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Enhancing the Stability of 2D/3D Hybrid Perovskite Solar Cells: Mechanisms, Challenges, and Future Perspectives

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Abstract. Among all photovoltaic technologies, perovskite solar cells (PSCs) have emerged as a standout, combining record-breaking efficiency with the promise of low-cost, scalable manufacturing. However, the poor stability of perovskite materials remains a major obstacle to their commercialization. To address this challenge, researchers have shifted focus from traditional three-dimensional (3D) PSCs to the development of two-dimensional/three-dimensional (2D/3D) hybrid structures, achieving remarkable progress. This review examines various strategies to improve stability, including constructing 2D/3D heterostructures, surface passivation, interface engineering, optimizing fabrication processes, and material design, with the aim of investigating the mechanisms underlying the enhanced stability of 2D/3D hybrid perovskite solar cells (PSCs) These methods effectively address issues such as ion migration, defect density, and environmental degradation. Key findings show that 2D/3D heterostructures and passivation layers significantly enhance device stability and efficiency, with some achieving power conversion efficiencies (PCEs) over 25%. However, challenges remain in large-scale production and long-term stability under extreme conditions. Future research should focus on developing scalable fabrication techniques, optimizing material systems for durability, and further improving charge transport efficiency to advance the commercial viability of 2D/3D PSCs.

Keywords: Renewable Energy, Photovoltaics, Perovskite Solar Cells(PSCs), Multidimensional 2D-3D perovskites, Stability

1. Introduction

Leveraging high efficiency, low cost, low weight, and mechanical flexibility, perovskite solar cells are steadily supplanting conventional silicon photovoltaics, accelerating the sector's shift toward high-performance, stable, and environmentally benign energy solutions [1]. Compared with traditional silicon-based solar cells, the stability problem of perovskite solar cells is more prominent, mainly manifested in ion migration of materials, chemical degradation, and environmental adaptability. Ion migration within the perovskite lattice can precipitate a swift collapse in device efficiency, while ambient humidity, illumination, and thermal stress act in concert to hasten irreversible material degradation [2]. Therefore, improving stability can not only extend the lifespan of devices and reduce maintenance costs, but also enhance market confidence in perovskite solar cells, promoting their wide application in the photovoltaic market.

At present, the stability of perovskite solar cells is being aggressively pursued through a diverse arsenal of strategies. For instance, Xie et al. enhance the stability of perovskite cells through interface enhancement and defect suppression [3]. Yang et al. pioneered the coupling structure of metal fullerene molecules, achieving in-situ encapsulation and enhancing stability and efficiency in complex environments [4]. Ye et al. have developed an anti-solvent seed layer strategy to address the issue of growth on rough surfaces and enhance the stability and efficiency of flexible batteries [5]. Among all the research methods, the construction of two-dimensional/three-dimensional (2D/3D) perovskite heterostructures is one of the key strategies. This structure combines the high stability of 2D perovskites with the excellent photoelectric performance of 3D perovskites, significantly enhancing the overall performance of the device. By capping the 3D perovskite with an ultrathin 2D layer, researchers seal surface traps and suppress ionic drift, markedly extending the device's operational lifetime [6,7].

However, although certain progress has been made in related research, long-term stability studies under extreme conditions are still insufficient, and the intrinsic connection between the internal microstructure of perovskite materials and macroscopic stability has not been fully revealed. Bridging these critical gaps is imperative if perovskite photovoltaics are to graduate from bench-top demonstrations to robust, market-ready products [8]. This work therefore targets the twin objectives of maintaining the technology's high power-conversion efficiencies while simultaneously extending its operational lifetime. By resolving the long-standing stability bottleneck, we aim to broaden both the practical application landscape and the commercial viability of perovskite solar cells. This not only meets the market's demand for efficient and stable renewable energy sources but also aligns with the global pursuit of sustainable and environmentally friendly technologies.

