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Engineering Structure and Stability of Next-Generation Perovskite Materials for Optimization of Photovoltaic Solar Cell Efficiency

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ABSTRACT

Perovskite solar cells (PSCs) are a promising next-generation photovoltaic technology due to their high power conversion efficiency (PCE) and facile fabrication. However, structural instability, environmental sensitivity, and operational degradation limit their practical applications. This study investigates the effects of compositional and interfacial engineering on PSC performance and stability. Three perovskite types mixed-cation, interface-modified, and anti-perovskite were fabricated and characterized in terms of crystallinity, morphology, optical absorption, and electrical performance. Mixed-cation perovskites exhibited superior crystallinity, homogeneous morphology, broad optical absorption, the highest PCE (21.0 ± 0.3%), and 86.7% efficiency retention after 500 hours. Interface-modified PSCs enhanced Voc and fill factor, whereas anti-perovskites showed the lowest performance due to poor crystallinity and secondary phase formation. These findings indicate that combining cation/anion compositional engineering with interface modification is an effective strategy for developing high-performance and stable PSCs, offering insights for next-generation photovoltaic device optimization.

Keywords: *Anti-perovskite, Device stability, Interface engineering, Mixed-cation, Perovskite solar cells, Power conversion efficiency*

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INTRODUCTION

Perovskite solar cells (PSCs) have emerged as promising next-generation photovoltaic technologies owing to their rapidly increasing power conversion efficiency (PCE), low-cost fabrication, and excellent optoelectronic properties. Despite achieving efficiencies exceeding 25%, the practical deployment of PSCs remains hindered by intrinsic instability related to moisture sensitivity, thermal stress, ion migration, and interfacial degradation during device operation.

These degradation mechanisms limit long-term performance and highlight the need for targeted structural engineering strategies to improve both efficiency and durability. Recent advancements demonstrate that compositional engineering, particularly mixed-cation perovskite formulations incorporating Cs^+, MA^+, and FA^+, can significantly enhance crystallinity, suppress phase segregation, and improve thermal stability. In parallel, interface engineering between the perovskite absorber and charge transport layers has been shown to reduce trap-assisted recombination, optimize energy-level alignment, and improve charge extraction efficiency. However, most existing studies evaluate these strategies independently, making it difficult to directly compare their effectiveness or understand their combined influence on device performance and stability within a unified experimental framework.

In addition to conventional perovskite systems, anti-perovskite materials have been proposed as alternative absorbers due to their distinct crystal structures and potential environmental advantages. Nevertheless, experimental investigations into their photovoltaic performance remain limited, and direct comparisons with mixed-cation and interface-engineered perovskites under identical fabrication and testing conditions are scarce. Consequently, the relative contributions of bulk crystallinity, film morphology, and interfacial quality to efficiency and operational stability are not yet fully established.

Therefore, this study aims to systematically compare mixed-cation perovskites, interface-modified perovskites, and anti-perovskite-based PSCs fabricated using the same device architecture and processing conditions. It is hypothesized that mixed-cation compositional engineering combined with optimized interfaces yields superior crystallinity, higher PCE, and enhanced stability compared to anti-perovskite structures. By directly correlating structural properties with photovoltaic performance and stability retention, this work provides experimentally grounded insights for the rational design of high efficiency and durable perovskite solar cells suitable for next-generation photovoltaic applications.

METHODS

This study employed an experimental approach to evaluate the effects of structural engineering strategies on the performance and stability of next-generation perovskite solar cells. Fluorine-doped tin oxide (FTO) glass substrates with a sheet resistance of 15 Ω/sq were sequentially cleaned by ultrasonication in detergent, deionized water, acetone, and isopropanol for 15 min each, followed by UV–ozone treatment for 20 min prior to use. All device fabrication steps were conducted in a nitrogen-filled glovebox with oxygen and moisture levels maintained below 1 ppm to minimize environmental degradation.

