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Research Progress on Strategies for Enhancing the Stability of Perovskite Solar Cells

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Abstract. Perovskite solar cells (PSCs) have achieved remarkable leaps in power conversion efficiency as an emerging photovoltaic technology. However, their inherent instability remains a major barrier to commercialization. This review focuses on this bottleneck, systematically summarizing recent advances in enhancing device stability through three primary strategies: material modification, encapsulation techniques, and defect passivation. Despite persistent challenges, synergistic optimization of materials, structures, and processes has led to substantial improvements in stability. Looking ahead, the development of dynamic adaptive materials, precise defect repair techniques, and intelligent encapsulation systems will be key to transitioning PSCs from the lab to large-scale deployment.

Keywords: perovskite solar cells, photovoltaic durability, material modification, encapsulation techniques, defect passivation

1. Introduction

As the world confronts the dual pressures of energy transition and climate change, efficiently harnessing solar energy has become a strategic priority for nations worldwide. Photovoltaic technology, as the core means of solar energy utilization, plays a pivotal role in optimizing energy structures and achieving sustainable development. In this context, perovskite solar cells have emerged as a standout representative of third-generation photovoltaics, owing to their high absorption coefficient, tunable bandgap, excellent charge carrier transport properties, and compatibility with low-temperature solution processing. Notably, their power conversion efficiency has skyrocketed from 3.8% to over 25% in just over a decade, signaling immense commercial potential [1]. Yet a critical challenge persists: PSCs degrade under real-world stressors such as humidity, light, and heat, making instability the final obstacle to industrialization [2].

Research teams worldwide conduct investigations across materials, interfaces, device structures, and encapsulation. There is encouraging progress: the addition of specific additives makes the vertical cations uniformly distributed, suppresses phase separation, and enables the device to maintain an initial efficiency greater than 92% after 2500 hours of use [3]. The bifunctional additive can passivate defects and optimize energy level alignment, thereby improving efficiency and environmental tolerance. In terms of interface/device development, in situ polymer strategy [4] and self-healing radical molecules [5] offer new approaches to inhibit ion migration and repair transport-layer damage, paving the way for flexible PSCs. Furthermore, the ISOS standard is used to establish a framework for evaluating the reliability of PSCs [6].

Against this backdrop, this review systematically examines representative studies on PSC stability enhancement over recent years. It focuses on material modification, defect passivation, device structure optimization, and encapsulation, summarizing the mechanisms and potential of each strategy to guide the development of high efficiency. Through the adopted approaches, stability and durability under long-term operation are improved, thereby extending service life in actual use and enabling more efficient and economical power generation.

2. Working principle and structure of perovskite solar cells

Understanding how PSCs work and how their structures have evolved is fundamental to stability research. Unlike traditional silicon solar cells that rely on p–n junctions, PSCs adopt a typical "sandwich-like" multilayer heterostructure. A standard device comprises five functional layers stacked sequentially: a transparent conductive oxide (TCO) substrate, an electron transport layer (ETL), a perovskite light-absorbing layer, a hole transport layer (HTL), and a metal electrode [7].

In Figure 1, the incident photons with energy above the bandgap are absorbed by the perovskite layer, generating electron-hole pairs. Due to low exciton binding energy, the carriers separate into free electrons (e^-) and holes (h^+). Driven by the built-in electric field, electrons move to the ETL (like SnO_2 or TiO_2) while holes are collected by the HTL (for example, Spiro-OMeTAD). Finally, they are collected by the electrode, and a photocurrent is generated in the external circuit.

