Performance Evaluation of Lead-Free $Cs_2CuSbCl_6$ Perovskite Solar Cells for > 21.67% Efficiency

Ajay Kumar[1], *Senior Member, IEEE*, Melvin Saji Thomas[1], Neha Gupta[2], and Aditya Jain[3], *Senior Member, IEEE*

[1]Department of Electronics and Communication, Jaypee Institute of Information Technology, Noida, India.
[2]Department of Applied Science and Humanity, ADGITM, New Delhi, India.
[3]Department of Electronics and Communication, Symboisis Institute of Technology, Pune, India

Abstract— **This work investigates the performance of $Cs_2CuSbCl_6$-based lead-free perovskite solar cells for photovoltaic applications. $Cs_2CuSbCl_6$ has a bandgap of 1.7eV and it is a durable and non-toxic material. $Cs_2CuSbCl_6$ can absorb more photons and thus obtain high efficiency. This work has been performed using SCAPS-1D software with the focus on optimizing the absorber layer thickness in terms of solar cell performance metrics such as efficiency (η), fill-factor (FF), open-circuit voltage (V_{oc}), and short-circuit current density (J_{sc}). The highest efficiency of 21.67% has been obtained for the optimized value of the absorber layer thickness of 900 nm, with values of 1.22 V, 21.19 mA/cm^2, and 83.19% for V_{oc}, J_{sc}, and FF respectively. Thus, $Cs_2CuSbCl_6$ -based solar cell paves as the safe alternative to lead-based solar cells for photovoltaic applications.**

Keywords— Efficiency, $FASnI_3$, Perovskite, PEDOT:PSS, SCAPS-1D.

I. Introduction

There is a growing demand for energy as a result of population expansion. Traditional energy sources, such as fossil fuels, offer energy while also contributing to the greenhouse effect. To address such issues, experts are looking for alternate energy sources that may both provide energy and aid in pollution reduction. Solar cells, also known as photovoltaic cells, appear promising since they generate energy from sunlight, which is renewable and abundant in nature [1]. Silicon-based solar cells are widely available, however on the other hand perovskite-based solar cells demonstrated great performance at extremely cheap costs, and their PCE was over 25% in a few years [2].

The lead-based metal halide is an appealing perovskite solar cell that reported great PCE among other perovskites [3]. Lead, on the other hand, is a very poisonous substance, and its presence in perovskite poses a threat to human health and to the environment. Lead-free perovskites such as the $Cs_2CuSbCl_6$ compound have shown promising photovoltaic characteristics. $Cs_2CuSbCl_6$ is a promising semiconductor with a suitable bandgap for solar cells, $Cs_2CuSbCl_6$ has an indirect bandgap of 1.7 eV [4]. The $Cs_2CuSbCl_6$ perovskite compound is a promising material with excellent optical, electrical, and photovoltaic properties, and it could eventually replace lead halide perovskite in photovoltaic applications. The SCAPS-1D simulator was utilized to numerically simulate the effects of several ETLs in this work, with Spiro-OMeTAD serving as the HTL [5].

The performance of experimentally developed perovskite solar cells based on ITO/TiO_2/$Cs_2CuSbCl_6$/Spiro-OMeTAD/Au was analyzed, and then PSC was optimized in terms of perovskite absorber layer thickness. The optimized design of the PSCs will now be investigated further for doping concentrations in the absorber layer.

II. Device Structure and Simulation Methodology

As illustrated in Fig. 1, we presented a structure that is divided into three layers in order: The first is the ETL layer, the second is the absorber layer, and the last one is the HTL layer. For the designing and analysis of the perovskite solar cell, SCAPS-1D software is employed. The topmost contact (front contact) ITO is considered [6]. The thickness of the ETL layer is t = 200nm and is composed of TiO_2. TiO_2 is cheaper than other optical materials. Titanium dioxide (TiO_2) is advantageous because it provides the high chemical stability, nontoxicity, high light transmission, low series resistance, and conductivity [7]. The absorber layer is responsible for the capture and absorption of photons and must be a material with a large bandgap. In our study, $Cs_2CuSbCl_6$ is used as the absorption layer. The thickness of the HTL layer is 200 nm and consists of Spiro-OMeTAD.

III. Result and Discussion

In the perovskite solar cells, the absorber layer has an important role in the performance of the device and the results. The changes can significantly cause the performance and result of the solar cell. The proposed solar cell model has been numerically analyzed for the thickness of the absorber layer because it plays a vital role in enhancing the efficiency of solar cells. Fig. 2(a) and Fig. 2(b) show the J-V characteristics of the proposed device and the corresponding quantum efficiency (QE) curve respectively with varied absorber layer thickness [6]. When the absorber layer thickness increases from 700 nm to 1300 nm then J-V characteristics and QE slightly reduce as reflected in Fig. 2(a) and Fig. 2(b) respectively. Fig. 3(a-d) reflects the impact of absorber layer thickness on the photovoltaic parameters. As the absorber layer thickness reduces, V_{oc} increases gradually and reaches 1.242 V as shown in Fig. 3(a). Fig. 3(b) shows J_{sc} is slightly increase with the increase in absorber layer thickness and reaches 21.75 (mA/cm^2). FF of the proposed device is reflected in Fig. 3(c) which reflects that the device has a higher value of FF (~84%) and reaches 83.81% for the 700 nm thickness of the absorber layer. Fig. 3(d) shows that PCE is higher at 700 nm thickness of the absorber layer and achieved 21.67% owing to the high absorption of the absorber layer, which absorbs more photons for higher wavelengths. Thus, the optimized values (700 nm) of absorber layer thickness are found by considering photovoltaic parameters.

