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# Applications of Two-dimensional Materials in Perovskite Solar Cells

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**Abstract:**

As a new type of solar cell, perovskite solar cells (PSCs) exhibit significant potential due to the high performance. In recent years, they have garnered substantial attention due to their impressive photovoltaic conversion efficiency, low production costs, malleability, and other advantageous characteristics. However, there remains considerable room for the improvement in the performance of perovskite solar cells. Key factors that critically influence their performance include the charge transport layer, electrode materials, and overall cell structure. Two-dimensional (2D) materials, as emerging substances, facilitate the modifications of PSCs and enhance the electronic conduction. In this paper, a concise overview of perovskite solar cells is provided, followed by a summary of the current progress in enhancing their performance. The applications of 2D materials in the solar cell sector are highlighted. Finally, the existing challenges and issues confronting perovskite solar cells are discussed. This work will help promote the application of 2D materials in PSCs.

**Keywords:** Perovskite solar cells; two-dimensional materials; application.

## 1. Introduction

At present, perovskite solar cells (PSCs) have garnered substantial attention as a critical area of study in the field of photovoltaics [1-3]. In comparison to conventional solar technologies, including dye-sensitized and silicon-based solar cells, perovskite solar cells (PSCs) are considered to offer greater potential for future innovation and development. The advantages of PSCs include their low manufacturing costs, high energy conversion efficiency (ECE), and remarkable flexibility. These characteristics position PSCs as formidable contenders in the diverse landscape of solar energy technologies. However, the stability of PSCs is poor. Meanwhile, the risk of lead leakage is also a limiting factor for the further development of PSCs. A lot of researches on this topic have been conducted. It is reported that the use of advanced nanomaterials in PSCs can improve their performance effectively.

As a kind of nanomaterials, two-dimensional (2D) materials exhibit only one or a few atoms in thickness. It is acknowledged that 2D materials are more convenient for chemical modification and electronic conduction. Meanwhile, the flexibility and transparency of 2D materials are also very impressive. The largest family of 2D materials is the MXene family. It consists of three-dimensional parent materials called MAX phases. In addition, it is created to be 2D materials by removing the element A with acid. According to previous researches, using this material in PSCs can help achieve improved performance. In recent years, this material has garnered considerable attention from researchers and has emerged as a prominent area of study. Consequently, investigating 2D materials and their potential applications in PSCs holds significant importance.

This paper discusses the advancements in PSCs. It also outlines various strategies aimed at enhancing their performance and explores the potential applications of 2D materials in this context.

## 2. Perovskite Solar Cells

### 2.1 The Development Status of PSCs

Perovskite was first discovered in 1839 by Von Perovski. Till now, hundreds of such materials with perovskite structure are known. It has a wide range of family members from conductors to insulators. Perovskite materials are characterized by the general formula $ABO_3$. In their research, Miyasaka et al. utilized the perovskite compounds $CH_3NH_3PbI_3$ and $CH_3NH_3PbBr_3$ as sensitizers in solar cells [4]. The dye-sensitized solar cells were fabricated by incorporating a solid polypyrrole-carbon black composite as the hole transport layer. It has been reported that the solar cell in its as-prepared state demonstrates an energy conversion efficiency (ECE) of 0.4% under one atmospheric mass of sunlight. In addition, a liquid $I^-/I_3^-$ electrolyte was utilized as the hole transporting material, achieving an ECE of 2%. $CH_3NH_3PbI_3$ was also employed by this team in PSCs combined with liquid $I^-/I_3^-$ redox pair as electrolyte. The ECE was reported up to 3.5% [4]. The surface treatment of $TiO_2$ and the preparation methods of perovskite materials were systematically optimized by Park [5]. As a result, the external charge extraction efficiency of the newly prepared solar cells attained an impressive 6.5%. However, perovskite-sensitized solar cells that utilize liquid electrolytes suffer a critical limitation. The liquid electrolyte can dissolve or decompose the perovskite material, leading to cell failure within minutes. An intriguing alternative to address this issue is the integration of a robust electrolyte as the hole transport layer, as it is suggested in the study conducted by Miyasaka in 2008 [6]. This research emphasized the efficacy of 2,2,7,7-tetrakis(N,N-dimethoxy-phenylamino)-9,9'-spirobifluorene (Spiro-OMeTAD), which is also known as a highly effective medium for hole transport. The energy conversion efficiencies achieved by solar cells sensitized with perovskite materials are largely enhanced. It is reported that ECE reached up to 8% in $CH_3NH_3Pb(I_xCl_{3-x})$ and 10% in $CH_3NH_3PbI_3$.

