COMPUTATIONAL MODELING AND OPTIMIZATION OF $(CH_3)_4NBiI_3$ PEROVSKITE SOLAR CELLS FOR ENHANCED PHOTOVOLTAIC EFFICIENCY

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Abstract

Lead toxicity remains a critical challenge limiting the large-scale adoption of conventional perovskite solar cells. This study presents a comprehensive COMSOL Multiphysics investigation of lead-free tetramethylammonium bismuth iodide ($(CH_3)_4NBiI_3$) perovskite solar cells, focusing on device optimization for improved photovoltaic performance. The proposed device architecture consisted of a fluorine-doped tin oxide (FTO) electrode, titanium dioxide (TiO_2) electron transport layer (ETL), $(CH_3)_4NBiI_3$ absorber layer, Spiro-OMeTAD hole transport layer (HTL), and gold (Au) back electrode. Systematic parametric studies were conducted to evaluate the influence of absorber thickness (200 to 600 nm), ETL thickness (30 to 70 nm) and HTL thickness (100 to 300 nm) on device performance under AM1.5G illumination (100 mW/cm²). Absorber thickness was identified as the most influential parameter: increasing it from 200 to 600 nm raised the short-circuit current density (Jsc) from 5.250 mA/cm² to 7.150 mA/cm² for the 30 nm TiO_2 device, while the open-circuit voltage (Voc) and fill factor (FF) decreased slightly, from 1.480 to 1.455 V and from 67.215% to 65.105%, respectively. ETL optimization identified 40 nm as the optimum TiO_2 thickness. The optimized TiO_2 (40 nm)/$(CH_3)_4NBiI_3$ (600 nm)/Spiro-OMeTAD (200 nm) architecture achieved a Voc of 1.453 V, Jsc of 7.140 mA/cm², FF of 65.812% and a power conversion efficiency (PCE) of 6.828%, compared with 5.223% for the initial design (30 nm TiO_2/200 nm absorber). Although this efficiency remains lower than that of lead-based perovskite solar cells, the lead-free $(CH_3)_4NBiI_3$ device eliminates lead toxicity, indicating its potential as a sustainable alternative for future photovoltaic technologies.

Keywords: Lead-free perovskite solar cells, $(CH_3)_4NBiI_3$, COMSOL Multiphysics, Thickness optimization, Photovoltaic performance