

Numerical Investigation of MA3Bi2I9-Based Lead-Free Perovskite Solar Cells: Impact

WGA Pabasara, GA Sewvandi¹

Selected Proceedings of the 3rd International Engineering Research ..., 2026 • books.google.com

Abstract

This study presents a comprehensive numerical investigation of leadfree perovskite solar cells (PSCs) employing methylammonium bismuth iodide (MA3Bi2I9) as the absorber material in an FTO/ETL/MA3Bi2I9/Cu2O/Ni device architecture. Using SCAPS-1D simulation software, the photovoltaic performance of three electron transport layers (ETLs), TiO2, SnO2, and ZnO was analysed under identical absorber thickness (1.4 μm) and defect density ($1 \times 10^{12} \text{ cm}^{-3}$). The resulting power conversion efficiencies (PCEs) were 16.16% for TiO2, 14.82% for SnO2, and 16.23% for ZnO, with all devices achieving high open-circuit voltages ($V_{oc} \approx 1.44 \text{ V}$). All three ETLs yield a CBO of + 0.26 eV and a VBO of -0.95 eV, both within the literature-reported optimal thresholds (CBO < 0.30 eV and VBO < 0.2 eV) for achieving high efficiency. This alignment enables efficient hole extraction and creates an ideal spike-and-cliff band structure that reduces interfacial recombination while maintaining effective carrier flow. Therefore, the overall band alignment in all configurations supports favorable operation, and the remaining performance disparities stem from charge transport and interface quality. This work promotes MA3Bi2I9 as a stable, non-toxic absorber and validates Cu2O/Ni contacts as effective, low-cost alternatives to spiro-OMeTAD/Au.

books.google.com

[SHOW LESS](#) ^

☆ Save  Cite [Related articles](#)

Showing the best result for this search. [See all results](#)