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Recent advances in polymer and perovskite based third-generation solar cell devices

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ABSTRACT

This review article begins with a comparative overview of the configurations, materials, fabrication methods, and energy conversion efficiency of polymer and perovskite solar cells' photovoltaic performances. Firstly, there has been a significant increase in the adoption of solar cells due to the growing need for renewable and clean energy. Among all photovoltaic technologies, polymer and perovskite solar cells have garnered considerable attention owing to their potential to be affordable, lightweight, easy to manufacture, and quick charging. Research on polymer solar cells has spanned over two decades, whereas the use of perovskite solar cells is just eight years old. This expanding topic offers a wealth of information to readers interested in polymers and perovskite. As a basic comparison, the best power conversion efficiency results are 21.6 percent for a 1 cm^2 perovskite solar cell and 15.2 percent for polymer solar cells. Finally, this article recommends necessary improvements and future research areas in polymer and perovskite solar cells.

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1. Introduction

Given the limited availability of fossil fuels and the severe worries about global warming and environmental protection, the quest for more efficient technologies that produce cheap, clean, and renewable energy is essential for sustaining society's economic prosperity. In order to create new photovoltaic technologies (PVs) that effectively convert solar irradiation into electric power [1], enormous research efforts have been made in academia and industry since the 1950 s [2]. The ever-increasing need for renewable and sustainable energy sources [3] has drawn a lot of attention [4] to developing novel materials for efficient solar cells. Sunlight is the most possible long-term energy solution since it is widely available, inexpensive, and environmentally benign. Ali and Alomar have done a technical–economic study to evaluate the productivity of photovoltaic (PV) solar systems that are grid-connected. This study demonstrated that investments in PV system technologies are extremely advantageous [5]. Solar cells, which directly transform sunlight into electricity, are the most efficient and practical method to harness solar power [6].

PVs can be regarded as the greenest and most sustainable source of energy since sunlight is the most plentiful, unlimited, and pure source of energy on the planet. Polymer solar cells, also called PSCs, are now one of the most exciting developments in photovoltaic technology. They have many advantages over other technologies, such as being light, flexible, and easy to make in large quantities at a low cost. Heeger et al. established it in 1995 [2] that the bulk-heterojunction (BHJ) structure was a viable method for fabricating PSCs. In a typical BHJ structure, the photoactive layer that absorbs solar radiation and converts it into electricity is a mixture of an electron donor (D) and an electron acceptor (A) (PC61BM or PC71BM, respectively). The continuous and interconnected nanoscale network architecture that is generated by the blending components is an interesting feature of this BHJ structure. This architecture delivers dense D/A interfaces in a bulk volume that is appropriate for simple solution processing (Fig. 1) [1].

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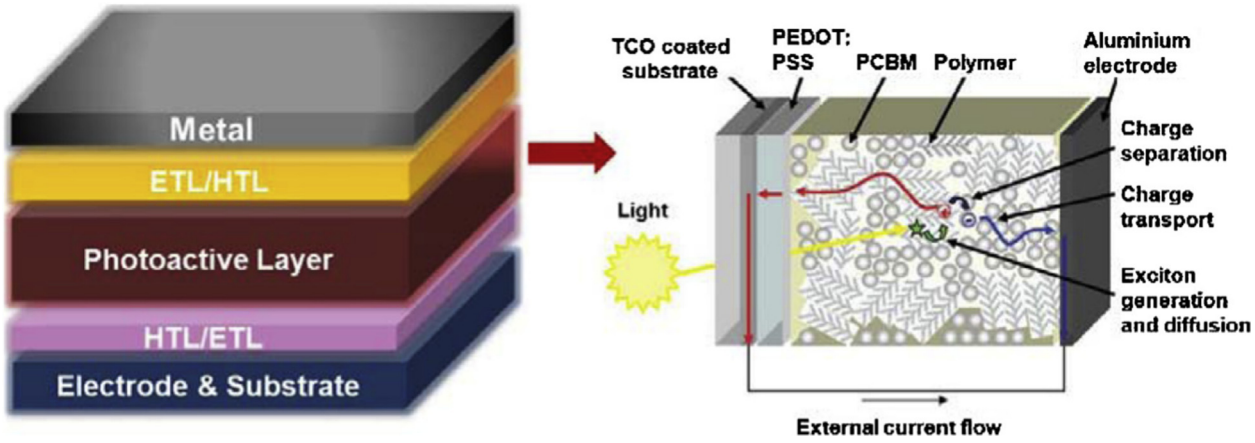