2. Analysis of stability issues of perovskite solar cells

2.1. Stability issues

Perovskite photovoltaics now command center stage in solar research, marrying record efficiencies with low-cost, solution-processable manufacturing. However, the poor stability of perovskite solar cells leads to structural decomposition and interfacial degradation during operation, resulting in device failure, shortened working life, and hindrance to large-scale application. These issues make it challenging to meet the demand for a long-term, stable power supply, and thus pose significant barriers to commercialization. Additionally, the preparation of perovskite solar cells often involves using lead-containing organic solvents, which are highly toxic. The instability and decomposition of these devices can pose threats to the environment and human health. Therefore, stability is crucial for the practical application of perovskite solar cells, as they need to operate stably for the long term in complex outdoor environments, such as high temperatures, high humidity, and continuous light exposure.

Currently, the stability parameters of perovskite solar cells are continuously being developed and optimized. Recent studies have demonstrated that the theoretical limit of the photoelectric conversion efficiency of perovskite solar cells (such as perovskite/silicon tandem cells) can reach 42.5%, while the highest efficiency achieved in the laboratory has reached 34.6%. This value exceeds the highest laboratory conversion efficiency of monocrystalline silicon solar cells (29.24%, with a theoretical limit of 29.4%), indicating significant potential for further performance improvement. However, when scaling up the cell area, the uniformity of perovskite film is difficult to control, leading to issues such as disordered crystal growth, increased defects, and poor film continuity. These issues significantly affect the stability and conversion efficiency of solar cells. For example, according to Huang et al., a laboratory-scale perovskite solar cell with an area of 0.06 cm^2 achieves a photoelectric conversion efficiency of 25.1%, but when the area is scaled up to 900 cm^2, the efficiency drops to 16.4%. This highlights the significant challenges faced by perovskite solar cells in large-area fabrication.

Moreover, the theoretical lifespan of perovskite solar cells is relatively short. Even under laboratory conditions, the longest continuous light exposure test for perovskite solar cells is only 10,000 hours, with a theoretical lifespan of approximately 6.8 years [9]. In practical applications, the lifespan is likely to be even shorter, compared with the 25-year theoretical lifespan of crystalline silicon solar cells. The industry generally believes that by 2030, a perovskite solar module with a photoelectric conversion efficiency of 17% needs to have a 34-years lifespan to be competitive with silicon technology in the market. This goal underscores the importance of stability research [10].

2.2. The causes of the stability problems of PSCs

Currently, a significant challenge for perovskite solar cells during long-term operation is how to maintain high photoelectric conversion efficiency while maximizing the stability of material, especially under the influence of environmental factors. These factors can induce chemical degradation and structural changes in perovskite materials, thereby causing a substantial decline in device performance [6]. Moreover, in 2D/3D perovskite heterostructures, photo-induced interfacial effects may lead to increased carrier recombination and reduced photovoltaic conversion efficiency due to factors such as interfacial defects and mismatches, quantum confinement effects, and the influence of interfacial electric fields [11]. The 2D perovskite layers, despite their unique layered structure that confers certain stability advantages, suffer from a relatively wide and difficult-to-tune bandgap. This results in a limited light absorption range, low charge separation and transport efficiency, and low carrier mobility, which become key factors restricting the overall charge transport efficiency of the device [12]. Additionally, ion migration within the perovskite material and the formation of defect states further exacerbate device performance degradation and long-term stability issues. In practical applications, the uniform coverage and thickness consistency of 2D perovskite layers are difficult to precisely control during the large-scale fabrication of perovskite solar cells. This not only affects the uniformity and stability of device performance but also reduces the reproducibility of the manufacturing process, thereby posing significant barriers to large-scale commercialization [13]. Therefore, it is crucial for the further development and practical application of perovskite solar cell technology to conduct in-depth research and find solutions to the environmental sensitivity and structural issues of perovskite materials.

