



Numerical Modelling of Efficient Lead-Free Inorganic Perovskite Solar Cell Using SCAPS-1D

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Abstract. Perovskite solar cells (PSCs) have become one of most emerging thin-film photovoltaic technologies. However, traditional lead-based perovskites face major limitations due to their toxicity and limited long-term stability, creating a strong need for environmentally friendly, lead-free alternatives. This work present, SCAPS-1D software is utilized to simulate a PSC based on a stable and eco-friendly inorganic absorber. To enhance carrier mobility, electron transport layer (ETL) is incorporated, and the commonly used PCBM is replaced with graphene oxide (GO), which also contributes to lowering the device cost. The key design parameters, such as thickness, acceptor concentration and defect density of active layer, metal work function and operating temperature are thoroughly examined. With GO functioning as the ETL, optimized device performance achieved includes a PCE of 25.27%, V_{oc} of 1.12 V, J_{sc} of 28.51 mA/cm², and an FF of 79.0%. The proposed lead-free PSC structure offers a promising way to addressing stability and toxicity concerns while improving overall device performance.

Keywords: Numerical simulation, SCAPS, ETL, HTL.

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I. Introduction

The rapid rise in global electricity demand has encouraged researchers to investigate substitutions to traditional energy sources. This increasing interest is attributed by the restricted accessibility of conventional energy resources, along with their environmental impacts, high costs, and practical limitations. These factors have enhanced the shift toward cleaner and more sustainable energy alternatives. Among the various renewable technologies, solar energy has developed as one of the most promising and efficient options. Silicon (Si) has long dominated the solar cell industry because of its stability, strong PCE, and excellent radiation resistance [1,2]. However, the development of conventional Si-based solar cells is constrained by inherent limitations, including silicon's indirect and optimum bandgap and the high production costs involved. Since 2009, mixed inorganic organic lead halide perovskites (OILHPs) have emerged as potential photovoltaic materials owing to their favourable attributes, such as low cost, suitable bandgaps, superior charge mobility, defect tolerance, and impressive PCE. Notably, the efficiency of PSC has mounted dramatically from an initial 3.8% in 2009 to about 26% by 2021[3].

The general composition of a PSC is represented by the composition AMX₃, where A corresponds to an inorganic or organic cation such as Rb⁺, K⁺, Cs⁺. The M site is occupied by a metal cation like Sn, Ge, or Pb, while X indicate a halide ion, typically I⁻, BF₄⁻, Br⁻, Cl⁻, or SCN⁻[4]. Vaibhava et al. investigated a lead-free based PSC with the layout FTO/PC₆₁BM/CsSn_{0.5}Ge_{0.5}I₃/Cu₂O/Au and achieved PCE of 12.37%, FF of 79.59%, V_{oc} of 0.8521 V, and J_{sc} of 18.24 mA/cm²[5].

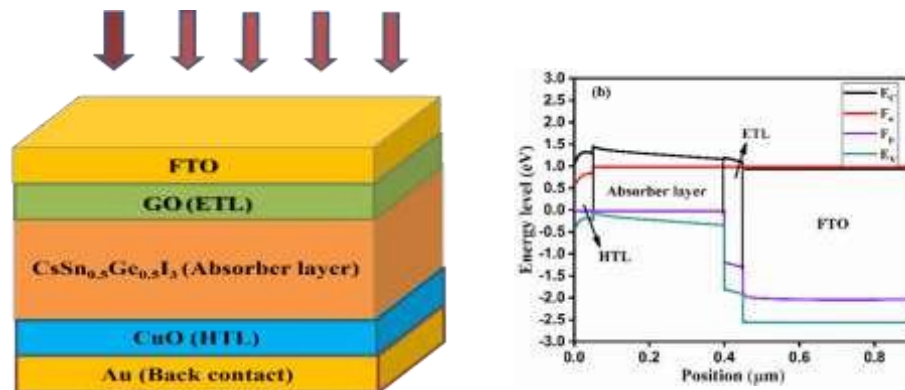
In this study, the influence of thickness, acceptor concentration, defect density of photoactive layer, temperature and metal work function of back contact on the performance of CsSn_{0.5}Ge_{0.5}I₃ based PSCs is examined. The main aim is to accurately optimize the device parameters to achieve higher PCE while simultaneously lowering overall fabrication costs.