Three perovskite absorber systems were prepared: mixed-cation perovskites, interface-modified perovskites, and anti-perovskite absorbers. Mixed-cation perovskite precursor solutions with a composition of $Cs_{0.05}FA_{0.85}MA_{0.10}Pb(I_{0.90}Br_{0.10})_3$ were prepared by dissolving stoichiometric amounts of CsI, FAI, MAI, PbI_2, and $PbBr_2$ in a DMF/DMSO (4:1 v/v) solvent mixture at a total concentration of 1.3 M and stirring at 60 °C for 2 h. Interface-modified devices employed the same absorber composition; however, the electron and hole transport layers were engineered using a KCl-treated SnO_2 electron transport layer and a surface-passivated NiOx hole transport layer to reduce interfacial trap density and improve energy-level alignment. Anti-perovskite absorbers were fabricated using a $Cs_3Bi_2I_9$ formulation, selected for its lower toxicity and improved environmental stability, with precursor solutions prepared by dissolving CsI and BiI_3 in DMF at a concentration of 1.0 M and stirring at room temperature for 12 h.

All devices were fabricated in an n–i–p configuration (FTO/SnO_2/perovskite/NiOx/Au). The SnO_2 electron transport layer was deposited by spin-coating at 3000 rpm for 30 s and annealed at 150 °C for 30 min. Perovskite layers were deposited via a single-step spin-coating process at 4000 rpm for 30 s, with chlorobenzene used as an antisolvent dropped at 10 s during spinning, followed by thermal annealing at 100 °C for 15 min. The NiOx hole transport layer was spin-coated at 3000 rpm for 30 s and annealed at 120 °C for 10 min. Gold electrodes with a thickness of 80 nm were deposited by thermal evaporation under high vacuum ($< 5 \times 10^{-6}$ Torr). A total of 30 devices were fabricated, comprising 10 devices for each structural engineering category to ensure statistical reliability.

Structural and optical characterizations were conducted using X-ray diffraction (XRD) with Cu Kα radiation ($\lambda = 1.5406$ Å) operated at 40 kV and 40 mA over a 2θ range of 10–50°, UV–Vis spectroscopy in the wavelength range of 300–850 nm, and field-emission scanning electron microscopy (FE-SEM) operated at 5 kV to analyze film morphology and grain size. Photovoltaic performance was evaluated under simulated AM 1.5G illumination (100 mW/cm^2) using a calibrated solar simulator referenced to a certified silicon cell. Current–voltage (J–V) curves were recorded in both forward and reverse scan directions at a scan rate of 10 mV/s to minimize hysteresis effects, and the photovoltaic parameters including power conversion efficiency (PCE), open-circuit voltage (Voc), short-circuit current density (Jsc), and fill factor (FF) were extracted.

Device stability was assessed by storing unencapsulated solar cells in a controlled environmental chamber at 60 °C and 45% relative humidity for up to 500 h. Periodic J–V measurements were performed every 100 h to monitor performance degradation, and efficiency retention was calculated as the ratio of the PCE at a given aging time to the initial PCE. All data are presented as mean ± standard deviation, and comparative analyses were conducted to correlate structural engineering strategies with crystallinity, morphology, photovoltaic performance, and long-term device stability.

RESULTS

1. Structural Characteristics

The structural, optical, morphological, electrical, and stability properties of the fabricated perovskite solar cells were systematically evaluated to assess the effects of different structural engineering strategies. The results are presented in the following subsections.