Fig. 1. Bulk-heterojunction polymer solar cells [1].

PSCs have attracted a great deal of attention due to their semi-transparency, inexpensive solution processing costs, lightweight weight, and adaptability. Using these benefits, PSCs have a bright future in the domains of wearable electronics, building-integrated photovoltaics, and portable electronics [7]. Over the last two decades, numerous studies have shown an immediate increase in PSCs' power conversion efficiency (PCE). The PCE of PSCs based on fullerene and non-fullerene small molecules has achieved 11 and 18 percent respectively, using suitable chemical methods and processing engineering [8]. Although the PCE has made significant progress, morphological and mechanical stability have remained a barrier. The limiting stability factors are water, oxygen, metastable morphology, irradiation, heating, mechanical stress, and diffusion of electrodes and buffer layers materials [9].

In contrast, all-polymer solar cells (APSCs) including acceptor and donor polymers exhibit morphological and mechanical stability, which are advantageous under thermal and mechanical stressors and are regarded as essential characteristics for future commercialization [2]. However, because of a dearth of high-performance acceptors, all-PSC devices' performance remains lower than that of innovative small molecule-based alternatives. Since the introduction of *n*-type polymers and their exploration in organic photovoltaics, several PSCs have shown excellent Photovoltaic System Efficiency [3]. The open-circuit voltage of perovskite solar cells (PKSCs) can be improved by inserting polymer passivation layers at the interfaces between the charge transport and perovskite layers [4].

The charge extraction capacity of inverted polymer solar cells (IPSCs) may be increased by utilizing thermally evaporated compact Ta_2O_5 as the cathode buffer layer (CBL) put on an indium tin oxide (ITO) substrate and adjusting the substrate temperature from 200 to 250 °C. When the substrate temperature is raised from 200 to 250 °C, current density–voltage tests reveal an increase in power conversion efficiency of 2.8 percent to 3.1 percent with a ratio/percentage increase of 10.7 percent [6]. Molybdenum oxide (MoO_3) and polyethyleneimine ethoxylated (PEIE) were used to form a double interfacial layer in polymer solar cells (PSCs). Using a MoO_3/PEIE bilayer, a high power conversion efficiency (PCE) of 3.69 percent was produced, which is 19.4 percent more than that of pristine devices [7].

Recently, multiple methods have been identified for enhancing the PCE of thin-film organic or polymer solar cells. The plasmonic effect is one such strategy that has been investigated in depth and shows promise for application in the development of PSCs. In PSCs, metal nanoparticles (MNPs) like gold and/or silver nanoparticles are implanted in the active layer, at the interface between these two layers, or the buffer layer in order to improve light absorption, hole-charge carrier production, and transport, which ultimately results in an increase in photocurrent. Therefore, the commercial manufacture of innovative polymer solar cells with desired features may be achieved by altering the location, size, and shape of NPs in different light-absorbing material layers by controlling the distribution, shape, and size of nanoparticles (NPs) inside the light-absorbing material's layers [8].