II. Materials parameter and device architecture

In this investigation, SCAPS-1D was employed due to its user-friendly interface, flexible control options, and capability to simulate device performance under both illuminated and dark conditions. The software also supports the construction of heterostructures with up to seven layers, making it suitable for detailed photovoltaic modeling. It was formed by Burgelman and his team at Ghent University in Belgium[6,7]. Fig. 1(a,b) illustrates the device configuration and band structure diagram.

Table 1. Electrical input parameter of PSC device[8,9].

Parameters	Units	FTO	GO	CsSn _{0.5} Ge _{0.5} I ₃	CuO
Electron affinity	(eV)	4.0	3.86	3.9	4.07
Effective DoS at VB	(1/cm ³)	1.80×10^{19}	2.20×10^{18}	3.10×10^{18}	5.5×10^{20}
Donor concentration	(1/cm ³)	2.0×10^{19}	1.0×10^{18}	1.4×10^{14}	0
Total defect	(1/cm ³)	1.0×10^{18}	1.0×10^{15}	1.0×10^{15}	1.0×10^{13}
Electron mobility	(cm ² /Vs)	20	100	974	100
Effective DoS at CB	(1/cm ³)	2.20×10^{18}	2.20×10^{19}	3.10×10^{18}	2.2×10^{19}
Acceptor concentration	(1/cm ³)	0	0	0	1.00×10^{20}
Bandgap	(eV)	3.5	3.0	1.5	1.5
Hole mobility	(cm ² /Vs)	20	25	213	0.1
Thickness	(cm)	500	50	350	50
Dielectric permittivity	ϵ	9.0	9.0	28	18.1


Fig.1 (a) Device configuration, (b) Band structure diagram

III. Results and analysis

A. Significance of absorber thickness

The efficiency of a PSC largely depends on absorber layer, as it is trustworthy for delivering charge carriers via light absorption. The thickness of this layer directly alters diffusion length and lifetime of photogenerated electrons and holes [10]. From Fig.2(a,b), to analyses how absorber thickness influences device behaviour, CsSn_{0.5}Ge_{0.5}I₃ layer was varied from 0.2μm to 0.9μm. As photoactive layer becomes thicker, J_{sc} increases up to 0.9μm due to enhanced photon absorption, after which it begins to decline. further thickening leads to higher recombination, raising the dark saturation current and causing V_{oc} to change only marginally beyond a certain point. The rising saturation current and recombination rate also contribute to gradual shifts in device behaviour. The FF reveal slight deviations with thickness variation. The overall PCE decreases until the absorber reaches 0.9μm, followed by a mild linear decrease at larger thicknesses. Thus, 0.2μm is identified as the optimal CsSn_{0.5}Ge_{0.5}I₃ layer thickness for subsequent simulations, yielding following performance parameters: V_{oc} (V) = 1.12, J_{sc} (mAcm⁻²) = 28.51, FF (%) = 79.0, and PCE (%) = 25.27.

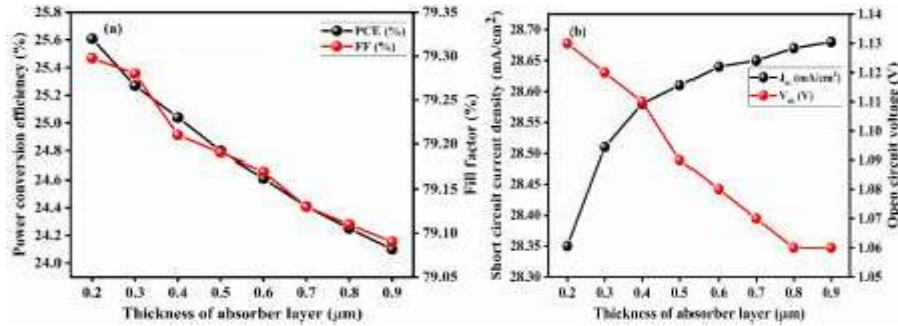


Fig.2 Thickness-dependent performance of photoactive layer

B. Role of defect density of photoactive layer

Defect density has a significant negative influence on performance of device. The overall PCE depends on how many charge carriers generated in perovskite layer successfully reach their individual electrodes. When the active layer contains a high number of defects, charge carriers recombine more readily, especially if the material quality is poor. These defects accelerate recombination, leading to notable reductions in all key photovoltaic parameters, with PCE and FF being the most severely impacted, as revealed in Fig. 3(a,b). Increasing defect density mitigate diffusion length of carriers and boosts recombination rate [11,12]. Based on this analysis, a bulk defect density of 10^{10} cm^{-3} was noted as ideal value, resulting in V_{oc} (V)= 1.03, $J_{sc}(\text{mAcm}^{-2}) = 28.55$, $\text{FF}(\%) = 77.81$, and $\text{PCE}(\%) = 22.96$.

