Application status of perovskite in solar cells

Xinle Du *

Jiangxi University of Technology High School, Nanchang, China

* Corresponding Author Email: 2961929707@qq.com

Abstract. Solar cells have emerged as a clean, sustainable, and efficient energy technology, playing a critical role in the global transition to renewable energy and carbon reduction. Among various types of solar cells, perovskite solar cells have gained significant attention due to their remarkable efficiency, tunable photoelectric properties, and cost-effective production methods. These advantages make perovskite solar cells a promising candidate for next-generation photovoltaic technologies. However, despite their immense potential, challenges such as stability, environmental adaptability, and long-term operational reliability must be addressed to enable their large-scale application. This review delves into the operational principles of solar cells, focusing on the ABX_3 structure of perovskite materials, which is essential for their superior performance. It further examines the complex degradation mechanisms, including UV-induced degradation, electrode ion migration, and material defects, that hinder device stability. By synthesizing recent research advancements, the paper provides a comprehensive understanding of perovskite material properties, degradation pathways, and strategies for performance optimization. These insights aim to support the development of durable, high-efficiency solar cells and contribute to sustainable energy solutions for global needs.

Keywords: Solar cells, perovskite materials, energy.

1. Introduction

Solar power is a process that uses the sun's light energy to convert it into electricity. It is a clean, renewable form of energy with many advantages. The principle of solar photovoltaic power generation is to convert sunlight directly into electricity through solar panels, solar panels are composed of multiple photovoltaic cells, and these cells are made of semiconductor materials, when the sun shines on the solar panel, the photons will excite the electrons in the battery, generating an electric current. It therefore produces no greenhouse gas emissions, helping to reduce the global carbon footprint and fight climate change. As a key technology for converting solar energy into electricity, solar cells are of great significance for realizing the efficient use of renewable energy, especially in the context of the global energy structure transformation and reducing carbon emissions, the research and application of solar cells are of great importance for promoting the development of green energy [1].

The perovskite structure, characterized by its distinctive ABX3 crystal configuration, is a semiconductor material renowned for its superior optoelectronic properties. These properties include high light absorption, significant carrier mobility, efficient energy conversion, and ease of fabrication. As a result, perovskites have garnered extensive attention and practical application in the field of solar cells, serving as a prime example of third-generation high-efficiency thin-film batteries [2]. Perovskite solar cells are seen as key contenders for sustainable energy solutions. At the heart of these devices lies the photovoltaic layer composed of perovskite material, which facilitates the conversion of solar energy into electrical power. The scope of applications for perovskite solar cells continues to broaden, encompassing areas such as the photovoltaic sector (including building-integrated photovoltaics, decentralized power plants, and ground-mounted stations) and the realm of new energy vehicles. The lightweight, flexible, and semi-transparent nature of perovskite batteries offers distinct advantages in building-integrated photovoltaic systems.

Despite its promising potential, the use of perovskite materials in solar cells presents certain challenges. One major issue is the stability of perovskite solar cells during prolonged operation, as these materials tend to decompose and degrade in humid and high-temperature conditions [3]. To

address this, inorganic perovskite materials can be employed, substituting inorganic cations for organic ones to enhance the long-term photostability and thermal stability of the cells. Additionally, ongoing research aims to refine the fabrication processes of perovskite materials to improve their environmental resilience. For instance, the ligand transformation strategy involving toluene-4-sulfonamide can regulate the crystallization of perovskite thin films at low temperatures, effectively reducing deep trap states by converting Sn^{4+} to Sn^{2+} [4].

2. How does perovskite solar work and its classification

2.1. The operational mechanism of a solar cell

Perovskite solar cells are a type of photovoltaic device that utilizes a perovskite structure material as the light-absorbing layer, sandwiched between two charge transport layers and connected to electrodes. They operate by absorbing sunlight, generating electron-hole pairs, and using an electric field to separate these charges, creating a flow of electrons that produces electricity. Perovskite materials, with their unique properties such as high optical absorption and charge carrier mobility, contribute to the efficiency of these solar cells. There are two main configurations for these cells: the conventional n-i-p and the inverted p-i-n structures, each with specific layers for electron and hole transport. The working mechanism of perovskite materials in solar cells is mainly as follows, which is divided into 6 steps: light absorption, electron and hole creation, electron field establishment, separation of electron and holes, electron flow, electrical output.

