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An optimized perovskite solar cell designs for high conversion efficiency

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Abstract

This paper reports the simulation and optimization of an organic/inorganic perovskite-based photovoltaic solar cell. Several structures for PSC are found in literature in order to enhance the conversion efficiency. The objectif of this work is to study and investigate different structures of solar cells based on perovskite materials to improve their performances. The simulated solar cell is made by sandwiching TiO_2/Perovskite/spiro-OMeTAD layers where TiO_2 is the electron transport layer (ETL), spiro-OMeTAD is the hole transport layer (HTL) and both $CH_3NH_3PbI_3$ $CH_3NH_3SnI_3$ are the perovskite (PVK) absorber layers. Therefore, the layer thicknesses of different materials are modified in order to find the better conversion efficiency of solar cells. The obtained results show that layer thicknesses that provide the maximum power conversion efficiency of 18.16% and 9.56% for both perovskite materials CH3NH3PbI$_3$ and CH3NH3SnI$_3$, respectively are 200 nm, 100 nm and 500 nm for spiro-OMeTAD, TiO2 and PVK materials, respectively. The numerical simulation was performed using the ATLAS device simulation software.

Introduction

In the last few years, there has been a surge of interest in the use of perovskite materials in photovoltaic solar cell research has developed exponentially [1], prompting researchers to invest in research to improve the performance of perovskite-based photovoltaic cells as well as trying to understand the various internal mechanisms that control several characteristics, including hysteresis [[2], [3], [4], [5], [6]], power conversion efficiency (PCE) [[7], [8], [9], [10], [11], [12]] and stability [[13], [14], [15], [16]].

Power conversion efficiency of perovskite-based solar cells was stepped from 3.8% in 2009 [17] up to 22.1% in 2016 [18]. In this context, experimental research investigations are made to increase conversion efficiency and enhance electrical performances of solar cells. Therefore, simulations efforts are also conducted to help sizing (thickness, doping density, band gap, …) and minimizing experiment costs of solar cells.

Recently, many authors have reported simulations for perovskite-based solar cell using free device softwares such as SCAPS [19,20], wxAMPS [21] and GPVDM [22] which are based on one physical model: the drift diffusion transport model. To reach a closer simulated model that describes experimental results, SILVACO ATLAS device software [23] presents a large multitude of physical models including drift diffusion transport model. It has different material models (for organic and inorganic) for recombination and mobility to help users doing the best choice for each material making them closer to experimental behavior. Furthermore, it is based on resolving of different equations mainly Poisson's equation and carrier continuity equations for electrons and holes.

In this work, numerical simulations of diverse structures of perovskite-based photovoltaic solar cells have been studied in order to improve the electrical performances of these devices. The key idea of this work is to find the better layer thicknesses of solar cell to enhance the conversion efficiency of them. For this reason, the effect of layer thickness of different materials (electron transport layer, hole transport layer and perovskite layer) on various electrical parameters of the solar cell is presented and discussed.

Section snippets

Device structure and simulation methodology

As can be seen from Fig. 1, the n-i-p perovskite-based planar heterojunction solar cell design is considered where TiO_2 is used as electron transport layer, spiro-OMeTAD is used as hole transport layer for both structures. $CH_3NH_3PbI_3$ and $CH_3NH_3SnI_3$ are used as absorber layer for the first and the second structure, respectively. All the work on the computer simulations was carried out using SILVACO ATLAS software to study the effect of different layer thicknesses on solar cell electrical…

Results and discussions

Simulations were carried out using parameters given in Table 1, Table 2 and the simulation methodology was presented in the last section. Fig. 2 shows the effect of $CH_3NH_3PbI_3$ (Pb) and $CH_3NH_3SnI_3$ (Sn) perovskite layer thickness on different electrical parameters. It is shown that J_{sc} (Fig. 2-a) increases with increasing of perovskite layer thickness in both cases ($CH_3NH_3PbI_3$ and $CH_3NH_3SnI_3$) to a saturation values of 23.99 mA/cm^2 and 19.03 mA/cm2, respectively. This can be explained by more…

Conclusion

In this paper, the effect of various layer thicknesses of perovskite-solar cells on different electrical parameters is presented. It is found that the perovskite layer thickness of both $CH_3NH_3PbI_3$-based solar cell and $CH_3NH_3SnI_3$-based solar cell has an important effect on electrical parameters in comparison with that of hole and electron transporting layers. Therefore, the obtained results show that perovskite based on $CH_3NH_3PbI_3$ has better electrical performances than perovskite based on CH_3NH_3…

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> …To solve these problems, Sn replacing Pb can be a decent approach that provides both toxic-free and better stable devices [3]. However, there are some problems with MASnI3 material because of its bandgap, which is almost 1.3 V and is much lower than traditional PVK material [14,15]. Having a lower bandgap, MASnI3 only absorbs photons with a smaller range of energy.…

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