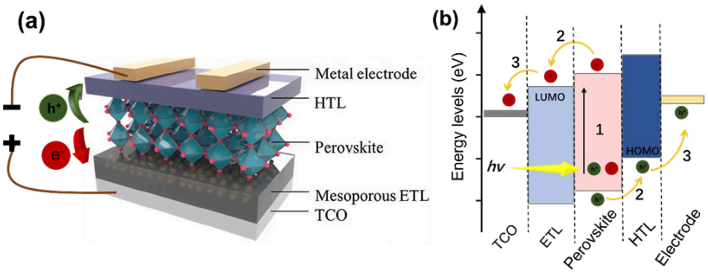

Figure 1. Schematic of PSCs operating principle [7]

From the perspective of structural evolution, the configurations of the main PSCs are divided into three categories. The first category is the mesoporous n-i-p structure, which originates from dye-sensitized solar cells. There is a mesoporous scaffold (such as TiO_2) on the conductive substrate to support the perovskite and help electron extraction. However, complex fabrication processes may affect stability. Secondly, the planar n-i-p structure, with each layer deposited planarly. This simplified design can reduce costs, but light absorption is relatively limited. Thirdly, the inverted p-i-n structure has attracted attention in recent years. Here, the charge transport layer is reversed: the HTL (NiO_x or SAM molecules) is at the bottom, and the ETL (PCBM) is on top. This structure has better process compatibility, weaker hysteresis effect, and better environmental stability, especially in moisture and oxygen resistance. Although its efficiency is slightly lower than that of n-i-p perovskite solar cells at present, it is easy to manufacture, compatible with flexible substrates, and can also be applied in series, which indicates significant potential as a promising commercial path.

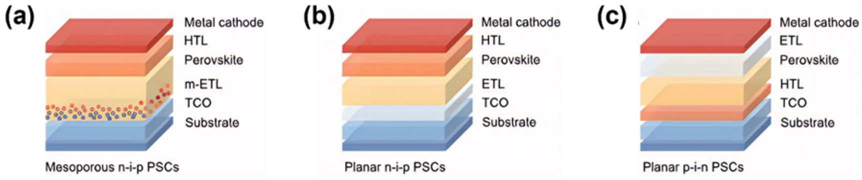

Figure 2. (a) Mesoporous n-i-p structure (b) Planar n-i-p structure (c) Inverted p-i-n structure [7]

3. Strategies for enhancing the stability of perovskite solar cells

3.1. Material modification

Perovskite materials have the "soft lattice" property, which makes them inherently unstable. Low lattice energy can lead to phase transitions and high ion mobility [8]. Under humidity, temperature, or light, these two factors will be exacerbated, accelerating degradation. To solve this problem, the material modification strategy primarily involves adjusting the lattice structure through ion doping. Entropy stabilization effects and lattice distortion control are used to suppress harmful phase transitions; they can also strengthen chemical bonds, limit ion migration, and improve stability [9].

Consider the case of the hybrid perovskite $MAPbI_3$, which is unstable because of low lattice formation energy. There are methods in the field of chemical engineering [10], and studies by Noh et al. show that placing Br at the I site can improve moisture resistance. Prepare thin films with different bromine contents. Observe for 20 days in an environment with 35% humidity at room temperature. Results: When the humidity suddenly rose to 55% on the 4th day, the light absorption rate of the low-bromine samples (x = 0, 0.06) decreased sharply, and the optical properties of the high-bromine samples (x = 0.20, 0.29) were relatively stable during the observation period (Figure 3). Appropriate bromine substitution inhibits the formation of the hydrated phase, thereby enhancing the material's ability to tolerate humidity fluctuations.

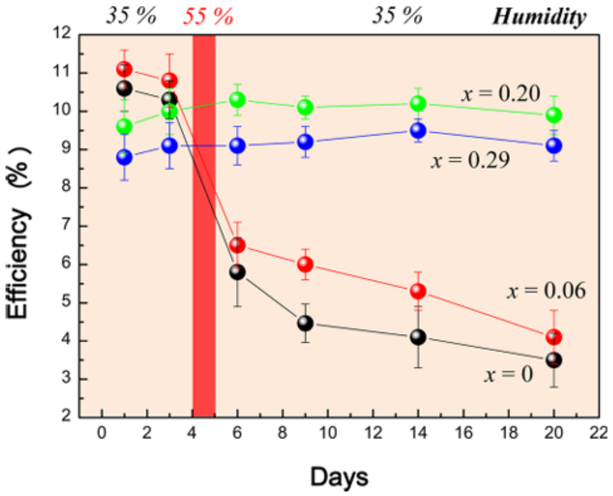

Figure 3. Performance of $MAPb(I_{1-x}Br_x)3$ (x=0, 0.06, 0.20, 0.29) over days under ambient air conditions without encapsulation. Humidity abruptly changed to 55% on day 4, and remained at 35% until day 20 [10]

