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NUMERICAL STUDY OF THE EFFECT OF DELAFOSSITE $CuAlO_2$ AND PEDOT:PSS AS HOLE TRANSPORT MATERIALS IN THE 3D/2D PEROVSKITE SOLAR CELL

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Metal halide perovskite solar cells have shown good performance in photovoltaic. Methylammonium lead iodide ($CH_3NH_3PbI_3$ or 3D-MAPI) is one of the most popular 3D metal halide perovskite materials. In this study, we numerically modelled metal halide perovskite solar cells having a p-i-n structure with intrinsic layers of 3D-MAPI and 2D monolayers of $CH_3NH_3PbI_3$ (2D-MAPI). However, the hole transporting material of the p-i-n perovskite solar cell can control the performance of the solar cell due to the recombination in the hole transporting layer (HTL). We simulated and observed how the delafossite $CuAlO_2$ and PEDOT:PSS (poly(3,4-ethylenedioxythiophene) polystyrene sulfonate) HTLs affect the solar cell model with the structure of Glass/p-PEDOT:PSS or p-$CuAlO_2$ (HTL)/i-3D-MAPI/i-2D-MAPI/n-PCBM (ETL)/Ag. The fullerene derivative (6,6)-phenyl-C61-butyric acid methyl ester (PCBM) was used as an electron transporting material (ETM). Firstly, the optimised solar cell model was simulated with a p-type PEDOT:PSS layer. Secondly, PEDOT:PSS was replaced with $CuAlO_2$ to observe its performance. The one-dimensional Solar Cell Capacitance Simulator (SCAPS-1D) has been used to model these solar cells under the AM1.5G solar spectrum. We have first obtained the results, with the power conversion efficiency (PCE) of 20.17%, open-circuit voltage (V_{OC}) of 1.10 V, fill factor (FF) of 76.08%, and short-circuit current density (J_{SC}) of 24.17 mA cm^{-2}. After replacing $CuAlO_2$, the solar cell performance improved, with the PCE of 23.17%, V_{OC} of 1.14 V, FF of 84.07%, and J_{SC} of 24.17 mA cm^{-2} since $CuAlO_2$ has shown high shunt-resistant value than PEDOT:PSS. Consequently, the 3D/2D metal halide perovskite solar cell model with $CuAlO_2$ has numerically shown better power conversion efficiency than the solar cell model with PEDOT:PSS since the low carrier recombination at the $CuAlO_2$ layer (HTL).

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Keywords: Hole-transporting material, Perovskite-based solar cells, Power-conversion efficiency, Recombination, SCAPS-1D