Furthermore, the conductivity of Spiro-OMeTAD experienced a substantial enhancement. An increase by an order of magnitude of conductivity is achieved due to the implementation of doping techniques. This advancement played a crucial role in significantly boosting the external conversion efficiency of solid-state dye-sensitized solar cells (SDSSCs). It rose to nearly 7.2%. A significant breakthrough occurred in 2012 when SDSSCs boasted an ECE of 9.7% under standard test conditions. Meanwhile, it also demonstrates remarkable stability.

Subsequently, PSCs that incorporated $Al_2O_3$ as a replacement for $TiO_2$ in the barrier layer, alongside the utilization of perovskite $CH_3NH_3PbI_2Cl$ as the sensitizing dye, achieved impressive ECE enhancement (~10%). The significant progress observed in SDSSCs in 2012 can largely be attributed to the incorporation of perovskite-structured materials as the active layer. Within this context, PSCs utilized perovskite as the dye, while poly-(triarylamine) (PTAA) acted as the hole transport layer (HTM). Notably, PSCs that employed PTAA as the HTM in combination with chalcocite as the dye realized an outstanding ECE of 12.3%. Additionally, a planar heterostructured PSC developed by Snaith et al., which similarly utilized perovskite as the dye, achieved a remarkable conversion efficiency of 15.4%.

### 2.2 Performance

Doping the intermediate layer of solar cells is a widely used approach for enhancing their overall performance. Zheng et al. presented a groundbreaking method that utilizes gold nanoparticles (AuNPs) to dope perovskite films, which led to enhanced performance in PCSs [7]. Through their extensive calculations, they achieved a notable power conversion efficiency of 19.01%. Furthermore, the mechanisms by which AuNPs enhance the quality of perovskite films were elucidated through simulations and spectral analysis techniques. Moreover, Jason et al. skillfully developed electron transport layers that are distinguished by optimal film coverage, thickness, and composition through careful modulation of the chemical bath deposition process for $SnO_2$ [8]. They successfully differentiated the passivation techniques applied to both the bulk material and the interfacial layers, which led to enhanced device performance and a significant decrease in energy band losses. Under forward bias conditions, the PSCs demonstrated an impressive external quantum efficiency for electroluminescence (~17.2%). Additionally, it also showed an exceptional electroluminescence external conversion efficiency (~21.6%). In terms of the performance of solar cell, these devices have achieved a certified power conversion efficiency of 25.2%. Meanwhile, there are some theoretical ways to improve their conversion efficiency which have not yet been put into practice. Luo et al. elaborated that due to the large number of non-radiative composite channels in practical PSCs, the vast majority of photogenerated carriers will preferentially composite via other non-radiative pathways [9]. The non-radiative complexation loss processes significantly diminish the steady-state concentration of photogenerated carriers within the cell. This reduction subsequently leads to a decreased energy level difference in the quasi-Fermi energy level splitting present in the metal halide perovskite layer. Ultimately, this phenomenon contributes to a substantial voltage loss in PSCs. Therefore, it is essential to identify strategies aimed at reducing these non-radiative recombination pathways. This will significantly improve both the open-circuit voltage and the photovoltaic conversion efficiency of the devices.