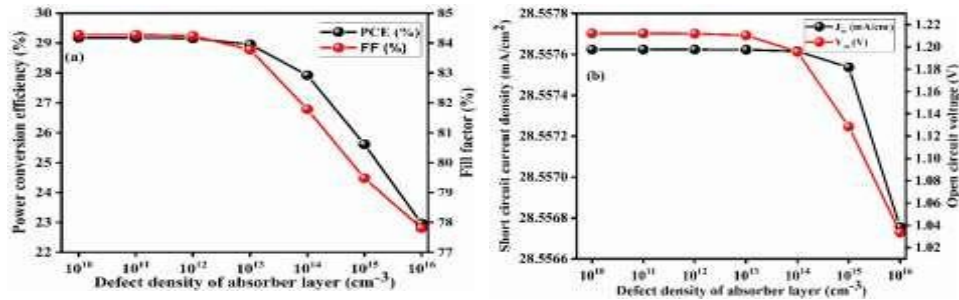


Fig. 3 Role of defect density on PV device performance.

C. Role of temperature

The temperature of PSCs plays a vital role in influential their long-term stability and performance under different environmental factors. Temperature variations affect several key physicochemical mechanisms, including charge generation, transport, and recombination. In addition, thermal effects modify the morphological, optical, and electronic characteristics of active layer such as grain size, crystallinity, bandgap, and dielectric behavior which in turn influence light absorption and charge generation efficacy.

Figure 4(a,b) presented how the photovoltaic parameters of structure change within the 300–510 K temperature range. The reduction in V_{oc} at higher temperatures is mainly due to increased recombination, influenced by enhanced carrier mobility and a surge in intrinsic carrier concentration. Although J_{sc} may remain nearly constant with increasing temperature owing to improved carrier mobility, elevated temperatures also enhance non-radiative recombination and improves the R_s . These combined effects lower the FF and ultimately decrease the PCE of device [13]. As the temperature increases, V_{oc} (V) decreases significantly from 0.97 to 0.48, while the $\text{FF}(\%)$ declines from 82.08 to 65.09, resulting in a reduction in $\text{PCE}(\%)$ from 22.74 to 9.04.

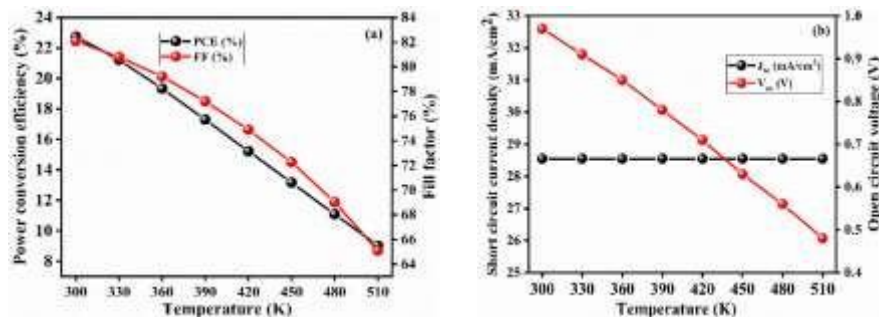


Fig.4 Influence of temperature on PSC

D. Impact of acceptor density of active layer

For p kind perovskite examined in the present work, choosing a suitable acceptor concentration (N_A) is essential for achieving high device performance. In this analysis, N_A in active layer was adjusted from 10^{15} to 10^{20} cm^{-3} , and resulting trends are presented in Fig.5(a,b). As doping level increases, the J_{sc} of both device configurations decrease, whereas V_{oc} , FF, and PCE show noticeable improvements. The reduction in J_{sc} is mainly due to intensified recombination associated with the higher carrier concentration in the absorber, which restricts the buildup of photogenerated carriers.

Figure5 further demonstrates that increasing N_A strengthens the built in electric field and lowers hole Fermi level, producing to an increase in V_{oc} . The rise in FF is linked to reduced series resistance and diminished interface recombination, both of which are facilitated by optimal doping levels. Together, the enhancements in V_{oc} and FF drive the overall increase in PCE [14]. The highest PCE obtained for the structure is 22.75% FF (%) = 82.09, $J_{sc}(\text{mAcm}^{-2}) = 28.55$ and $V_{oc}(\text{V}) = 0.97$.