2.1.1. Light absorption:

Upon exposure to sunlight, the cell captures the energy primarily carried by photons. This interaction predominantly takes place in the top layer of the solar cell, which features an anti-reflective coating designed to minimize reflection and maximize the entry of light particles into the cell. The semiconductor material then absorbs these photons, effectively harnessing the sun's energy.

2.1.2. Electron and hole creation:

Once the photon energy is absorbed by the semiconductor within the solar cell, electrons, initially situated in the valence band (a lower energy level), absorb the photon energy and transition to the conduction band (a higher energy level). This transition results in the formation of free electrons and holes. A hole represents the positive charge that remains in the valence band when an electron is excited to a higher energy state. This phenomenon is illustrated in **Figure 1** with the caption "Sunlight provides the energy necessary to release more electrons and create more positive holes".

2.1.3. Electric field establishment:

Within the solar cell, a p-n junction exists, which a boundary is created by introducing different impurities into the material to produce p-type and n-type semiconductors. In p-type semiconductors, the primary charge carriers are holes (the absence of electrons), whereas in n-type semiconductors, the main charge carriers are free electrons. This junction inherently generates an electric field [5].

2.1.4. Separation of electrons and holes:

When p-type semiconductors and n-type semiconductors are in close contact, a special region is formed between them, that is, the p-n junction. In this region, due to the difference in the carrier concentration of the two semiconductors, a built-in electric field is created that prevents the holes in the p region from entering n. It also prevents the electrons in the n region from entering the p region. This separation creates an electric potential difference near the boundary [6].

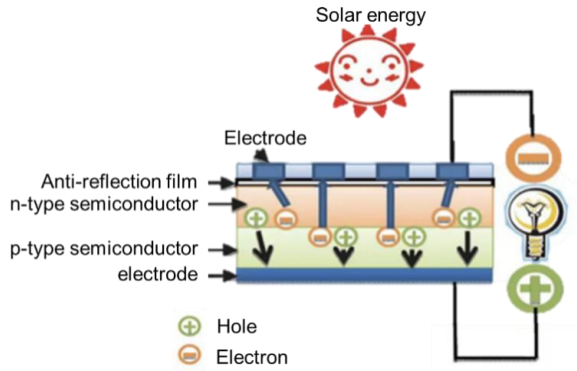

Figure 1. The basic structure of solar cells.

2.1.5. Electron flow:

Due to this potential difference, electrons will flow from the N-type semiconductor to the P-type semiconductor through the external voltage, resulting in an electric current. **Figure 2** shows the external circuit and notes "electrons move through the external circuit".

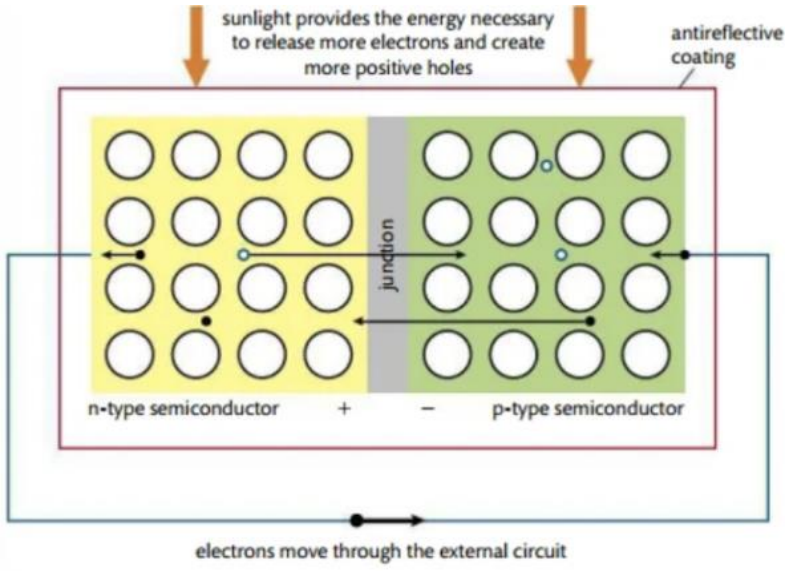

Figure 2. Movement of electrons in a battery [7].

