | Voc (V) | Ref. |
|---|---|---|---|---|---|---|
| **PM6:ITC-2Cl** | PEDOT:PSS | 13.60 | 74.1 | 20.10 | 0.91 | Ma et al. 2021 |
| **PM6:Y6** | PEDOT:PSS-DA | 16.55 | 77.1 | 25.52 | 0.84 | Lee, et al., 2015 |
| **PM6:Y6-BO** | 2PACz-BHJ | 17.8 | 78.4 | 26.0 | 0.832 | Jing, et al., 2021 |
| **P3HT:PCBM** | Au thin film | 1.83 | 0.49 | 6.75 | 0.55 | Yambem, et al., 2011 |
| **PTB7-Th:PC71BM.** | V2O5:PEDOT:PSS | 9.44 | 70.14 | 16.83 | 0.80 | Li et al., 2020 |
| **$TQ_1/PC_{70}BM$** | MoO3-PEDOT:PSS (10 nm thickness) | 6.4 | 0.65 | 10.3 | 890 | Shao, et al., 2012 |
| **PM6:N3** | MoO3/Ag/MoO3 (100nm Ag/0 nm MoO3) | 13.79 | 66.91 | 25.29 | 0.82 | Chang, et al., 2020 |
| **$PCDTBT:PC_{70}BM/TiO_X/Al$** | $ZnI_2$/PEDOT:PSS (2% $ZnI_2$ additive volume) | 2.42 | 0.47 | 6.28 | 818 | Krobthong, et al., 2023 |
| **PBDB-T-2Cl:IT-4F** | Ag NWs/PEDOT:PSS | 13.53 | 0.75 | 20.76 | 0.868 | Peng, et al., 2019 |
| **PBDB-TF:IT-4F** | WOx:PEDOT:PSS | 14.57 | 80.8 | 20.73 | 0.87 | Ha, et al., 2018 |

improvement was attributed to 2D-Ti3C2TX's superior hydrophilicity, high metallic electrical conductivity, large surface area, and outstanding transparency. The composite layers showed higher conductivity and improved long-term stability. Zinc phosphotungstate (ZnPW) serves as an anode interfacial material to enhance energy level matching, lower contact resistance, boost light absorption, and prevent charge recombination. The ZnPW-modified device achieved a PCE of 18.67% and a fill factor of 80.29%, outperforming PEDOT/PSS-modified devices. ZnPW-modified devices also excelled in photostability and storage stability (Feng, et al., 2023). Table 2 summarizes the performance of organic solar cells with various anode and active layers.

**4.1.2 Cathode interfacial layers**.

Organic solar cells (OSCs) utilize a range of cathode contact materials to enhance their performance. Nonetheless, many of these materials fall short in terms of optimizing the stability and efficiency of OSCs. Recent studies suggest that altering the cathode interfacial layer is essential for enhancing the efficiency, durability, and charge transport of OSCs. The most used materials for modifying cathode buffer layers are either organic or inorganic. Cathode interfacial layers can be composed of metal oxides such as TiO2, ZnO, and Al2O3, conductive polymers including PEDOT:PSS, PANI, and PPy, self-assembled monolayers (SAMs), or extremely thin metal films like LiF, Ca, and Ba (Brabec, et al., 2002; Wen, et al., 2019; Yu et al., 2016). Their remarkable electron mobility, stability, conductivity, and flexibility make them valuable, while ultrathin metal films boost electron injection. The development of OSCs encounters obstacles, such as long-term stability, which is often overlooked in reports of high-efficiency devices. The main strategy for prolonging the lifespan of OSCs involves creating methods to minimize damage from oxygen and moisture. Research on modifying the cathode interface layer is vital for simultaneously enhancing device stability and efficiency, and several techniques addressing these issues are outlined below.