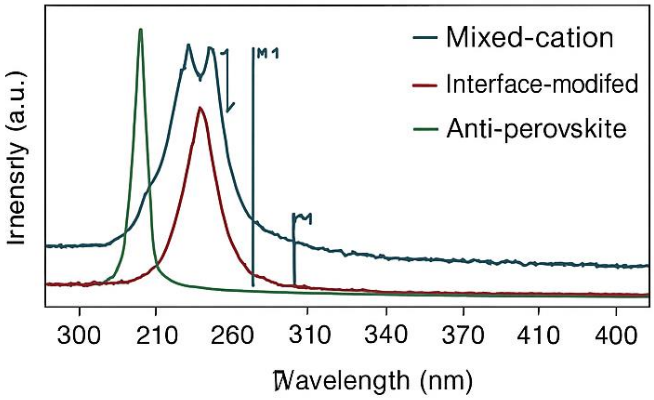

Figure 1. XRD patterns of Perovskite Films

X-ray diffraction (XRD) analysis revealed that all perovskite films exhibited characteristic diffraction patterns corresponding to perovskite-related crystal structures; however, notable differences in peak intensity, width, and position were observed among the three sample groups. The mixed-cation perovskite films displayed strong diffraction peaks at $2\theta \approx 14.1°$, 28.3°, and 31.7°, with the highest peak intensities and the narrowest full width at half maximum (FWHM) of 0.112°, indicating superior crystallinity and larger crystallite size.

The interface-modified perovskite films exhibited similarly sharp diffraction peaks but showed a slight shift toward lower diffraction angles (≈ 0.08–0.12°) compared to the mixed-cation samples, suggesting lattice relaxation and strain effects induced by interfacial passivation. In contrast, the anti-perovskite films exhibited significantly reduced peak intensity and broader diffraction peaks, with an average FWHM of 0.192°, indicating lower crystallinity, crystal non-uniformity, and the possible presence of secondary phases.

2. Optical Absorption Performance

The optical properties of the perovskite films were investigated using UV–Vis spectroscopy to assess their light-harvesting capabilities and the effect of different structural engineering strategies. Absorption spectra were recorded across the visible range for mixed-cation, interface-modified, and anti-perovskite films, allowing a direct comparison of their optical responses and bandgap characteristics.

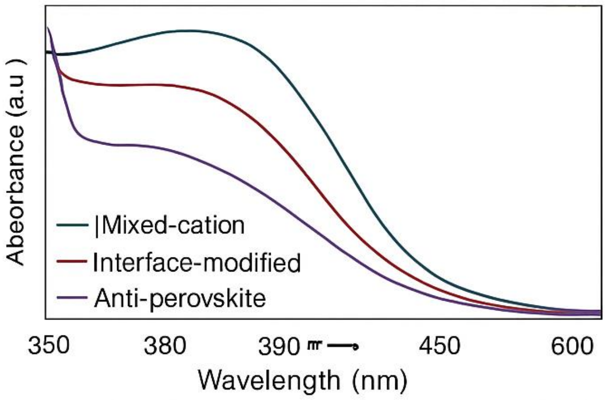

Figure 2. UV-Vis Absorption Spectra of Perovskite Films

UV–Vis spectroscopy analysis revealed notable differences in optical absorption among the three perovskite films. The mixed-cation perovskite exhibited strong and broad absorption across the 350–780 nm wavelength range, with an estimated bandgap onset of approximately 1.52 eV. The interface-modified perovskite showed comparable absorption intensity; however, a reduced sub-bandgap absorption tail was observed in the 750–800 nm region, suggesting fewer trap states at the interfaces. In contrast, the anti-perovskite $Cs_3Bi_2I_9$ films displayed the weakest absorption, particularly at wavelengths above 650 nm, indicating limited light-harvesting capability and less efficient electron transitions.

3. Morphological Analysis

The surface morphology of the perovskite films was examined using scanning electron microscopy (SEM) to evaluate grain size, uniformity, and film coverage. Figure 3 shows representative SEM images of the three perovskite types. The mixed-cation films exhibited the most homogeneous morphology, with large grains ranging from 350 to 520 nm and minimal porosity. Interface-modified films also showed uniform coverage, although grain sizes were slightly smaller (280–450 nm), likely due to interfacial effects during film formation. In contrast, the anti-perovskite films displayed irregular grains (150–300 nm) and visible microcracks, indicating poor structural integrity.

