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A numerical simulation of the effect of the surface defect layer (SDL) properties on 3D/2D perovskite solar cell performance

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Organic-inorganic hybrid perovskites have become one of the promising solar cell materials in photovoltaic because of their low cost and excellent performance. In this study, we have modelled a hybrid organic-inorganic perovskite thin-film solar cell having p-i-n structure, with intrinsic layers of 3D methylammonium lead iodide ($CH_3NH_3PbI_3$) (MAPI) and 2D monolayers of $CH_3NH_3PbI_3$. The 2D layer is mainly used to improve the stability of the 3D $CH_3NH_3PbI_3$ layer. The p-type layer is an organic hole transporting material (HTM) called Poly (3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS). The material fullerene derivative (6,6)-phenyl-C61-butyric acid methyl ester (PCBM) is used as an organic electron transporting material (ETM) and this is the n-type layer. This numerical simulation study of a 3D/2D hybrid perovskite solar cell model has been carried out by using Solar Cell Capacitance Simulator (SCAPS-1D). In this study, we have intentionally included the surface defect layer (SDL), which is p-type, in between 3D-MAPI and 2D-MAPI layers to improve the performance of the 3D/2D perovskite-based thin-film solar cell model. The effect of the surface defect layer (SDL) is analyzed by changing the thickness, bandgap, and neutral defect density. According to the simulation results, the optimum thickness of SDL is in the range of 160-170 nm with the optimum SDL bandgap of 1.4 eV, has shown higher power conversion efficiency of the cell model. The neutral defect density of the SDL has been changed to identify the effect on the power conversion efficiency of the solar cell. We have also identified that the neutral defect density of the SDL should be kept less than 10^{13} cm^{-3} to get better performance. According to the results, we have observed the improvement of the solar cell efficiency of the cell structure, p-PEDOT:PSS/i-3D-MAPI/p-SDL/i-2D-MAPI/n-PCBM/Ag, with the efficiency of 21.41%, open-circuit voltage (V_{OC}) of 1.1034 V, short-circuit current density (J_{SC}) of 25.59 mA/cm^2, and fill factor (FF) of 75.80%. This 3D/2D perovskite solar cell structure with SDL has shown good power conversion efficiency than that of the cell model that does not contain SDL, which is 19.65%. We have numerically simulated that the SDL can improve the efficiency and the performance of the cell model.

Keywords: Defect density, Perovskite-based solar cell, Power conversion efficiency, Surface defect layer (SDL), Thin-films

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