**A. Double cathode modification**

The performance of OSCs is greatly influenced by the electrical configuration, the energy offset at the junction, and the application of electrode modification materials that have a compatible energy band alignment (Chang, et al., 2020a). Lin et al. (2019) enhanced charge transfer and stability in OSCs within the PM7:IT-4F framework by employing a dual cathode modification. They introduced a $SnO_2$/ZnO double layer to a non-fullerene OSC based on PM7:IT-4F to explore its underlying mechanisms. This layer merges the advantages of ZnO and $SnO_2$ films, greatly improving device stability and presenting innovative ideas for cathode layer modification. The $SnO_2$/ZnO buffer layer elevates the OSC's PCE to 12.91%, with an FF of 70%, Jsc of 20.04 mA/cm$^2$, and Voc of 0.92 V, surpassing a single cathode layer. Studies on charge transport and extraction using photo-CELIV, TPV/TPC, and $V_{oc}/J_{sc}$ dependence on light intensity reveal fewer traps near the interface and a reduced energy barrier between the electrode and active layer. This leads to efficient charge transfer and collection at the active layer/($SnO_2$/ZnO) interface and diminished charge recombination. The denser $SnO_2$/ZnO layer hinders oxygen and water from penetrating the interface and prevents active material from seeping into the electrode, significantly reducing the dark deterioration rate to 17% in air and 7% in nitrogen. This research clarifies the processes that enhance device efficiency and stability through cathode modification, encouraging further exploration and demonstrating the effectiveness of a double-cathode layer for OSC stability and efficiency.

Liang et al. (2019) investigated the use of double-sided modified ZnO layers as electron-transporting layers (ETLs) to enhance the photovoltaic efficiency of inverted organic solar cells. Their research demonstrated that devices incorporating modified ZnO interfacial layers achieved higher power conversion efficiencies than those with unmodified layers. Specifically, the PCE increased from 3.42% to 4.23% in the P3HT:PC61BM active layer and from 7.57% to 8.61% in the PTB7:PC71BM blend system. These improvements are attributed to better interface contact quality and optimized energy-level alignment between the ETL and active layer, which reduce the interfacial energy barrier with the indium tin oxide electrode and improve electron collection and transport efficiency. This dual surface modification strategy holds potential for use in various photoelectric devices, such as organic light-emitting diodes, quantum dot solar cells, and perovskite solar cells. The enhanced performance is due to improved interface contact and optimized energy level alignment, which facilitate electron collection and transport.

The adoption of twin cathode modification brings notable benefits in aligning energy levels and providing protection, thereby improving light absorption and dispersion in the active layer. Huai et al. (2018) illustrated this by integrating three alcohol-soluble cathode interfacial materials with bathocuproine (BCP) to develop multifunctional bilayer cathode buffers for traditional organic solar cells (OSCs). This method led to a device achieving a power conversion efficiency (PCE) of over 10.11% and enhanced stability. Double interlayers were also utilized to boost light absorption and dispersion within the active layer. These interlayers enable efficient charge collection, alcohol treatment, and advantageous energy-level alignment, which help decrease leakage current and mitigate recombination. The stability of the OSCs device was enhanced due to the BCP-metal electrode complex's blocking effect and the protective qualities of the alcohol-soluble components. The dual interlayer approach is a novel technique for maximizing the potential of OSCs, offering broad applicability because alcohol-soluble organic electrolytes are commonly used as cathode buffer layers, and the double cathode layers have demonstrated their superiority.

B. Modification through doping

Zinc oxide (ZnO) amorphous films, created through sol-gel techniques, are widely utilized as cathode interfacial layers (CILs) (Huang, et al., 2018; Nian, et al., 2015). ZnO is known for its excellent electron-transporting and hole-blocking properties, along with its stability, transparency, and suitable energy levels, meeting the key requirements for CILs. Nonetheless, the chemical incompatibility between ZnO and organic/polymer-based photoactive layers often leads to adverse electron extraction, which increases the series resistance (Rs) and charge recombination in ZnO-based organic solar cells (OSCs) (Woo. et al., 014; Liang et al., 2015). The thickness of the ZnO layer plays a crucial role in device performance, as the low conductivity of ZnO processed from an aqueous solution impedes optimal performance in thicker layers, such as those measuring 100 nm (Wen et al., 2019). Luo et al. (2020) enhanced hybrid photoconductive interlayer materials by incorporating perylene bisimide dyes into ZnO, creating an ionic connection between the organic additives and the inorganic framework. This modification improved the hole-blocking and electron-transporting properties of aqueous solutions. The introduction of benzenesulfonic acid groups to the perylene bisimide dyes increased their water solubility and promoted ionic bonding with zinc atoms during the formation of hybrid thin films. This ionic bonding led to molecular dispersion, which enhances hole blocking through photoinduced electron transfer from the organic dye molecules to the conduction band of ZnO. The improved hole blocking and electron transport enhance the fill factors in organic solar cells by increasing the charge selectivity of the cathode interlayer. With PM6:Y6 as the active layer, a hybrid interlayer treated with an aqueous solution achieved a PCE of up to 15.4%. Hybrid thin films can be manufactured at 150 °C, an optimal thermal annealing temperature for flexible device applications.