3. Strategies for enhancing the stability of perovskite solar cells

3.1. Construct 2D/3D perovskite heterostructures

A 2D/3D perovskite heterojunction seamlessly integrates an ultrathin two-dimensional perovskite overlayer with an underlying three-dimensional perovskite bulk, creating a stratified architecture that capitalizes on the complementary strengths of each dimension. The 2D perovskite layer typically adopts the Ruddlesden-Popper (RP) phase, which is a structure of periodically stacked perovskite layers. These layers within the RP phase are connected by weak van der Waals forces or ionic bonds, endowing the material with good ionic conductivity and high stability. In contrast, the 3D perovskite layer, characterized by its 3D network structure, generally exhibits high carrier mobility and excellent light absorption capability. The ultrathin two-dimensional perovskite capping layer functions as both a molecular raincoat and a crystallographic scaffold: it shields the three-dimensional bulk from moisture and airborne contaminants while steering the nucleation and growth of the underlying film, thereby suppressing bulk and interfacial defects. Concurrently, the thicker 3D layer furnishes ample absorption depth. This dual-layer architecture markedly extends device endurance under humidity, heat, and illumination by blocking ionic migration and chemical erosion. Moreover, judicious tuning of the 2D/3D thicknesses and compositions provides precise band-gap engineering, enhancing photon harvesting and charge extraction and ultimately driving a substantial gain in power-conversion efficiency [6]. The 2D/3D structure can be fabricated into large-area perovskite films via solution processing, enabling large-scale production, reducing manufacturing costs, and enhancing economic feasibility [14]. According to Sidhik et al., the 3D/PP-2D HaP bilayer device exhibited almost no degradation in efficiency after T99 exceeding 2000 hours under conditions of 60 ± 5°C and relative humidity of 70 ± 5%, whereas the pure 3D device retained only 75% of its initial PCE after 2000 hours [15]. However, Yu et al. believe that the constructed 2D/3D perovskite model indicates that this heterojunction is a PN heterojunction, with the potential for anomalous photo-induced effects at the interface. These effects may significantly enhance the built-in potential under illumination, forming barriers that impede the transport of photogenerated carriers. Moreover, 2D perovskites with low n values (n=1 or 2) hardly participate in energy transfer but instead act as recombination centers, further reducing charge transport efficiency [11]. In summary, the 2D/3D perovskite heterojunction has proven to be an effective strategy for enhancing the stability of perovskite solar cells. By leveraging the protective and stabilizing properties of the 2D perovskite layer, significant improvements in durability and performance have been achieved, particularly under harsh environmental conditions.

3.2. Surface passivation technology

Surface passivation harnesses a 2D perovskite overlayer that chemically coordinates with dangling bonds and under-coordinated ions on the 3D perovskite surface. By plugging vacancies, neutralizing trap states, and forming a dense, hydrophobic barrier, this strategy suppresses non-radiative recombination, curbs ionic migration, and repels moisture and oxygen—collectively extending carrier lifetimes and markedly boosting both efficiency and long-term stability. This process enhances the open-circuit voltage (VOC) of the device, thereby improving the photoelectric conversion efficiency. Common passivators include pure 2D perovskite (A′2An-1PbnI3n-1), ammonium salts (A′X, where X is a halide), and large amine molecules (A′). Passivation of the substrate can be achieved through methods such as spin-coating, dip-coating, vacuum deposition, or mechanical pressing. After passivation, the surface of the perovskite film becomes more uniform and dense, with increased grain size and reduced surface roughness, which is conducive to improving carrier extraction efficiency [16]. Li et al. used phenethylammonium (PEA) lead iodide to construct an ordered 2D perovskite passivation layer on the 3D perovskite FA0.8Cs0.2PbI3. When the optimal content of FPEA passivation was 16.67%, an ultralong photoluminescence (PL) lifetime of 1.3 μs, a high carrier mobility of approximately 18.56 cm2V-1s-1, and a long carrier diffusion length of about 7.85 μm were achieved [7]. This approach also reduced the formation of defect states, suppressed ion migration, and slowed down the degradation rate of the materials, thereby enhancing its stability. Yang et al. improved the hydrophobicity of the device surface by using cesium-ethylammonium iodide (CEAI) to passivate the 3D perovskite, resulting in a fill factor (FF) of 82.6% and a power conversion efficiency (PCE) of 23.57%. After 1500 hours under one-sun illumination, the remaining efficiency was still over 96%, indicating excellent stability [17]. It can be concluded that surface passivation technology, by reducing surface defects and inhibiting ion migration, has been proven to effectively enhance the stability of perovskite solar cells.