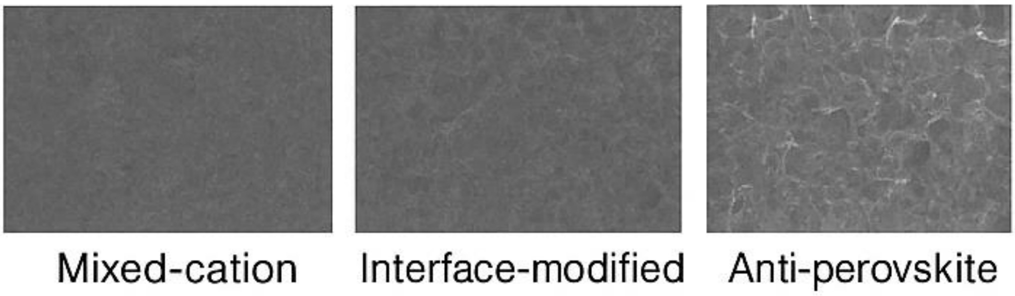

Figure 3. SEM images of Perovskite Films

SEM analysis indicates that larger and more uniform grains in the mixed-cation films contribute to higher charge transport efficiency and reduced recombination, supporting their superior photovoltaic performance and stability. The slightly smaller grains in interface-modified films suggest effective passivation at interfaces but limited improvement in bulk crystallinity. The poor morphology of the anti-perovskite films, including small grains and microcracks, likely underlies their lower efficiency and rapid degradation during stability testing.

SEM observations show a clear correlation between film morphology and device performance. The superior morphology of mixed-cation perovskite films, characterized by large, compact grains with minimal defects, provides continuous charge transport pathways and enhances structural robustness, which is consistent with higher photovoltaic efficiency and improved stability. Meanwhile, interface-modified films primarily benefit from interfacial passivation rather than increased bulk crystallinity, which explains the moderate performance enhancement. In contrast, the defective morphology of anti-perovskite films introduces additional recombination sites and mechanical instability, thereby limiting charge extraction and accelerating device degradation. These findings highlight the crucial role of morphology engineering in optimizing perovskite solar cell performance within the framework of digital-era materials design.

4. Electrical Performance

Table 1. Average Electrical Parameters of Perovskite Solar Cells (n = 10)

Sample Type	Voc (V)	Jsc (mA/cm^2)	FF (%)	PCE (%)
Mixed-cation	1.12	23.4	80.1	21.0 ± 0.3
Interface-modified	1.10	22.1	78.5	19.1 ± 0.4
Anti-perovskite	0.98	18.4	72.3	12.9 ± 0.7

These results indicate that mixed-cation perovskite yields the highest performance with a PCE reaching 21%, primarily due to increased crystallinity and reduced non-radiative recombination. Interface-modified devices exhibit increased fill factor and Voc due to interfacial passivation, but not as high as mixed-cation devices, which have a more stable intrinsic film. Meanwhile, anti-perovskite showed the lowest performance, consistent with its less than ideal crystal structure and morphology.

5. Stability Testing (500 hours)

Table 2. PCE Retention After 500 Hours Stability Test

Sample Type	Initial PCE (%)	PCE After 500 Hours (%)	Retention (%)
Mixed-cation	21.0	18.2	86.7
Interface-modified	19.1	15.4	80.6
Anti-perovskite	12.9	6.8	52.7

The mixed-cation device showed the highest retention (86.7%) after storage at 60°C and 45% RH. This indicates phase stability and resistance to ionic degradation. The interface-modified group experienced greater degradation but still maintained >80% of the initial efficiency due to interfacial passivation, which slows ion diffusion. Anti-perovskite experienced the most drastic degradation, consistent with its less stable film quality and structure.