Direct interaction between n-doped cathode-modifying layers and active layers negatively impacts photovoltaic performance. To mitigate this issue, Li et al. (2024) introduced a thin interlayer between these components to boost OSC performance. They employed thermally evaporated bathocuproine (BCP) and ytterbium-n-doped BCP (BCP:Yb) to modify the interfaces between the cathode and active layers. A device featuring a 1 nm BCP/9 nm BCP:Yb configuration demonstrated an open-circuit voltage of 0.793 V, similar to that of a 10 nm BCP. These devices achieved higher short-circuit current densities and enhanced PCE, despite having lower fill factors. Zhou et al. (2020) explored the use of polyethylenimine ethoxylated (PEIE), aluminum nitrate (Al(NO3)3), and Al(NO3)3: PEIE-doped ZnO cathode interlayers to optimize the efficiency of inverted organic solar cells. Devices with an Al:PEIE dual-doped ZnO cathode interlayer exhibited an improved power conversion efficiency (PCE) of 9.51%, which is 14.99% higher than that of pristine ZnO (8.27%). This improvement was attributed to better photon absorption, utilization, and enhanced light transmittance. The performance

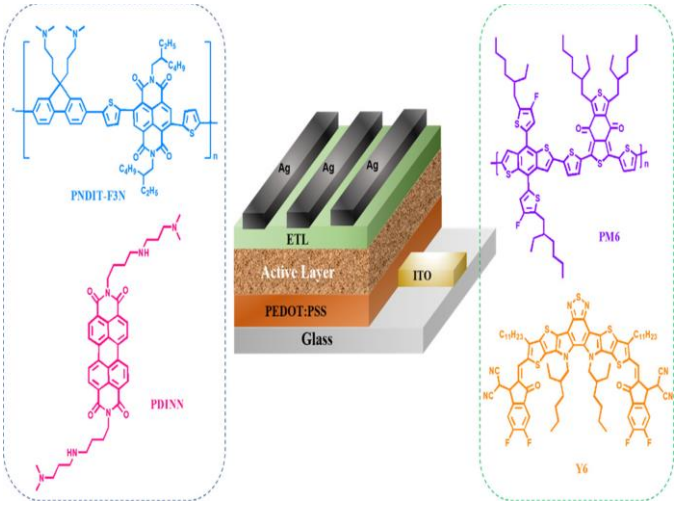



**Figure 10** Chemical structures of PDINN and PNDIT-F3N and their device configurations [110]. (ACS Appl. Mater. Interfaces 2021, 13, 43, 51078-51085)

enhancement was due to a reduced work function and improved interfacial contact, potentially enhancing charge transfer and reducing exciton recombination. Stability assessments indicated that devices with a doped ZnO interlayer demonstrated superior stability compared to those with pure ZnO.

**C. Modification using novel materials and nanoparticles**

Liu et al. (2022b) explored the use of a self-assembled monolayer of aromatic organophosphonic acid (2PACz) on the cathode, which enhanced both PCE and stability in air. Through ultraviolet photoelectron spectroscopy, it was revealed that this adjustment improved the work function of the cathode interlayer for electron extraction and lowered the surface energy without affecting the deposition of the layer. The organic solar cells (OSCs) created with PBDB-T:IT-M exhibited excellent PCE and air stability, retaining 88% of their initial PCE after 555 hours of exposure. Li et al. (2019) introduced a gradient composite film for OSCs by merging zinc oxide (ZnO) with the non-fullerene organic semiconductor ITIC, forming the G-ZnO/ITIC film. This innovative film demonstrated increased surface hydrophobicity and a smooth morphology, which enhanced the interfacial contact between the organic photoactive layer and the inorganic interfacial layer. The OSCs utilizing G-ZnO/ITIC in combination with PTB7-Th:PC71BM achieved a PCE of up to 8.73%, surpassing the performance of conventional ZnO-based devices. This development is promising for advancing high-performance charge-injection layers in OSCs.