Further research shows that higher Br content helps suppress the decomposition of $MAPb(I_{1-x}Br_x)_3$ in the dark and under light; most components can still maintain their original crystal phase under high humidity (67 ± 5% RH) [10]. The stability stems from the fact that the increase in Br content enhances hydrogen bonding between NH_3^+ and halide anions, locks the skeleton of 3D octahedra, and improves resistance to moisture intrusion.

In addition to halogen mixing, cation engineering is also crucial. Lee et al. introduced Cs^+ into $FAPbI_3$ to prepare $FA_{1-x}Cs_xPbI_3$ solid solution. The smaller ionic radius of Cs^+ will reduce the lattice and can also enhance the interaction between the cations and halogen ions. For example, the H bond will be enhanced by Br substitution, ultimately improving moisture resistance.

For all-inorganic $CsPbI_3$ perovskites, researchers have explored B-site doping with smaller metal cations (Mn^{2+}, Ge^{2+}, Sn^{2+}, Sb^{3+}, Bi^{3+}, Eu^{3+}), aiming to adjust the tolerance factor and stabilize the photoactive phase. The method is verified through experimental results: the device efficiency reaches 13.21% when 4 mol% of Bi^{3+} is doped ($CsPb_{0.96}Bi_{0.04}I_3$), and it still retains 68% of the initial performance after being placed in the air for 168 hours; the device doped with Eu^{3+} maintains 93% efficiency after 370 hours of white light irradiation. Although Mn^{2+} was also attempted, its ionic radius differs significantly from that of Pb^{2+} (0.70 Å vs. 1.19 Å), which hinders the ideal lattice matching. The radius of Sn^{2+} is relatively close to that of Pb^{2+} (1.18 Å), which can be used to adjust the tolerance factor, but its direct use is limited due to oxidation sensitivity. To solve this problem, Br^- is reintroduced to prepare $CsPb_{1-x}Sn_yI_{3-x}Br_x$ solution, significantly improving their phase stability.

In short, the main ways of material modification are to improve the performance of perovskite: the mixed halide makes the hydrogen bond network in the crystal lattice stronger and the structure harder; cation doping optimizes the stability of the crystal phase by adjusting the tolerance factor. These methods work synergistically at the atomic layer level, laying the foundation for high-performance PSCs.

3.2. Encapsulation technology

Initially, the modification of the intrinsic material can improve the tolerance of perovskite. In practical applications, physically separating the active layer from environmental aggressors (such as water vapor and oxygen) is still crucial for the long-term stability of the device. Encapsulation achieves this goal by constructing a dense barrier around the device to delay or block the degradation pathways.

Leijtens et al. divided the encapsulation strategies into three categories: inserting a blocking layer between the perovskite and HTL, using HTL materials with moisture-proof properties, and replacing the metal electrode with a hydrophobic carbon electrode [11].

Common HTL materials like Spiro-OMeTAD, PTAA, and P3HT have moisture barriers. Hygroscopic dopants such as Li-TFSI can cause hydrolysis of the perovskite layer (Figure 4a). To avoid this, there are alternative HTL materials that do not use hygroscopic dopants. For example, the derivative TTF-1 has inherent hydrophobicity and hole transport ability, like Spiro-OMeTAD, which does not use chemical doping. The stability of TTF - 1 devices in a humid and hot environment is about 3 times better than that of traditional doped devices (Figure 4b). A more complex method is to embed single-walled carbon nanotubes in a polymer matrix and combine it with a PMMA/PC double - layer structure to prepare a multi-layer barrier composite material. This system can operate stably for more than 100 hours in a humid, hot, and light environment, and can maintain basic functions when directly sprayed with water, and has excellent encapsulation performance [12].

