ABSTRACT

Organic-inorganic lead halide perovskite solar cells (PSCs) have emerged as a highly promising technology for solar energy conversion, achieving impressive power conversion efficiency over 27% by 2025. This remarkable performance is driven by the excellent optoelectronic properties of halide perovskites, coupled with advances in various fabrication strategies such as composition optimization, additive incorporation, interface modification etc. However, despite these achievements, the long-term stability remains a major challenge, as PSCs are vulnerable to degradation from environmental factors like heat, moisture, UV exposure etc. Furthermore, the fabrication of PSCs typically requires a controlled environment, such as a glove box, making large-scale commercial production difficult. Therefore, addressing these challenges is crucial for the widespread adoption of perovskite-based technology.

Mixed cation/halide perovskites demonstrate enhanced stability as well as efficiency compared to single cation/halide perovskites. This thesis focuses on addressing instability issues of PSCs through compositional and interfacial engineering strategy in $FA_{1-y}Cs_{y}Pb(I_{0.85}Br_{0.15})_3$-based perovskite. Optimum perovskite composition is required to make perovskite both intrinsically and extrinsically stable. In this study the structurally stable perovskite film with Cs 10% has shown enhanced thermal stability when exposed to 85 °C under controlled humidity conditions (relative humidity of~30%) in ambient air. Furthermore, the interfacial engineering using tetraoctylammonium bromide (TOAB) at the hole transporting layer (HTL)/perovskite interface has been employed to improve the moisture instability of PSCs. TOAB serves a as multifunctional agent by passivating trap states, imparting hydrophobicity, reducing energy mismatch between perovskite and HTL, and facilitating efficient hole extraction through interaction with HTL. The unencapsulated TOAB-coated device showed enhanced stability retaining above 67% of its initial PCE after 1200 hours under ambient air in 70% relative humidity (RH). Also, excellent shelf-life was found for the TOAB-coated device, retaining above 74% after 400 days under dark storage in air under 30% RH conditions. Lastly, considering $FA_{0.90}Cs_{0.10}Pb(I_{0.85}Br_{0.15})_3$ as a photoactive layer the device has been tested for self-powered photodetector applications by characterizing its various figure of merits. In addition, in the entire study a relatively cheap, stable, less explored HTL material (TOP-3) has been employed in the devices. Also, the devices were fabricated in air ambient conditions with controlled humidity (20% < RH < 35%, room temperature) which help to bridge the gap between lab-scale fabrication and commercial production.

Keywords: Perovskite solar cells, Air ambient fabrication, Compositional tuning, Interface engineering, Efficiency, Stability, Self-powered perovskite photodetector

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