Mech et al. (2022) studied the effect of cathode materials on PTB7:PC70BM bulk heterojunction OSCs, focusing on efficiency, work function, Voc, electrical characteristics, and stability. They assessed 12 cathode materials: Al, Ag, In, InAl, Al3004 alloy, CaAl, MgAl, ZnAl, Sn, Ti, Au, TiAu, and Ni. The

results showed that Al3004 alloy, Sn, In + Al, and In cathodes performed best. The In + Al cathode achieved a PCE of 4.9%, significantly boosting efficiency. A correlation was noted between cathode work function, Voc, and efficiency. Longevity tests showed the In + Al bilayer cathode had the highest PCE compared to pure Al, doubling cell stability and reducing using toluene as a non-halogenated solvent, combined with state-of-the-art all-polymer technology.

Zinc oxide nanoparticles (ZnO NPs) serve as outstanding electron transport materials in high-efficiency OSCs, thanks to their wide bandgap, excellent electron mobility, easy synthesis, and low-temperature solution processing (Wang, et al., 2024).

**Table 3** Comparative overview of the interfacial layers' modification of OSCs

| Modification Type | Approach | Performance benefits | Commercialization Prospect | Challenges |
|---|---|---|---|---|
| **Surface Energy Engineering** | Modifying surface energy using self-assembled monolayers, chemical functionalization or plasma treatment. | Enhanced wettability, and improved film morphology, leading to better charge extraction and reduced combination losses. | Generally scalable but involves additional processing steps and costs. | Process complexity, Uniformity |
| **Doping/Chemical modification** | Doping interfacial layers with materials such as metal oxides, fullerene derivatives and ionic liquid to tailor work function and conductivity. | Higher Voc/FF, Better energy alignment, and reduced contact resistance. | Cost-effective dopants. Compatible with solution-processing | Material stability, environmental impact |
| **Novel Materials** | Employing new materials such as 2D materials, hybrid organic-inorganic compounds and conjugated polyelectrolytes. | Superior stability and energy alignment, environmental robustness | Material cost, availability, and compatibility with roll-to-roll processes | Cost, material sourcing |
| **Nanostructuring and morphological control** | Introducing nanostructured interlayers such as nanorods, nanoparticles or porous films. | Enhanced interfacial area, and charge selectivity, reduced recombination and higher PCE. | Potential for high performance, fabrication complexity | Scalability, reproductivity |
| **Passivation/Defect Engineering** | Passivating defects at the interface using insulating layers or functional molecules. | Reduced recombination. Increase stability and improve operational lifetime | Compatible with existing processing methods, aiding scalability and commercialization | Potential for added layer complexity |

degradation. OSCs with Ti and TiAu alloy cathodes showed increased efficiency over 34 weeks, suggesting potential for improved air stability.

A combination of PDINN and PNDIT-F3Z electron transport materials enhances the power conversion efficiency (PCE) of non-fullerene organic solar cells, as shown in Figure 10 (Ding, et al., 2021). This approach creates a complex electron transfer layer (ETL) that improves the PCE of PM6:Y6-based organic solar cells (OSCs). The properties and efficiencies of pure PDINN (16.66%) and pure PNDIT-F3N (15.98%) were key factors in selecting this combination. A blend of PNDIT-F3N and PDINN (0.9:0.1 weight ratio) produced a novel ETL with 17.20% efficiency and a fill factor exceeding 78%, making it one of the most effective PM6:Y6-based binary devices. The study showed improved charge extraction efficiency due to reduced charge recombination, enhanced surface morphology, and increased selectivity. The mixed ETL achieved optimal charge extraction, reaching a PCE of over 16% for binary all- polymer solar cells