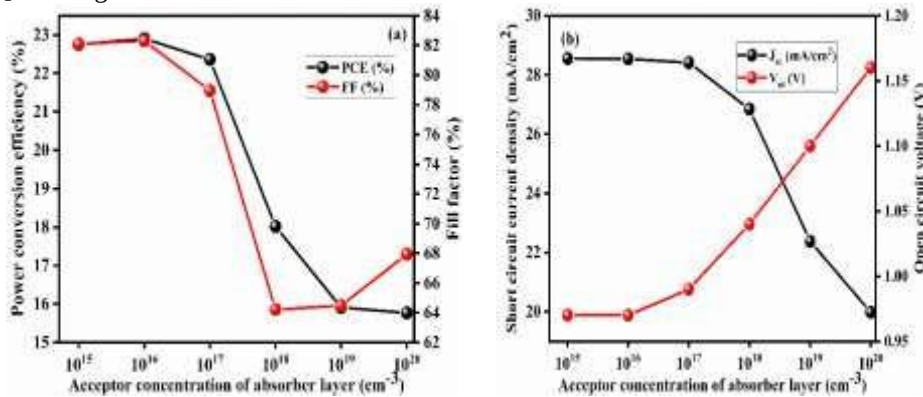


Fig.5 Role of acceptor density on absorber layer performance.

E. Impact of various back-contact materials on solar cell performance

The back contact plays a vital role in a solar cell, as it collects and transports charge carriers to the external circuit. Together with the front contact, it forms the conductive pathway through which the generated electrical energy is extracted. For efficient operation, the back contact (W_F) must provide a low resistance route for carrier flow to minimize power losses. In this study, several back contact materials were evaluated for the “Glass/FTO/GO/CsSn_{0.5}Ge_{0.5}I₃/CuO/back contact” structure. As revealed in Fig.6 (a,b), the optimal PCE is attained when gold serves as back contact, owing to its work function of 5.10 eV. Gold’s low electrical resistance, strong reflectivity, and excellent chemical stability make it an effective back contact material for solar cells. Although silver offers even higher optical reflectivity, its electrical conductivity is lower than that of gold. Additionally, gold’s superior resistance to environmental degradation further enhances its suitability for photovoltaic applications [10,11,15]. The resulting PCE (%) = 22.74, $J_{sc}(\text{mAcm}^{-2}) = 28.55$, FF (%) = 82.08 and $V_{oc}(\text{V}) = 0.97$ are accomplished for W_F of 5.1 eV.

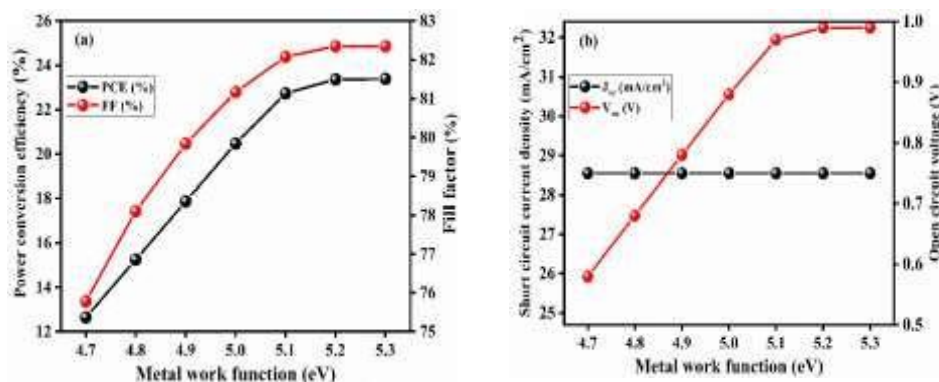


Fig. 6 Role of metal work function in PSC behavior

IV. Conclusion

In conclusion, the device structure FTO/GO/CsSn_{0.5}Ge_{0.5}I₃/CuO/Au was analyzed numerically employing SCAPS-1D simulator. The significance of such as thickness, acceptor concentration and defect density of active layer, metal work function and operating temperature on cell performance was systematically evaluated. With GO employed as the ETL, the optimized photovoltaic parameters obtained were: PCE(%) = 25.27, $V_{oc}(V) = 1.12$, $J_{sc}(mAcm^{-2}) = 28.51$, and FF(%) = 79.0. These simulation outcomes provide valuable findings for improving the PCE of CsSn_{0.5}Ge_{0.5}I₃ based all-inorganic PSC and for developing a clearer understanding of their operational behaviour.

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