Insert an ultra-thin insulating layer between the perovskite and the HTL. For example, an Al_2O_3 layer prepared by atomic layer deposition. Dong et al. found that a few nanometers of Al_2O_3 can significantly delay the permeation of water vapor; under dark and high-humidity conditions, the device still maintains more than 90% of the initial performance after 24 days of testing [13].

In the device structure without HTL, the encapsulation performance of the three-layer mesoporous structure based on carbon electrodes is relatively good (Figure 4c) [14]. Mei et al. said that the unsealed device can work stably for more than 1000 hours under full-spectrum illumination. For the encapsulated device, there is no obvious degradation phenomenon after 7 days of outdoor testing or storage in a dark environment at 80 - 85 °C for 90 days. This shows that the hydrophobicity of the carbon material itself and the compactness of the structure provide reliable stability for the design without HTL.

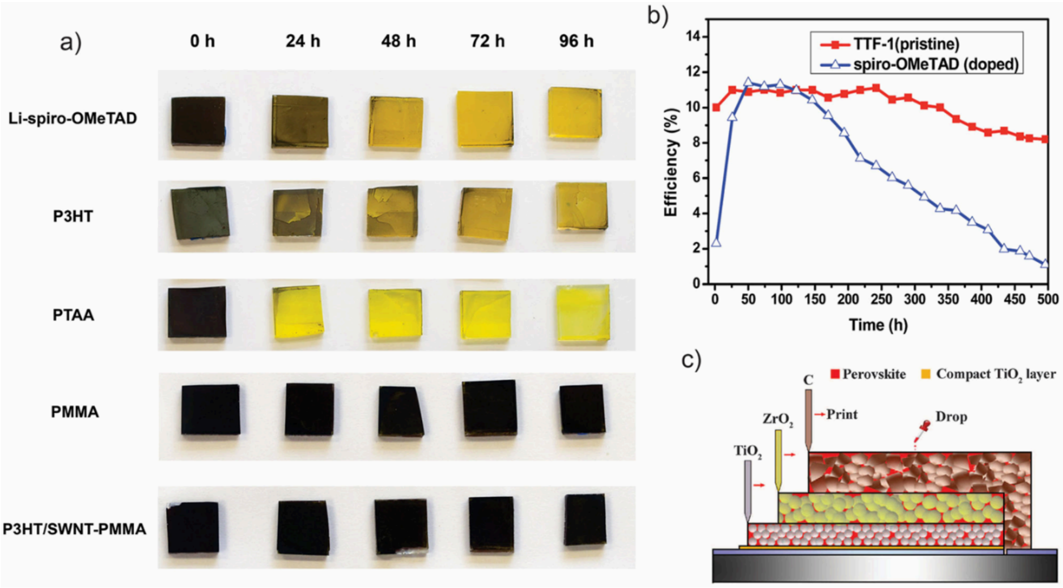

Figure 4. a) Observation of effective phase evolution over time for a series of hole transport materials exposed to ambient air at 80°C b) TTF-1 device performance significantly surpasses conventional doped devices c) Three-layer device structure without hole transport materials [11]

In summary, encapsulation technology establishes a robust external protective barrier for perovskite solar cells through physical barrier layers, hydrophobic material innovations, and HTL-free device designs, endowing them with outstanding environmental stability.

3.3. Defect passivation

Defects such as lead vacancies, iodine vacancies, and uncoordinated ions exist in the low-temperature solution process of perovskite films [15]. These defects reduce the photogenerated carrier collection efficiency and accelerate performance decay with environmental degradation. Defect passivation is the key to improving the efficiency and stability of perovskite solar cells.