Nonetheless, their surface defects and catalytic characteristics present notable challenges. Yan et al. (2023) developed ZnO nanoparticles (ZnO@C NPs) coated with carbon. The carbon layer surrounding the ZnO NPs provided UV absorption and hydrophobic properties, reducing water and oxygen adsorption, addressing surface defects, and limiting the formation of hydroxyl radicals. Organic solar cells (OSCs) using ZnO@C achieved a power conversion efficiency (PCE) of 17.55%, which is higher than the 16.92% seen in devices based on ZnO. The ZnO@C NP-based OSCs showed improved stability against air and UV exposure. The ZnO@C NPs enhanced ohmic contact with the active layer and decreased interfacial exciton recombination, thanks to their increased monodispersity, fewer surface defects, and a more appropriate work function (WF) of 3.89 eV. This study underscores the promise of ZnO@C NPs in creating efficient and stable OSCs. Chen et al. (2021) improved the performance of OSCs by modifying the cathode interlayer with metal oxide ($TiO_2$) nanocrystals. While metal oxide nanocrystals have a

suitable work function and conductivity for use as CILs, their tendency to aggregate significantly impedes the creation of uniform films. To address this, researchers treated the surfaces of TiO2 nanoparticles with 4-dimethylamino benzoic acid, which minimized aggregation and allowed for a consistent $TiO_2$-N coating. This $TiO_2$-N coating showed better energy-level alignment with the photoactive layer due to its decreased work function. Utilizing $TiO_2$-N as a CIL facilitated efficient charge generation and minimized charge recombination. OSCs utilizing PM6:BTP-4Cl and PM6:IT-4F blends achieved higher PCEs with TiO2-N as the CIL compared to those using unmodified $TiO_2$. Table 3 gives a comparative overview of the different interfacial layer modification, assessing their impact on charge extraction, energy level alignment, device longevity, OSCs performance and prospects for commercialization.

### 4.1.3 . Modification of the active layer

Early OSCs used planar heterojunction (PHJ) structures with distinct donor and acceptor layers (Tang, et al., 1986). Donor–acceptor heterojunctions have emerged as the most effective method for exciton separation in OSCs, and selecting the right donor and acceptor materials is crucial for boosting OSC efficiency. Polymer donors such as D18, PTQ10, PM6, P3HT, and PffBT4T-2OD have exhibited remarkable photovoltaic performance (Lv, et al., 2024). Conventional OSC architectures using fullerene derivatives as electron acceptors face limitations in performance optimization because of the lack of donor-acceptor interfaces, instability, voltage loss, and inadequate light harvesting (Huang, et al., 2021). Despite progress in bulk heterojunction (BHJ) technology, achieving precise morphological control remains challenging. The vertical distribution of donor-acceptor components affects charge extraction and transmission (Zhang et al., 2021). Efforts to enhance the efficiency have focused on developing ideal architectures with selective carrier transport and controlled recombination. Hong and Ge (2021) introduced a hybrid planar/bulk heterojunction structure for OSCs, incorporating a BHJ of p-type polymer (PTO3) and n-type naphthalene imide small molecule (NDI-i8), with acceptor enrichment at the cathode and donor enrichment at the anode, sandwiched between a BHJ donor and acceptor blend. This configuration improved charge transport, extraction, and recombination, resulting in a 23 meV reduction in nonradiative energy loss, increased Voc from 0.843 to 0.866 V, and a maximum PCE of 18.5%. in another study, Jiang et al. (2021) developed pseudo-bilayer (PB) architecture for OSCs, fabricating a PB film based on PM6:N3:PC71 using the SD processing method. This novel active layer achieved a PCE of 17.42%, surpassing the conventional bulk heterojunction architecture (16.44%) because of the higher FF and Jsc values, which are attributed to more efficient exciton dissociation and charge transport.

