Abstract

Over the last few years, considerable efforts have been invested in designing solar cell modules that are envisaged to revolutionize photovoltaic technology towards clean and sustainable energy. Solid-state dye-sensitized solar cells (ssDSSCs) have gained considerable attention because of their robust light harvesting capabilities. Herein, we investigate the performance of a hole transport layer-free (HTL-free) ssDSSC architecture of the configuration ITO/$PC_{61}BM$/N719 Dye/Ni HTL-free by device simulation using the solar cell capacitance simulator (SCAPS-1D). The results show viable power conversion efficiency (PCE) of 14.51%, coupled with an impressive fill factor (FF) of 84.58%, indicative of effective charge extraction mechanisms and minimal recombination losses within the device structure. Furthermore, the short-circuit current density (J_{sc}) and open-circuit voltage (V_{oc}) attained remarkable values of 22.37 mA/cm^2 and 0.7665 V, respectively. This work also found that the optimal defect density of the absorber was 1.0×10^{14} cm^{-3}, whereas the optimal donor and acceptor densities were 1.0×10^{16} cm^{-3} and 1.0×10^{19} cm^{-3}, respectively. These findings underscore the excellent light absorption, efficient charge generation, and good electron–hole separation at device interfaces. The findings of this work accentuate the promise of HTL-free ssDSSCs as high-performing solar cells characterized by simplified device architectures. The elimination of the HTL not only streamlines fabrication processes but also imparts cost efficiencies and enhances device stability. This study thus contributes invaluable insights to the advancement of efficient and commercially viable ssDSSCs, thereby inspiring progress towards a greener and more sustainable renewable energy landscape.