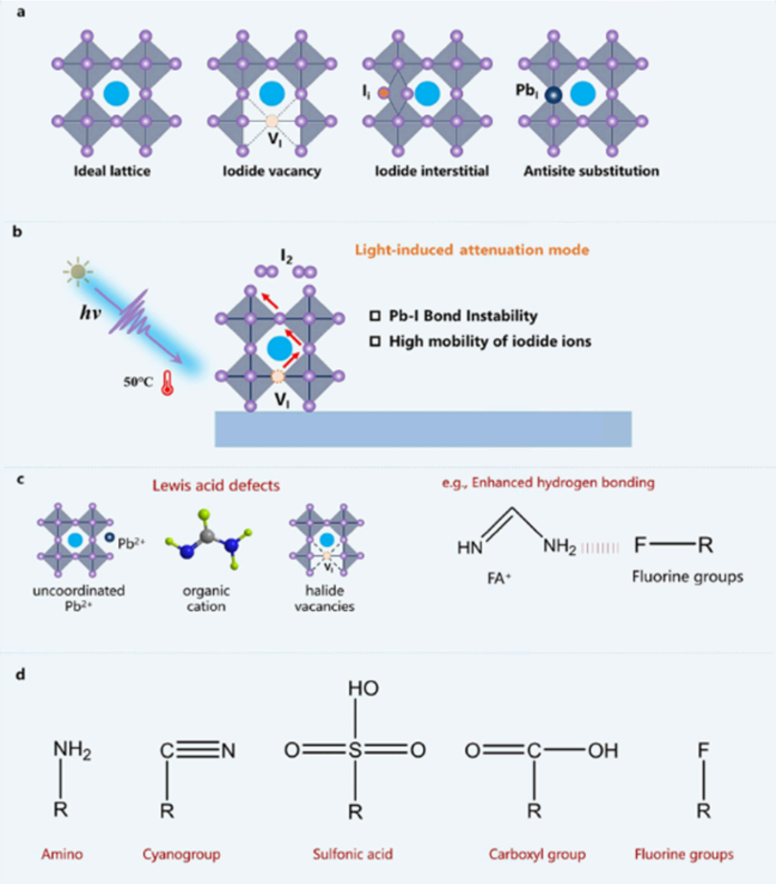

Figure 5. (a) Common vacancies, interstitial atoms, and anti-site defects in the perovskite lattice; (b) Iodine vacancies (V_I) and excess iodine (I_2) defects; (c) Lewis acid defects (uncoordinated Pb vacancies) commonly found in perovskite films; and (d) Passivator functional groups frequently observed in perovskite films [15]

Karim et al. discovered using secondary ion mass spectrometry that device performance is quite sensitive to defect density [16]. For example, in the $CH_3NH_3SnI_3$ battery, the bulk defect density in the absorption layer increases from 10^{14} cm^{-3} to 10^{18} cm^{-3}, and the power conversion efficiency (PCE) plummets from 31.68% to 1.91%; in addition, when the defect density at the ETL/perovskite interface increases, the efficiency also decreases by 30%, reducing from 72% to 0.49%. The results show that defect passivation plays an important role in suppressing trap-assisted recombination and improving carrier collection efficiency.

Andrei et al. managed to incorporate IM at site A to improve the performance of $MAPbI_3$ devices [17]. Experiments show that the incorporation of IM not only increases the PCE but also greatly improves the stability of the devices in a humid and high-temperature environment. The mechanism is that the two N atoms on the IM ring act as Lewis base sites, forming coordination bonds with uncoordinated Pb^{2+} and other Lewis acid defects. In this way, the defect charges are neutralized, and the contact between environmental molecules and active sites is also blocked (Figure 6).