#### A. Non-fullerene acceptors

Fullerene derivatives (PC61BM and PC71BM) serve as acceptors in most BHJ OSCs owing to their superior electron affinity, isotropic charge transport, and remarkable electron mobility (Nian, et al., 2016; Collins, et al., 2017). However, these fullerene-based acceptors have inherent limitations that impede PCE advancements, including poor visible-light harvesting, high costs, limited architectural adaptability, morphological instability in thin films, and substantial energy loss. Non-fullerene acceptors (NFAs) have enabled OSCs to exhibit exceptional PCE. Optimal OSC performance requires an appropriate film morphology in the photoactive layer to balance the charge transfer and exciton dissociation. OSCs with polymeric donors and fullerene-derived acceptors have been successful because of their bulk heterojunction (BHJ) architecture, which overcomes the short exciton diffusion length in polymer donor materials and establishes an interpenetrating donor/acceptor (D/A) network (Tokmoldin, et al., 2020; Siegmund, et al., 2017; Clarke, and Durrant, 2010). However, BHJ OSCs based on fullerene derivatives are hindered by inefficient charge transmission within complex D/A networks. NFAs have addressed the optical, photophysical, and stability challenges of fullerene acceptors in OSCs, thereby enhancing their overall performance (Karki, et al., 2021; Armin et al., 2021). Extensive research has focused on developing novel donors and NFAs and optimizing devices for fullerene-free OSCs (Wu et al., 2016; Tokmoldin, et al., 2020; Yao, et al., 2018). The collaborative effect of innovative NFAs and donor materials in BHJ OSCs has improved light absorption and reduced energy loss, resulting in certified PCE exceeding 17% (NREL). Despite significant advancements, interface materials that are solution-processable on top of the active layer, compatible with innovative NFAs, and that demonstrate sufficient long-term stability remain unavailable.

The use of PEDOT:PSS as the top layer in inverted devices consistently results in a diminished open-circuit voltage (Voc) owing to energy level misalignment at the active layer-PEDOT:PSS interface. This occurs despite the potential advantages of PEDOT: PSS as a solution-processed hole transporting layer (HTL) material for OSCs (Han, et al., 2019). Additionally, surfactants needed to enhance the wettability of PEDOT: PSS negatively impact device stability and performance. To address these issues, Xu et al. (2024) developed an innovative OSC architecture with a non-fullerene acceptor as the HTL within a solution-processed polymer bilayer incorporating a standard acidic PEDOT-PSS. This novel bilayer HTL comprised doped poly[bis(4-phenyl)(2,5,6-trimethylphenyl)amine (PTAA) nanoparticles and PEDOT:PSS, eliminating additional surfactants. PEDOT:PSS forms a thick protective layer over the active layer and enables Ohmic contact with the Ag electrode, whereas doped PTAA nanoparticles (D-PTAAnp) act as a buffer layer, ensuring proper hole-transport level alignment and efficient

extraction. Testing with various active layers and ETLs showed that this HTL configuration improved the stability and efficiency, matching or surpassing other HTL systems. The inverted OPV cells based on PM6:BTPeC9:L8-BO achieved a PCE of 17.1%. These devices demonstrated exceptional operational stability under metal-halide lamp irradiation, maintaining 93% of initial performance after 1,800 hours at 60 °C and 95% after 1,600 hours at room temperature. AgNW electrode-based all-solution-processed devices exhibit remarkable stability and efficacy. The top PEDOT:PSS layer provides a crucial mechanism for industrially scalable PM6: Y6 modules, as evidenced by the stability and performance values obtained. The high PCE of approximately 18% can be attributed to the exceptional properties of the synthesized non-fullerene acceptor Y6 (Zhu, et al., 2020; Zhang, et al., 2020). The chemical structure and alkyl chains of Y6 differ significantly from those of the previously identified pentacyclic ladder-type indacenodithiophene (IDT)-based NFAs. Although the IDT-based NFAs were centrosymmetric, Y6 exhibited an axisymmetric crescent-shaped configuration. In IDT-based NFAs, p-hexylphenyl typically serves as an alkyl chain attached to two sp3-hybridized carbon (C) atoms of the IDT unit. These long side chains contribute to solubility but introduce a steric barrier between the IDT units, resulting in end-group π (π–π) stacking and linearly stacked molecular packing (Zhang, et al., 2020). The modification of the branched alkyl chains in Y6, as reported by Abbas et al. (2022), improved the morphology and performance of inverted organic solar cells using non-halogenated solvents. This alteration enhanced Y6's processability and solubility, resulting in an optimal bulk heterojunction (BHJ) morphology. Organic solar cells incorporating modified Y6 molecules and o-xylene achieved a power conversion efficiency of 17.4% and fill factor of 77.9%. Zhu et al. (2020) explored the solid-state structure underlying high efficiency of BHJ blends, offering insights into enhancing film morphology and creating effective donor-acceptor mixtures. Their findings revealed that Y6 could form a distinctive two-dimensional packing structure with a conjugated backbone resembling a polymer oriented perpendicular to the substrate when the processing solvent and thermal annealing parameters were controlled. This structural arrangement was elucidated through morphological investigations. The optimized device demonstrated a power conversion efficiency of 16.88% (16.4% certified), exhibiting balanced short-circuit current density, fill factor, and open-circuit voltage in a single-layer binary BHJ mixture. This morphology facilitates efficient carrier transfer and transport, indicating promising prospects for organic photovoltaic development. This study emphasizes the critical role of film morphology in device performance, highlighting how the morphology and crystal packing of Y6 acceptor-based high-efficiency devices in BHJ blends significantly impact the overall performance.