## 3. Applications of 2D Materials in PSCs

2D materials have garnered significant interest from the scientific community, owing to their remarkable properties. 2D materials are only one or a few atoms in thickness, with a lateral size of a few micrometers. Electrons in these materials are confined to 2D space, which gives rise to novel physical, electronic, and chemical properties. Graphene, one of the most significant 2D materials, has attracted substantial interest. The techniques utilized for its synthesis encompass mechanical exfoliation (ME), liquid phase exfoliation (LPE), and chemical vapor deposition (CVD). The largest family of 2D materials is the MXene family, which consists of three-dimensional parent materials known as MAX phases.

### 3.1 Graphene

Zhang et al. proposed graphene can be used as a charge-transport layer material for PSCs [10]. This method significantly improved the trapping efficiency of photogenerated electron and hole pairs. It was found that in graphene composite charge transport materials, the specific performance of added graphene can be demonstrated when the graphene mass ratio is within the range from 0.4% to 7%. Graphene composite charge transport materials also exhibit good technological economy. Therefore, graphene composites will become a new driving force to promote the development of PSCs.

Wang et al. prepared a dense layer by spin-coating ultrasonically dispersed graphene and $TiO_2$ composite sol on the surface of a conductive glass, which required an annealing temperature of less than 150°C [11]. The dense layer that was formed showcased graphene, which served as a continuous 2D conductive framework. Furthermore, $TiO_2$ nanoparticles were attached to graphene nanosheets. This arrangement demonstrated that graphene effectively reduced series resistance and minimized charge compounding losses, leading to an enhanced battery efficiency of 15.6%.

Han et al. employed a nanocomposite film composed of reduced graphene oxide (RGO) and mesoporous $TiO_2$ to serve as the electron transport layer. This innovative approach yielded an 18% increase in photovoltaic conversion efficiency when RGO comprised 0.4% of the volume fraction of the composite film [12].

### 3.2 MXene Material

In addition, if carbon is used as a substitute for expensive metal materials such as gold and silver, costs can be effectively reduced while maintaining the same performance [13]. Carbon electrodes contain a large number of carbon particles, resulting in a smaller contact area with the active layer, which in turn generates a larger contact resistance and adversely affects transmission[14]. To address this issue, Mi et al. added 2D $TiC_2T_x$ and carbon nanotubes to a commercial carbon paste to form a hybrid carbon electrode in perovskite thin-film solar cells, as shown in Fig. 1. While contributing its high conductivity properties to the hybrid electrode, $TiC_2T_x$ also provides a lattice structure and a three-dimensional charge transfer pathway [15].

Cao et al. sprayed $TiC_2T_x$ paste on the light-absorbing layer of perovskite, and then formed the back electrode after pressing it using the hot pressing method [16]. The results showed that the average resistance of $TiC_2T_x$ back electrode was only around 25 Ω, which is only 1/6 of that of the carbon electrode. It demonstrated significantly improved electrical conductivity. Furthermore, it established a secure interface between the electrode and the perovskite layer, thereby enhancing the stability of the PSCs [17].

MXene is utilized as an additive in PSCs to enhance their crystallinity. The excellent conductivity of MXene facilitates a charge transfer channel to the active layer of the perovskite material. In 2008, MXene was used as an additive to $MAPbI_3$ perovskite. It was observed that MXene can enhance the nucleation time of $MAPbI_3$. Besides, the light absorption capacity of its light-absorbing layer is significantly increased. In addition, electrochemical impedance test (EIS) showed $TiC_2T_x$ increased the carrier mobility inside the device. Guo et al. increased the $MAPbI_3$ conversion efficiency from 15.5% to 17.4% after the addition of 0.03% $TiC_2T_x$.below [18].