The benefits of metal halide perovskite materials, such as low charge recombination loss, long carrier diffusion lengths, and high defect tolerance, have led to a dramatic increase in PKSCs' power conversion efficiency (PCE) over the last decade, from 3.8 % to over 25 % [10]. Commercial production of perovskite solar cells requires that they meet or surpass established requirements for efficiency, durability, and longevity in the field. Long-chain carbon-based organic spacer cations have been discovered to increase device performance and stability in 2D-3D perovskite solar cells, for instance. In this paper, the latest research results on mixed-dimensional perovskite solar cells are presented and discussed to provide a critical evaluation of the sources of stability and performance improvement. When theoretical and experimental data are compared, we can better understand the role that factors like perovskite composition, film formation processes, solvent, and additive engineering play in determining efficiency and stability and so direct future research efforts toward the most promising avenues for improvement.

PKSCs are one of the most interesting photovoltaic technologies that are now in the process of development. They have an exceptional power conversion efficiency (PCE) and use a solution approach that is simple and inexpensive. By 2020 [11], approved PSC efficiencies are expected to reach 25.2 %, making them a competitive option for application as both standalone photovoltaic modules and as component cells in high-efficiency perovskite silicon tandem solar cells [12]. Perovskites typically have the structural formula ABX_3, where A is a monovalent organic (CH_3NH_3 (MA: methylammonium)) or inorganic (Cs and Rb) cation, X is a halogen anion (Cl, I, or Br) and B is a divalent metal ion (Bi, Pb, and Sn) [13]. Two different kinds of third-generation solar cells, namely BHPSCs (Bulk heterojunction polymer solar cells) and PKSCs, have been introduced. The configurations, materials, mechanisms, and present state were summarized, revealing their similarities and differences.

2. The efficiency improvement of solar cells

In recent years, organic photovoltaics and perovskite solar cells have both seen significant increases in their power conversion efficiencies, reaching around 18 % [14] and 25 % [15], respectively. It explains how the use of these material systems has improved fun-

damental photophysical processes and the reliability and durability of devices. These 2D material systems, with their high environmental stability, high mechanical flexibility, low environmental impact, and low electrical resistance, have the potential to be used to develop lightweight, cost-effective, high performing, environmentally friendly, and flexible solar cells in the future [13]. High power conversion efficiency (PCE) is often attained on device areas less than 0.1 cm^2 in organic photovoltaics. Liu and his team described solar cells with a certified PCE of 15.24 percent based on D18:Y6 absorber layers. It is common to find that the aperture or specified area of organic photovoltaics (OPV) devices with high PCE is less than 0.1 cm^2 and, in most instances, less than 0.05 cm^2 [16]. A graphic produced by the National Renewable Energy Laboratory (NREL) and tables detailing solar cell efficiencies is used by scientists to compare the efficiency records of various photovoltaic systems under "1 sun" (the worldwide AM1.5 spectrum) [17].

3. Device fabrication and measurements

BHPSCs and PKSCs have been discussed before, and their parallels and contrasts in their photovoltaic capabilities are outlined in this section. The value of the open-circuit current (VOC) defines the photovoltaic performance of a solar cell, the short circuit current (Jsc), the fill factor (FF), and PCE, which are taken from the current–voltage characteristics. PCE is mainly determined by solar cells' VOC, a crucial photovoltaic property. Previous research has shown that in heterojunction polymer devices, the VOC is mostly dictated by the energy gap between the acceptor's lowest unoccupied molecular orbital (LUMO) and donor's highest occupied molecular orbital (HOMO) [18,19].

Techniques for fabricating BHPSCs and PKSCs are available in various ways. Polymer and Perovskite films are often deposited using solution-processed techniques. Spin-coating, printing, or spray-coating are examples of processes that use solvents to dissolve and deposit precursors onto a substrate [19]. Donor and acceptor are dissolved in a common solvent, such as chlorobenzene, in polymer devices before being deposited in a single step. In contrast, the absorbers in perovskite devices are deposited in a single or a two-step procedure, as shown in Fig. 2. Spin-coating the substrate with a solution of CH_3NH_3I and PbI_2 is a standard one-step procedure. PbI_2 solution is first coated, and then a solution of MAI is spun on top of it in a two-step procedure. Even though the one-step approach is more challenging to manage than the two-step method for perovskite film morphology, it is the most cost-effective and accessible technology. dimethylformamide (DMF) and γ -butyrolactone are the solvents used for perovskite materials [20,21]. Laser-based methods and the previously described desired solution procedures are commonly used to create large-area modules of these devices [21,19].