Zhao et al. (2022) examined hybrid plasmonic nanostructures in non-fullerene organic solar cells (OSCs). These structures incorporate metal nanostructures (MNS) of gold nanobipyramids (AuNBPs) and gold nanospheres (AuNSs) to enhance the near-infrared photoresponse. Researchers engineered the synergistic localized surface plasmon resonance (LSPR) of hybrid MNS to align with the absorption range of the non-fullerene photoactive layer, particularly in the near-infrared (NIR) spectrum. This alignment enhanced the photoresponse and light-harvesting capabilities. The study used experimental data and theoretical models to analyze the plasmonic enhancement mechanisms. The findings showed that the hybrid MNS exhibited significant broadband near-field enhancement and scattering effects with electrical advantages that facilitated charge extraction and transport. The synergistic plasmonic influence of the hybrid MNS increased power conversion efficiency (PCE) from 15.46% to 16.62% in PM6:Y6-based OSCs. This study yielded high-performance OSCs utilizing plasmonic MNS with adaptable optical properties.

**B. Nanoparticles and nanomaterials in the active layer**

The incorporation of transition metal nanoparticles, such as gold (Au) and silver (Ag), into the active layers of organic solar cells (OSC) has been explored to enhance their performance. Kaçuş et al. (2021) examined Au and Ag nanoparticle effects on a PP3HT:PCBM photoactive layer in OSCs. They found that Ag nanoparticles reduced the active layer absorption, whereas Au nanoparticles increased it. The power conversion efficiency (PCE) of the OSCs improved by 3.50% and 3.35% with 0.5 and 1 wt. percent of Ag and Au NPs, respectively. Nanoparticle integration enhances the OSC performance by extending the carrier lifetimes and increasing the optical path length within the active layer. PCE improvements were attributed to enhanced far-field light scattering at the localized surface plasmon resonance (LSPR) facilitated by highly localized fields surrounding the Ag and Au NPs.

Piralaee et al. (2020) examined the plasmonic effect of randomly dispersed Ag NPs on the active layer to optimize BHJ OSC system performance. The reference devices exhibited optoelectrical characteristics with Jsc, Voc, and FF values of 30.54 A/cm2, 0.71V, and 0.60 for the P3HT: PCBM and 49.08 A/cm2, 0.83V, and 0.65 for PCDTBT: PCBM mixtures, yielding PCEs of 1.22% and 2.43%, respectively. Incorporating Ag NPs at a 0.05 fraction into the active layer improved efficiency by 32% and 28%, respectively. Increasing the Ag NP concentration to 0.1 led to enhancements of 65.6% and 56.4% in blend-based device efficiency. The observed increase in the absorption coefficient corresponds to the improved external quantum efficiency (EQE) of the OSC devices, which is attributed to the localized surface plasmon resonance (LSPR) phenomenon of Ag NPs.