2.1.6. electrical output:

The external circuit is connected to a load (such as a light bulb or battery), and the electrons release energy as they flow through the load, and then return to the P-type semiconductor to complete the circuit.

2.2. The mechanism of perovskite in solar cells

Perovskite materials originate from the calcium titanate ($CaTiO_3$) structure, which is characterized by an ABX3 molecular configuration. These materials have garnered significant interest due to their cubic lattice structure that features an octahedral layering, as well as their distinctive properties in terms of optics, thermal behavior, and electromagnetics [8]. In the context of solar cells, perovskites are organic-inorganic hybrid metal halides that maintain the perovskite structure. Within this structure, Group A consists of organic cations such as methylammonium (MA^+) or formamidinium (FA^+), which are positioned at the corners of a cubic lattice that is centered on each face. Meanwhile, the metal cation B, which could be lead (Pb^{2+}) or tin (Sn^{2+}), and the halogen anion X, which could be chlorine (Cl^-), bromine (Br^-), iodine (I^-), or a mixture of halogens, are situated at the center and the tips of the octahedra, respectively. These metal-halogen octahedra interconnect to create a robust three-dimensional framework. A visual representation of the crystal structure can be found in Figure3

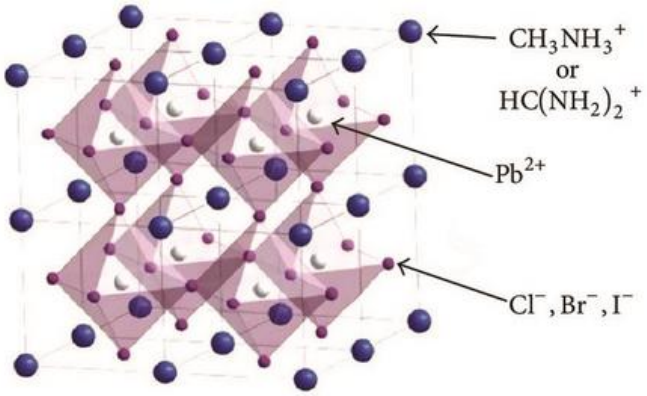

Figure 3. Metal-halogen octahedra interconnect crystal structure of Perovskite materials [9].

These materials exhibit four key features. Firstly, they are endowed with superior photoelectric properties, which include a reduced exciton binding energy and an enhanced optical absorption coefficient that can reach up to 10^4 cm^{-1}. Secondly, when employed as the light-absorbing layer, perovskites demonstrate an exceptional ability to harness solar energy efficiently. Thirdly, these materials are characterized by a high dielectric constant, which facilitates the effective transmission and collection of both electrons and holes. Lastly, the simultaneous transport of electrons and holes is possible, with the distance they can travel being significant, extending to 100 nm or greater, and in some cases, exceeding 1 μm [10].

In the realm of solar cell technology, materials with a particular structure exhibit several notable characteristics that significantly enhance their performance. These attributes result in elevated open-circuit voltages (Voc) and short-circuit current densities (Jsc) when integrated into solar cell devices. Upon sunlight exposure, the perovskite layer is responsible for the initial absorption of photons, which leads to the creation of excitons, or electron-hole pairs. The exciton binding energy in perovskite materials varies, allowing these excitons to either dissociate into free carriers that generate current or recombine into excitons. The low recombination rates of carriers in materials such as $CH_3NH_3PbI_3$ ($MAPbI_3$) and other perovskites, coupled with their high carrier mobility, result in extended diffusion distances and lifetimes for the carriers. For instance, the carrier diffusion distance in $MAPbI_3$ is at least 100 nm, and exceeds 1 μm in $MAPbI_{3-x}Cl_x$. These extended distances and lifetimes contribute to the superior performance of perovskite solar cells. Subsequently, the free electrons and holes are collected by electron transport materials (ETM) and hole transport materials (HTM), respectively. Electrons are transferred from the perovskite to TiO_2, which is utilized in ETM layers and ultimately collected by FTO glass. Concurrently, holes are transferred to the HTM layer and gathered by the metal electrode. Ultimately, the connection between FTO glass and the metal electrode completes the circuit, enabling the generation of photocurrent in the external circuit.