3.1. Utilization of noble metals and metal oxides in polymer solar cell devices

Integrating noble metal nanostructures into organic solar cells can enable them to function better by dispersing the incoming light to the active layer. To maximize the effect of the extra photons absorbed in the active layer, the active optical route length of the incoming photons should be as long as possible. Nanostructured metal oxides and noble metals are now included into the design of bulk heterojunction polymer solar cells (BHJ PSCs). PCSs use fullerene electron acceptors, and their performance, optical and structural features will be presented in this review. Theoretically interpreted effects of gold (Au) and silver (Ag) metallic nanoparticles (NPs) integration on PSC performance are discussed. Additionally, we examine the impact of adding metal oxide nanoparticles, such as ZnO and TiO_2, into organic solar cells [22,23].

3.2. Role of polymers in perovskite solar cell devices

The polymer approach is frequently employed, for example, by including polymer additives into the perovskite active layer AL, by utilising polymeric charge transport layer (CTL), incorporating polymer dopants into the CTL (i.e., hole transport layer (HTL) and the electron transport layer (ETL)), by capping polymer encapsula-

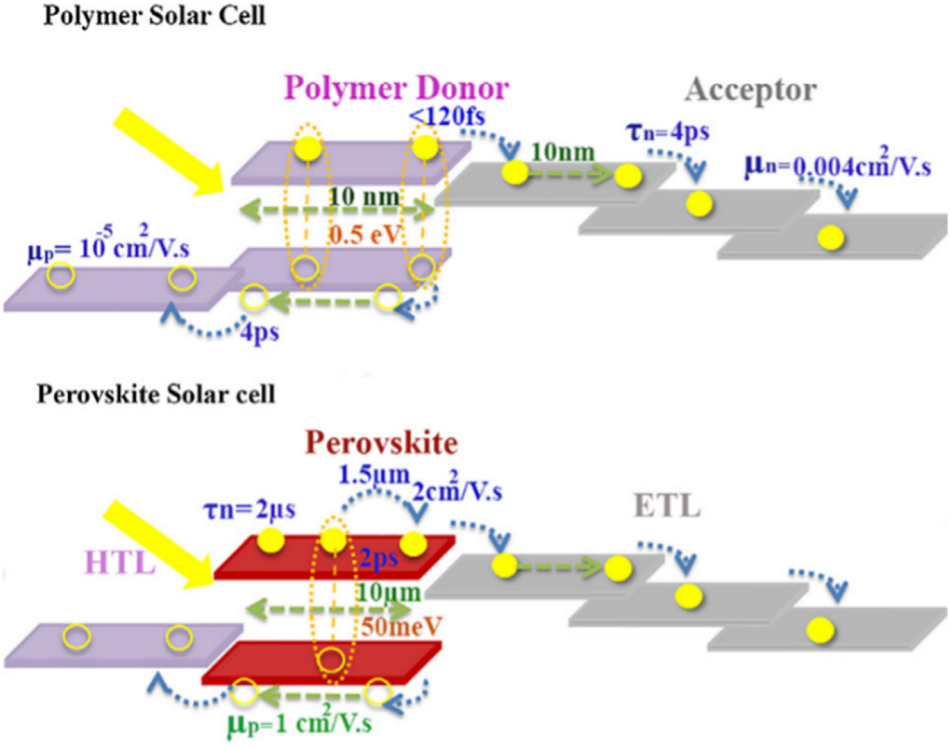

Fig. 2. Schematic representation of exciton formation and dissociation in V and PKSCs and their properties [21].

tion layers (EL), and by inserting polymeric interface layers (IL). Studies have also shown that polymer additives to charge transport layer materials, including small organic molecules, inorganic metal oxides, and polymeric semiconductors, can enhance PSC performance and stability. Another polymer strategy uses a polymer as a CTL material. ETL (non-fullerene-based, fullerene-based, and inorganic material base ETL) and HTL (small organic molecules-based inorganic metal oxides-based, and polymer-based HTL) polymer additives are summarised in [24].

