

## Design and Numerical Simulation of Azetidinium-based Multi-Layer Perovskite Solar Cells Using SETFOS

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**Abstract:** Solar photovoltaic technology continues to advance toward higher efficiency and lower-cost energy solutions, with metal–halide perovskites emerging as leading candidates for next-generation solar cells. While conventional perovskite absorbers offer excellent optoelectronic properties and have rapidly achieved efficiencies above 26%, their long-term instability remains a major barrier to commercialisation. Multi-absorber and tandem perovskite architectures present an effective strategy to enhance spectral utilisation and device durability beyond the single-junction limit. In this study, we explore Azetidinium (AZ<sup>+</sup>) as a novel A-site cation for stabilising multi-absorber perovskite structures. The unique four-membered cyclic geometry of AZ<sup>+</sup> improves lattice rigidity, enhances moisture and thermal resistance, suppresses ion migration, and promotes uniform crystallisation. These characteristics yield reduced defect density and improved carrier transport, making AZ-based perovskites highly suitable for high-efficiency, stable tandem configurations. Our findings highlight Azetidinium as a promising pathway toward robust, commercially viable next-generation perovskite photovoltaics. The proposed configuration of the PSC consists of FTO/SnS<sub>2</sub>/AZSnBr<sub>3</sub>/AZSnI<sub>3</sub>/Cu<sub>2</sub>O/Au. Where Azetidinium Tin Bromide (AZSnBr<sub>3</sub>) and Azetidinium Tin Iodide (AZSnI<sub>3</sub>) are the absorber layers. Tin Disulfide (SnS<sub>2</sub>) and Cuprous Oxide (Cu<sub>2</sub>O) are the electron transport layer (ETL) and hole transport layer (HTL), respectively. Fluorine-doped Tin Oxide (FTO) and Gold (Au) are typically utilised as top and bottom electrodes, respectively. Using the Semiconducting Thin Film Optics Simulation (SETFOS) 5.3 software, the thicknesses of each layer were optimised to achieve a PCE of 23.91%, Fill Factor (FF) of 78.73%, Open Circuit Voltage (V<sub>OC</sub>) of 0.74 V, Short Circuit Current Density (J<sub>SC</sub>) of 40.99 mA/cm<sup>2</sup>, and External Quantum Efficiency (EQE) of 93.68%.