Pereira et al. (2019) investigated the longevity, stability, and efficiency of inverted flexible OSCs manufactured via a semi-industrial blade coating process using non-halogenated solvents, focusing on cobalt ferrite ($CoFe_2O_4$) nanoparticles ranging from 4

to 10 nm in size. $CoFe_2O_4$ NPs were incorporated into a blend of [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) and poly(3-hexylthiophene-2,5-diyl) (P3HT) at a 1:0.99 weight percentage ratio as a substitute for P3HT. Devices enhanced with cobalt ferrite nanoparticles showed a 10% increase in PCE compared with their nanoparticle-free counterparts. This improvement was attributed to the magnetic moments in the active layer, leading to increased diffusion length and exciton lifetime, as well as enhanced intersystem crossing efficiency (González et al., 2015). The coercive electric field (CEF) from dipole interactions between CFO nanoparticles may facilitate charge carrier absorption by the intrinsic electric field of the electrodes (Akhatova, et al., 2023b). Metal-oxide nanoparticles are susceptible to pinhole formation during film coating, potentially causing device shunting. Therefore, there is a need to develop stable and robust HTLs that can be solution-processed to advance the commercialization of all-solution-processed OPVs. Siddiqui et al. (2020) explored the performance of bulk heterojunction solar cells (BHJ-SCs) using wet chemically synthesized copper oxide nanoparticles (CuO-NPs) as the active layer. Their findings showed an increase in the PCE from 2.85% to 3.82%, without negatively affecting the fill factor or open-circuit voltage. The enhanced PCE of 3.82% with the optimal concentration of CuO NPs in P3HT:PC70BM is attributed to improved excitation generation, light absorption, and photoexcited charge separation and collection. The EQE experiment provided further evidence that CuO nanoparticles can effectively enhance device performance when incorporated into the P3HT:PC70BM blend.

Plasmonic metal nanoparticles can significantly enhance the electrical properties and light absorption in organic and perovskite solar cells, improving device performance. The enhancement mechanisms include near-field plasmonic enhancement, enhanced light scattering, improved exciton dissociation, and enhanced charge transport and collection. Modulating the nanoparticle size, shape, distribution, and surrounding media can further enhance the performance of organic solar cells (OSC). As the MoS2 concentration increased, the resistance of the bulk heterojunction (BHJ) layer increased, impairing device functionality. The recombination resistance decreases with further MoS2 concentration development, suggesting an increase in the charge recombination rate (Akhatova, et al., 2023). Mao et al., (2018), reduce the leakage of current in thin active layer of OSCs by developing a novel strategy to patch the defect. The defeat was patched using by coating an insulating polymer using the Maobi tools. Insulating polymers such as polymethylmethacrylate (PMMA), polyvinyl alcohol (PVA), and polyethylenimine (PEI) were used to patch the defect. The patching strategy is applicable to both fullerene-based and non-fullerene-based solar cells and can effectively restore the photovoltaic properties of the active layers with defects.

## 5.0 Conclusion

Solar energy technologies such as photovoltaic (PV) solar cells have evolved to address energy and environmental challenges. Organic solar cells show lower power conversion efficiency (PCE) than inorganic solar cells, requiring research on device physics, design optimization, stability, large-scale manufacturing, and the integration of novel concepts. Advancements have been developed to enhance light absorption, reduce optical losses, inhibit exciton recombination, facilitate charge transfer, improve stability, and enhance PCE. Improvements in photovoltaic materials and OSC architectures have contributed to improved performance and stability. Defects and disordered states within devices can lead to degradation caused by synthetic impurities, conformational changes, or molecular defects resulting from suboptimal synthesis. Further research is needed to understand these issues and develop improved devices. Understanding the charge generation, dissociation, and recombination processes is essential for optimizing efficiency. Additionally, introducing metal and semiconductor nanoparticles into organic layers enhances electronic and photonic properties, promoting OSC commercialization to improve efficiency, scalability, and stability.

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## Declaration of conflict of interest

The authors have collectively contributed to the conceptualization, writing and reviewing the manuscript. This manuscript has not been previously submitted or reviewed by any other journal or publishing platform. The authors declare that there are no conflicts of interest regarding the publication of this manuscript.

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