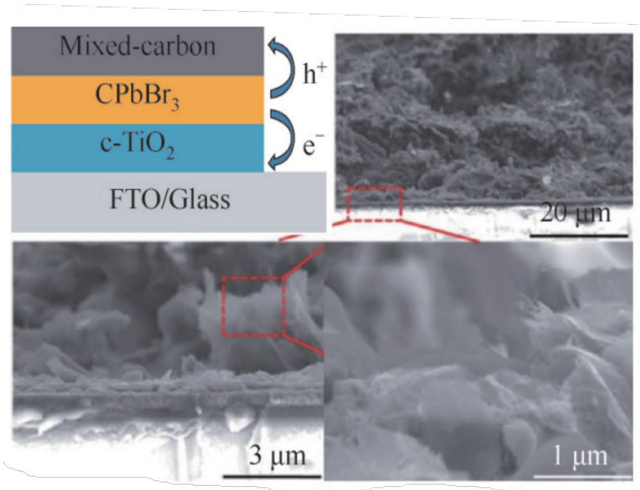


**Fig. 1 Device structure of a PSCs using a hybrid carbon electrode and SEM image of the cross-section of the hybrid carbon electrode [18]**

### 3.3 2D III-V Group Heterogeneous Materials

Gallium Arsenide (GaAs) is recognized as an exceptional semiconductor material, primarily due to its direct bandgap and its classification within the III-V group of materials. Significantly, GaAs solar cells have exhibited unparalleled photovoltaic conversion efficiencies when compared to other single-junction solar cells. In recent years, there has been a steady progression in the efficiency benchmarks of GaAs solar cells. A predominant number of high-efficiency GaAs solar cells documented in the literature employ semiconductor materials that feature relatively thick absorbers in conjunction with smooth top surfaces. In a prominent study conducted by Steiner et al., high-quality GaAs solar cells were developed with an integrated backside reflector, which led to high conversion efficiencies (~27.8%). These solar cells capitalize on the photon recycling effect to achieve the enhancecment of equilibrium density of photogenerated carriers.

Indium phosphide (InP) crystals are a significant category of ternary compound semiconductors, boasting a band gap of 1.35 eV, which is near the ideal threshold for single-junction solar cells. Nevertheless, the photoelectric conversion efficiency of InP-based solar cells is relatively lower compared to GaAs solar cells. This discrepancy in performance can primarily be attributed to factors such as their reduced open-circuit voltage and lower fill factor. Despite these challenges, InP solar cells offer a promising solution for space-related applications, particularly when employed in multi-junction solar systems, which sets them apart from solar cells. Furthermore, the enhanced radiation resistance of InP provides a notable advantage over GaAs and silicon materials in the context of space applications.

## 4. Challenge

The most significant challenge facing the widespread adoption of perovskite crystal materials lies in their low stability. To precisely assess the stability of perovskite devices, it is crucial to take into account a range of degradation factors and mechanisms. These factors include variations in temperature, humidity levels, halide concentrations, and the movement of dopants. Conducting tests on these devices at elevated temperatures which exceed 60°C can precipitate substantial degradation. Notably, the thermal instability of methylammonium (MA) cations within perovskite films is identified as the primary contributor to thermal degradation.

During the development of PSCs, it was inevitable to consider the leakage of the element Pb. Pb-based perovskite are converted to $PbI_2$ when it is degraded. Afterwards, $MAPbI_3$ undergoes a spontaneous and irreversible dissolution process when it encounters $H_2O$. The typical decomposition products are $CH_3NH_2$, HI, and $PbI_2$. Among these products, HI is formed by the presence of light or oxygen. It is also shown that $H_2O$ reacts with the Pb sites, exposing I element by rapid dissolution on the surface of the perovskite and forming stronger Pb-I bonds on the surface. Subsequently, hydrated phases are formed which lead to faster dissolution of the perovskite. The final result is $PBI_2$ or monomeric Pb. As $Pb^{2+}$ from the decomposition of perovskite gradually diffuses into the environment, it can cause serious damage to the human blood system and nervous system. Therefore, the toxicity of Pb and the harm it causes cannot be ignored [19].

## 5. Conclusion

Overall, PSCs have made impressive development in recent years. Its highest certified photovoltaic conversion efficiency has reached more than 26%. Compared with mainstream silicon solar cells, PSCs have a low manufacturing cost, available solution processing, high flexibility. 2D materials are also one of the new materials in recent years. This study explores the utilization of two-dimensional materials in PSCs, including graphene and MXene. It is demonstrated that combining 2D materials with perovskite cells can further improve the performance of PSCs.

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