

Abstract

The primary aim of this work is to investigate the use iron di-silicide (FeSi_2) as a photoactive layer in order to achieve superior performance in the solar cell architecture—ITO/ TiO_2 / FeSi_2 /CuSCN/Ni. The optimum thickness of the absorber layer was found to be 1000 nm, which gave optimal properties of the proposed cell—a short-circuit current density (J_{sc}) of 51.41 mAcm^{-2} , an open-circuit voltage (V_{oc}) of 0.93 V, a fill factor (FF) of 77.99%, and power conversion efficiency (PCE) of 37.17%. The introduction of an ultrathin interfacial layer between the electron transport layer (ETL), the perovskite interface, and the hole transport layer (HTL) enhanced the electrical output of the proposed solar cell. The J_{sc} increased to 51.86 mAcm^{-2} , V_{oc} rose to 0.97 V, while FF and PCE increased to 82.86% and 41.84%, respectively. Accordingly, the proposed cell architecture is promising and can be introduced into the manufacturing workflow for commercial applications. Moreover, because of its exceptional photon absorption capabilities, FeSi_2 is a potentially excellent photoactive material for solar cell fabrication. The detailed findings of this study have therefore indicated that high-performance FeSi_2 -based solar can be achieved in future.