3.3. Interface engineering strategy

In solar cells, the separation and transport of photogenerated carriers (electrons and holes) are crucial processes for achieving photoelectric conversion. In practical devices, carriers may encounter and recombine at material interfaces during transport, thereby consuming carriers and degrading device performance. Interface engineering, which optimizes the materials and structures at interfaces to reduce interface states, ion diffusion, and energy level mismatches [18], has emerged as a promising solution. Luo et al. utilized EDMA and POSS to fabricate highly crosslinked CLP, forming a thin film between 3D and 2D perovskites that effectively suppresses ion diffusion. 3D/CLP/2D heterojunction perovskite solar cells deliver a champion power-conversion efficiency of 21.2 % and retain 90 % of their initial output after 4,390 h of continuous operation at 60 °C [19]. Sutanto et al. investigated 2D perovskite materials based on thienyl-based bulky organic cations, regulating the overall interface energy alignment by adjusting their halide counterions. By spin-coating the 2D perovskite layer onto the 3D perovskite layer and combining UPS analysis, it was found that a p-n junction formed between the 2D and 3D perovskites, effectively promoting hole extraction, blocking electrons, and reducing interface recombination. The optimized PSCs achieved a photoelectric conversion efficiency of 20.82% with an open-circuit voltage of 1.19 V, approaching the theoretical limit. Moreover, the 2-TMAbr-based devices retained 75% of their initial efficiency after continuous illumination for 1000 hours [20]. In summary, by precisely tuning the interfacial characteristics and reducing recombination losses, interface engineering has become a powerful technological means to enhance the stability and performance of perovskite solar cells.

3.4. Optimization of fabrication processes

Optimizing the fabrication process of PSCs is crucial for enhancing their performance and stability. Common strategies for process optimization include the preparation methods of perovskite films, solvent selection and treatment, and post-treatment of perovskite films.

Regarding the preparation of perovskite films, the emerging solid-phase interfacial growth (SIG) method can be employed. This method enables the growth of 2D perovskites on 3D surfaces through physical contact, as well as the application of pressure and temperature. It avoids the common issues of phase mixing and defect formation encountered in traditional solution-based methods, thereby improving the performance and stability of the devices. This method can achieve precise control over the thickness of 2D perovskites, high phase purity, and uniform growth [14]. In experiments, the SIG method was used to grow BA2PbI4 (n=1) 2D layers on FAPbI3 surfaces, resulting in a PCE of 24.5% and a T99 (time to 99% of initial efficiency) exceeding 2000 hours [21].

Strategic solvent engineering offers a powerful lever for optimizing perovskite-film quality. For example, Shan et al. formulated a 2D-interlayer ink in which isopropanol (iPA) serves as the primary solvent, augmented with just 1 % dimethyl sulfoxide (DMSO) to refine wetting, slow crystallization, and ultimately yield a denser, more uniform cationic (DFP) overlayer [13]. This combination not only promoted the diffusion and reaction of DFP within the 3D perovskite but also formed high-quality 2D layers (denoted as DFP-MIX). After DFP treatment, the perovskite films were annealed at 100°C to facilitate secondary crystallization growth on the surface, further optimizing the quality of the 2D layers. As a result, the fill factor increased to 85%, representing a 6.9% improvement. The open-circuit voltage reached 1.17 V (DFP-MIX), and the PCE was enhanced from 20.13% to

24.03%. The DFP-MIX devices maintained nearly constant efficiency during thermal cycling tests (85°C, 10 cycles) and retained high efficiency even after 10 hours in an environment with 70% relative humidity [13].

In summary, the improvements in the fabrication process of perovskite solar cells, particularly through the application of advanced techniques like solid-phase interfacial growth (SIG) and meticulous solvent selection, have demonstrably bolstered both the stability and performance of these devices. These strategies not only address typical challenges such as phase mixing and defect generation but also bolster the devices' operational longevity and efficiency across diverse environmental settings.

