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Theoretical study on the effect of electron transport layer parameters on the functionality of double-cation perovskite solar cells

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ABSTRACT

Here, device modeling of $FA_{0.83}Cs_{0.17}Pb(I_{0.6}Br_{0.4})_3$ perovskite solar cell was performed. The band gap energy, electron affinity, and carrier concentration of the electron transport layer (ETL) have been investigated. Furthermore, ETL/perovskite interface defect density has been varied for this study. The study on electrical properties and the photovoltaic parameters of the perovskite solar cell showed that conduction band offset plays a vital role in cell performances. Furthermore, by increasing the electron affinity of ETL the cell performance decreased drastically, we attributed this result to an effective increase in the photogenerated carrier recombination in the ETL as well as ETL/front contact interface. Furthermore, simulation results disclosed a great dependence of PCE on the defect density at ETL/perovskite absorber interface layer. It was found that the role of interface trap density on decrement of Voc is dominant.

1. Introduction

High performance perovskite solar cells have attracted significant attention of researchers in the green and renewable energy field [1]. A conventional planar perovskite solar cell, which has high efficiency, typically consists of a transparent conducting oxide (TCO) layer, an electron transport layer (ETL), which normally is a wide bandgap n-type semiconductor, a perovskite absorber layer, a hole transport layer (HTL) which is a p-type semiconductor, and a proper back contact [2].

The perovskite materials, which can consist of organic-inorganic hybrid compounds, are used as the light absorber in solar cells. The compounds have chemical formula of ABX_3, where A is an organic or inorganic cation (such as Methylammonium ($CH_3NH_3^+$)), Ethylammonium ($CH_3CH_2NH_3^+$), formamidinium ($[NH_2CH]NH_2^+$), or CS^+, B is a divalent metal cation (like Pb^{2+}, Sn^{2+}, Ge^{2+}), and X refers to a halogen anion (such as I^-, Br^-, Cl-, F-). Among all of the different perovskite compounds, methylammonium lead iodide ($MAPbI_3$) is one of the firstly used and the most popular perovskites used in perovskite solar cells [3–5]. However, $MAPbI_3$ has some problems such as thermal instability, degradation over time and lake of long-term stability. Finding suitable alternative compounds to improve cell efficiency by increasing the absorption coefficient, increasing the electron and hole diffusion length, and reducing carrier recombination, are among the researches in the world [6].

Various approaches have been proposed for this purpose. Replacing the A Cation as well as X halide is a one common strategy. For instance, compared to methylammonium lead halide, Formamidinium lead halide has attracted greater attention due to its broad

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