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A NUMERICAL SIMULATION STUDY OF THE PERFORMANCES OF 3D/2D PEROVSKITE SOLAR CELL AFTER INTRODUCING THE DEFECTS IN THE 3D PEROVSKITE LAYER

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Abstract

This is a numerical simulation study of a thin film hybrid organic-inorganic perovskite solar cell with a p-i-n structure. The p-type semiconductor layer is an organic hole transporting material (HTM) called Poly (3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS). In this new device structure, we have intentionally included a double intrinsic layer (i) of 3D Methylammonium Lead Iodide ($CH_3NH_3PbI_3$) (MAPI) and the 2D monolayer of $CH_3NH_3PbI_3$ to minimize the degradation of the device, and also embedded deep and shallow defects in the 3D-MAPI layer. The n-type material, fullerene derivative (6,6)-phenyl-C61-butyric acid methyl ester (PCBM) is used as an organic electron transporting material (ETM). The solar cell performance has changed after including defects in the 3D-MAPI since the defects can alter the dark saturation current of the device. The simulation results show that the shallow defects and deep defects of 3D-MAPI can alter the open-circuit voltage of the perovskite solar cell model. The open-circuit voltage of the solar cell model depends on the dark saturation current, which indicates how much recombination is occurring in a semiconductor. The deep defects of 3D-MAPI should be minimized to increase the cell performance since the high dark saturation current decreases the open-circuit voltage of the solar cell. We have observed that Shockley-Read-Hall recombination is the most predominant recombination mechanism for the deep defects in the 3D-MAPI materials.

Keywords: perovskite-based solar cell, recombination, thin-films, dark saturation current, defects