Analysis of Cs_2TiBr_6 Single-Halide Perovskite Solar Cell by introducing IDL

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***Abstract*– Lead-based perovskite solar cells (PSCs) are popular in the photovoltaic industry for their remarkable properties, but issues like toxicity and instability limit their use. To address these problems, eco-friendly, lead-free, and stable Cesium Titanium Bromide (Cs_2TiBr_6) absorber material has been introduced. This work simulates an FTO/SnO_2/IDL_1/Cs_2TiBr_6/IDL_2/MoO_X/Au structure using SCAPS-1D incorporating the use of interfacial defect layer (IDL), examining factors such as layer thickness, doping, defect density, and quantum efficiency. The optimized structure achieves a power conversion efficiency (PCE) of 20.11%, having a fill factor of 82.17, V_{OC} of 1.488 V, and J_{SC} of 16.34 mA/cm². This research supports the development of efficient, low-toxic, and stable PSCs for the solar industry.**

***Index terms* – Single-halide, Power Conversion Efficiency, IDL, Cs_2TiBr_6, MoO_X, SnO_2.**

I. INTRODUCTION

Recently, lead-based PSCs have attracted global attention in solar industry due to its extraordinary properties that includes a suitable wide band gap, high absorption coefficient, high carrier mobility, extended carrier lifetime, significant diffusion length and ease of manufacturing which reported its PCE upto 22 % [1]. Yet, the environmental concern primarily revolves around the presence of toxic elements such as Pb and heavy metals throughout the lifecycle of PSCs. So, researchers and industrial professionals have made significant efforts to explore non-toxic materials for the perovskite photovoltaic market. Fortunately, many non-toxic absorber materials such as Ge, Sn, Ti, Sb, Bi acted as a promising candidate for the replacement of toxic materials [2]. Among the non-toxic materials, the titanium (Ti)-based single halide Cs_2TiBr_6 has become a potential candidate in the photovoltaic sector for its low toxicity, thermal stability, and biocompatibility [3]. Numerous researchers have reported that lead-free inorganic single-halide Cs_2TiBr_6 compound-based PSCs have achieved stable efficiencies in recent years, attributed to its tunable bandgap and vacancy-ordered double perovskite structure. The aim of this work is to present a systematic approach of a novel planar p-n heterojunction PSC with stable single-halide Cs_2TiBr_6 by considering the interfacial defect layers (IDL) that can potentially enhance charge extraction and reduce recombination at the interfaces to mitigate electronic defects and improve carrier lifetime. Through a comparative analysis of proposed novel PSC and early reported Cs_2TiBr_6 based PSCs, the external quantum efficiency, V-I performance of perovskite cell, the effect of absorber layer thickness and its doping concentration have been studied on the various parameters. In addition to that, the study helps in understanding major benefits of IDL in enhancement of device performance and stability through optimized values of open-circuit voltage (V_{OC}), fill factor, short circuit current density (J_{SC}) and PCE.

II. DESIGN OF PEROVSKITE BASED SOLAR CELL

Fig.1 depicts the layered structure of the novel FTO/SnO_2/IDL_1/Cs_2TiBr_6/IDL_2/MoO_X/Au PSC. The structure's top layer, a contact layer, is made of highly conductive fluorine-doped tin oxide (FTO), which allows sunlight to pass through and reduces electrical losses while enhancing conductivity. Beneath this contact layer, a heavily doped 0.05 µm thick SnO_2 region (n-type) acts as an efficient electron transport layer (ETL) due to its high optical transmittance and high electron mobility. The p-type Cs_2TiBr_6 absorption layer is positioned between the ETL and hole transport layer (HTL). The p-type MoO_X (Molybdenum Oxide) serves as a HTL, characterized by a 3.0 eV band gap, that provides high hole mobility, enhanced stability and minimum valence band offset with absorber Cs_2TiBr_6. Au (gold) as back metal contact (BMC) layer connected to HTL.

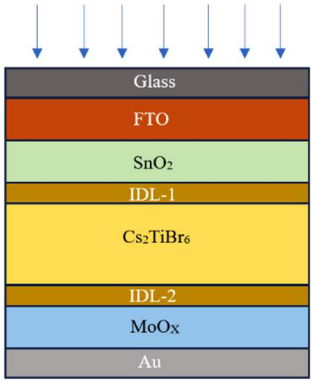
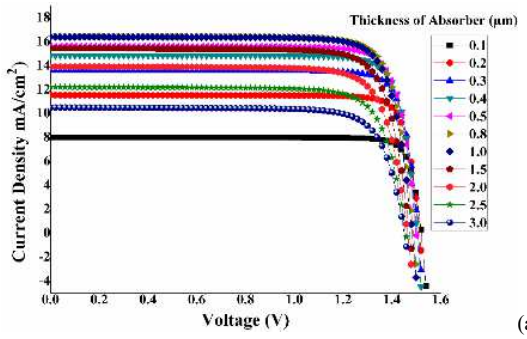


Fig 1: Proposed planar heterojunction FTO/SnO_2/IDL_1/Cs_2TiBr_6/IDL_2/MoO_X/Au PSC.