Perovskite solar cells are primarily structured in two configurations: the conventional n-i-p structure (**Figure 4**) and the inverted p-i-n structure (**Figure 5**). In the conventional n-i-p structure (**Figure 4**), the device is composed of several layers stacked in a specific order. The bottom electrode serves as the electron transport layer (ETL), typically made of materials such as tin oxide (SnO_2), titanium oxide (TiO_2), or PCBM. These materials are chosen for their ability to efficiently transport electrons and block holes, thereby reducing recombination losses. Above the ETL, the perovskite active layer is deposited. This layer is crucial as it absorbs sunlight and generates electron-hole pairs. The quality of the perovskite layer, including its crystal structure and defect density, significantly impacts the device's performance. Next, the hole transport layer (HTL) is placed above the perovskite layer. Common HTL materials include Spiro-OMeTAD, an organic compound known for its good hole transport properties, and inorganic materials like nickel oxide (NiO). The HTL facilitates the movement of holes towards the top electrode, ensuring efficient charge separation. Finally, the top electrode is typically made of noble metals such as gold (Au) or silver (Ag), chosen for their excellent conductivity and stability. This electrode collects the holes and completes the electrical circuit, allowing the device to generate power [11].

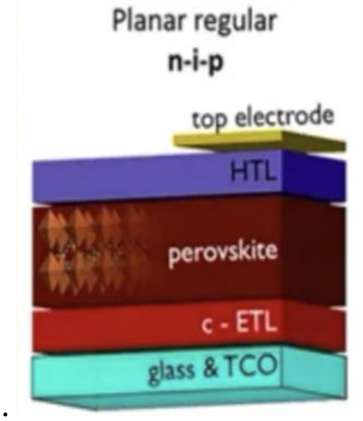

Figure 4. Configurations and application demonstration of PSCs. TCO: transparent conducting oxide; HTL: hole transport layer; ETL: electron transport layer [12].

In the inverted (p-i-n) structure of perovskite solar cells (**Figure 5**), the layers are arranged in a specific sequence to optimize charge transport and minimize recombination losses. The bottom electrode serves as the hole transport layer (HTL), which is crucial for the initial step of charge separation. Poly (3, 4-ethylene dioxythiophene) doped with poly (styrene-sulfonate) (PEDOT: PSS) is commonly used as the HTL due to its excellent hole transport properties and good compatibility with the perovskite layer. Alternatively, inorganic materials such as nickel oxide (NiO) can also be employed as the HTL, offering advantages in terms of stability and thermal resistance.

Above the HTL, the perovskite active layer is deposited. This layer is responsible for absorbing sunlight and generating electron-hole pairs. The quality of the perovskite layer, including its crystal structure and defect density, is critical for the overall performance of the solar cell. The perovskite layer must be well-aligned with the HTL and ETL to ensure efficient charge transport and minimal recombination.

The electron transport layer (ETL) is placed above the perovskite layer. Common materials used for the ETL in inverted structures include phenyl-C61-butyric acid methyl ester (PCBM) and zinc oxide (ZnO). These materials are chosen for their ability to efficiently transport electrons and block holes, thereby reducing recombination losses. The ETL plays a vital role in extracting electrons from the perovskite layer and transporting them to the top electrode.

Finally, the top electrode is typically made of metals such as aluminum (Al) or silver (Ag). These materials are chosen for their good conductivity and compatibility with the ETL. The top electrode collects the electrons and completes the electrical circuit, allowing the device to generate power. The inverted structure offers several advantages, including improved stability and flexibility in processing conditions, making it a promising architecture for the development of high-performance perovskite solar cell.