Conducting polymers has boosted perovskite solar cells' environmental stability and performance by being used as nanocomposites, CTL, and passivation. Perovskite solar cells use various conducting polymers to fine-tune their shape and passivate their charge trap sites. To enhance the efficiency and durability of perovskite solar cells, researchers have recently turned to hybrid structures made of perovskite and conducting polymer. In these PSCs, the perovskite absorber layer generates charges when it encounters light, resulting in the creation of excitons. They also diffuse across the hole and electron selective contacts [25]. The energy levels provide a path with the least amount of loss in the layers of solar cells. Once at the electrodes, the charges may be used to power an external load through a connecting circuit. Fig. 3 depicts the PSC's schematic energy levels and functioning principles [26].

Perovskite materials have made great advancements in solar cells, but their susceptibility to water, oxygen, and UV irradiation has hindered their commercialization. Perovskites are hydrophilic and absorb water to form hydrates [27]. These compounds might also break into the lead and organic salts if exposed to dampness. At higher temperatures, perovskites' photostability becomes an issue. When these substances are heated, they decompose into lead salts. This causes perovskite solar cells to lose their photostability and performance at higher temperatures. CsFAMA perovskite film performance was further studied by Chen et al. by investigating the influence of a poly(bithiophene imide) (PBTI), conjugated polymer addition [28]. As demonstrated in Fig. 4, PBTI's polythiophene backbone played a vital role in passivating grain boundary defects by forming PbeS coordination, which enhanced film performance and stability while preventing ion migration.

By means of electrochemical polymerization, three hole-transporting materials (HTMs) with distinct work functions, including poly(p-phenylene) (PPP), polythiophene (PT), and poly (4,40-bis(*N*-carbazolyl)-1,10-biphenyl) (PPN), have been easily synthesised. The polymers were very compatible and wettable in dimethylformamide (DMF) solution. As shown in Fig. 5, DMF had

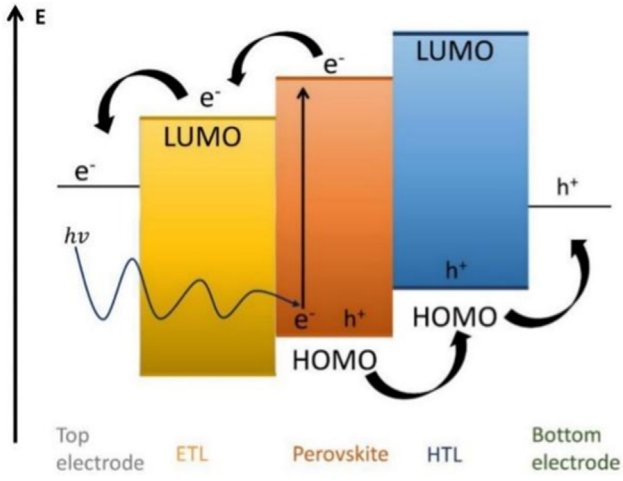

Fig. 3. A typical perovskite solar cell's energy levels and working principle [26].

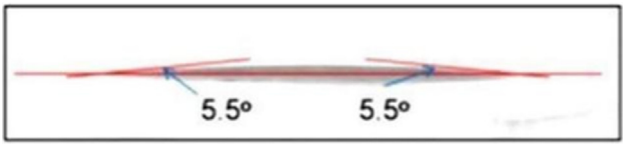

Fig. 5. Dimethylformamide contact angle of poly(p-phenylene) film [30].