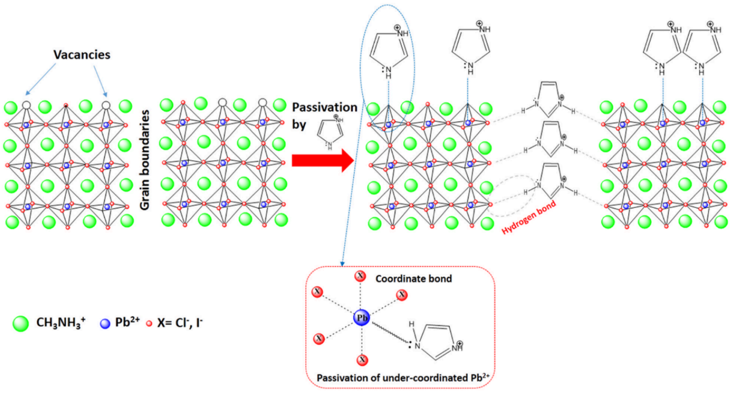

Fig. 6. Mechanism for passivation of $MA_{1-x}IM_xPbI_{2.6}Cl_{0.4}$ defects by IM doping.

Figure 6. Mechanism of IM doping for defect passivation in $MA_{1-x}IM_xPbI_{2.6}Cl_{0.4}$ [17]

Zhu et al. summarized the passivation strategies of lead perovskite defects in the review [18]. For uncoordinated Pb^{2+}, the coordination filling is carried out by using Lewis base additives with lone-pair electron functional groups. For example, additives containing fluorine or sulfonyl groups coordinate with Pb^{2+} through pyridine nitrogen atoms and fill the defective iodine vacancies with sulfonyl groups. After 1000-hour MPP tracking, the device efficiency reaches 21.96% and still maintains 83% of its initial performance. In another study, the P=O and O=C groups of the DPPP additive will coordinate with Pb^{2+} and also play a role in inhibiting the formation of iodine vacancies; the device modified by DPPP did not show a decrease in efficiency after 3500 hours of MPP test.

The low-dimensional perovskite reconstruction strategy has unique advantages in terms of grain boundary defects. PTAI in situ forms a 2D PTA_2PbI_4 phase at the $CsPbI_3$ grain boundary, fills the gaps and passivates the I vacancies. In addition, adding 4-aminobutyric acid or 3-amino-1-propanesulfonic acid at the $CsPbI_3/TiO_2$ interface constructs a chemical bridge with a dipole, optimizing the energy level arrangement and the interface defect density, and achieving double improvement of passivation and charge transport.

4. Conclusion and outlook

Research on perovskite solar cells is opening new pathways to address energy and environmental challenges. This review has outlined the fundamental operating principles and structural evolution of PSCs, highlighting that inverted p-i-n architectures are gaining research momentum due to simplified fabrication and superior properties. Regarding the long-standing stability hurdles that impede commercialization, we have summarized representative strategies across three dimensions: material modification, encapsulation, and defect passivation. Material modification optimizes the lattice structure by introducing cations and anions of varying sizes to enhance intrinsic stability; encapsulation employs physical barriers or inherently hydrophobic layers to effectively isolate water and oxygen; defect passivation fills or eliminates lattice defects through chemical coordination or interface reconstruction, thereby suppressing non-radiative recombination and environmental degradation.

It is worth noting that at the 8th China International Photovoltaic and Energy Storage Industry Conference held in 2025, "Father of Solar Energy" Martin Green also said that stability is the key challenge of current perovskite solar cells. In terms of material design, in the future, "dynamic adaptive lattice engineering" can be carried out, for example, using multifunctional ligands with reversible coordination ability, or constructing a halide gradient doping structure, which may enable the perovskite framework to have a stress buffering function. This design can help alleviate lattice distortion, ion migration, and phase separation under temperature changes or light. In terms of defect passivation, the research needs to develop in the direction of "precise targeting and interface integration". Advanced in-situ characterization technologies, such as in-situ KPFM and cryo-TEM, can dynamically track the evolution of defects under light, heat, and humidity, helping the targeted design of passivation molecules. Packaging has transformed from a "single-layer barrier" to an "intelligent packaging system" with humidity response and self-healing functions, which can provide comprehensive protection, enabling PSC to operate stably for a long time in diverse scenarios. With these paths advancing synergistically, PSC is expected to be widely applied in photovoltaic power stations, building-integrated photovoltaics, and portable energy systems, becoming a key supporting technology for the global clean energy transition.

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