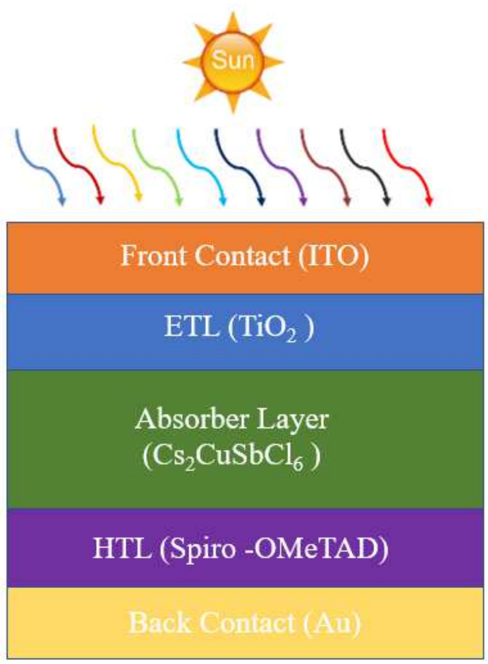

Fig. 1. The proposed structure of $Cs_2CuSbCl_6$ perovskite solar cell.

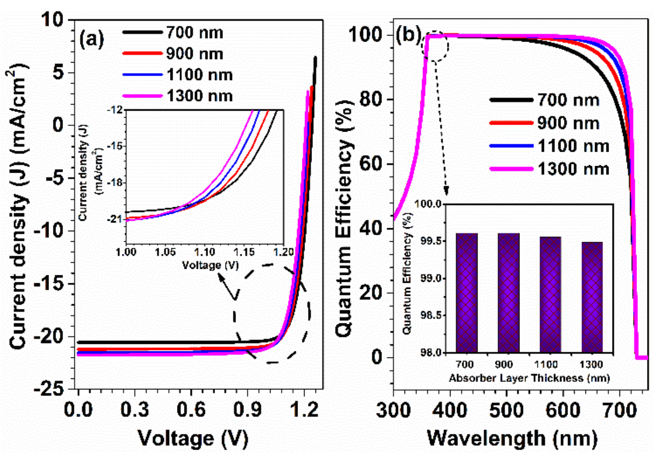

Fig. 2. (a) Current density and (b) Quantum efficiency of $Cs_2CuSbCl_6$ perovskite solar cell.

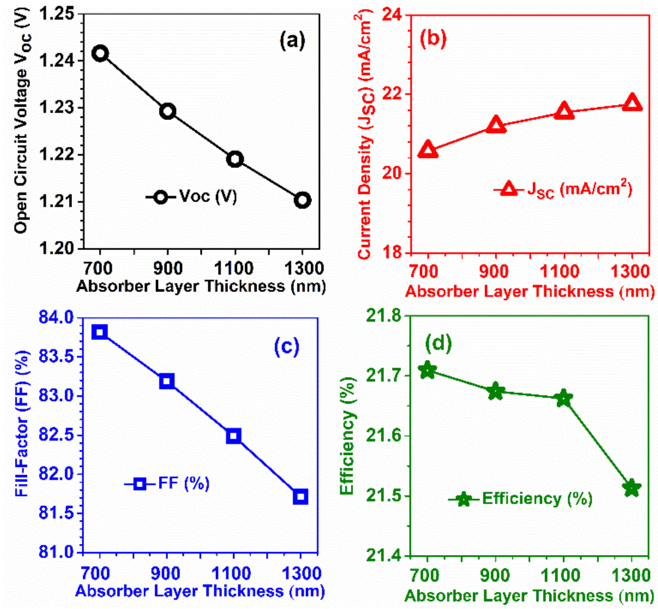

Fig. 3. (a) V_{oc}, (b) J_{sc}, (c) FF, and (d) η; for the different absorber layer thickness of $Cs_2CuSbCl_6$ perovskite solar cell.

IV. Conclusion

In the present work, $Cs_2CuSbCl_6$ based solar cell has been proposed for lead free photovoltaic applications. The variations of absorber layer thickness on $Cs_2CuSbCl_6$ based solar cells is observed to optimize its thickness, and it was found the maximum efficiency of 21.67% is achieved with optimized values for absorber layer thickness at 700 nm. Other performance parameter values: V_{oc} is 1.242 V, J_{sc} is 21.75 (mA/cm^2), and FF is 83.81% are obtained. This work could be helpful for the fabrication of lead-free perovskite solar cells for photovoltaic applications.

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