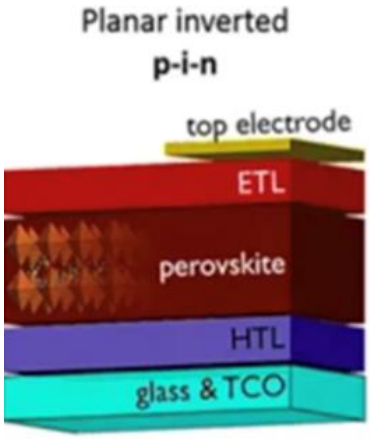

Figure 5. Configurations and application demonstration of PSCs. TCO: transparent conducting oxide; HTL: hole transport layer; ETL: electron transport layer [12].

2.3. Solar cell failure

About how the failure of solar cells is affected by perovskite materials, it is mainly reflected in the following aspects. Under ultraviolet (UV) irradiation, the titanium dioxide (TiO_2) electron transport layer in perovskite solar cells absorbs UV light, exciting electron-hole pairs. This process reduces the photoelectric conversion efficiency of perovskite solar cell devices. Additionally, UV irradiation causes the grain boundaries of the perovskite film to widen, leading to the decomposition of perovskite into lead iodide (PbI_2) [13]. The presence of gold (Au) nanoparticles accelerates this decomposition, contributing to the rapid degradation of perovskite solar cells. Metal Electrode Migration Problem: In perovskite solar cells, the gold (Au) element can migrate from the metal electrode to the interface between tin dioxide (SnO_2) and methylammonium lead iodide ($MAPbI_3$) [3] This migration affects electrode coverage and electron transport, leading to a continuous decline in device performance parameters. The interaction between Au and iodide (I^-) ions results in the formation of gold iodide, which releases electrons. The instability of AuI leads to its decomposition into metallic Au and elemental iodine (I_2), further deteriorating battery performance. The Field Shielding Effect Caused by Mobile Ions: The influence of mobile ions on field shielding is a key contributor to the performance degradation of perovskite solar cells [14]. A rise in the density of mobile ions (nION) markedly diminishes the steady-state power conversion efficiency (PCE). Furthermore, intensified field shielding exacerbates the discrepancy between the open circuit voltage (VOC) and the quasi-Fermi level splitting (QFLS). Failure mechanism under reverse bias: When a perovskite solar cell is subjected to reverse bias, it can lead to the injection of holes into the cathode, causing iodide oxidation. The resulting iodine (I_2) can then react with the metal electrode, such as copper, leading to electrode corrosion. This process generates metal ions, like Cu^+, which can migrate and reduce, ultimately causing a short-circuit failure in the device. Defects in perovskite materials, including reverse and gap defects, can significantly impact the performance and stability of devices. Exposure to light can induce the formation of metastable deep-level defect states within the energy gap, leading to a gradual decrease in photocurrent. Doping with elements like Cl ions can enhance the photostability of perovskite materials and mitigate the formation of deep-level defects. Overall, the degradation mechanisms of perovskite materials are multifaceted, involving various factors such as light, temperature, humidity, and material migration, which shown in **Figure 6**, all of which collectively contribute to the reduced performance and failure of perovskite solar cells [15].

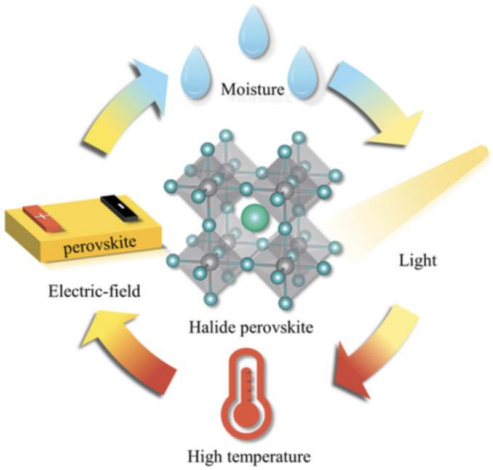

Figure 6. Factors affecting the application of halide perovskite [13].