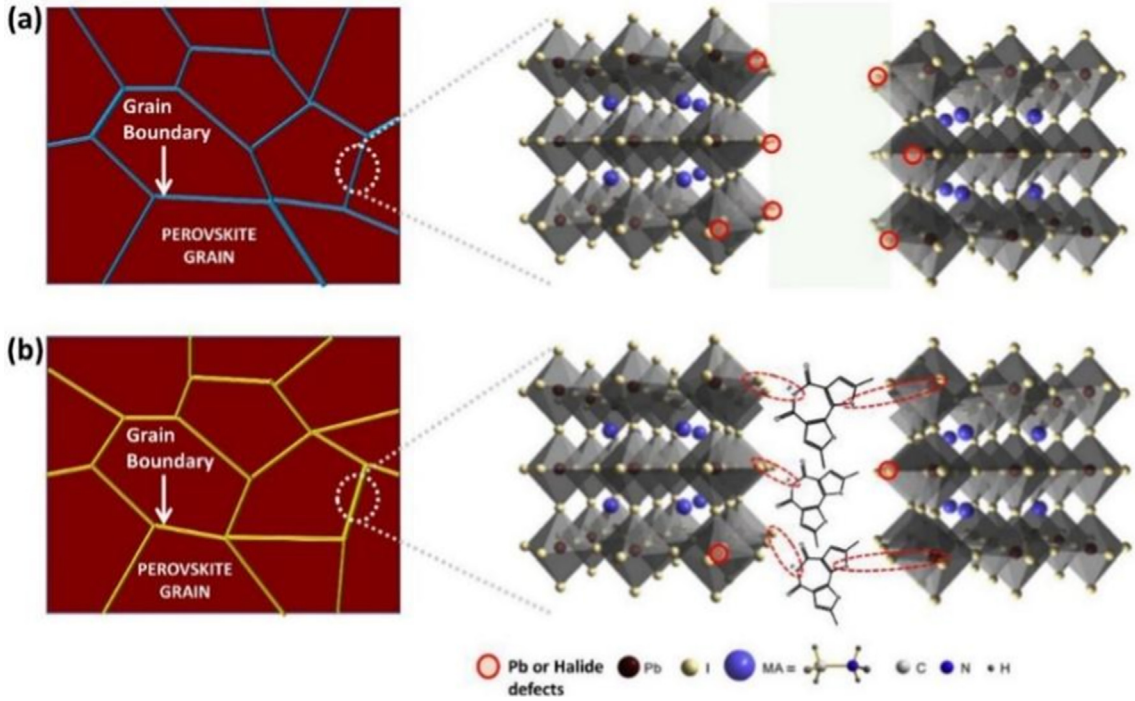

Fig. 4. Schematic depiction of the grain boundaries and associated defects in (a) chlorobenzene treated and (b) PBTI treated Perovskite films [28].