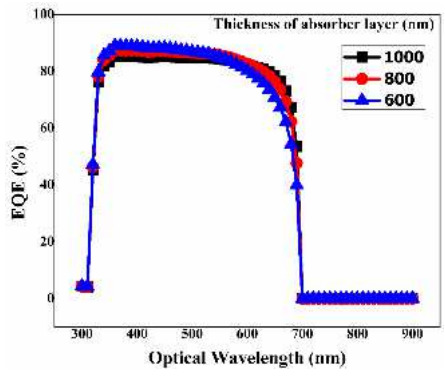
III. RESULTS AND DISCUSSION

Fig. 2 (a) depicts the current-voltage characteristics of the PSC under solar illumination of 1.5 G. This shows that the the Jsc drastically rises up to 800 nm absorber thickness and then suddenly falls when altering the thickness from 900 to

3000 nm. Above 800 nm active layer thickness, there is an abrupt decrease in Jsc because of the increase in series resistance value and back metal contact recombination. It was noted that all Voc values coincide at a common point. While varying the thickness from 100 nm to 800 nm, Jsc improves from 8 mA/cm^2 to 16.34 mA/cm^2. Therefore, the optimal light harvesting layer (Cs_2TiBr_6) thickness yielding a maximum efficiency of 20.11 %, is 800 nm. Fig. 2(b) highest peak is obtained at absorber thickness of 350 nm. Thus, more photo absorption take place with better EQE. Moreover, as the absorber thickness increases above 800 nm, the increase in photo absorption was smaller. Thus, longer wavelength light absorption is obtained at 800 nm absorber thickness when varying the thickness from 300 nm to 3000 nm.



(a)



(b)

Fig. 2 (a) I-V characteristics of PSC with Cs_2TiBr_6 absorber thickness variation (b) EQE in contrast to wavelength of PSC.

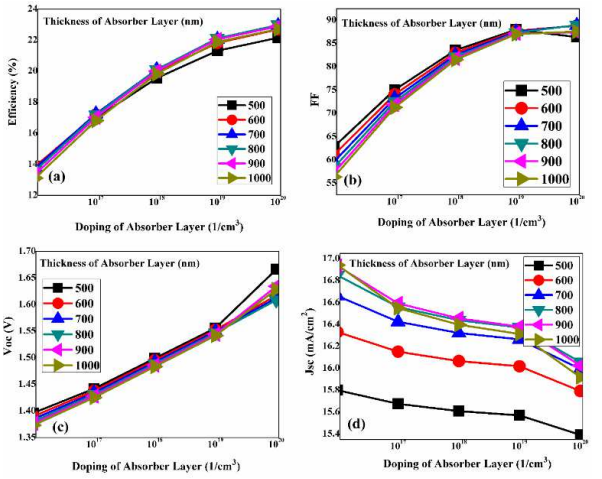


Fig. 3 Effect of doping density of Cs_2TiBr_6 while varying its thickness from 500 to 1000 nm on (a) PCE (b) FF (c) Voc (d) Jsc.

Fig. 3 shows the study of doping density of absorber when altered from 10^{16} cm^{-3} to 10^{20} cm^{-3}. In fig. 3 (a, b and c), the Voc, PCE, and FF also gradually keep on increasing as the shallow acceptor impurity increases. However, in fig. 3 (d), Jsc drops significantly while increasing doping density. This is because of the substantial increase in the recombination of photo generated charge carriers. which reduces the carrier mobility, diffusion length and minority carrier concentration. Further, increase in Voc (fig. 3 (c)) is due to the increase in conductivity which ensures the higher built-in potential hence gives the higher Voc. Thus, optimal value of doping can be studied by considering all these doping factors. So, 10^{18} cm^{-3}, considered as the optimum value of doping of light harvester layer thickness 800 nm to get the better efficiency (20%) of the device structure.

Table 1: Comparative study of proposed PSC with early reported structures

Structure	J_{sc} (mA/cm^2)	V_{oc} (V)	FF (%)	Efficiency (%)
Ref. [4] Experimental	3.87	0.89	59.5	2.15%
Ref. [4] Experimental	5.75	0.99	54.9	3.12%
Ref. [5] Simulation	8.66	1.53	86.45	11.49%
Proposed work	16.34	1.488	82.17	20.11%

IV. CONCLUSION

In this study, the structure employing FTO/SnO_2/ Cs_2TiBr_6/MoOx/Au with IDL has been completely investigated by SCAPS-1D. Through a comparative analysis of proposed structure and already developed experimental and simulated structures, the study examines the proposed device performs better and gives the higher PCE of 20.11% at a thickness of 800. By doing simulations, it has been observed that with the incorporation of IDL, the device performed better as compared to other existing structures without IDL. As a result, maximum PCE reached upto 20.11% along a FF (82.17), Voc (1.488 V), and Jsc (16.34 mA/cm^2).

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