3.5. Material design and modification

Material design and modification have significantly enhanced the stability of PSCs through various mechanisms. Interface modification can passivate defects and strengthen interfacial bonding, thereby improving the device's resistance to environmental erosion. Material modification can also optimize the crystallization quality of perovskite, reduce defect density, and enhance hydrophobicity, thereby mitigating the impact of moisture on the device. Additionally, through elemental doping and gradient design, the lattice stability of perovskite can be enhanced, the energy level structure can be optimized, and carrier recombination can be reduced. The introduction of multifunctional molecules and chiral structures can simultaneously achieve multiple functions, further improving the overall performance of the device. These design and modification strategies not only improve the stability of PSCs under various environmental conditions but also ensure their high efficiency during long-term operation, providing important support for the commercial application of perovskite solar cells. Li et al. doped 1,8-ND into perovskite to optimize the electronic structure and optical properties, and the device still maintained 83.2% of its initial PCE after 50 days [22]. Yu et al. introduced n-butylammonium acetate to replace the traditional organic ammonium iodide, altered the crystallization kinetics of perovskite, and achieved the preparation of phase-pure films. For the phase-pure film with n=4, the PCE increased from 13.81% to 16.25%, which indirectly enhances stability [11]. In addition, the work function of the 3D perovskite doped with alkali cation Rb+ decreased from 4.73 eV (undoped) to 4.53 eV, which helps to improve charge transport performance and device stability. The unencapsulated doped device maintained 81% of its initial PCE after 60 days in an environment with 50% RH, while the unencapsulated undoped device experienced a 65% drop in PCE [18].

Targeted material design and judicious interface engineering have now tamed two of the technology’s most stubborn weaknesses—high defect densities and moisture susceptibility—delivering simultaneous gains in efficiency and durability. Recent demonstrations confirm that such strategies can extend operational lifespans without sacrificing record power-conversion efficiencies, underscoring their pivotal role in propelling perovskite photovoltaics toward commercial reality.

4. Discussion

The future development of 2D/3D perovskite solar cells needs to focus on solving key problems such as large-scale production, stability enhancement, interface engineering, and material optimization. Firstly, developing large-scale preparation technologies (such as roll-to-roll printing) and optimizing solvent treatment processes (such as DMSO-assisted solvent regulation) are necessary conditions for achieving large-scale production [13]. Secondly, to enhance the long-term stability of the device in extreme environments such as high humidity, high temperature, and intense light, it is necessary to conduct in-depth research on degradation mechanisms and develop more durable material systems [9]. In addition, interface engineering and carrier dynamics optimization are the keys to enhancing performance. It is necessary to suppress ion diffusion and improve charge transport efficiency through cross-linked polymers or novel organic ligands [3]. Finally, further reducing production costs and improving devices repeatability are fundamental prerequisites for commercial applications. Through breakthroughs in these research directions, 2D/3D perovskite solar cells are expected to move from the laboratory to practical applications.

5. Conclusion

This review offers a systematic appraisal of 2D/3D hybrid perovskite solar cells, centering on the mechanistic origins of their markedly improved stability. By marrying the robust moisture and thermal resilience of two-dimensional perovskites with the outstanding optoelectronic performance of three-dimensional absorbers, the heterostructure architecture simultaneously raises efficiency and extends operational lifetime. Studies converge on a single conclusion: the ultrathin 2D capping layer functions as a multifunctional interface—passivating surface traps, arresting ion migration, and suppressing non-radiative recombination—thereby anchoring long-term device integrity. Furthermore, through the optimization of interface engineering, material design, and preparation processes, the photoelectric conversion efficiency of 2D/3D PSCs has exceeded 25%, approaching the level of commercial photovoltaic technology. However, despite the significant progress made under laboratory conditions, 2D/3D PSCs still face challenges in large-scale production and long-term stability.

While this review distills key advances, it is not exhaustive. Firstly, the scope of the discussion may not be comprehensive. Given the vast array of strategies available for enhancing the stability of 2D/3D perovskite solar cells (PSCs), this review has focused on only five representative techniques. Secondly, the review lacks reproducibility experiments to verify the reliability of the data presented. Lastly, the number of references is somewhat limited. Future work should aim to address these limitations by incorporating a wider array of techniques, conducting reproducibility studies, and expanding the range of references to ensure a more thorough analysis.

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