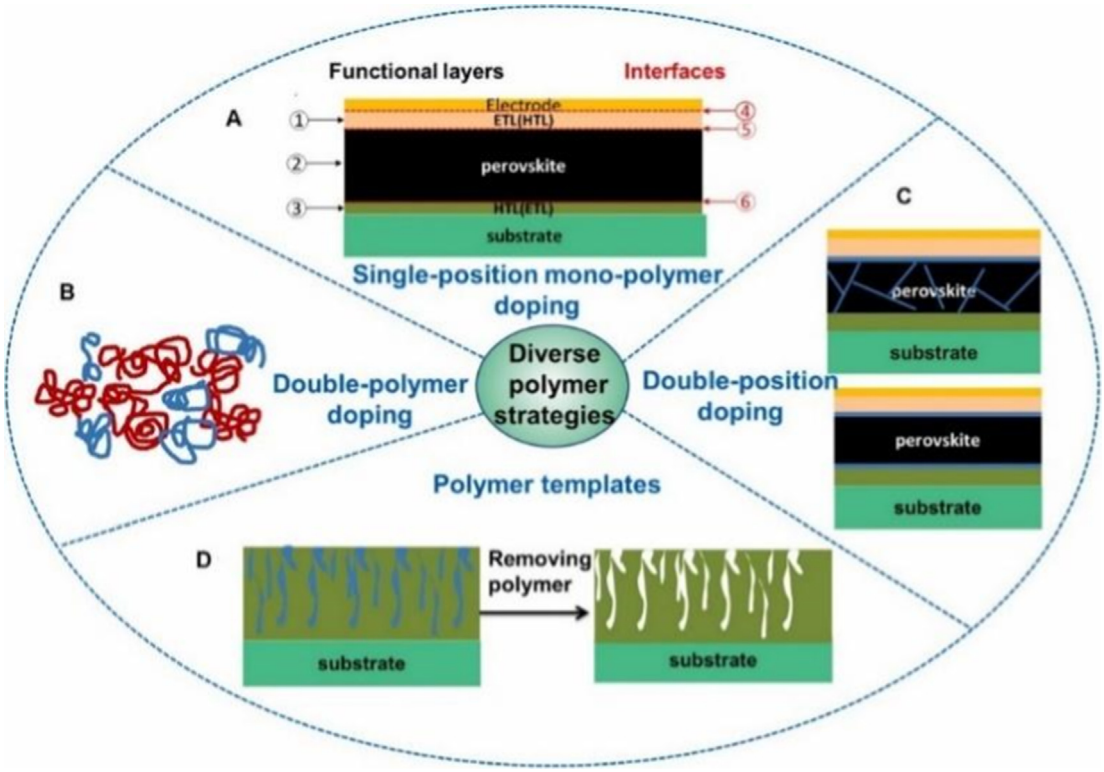

Fig. 6. Diagrams showing the many ways in which polymer techniques are used in PKSCs. There are four types of polymer doping: (a) single-position mono-polymer doping, in which a single polymer is introduced into a single functional zone (the perovskite layer, the HTL, or the ETL), or inserted into an interface (the perovskite layer, the HTL, the ETL, or the electrode). (b) double-polymer doping, in which polymer mixtures are used. (c) doping in two functional regions (double-position doping). (d) a polymer acting as a sacrificed template [29].

a contact angle of 5.5° with PPP, whereas the contact angles for PPN, PEDOT: PSS, and PT were 6.5°, 5.7°, and 2.6°, respectively. This enabled us to fabricate perovskite films with high crystallinity and a smooth surface [29,30].

The polymer approach has a great capacity to improve device performance and strengthen device stability. PMMA was utilised as a template to regulate crystal development and nucleation by Bi et al. [31]. As a result, the device's stability was improved, and its PCE could reach 21.6 % without exhibiting any J-V hysteresis behaviour at all. PMMA and polystyrene PS have been introduced into the perovskite/HTL and perovskites/ETL interfaces by Wu et al. & Peng et al. Consequently, the PCE values of the PKSCs were 21.89 percent and 20.8 percent, respectively, with no J-V hysteresis [32,33].

Perovskite anode layer, charge transfer layers (both HTL and ETL), and electrodes are typical components in PKSCs. This is true regardless of whether the configuration is *n*-i-p or p-i-n. Interfaces between the electrode and the ETL, the ETL and the perovskite, the perovskite and the HTL, and the HTL and the electrode are all present in these devices. The overall device performance is determined by the individual functional layer and interface levels. The ease with which polymer may be included into PSCs means that polymer methods can be used to optimise any functional layer or interface, leading to improved final device performance (Fig. 6a). Using more than one polymer is another way to enhance PKSCs (Fig. 6b).