3. Conclusion

This paper systematically studies the efficiency and stability of perovskite solar cells, summarizes recent advancements, and offers insights into current challenges. It details the six key steps of solar cell operation: light absorption, electron and hole generation, electric field formation, separation of electrons and holes, electron flow, and electrical energy output. The paper also discusses the structural

features of perovskite solar cells, including n-i-p and p-i-n structures, and analyzes failure mechanisms such as UV irradiation, metal electrode migration, and material defects. The study provides new ideas for improving stability and efficiency and aims to advance solar cell technology for sustainable energy solutions.

References

[1] Askari Mohammad Bagher, Mirzaei Mahmoud Abadi Vahid, Mirhabibi Mohsen, et al. Types of Solar Cells and Application. American Journal of Optics and Photonics, 2015, 3(5), 94-113, 2330-8494.

[2] Chuantian Zuo, HenkJ Bolink, Hongwei Han, et al. Advances in Perovskite Solar Cells. Advanced Science, 2016, 3, 7, 1500324.

[3] Juan-Pablo Correa-Baena, Michael Saliba, Tonio Buonassisi, et al. Promises and challenges of pero vskite solar cells. Science. 2017, 358, 6364, 739744.

[4] Shurong Wang, Huanhuan Yao, Weike Zhu, et al. Stabilization of Perovskite Lattice and Suppression of Sn2+/Sn4+ Oxidation via Formamidine Acetate for High Efficiency Tin Perovskite Solar Cells. Advanced Functional Materials, 2022, 33, 17, 2215041.

[5] Shruti Sharma, Kamlesh Kumar Jain¹, Ashutosh Sharma, et al. Solar Cells: In Research and Applications. Materials Sciences and Applications, 2015, 6, 12, 612113.

[6] Christopher M. Proctorb, Martijn Kuik, Thuc-Quyen Nguyen, et al. Charge carrier recombination inorganic solar cells. Progress in Polymer Science, 2013, 38, 12, 1941-1960.

[7] Ran Xu, Qing Zhang, Jing Yuan Wang, et al. Direct current triboelectric cell by sliding an n-type semiconductor on a p-type semiconductor, Nano Energy. 2019, 66, 104185.

[8] Dian Wang, Matthew Wright, Naveen Kumar Elumalai, et al. Stability of perovskite solar cells. Solar Energy Materials and Solar Cells, 2016, 147, 255-275.

[9] Di Zhou, Tiantian Zhou, Yu Tian, et al. Perovskite-Based Solar Cells: Materials, Methods, and Future Perspectives. Journal of Nanomaterials, 2018, 1, 814807.

[10] Martin A. Green, Anita Ho-Baillie, Henry J. Snaith, et al. The emergence of perovskite solar cells. Nature photonics, 2014, 8, 506–514.

[11] Drajad S. UtomoLauryna M. SvirskaiteAdi Prasetio, Nonfullerene, Self-Assembled Monolayers As Electron-Selective Contacts for n-i-p Perovskite Solar Cells. ACS Energy Letter, 2024, 9, 4, 1682–1692.

[12] Yaoguang Rong, Yue Hu, Anyi Mei, et al. Challenges for commercializing perovskite solar cells. Science, 2018, 361, 6408.

[13] Caixin Zhang, Tao Shen, Dan Guo, et al. Reviewing and understanding the stability mechanism of halide perovskite solar cells. InfoMat, 2020, 2, 6, 1034-1056.

[14] Boris Rivkin, Paul Fassl, Qing Sun, et al. Effect of Ion Migration-Induced Electrode Degradation on the Operational Stability of Perovskite Solar Cells. ACS Omega, 2018, 3, 8, 10042–10047.

[15] Lucy J. F. Hart, Fraser J. Angus, Yin Li, et al. More is different: mobile ions improve the design tolerances of perovskite solar cells. Energy & Environmental Science, 2024, 17, 7107-7118.