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Abstract

Decarbonizing the world's energy system has set the stage in favor of renewable energy alternatives such as the more reliable, abundant, inexhaustible, and sustainable solar energy. However, the photovoltaic technology faces significant stability, longevity, and scalability challenges. These difficulties can be overcome by judicious optimization of interfacial engineering of the solar cell architecture that will decrease the cost of fabrication and enhance the solar cell performance and durability. Herein, a comprehensive analysis of a novel high-performance hole transport layer-free (HTL-free) perovskite solar cell (PSC) of the configuration, ITO/$PC_{61}BM$/$CH_3NH_3SnI_3$/Pt, was investigated by device simulation while optimizing electron transport materials, metal back contacts, front contact materials, and buffer layers. The focus is on enhancing device performance by introducing various types of buffer layers, such as cadmium sulphide (CdS) in the proposed solar cell model. By fine-tuning the ETL layers and manipulating perovskite acceptor and donor densities, better device performance was achieved. Furthermore, the Mott-Schottky capacitance analysis yielded critical insights into the interface properties and dynamics of charge carriers within the solar cell structure. Optimizing back contacts also play a critical role in charge extraction and reduced recombination losses. Leveraging a sophisticated simulation platform, SCAPS-1D, the study assesses how design strategies impact photovoltaic electrical outcomes such as open-circuit voltage (V_{oc}), power conversion efficiency (PCE), short-circuit current density (J_{sc}), and Fill factor (FF). The proposed HTL-free device posted remarkable results – PCE of 38.11 %, J_{sc} of 35.32 $mAcm^{-2}$, FF of 88.67 %, and V_{oc} of 1.2168 V. Accordingly, this work inspires the promising prospects of HTL-free PSCs in achieving robust solar harvesting capabilities while streamlining device affordability. Therefore, the proposed device architecture stimulates the journey towards affordable and high-performance scalable solar cell modules.