Furthermore, The combination of rigid PMMA and pliable PS in the perovskite active layer was reported to enhance crystal formation and pliability by Yao et al [34]. Adding both PFNOX and PS as polymers to ETL films, as was done by Zhu et al., may boost both the films' electron transport performance and their morphology [35]. poly(methyl methacrylate) (PMMA) and Poly (3-hexylthiophene) (P_3HT) polymers, which may be added to single-walled carbon nanotubes (SWNTs) to create a superior moisture- and heat-resistant HTL, were proven by Habisreutinger et al. [36]. PKSCs may also be improved by introducing the same polymer into several components (Fig. 6c). To improve defect passivation, At the interfaces between the perovskite and ETL and the perovskite and HTL, Peng et al. used ultrathin PMMA films. At open-circuit voltages up to 1.22 V, the second interfacial layer suppressed non-radiative recombination on perovskite surfaces and grain boundaries [33]. Coatings of polarised ferroelectric (PFE) polymer were applied to the perovskite layer as well as the interfacial dipole layer that was located between the perovskite and the HTL layer [37]. This resulted in a PCE of 21.38 percent and an open-circuit voltage of 1.14 V for the PSCs. Polymers are added to the functional layer and then left there. After the functional layers are constructed, specific polymers must be removed (Fig. 6d) [29].

4. Conclusions and prospect

BHPSCs and PKSCs, two types of third-generation solar cells, were presented in comparison. An overview of their configurations (materials, mechanisms, and present condition) highlighted the similarities and variations between them. For instance, donors and acceptors of BHPSCs such as P_3HT and PCBM are being investigated for PSCs potential HTM and ETM. Several of the same components, such as high-temperature laminates, electrolytic layers, and contacts, are in use in both devices, as has already been highlighted. The absorber layers' optical and electrical characteristics were the primary influence, and they were shown to have a large impact on the device's performance. It is possible to attribute the better electrical characteristics of Perovskites to the increased per-

formance of PSCs compared to BHPSCs. MXene 2D transition metal entered the solar cell manufacturing process in 2018 to improve the efficiency of energy generated and the stability of solar cells. A PKSC efficiency greater than 23.3 % was recently discovered by Yang et al. [38,39].

This review focuses on the basic features of introducing metal oxides and noble metals nanostructures into the BHJ PSCs, emphasising solar cell performance and optical and structural properties. The noble metals may be easily included in OSCs regardless of their location inside the device. Finally, in OSCs, plasmonic-assisted architectures have greatly improved device performance, mainly when applied to low bandgap polymer OSCs. It is possible to increase the infrared absorption of low bandgap polymers.

Nonetheless, a significant impact on the PCE in OSCs requires the careful manufacturing and adjustment of noble nanostructures. For a long-term stable device, it was necessary to consider the effects of solar deterioration as well as electron/hole mobility and energy level misalignment. With the recent efficiency of more than 15.19 % for PSC [40] and 23.3 % for PKSC [39], the resultant SCs demonstrated a steady-state power conversion efficiency and exceptional stability against humidity and light soaking for the related solar cells.

In conclusion, conducting polymers, such as poly[(thiophene)-*alt*-(6,7-difluoro-2-(2-hexyl-decyl oxy)-quinoxaline)] (PTQ10) and poly[3-(4- carboxybutyl)-thiophene-2,5-diyl] (P_3CT), continue to play an important role in the development of efficient and stable perovskite solar cells. As a result, conjugated polymers with multifunctional capabilities will be beneficial in lowering total material utilisation and achieving cost-effective perovskite solar cells.

Even though PKSCs' efficiency has increased to above 25 %, their commercialisation has been limited by the devices' inherent instability. While research has increased the lifetime of PKSCs between a few minutes and hundreds of hours, the approaches remain inadequate for practical deployment. The use of the polymer approach has the potential to help achieve this aim, but there are two significant obstacles to overcome. First, physical blending is by far the most common method for implementing polymer strategy. Because of poor polymer and ionic perovskite compatibility, the polymer/perovskite layer will have an inhomogeneous and micro void-containing morphology in PKSCs. Therefore, the polymer-host material phase separation may harm the device's performance and stability. Second, device performance is highly dependent on the included polymer concentration or thickness since available polymers have limited charge mobility and electrical insulation.

Data availability

No data was used for the research described in the article.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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