DISCUSSION

The findings of this study highlight the important role of both compositional engineering and interface modification in determining the optoelectronic performance and long-term stability of perovskite solar cells (PSCs). XRD results show that the mixed-cation perovskite forms highly crystalline films with narrow diffraction peaks (FWHM 0.112°), indicating larger and more uniform grains. Such high crystallinity is typically associated with lower defect density and fewer deep trap states, which facilitate efficient charge transport and enhance device stability. These observations are in line with previous reports suggesting that mixed-cation systems, such as Cs/FA/MA perovskites, help stabilize the α-phase, suppress halide segregation, and reduce ion migration, all of which are critical for minimizing hysteresis and performance degradation (Sandhu & Park, 2024; Saidani et al., 2025). In contrast, the anti-perovskite films showed broader diffraction peaks (FWHM 0.192°), reflecting smaller, less uniform grains and secondary phase formation. Such structural disorder can introduce defect states that act as non-radiative recombination centers, limiting charge extraction and reducing device efficiency (Kalita et al., 2024).

Optical measurements support these structural findings. Mixed-cation perovskites exhibit the strongest and broadest absorption with a bandgap around 1.52 eV, consistent with the observed high short-circuit current density (Jsc 23.4 mA/cm^2). Interface-modified films show reduced absorption tails in the 750–800 nm range, suggesting fewer trap states at the interfaces. This is consistent with previous studies showing that interface passivation using self-assembled monolayers or fullerene derivatives can suppress interfacial recombination, thereby improving Voc and fill factor (Tian & Zhang, 2025; Gao et al., 2022). It should be noted, however, that trap densities were not directly measured in this work, so the interpretation of trap suppression remains inferred rather than directly proven.

Morphological analysis using SEM shows that mixed-cation films have large, uniform grains (350–520 nm), which reduce recombination pathways and enhance charge collection. Interface modified films show slightly smaller grains (280–450 nm) but smoother surfaces, indicating that passivation can partially compensate for grain size effects by reducing recombination at boundaries. Anti-perovskite films, on the other hand, have smaller, non-uniform grains (150–300 nm) with micro cracks, which likely serve as additional recombination sites, explaining their lower PCE and poorer stability.

Electrical measurements confirm these trends: mixed-cation devices achieve the highest PCE (21.0 ± 0.3%), followed by interface-modified (19.1 ± 0.4%) and anti-perovskite (12.9 ± 0.7%) devices. The superior performance of mixed-cation films can be attributed to their high crystallinity, low defect density, and efficient charge transport. Interface engineering enhances Voc and fill factor by passivating surface and interfacial defects, but it cannot fully compensate for limitations in the underlying film quality (Gao et al., 2022; Tian & Zhang, 2025).

Stability testing over 500 hours shows that mixed-cation devices retain 86.7% of their initial efficiency, interface-modified devices 80.6%, and anti-perovskite devices only 52.7%. The enhanced stability of mixed-cation films likely arises from improved phase stability and reduced ion migration, whereas interface passivation provides additional, though partial, stabilization. The poor stability of anti-perovskite films underscores the challenges in achieving durable performance with alternative perovskite compositions (Kalita et al., 2024; Alsulami et al., 2025).

In conclusion, these results suggest that a combination of cation/anion compositional engineering and interface modification offers a promising pathway to high-performance, stable PSCs. The mixed-cation approach consistently delivers superior crystallinity, morphology, optical absorption, electrical performance, and long-term stability, while interface passivation acts as a complementary strategy to improve Voc and suppress interfacial recombination. Future studies employing direct measurements of trap states, ionic transport, and recombination dynamics would further clarify the mechanisms governing device performance and degradation.

CONCLUSIONS

This study demonstrates that compositional and interfacial engineering play crucial roles in determining the performance and stability of perovskite solar cells (PSCs). Mixed-cation perovskites achieved the highest power conversion efficiency (PCE: 21.0 ± 0.3%) and exhibited superior long-term efficiency retention (86.7%), highlighting their intrinsic structural and optoelectronic advantages. Interface-modified devices improved open-circuit voltage (Voc) and fill factor, but their performance was limited by the quality of the underlying perovskite film. Anti-perovskites showed the lowest performance, attributed to poor crystallinity and secondary phase formation. Overall, these results suggest that combining cation/anion compositional engineering with interface modification provides a promising strategy for developing high-performance and stable next-generation PSCs. Future work should focus on direct characterization of trap states, ionic mobility, and interfacial recombination to further optimize device performance and durability.

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