Eco-Friendly Lead-free Perovskite Solar cell with Graphene Oxide ETL and CZTS HTL

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Abstract. In this study, numerical simulations were carried out using the SCAPS-1D software to analyze the performance of a lead-free Potassium germanium chloride ($KGeCl_3$) based PSC. The device architecture incorporates GO as ETL, CZTS as HTL, and Au as back contact. The effects of operating temperature and defect density of absorber layer were systematically examined under varying conditions. The optimised device configuration demonstrated a maximum power conversion efficiency of 30.41%, with a fill factor of 80.57%, short-circuit current density of 43.53 mA/cm², and open-circuit voltage of 0.86 V. Additionally, thermal stability analysis revealed that the device maintains stable performance at an operating temperature of 300 K.

Keywords: Efficiency, Perovskite, SCAPS-1D, ETLs and HTLs.

1 Introduction

Energy plays a crucial role in our daily lives. With the rising population and im-proving living standards, energy consumption has surged significantly. The increasing demand for energy around the world coupled with rising environmental protection concerns has added fuel to the fire to find sustainable and environment-friendly energy technologies. The increased use of fossil fuels has led to severe environmental problems like emission of carbon dioxide, pollution of the atmosphere, and climate change in the world; hence, the need for more sustainable energy resources. Among the different types of available renewable energy resources, solar energy seems to be a promising source due to the abundance and sustainability of the energy. Photovoltaic technology is a procedure that uses solar power as a source of energy to generate electricity. This kind of technology is gaining popularity as a clean source of power and is environmentally friendly [1,2]. Currently, the use of halide materials in perovskite photovoltaic cells is giving exceptional results due to the enhanced optoelectronic properties as well as cost-effective fabrication techniques. PSC is a PV cell made of thin film materials, which are all characterized under the perovskite structure. An astounding growth rate in regard to PCE for PSCs has been observed in a short time, achieving a PCE of more than 27%. Therefore, PSCs have unique characteristics, which enable it to compete favorably against other conventional PV cells, which are made of silicon material. To start with, PSCs have attractive optical proper-ties, allowing it to trap a higher percent of sunlight irradiance. Secondly, PSCs have charge carriers with long diffusion length. Thirdly, PSCs have adjustable bandgaps, which enable them. Furthermore, the ability to be made at low temperatures makes them promise a lot [3].

Potassium germanium chloride ($KGeCl_3$) has recently gained attention as an emerging perovskite material for PV applications, owing to its distinctive optoelectronic characteristics and superior stability relative to conventional organic cation–based perovskites. In the $KGeCl_3$ lattice, potassium (K^+) occupies the A-site, germanium (Ge^{2+}) resides at the B-site, and chloride (Cl^-) fills the X-site, forming a stable ABX_3 crystal framework. This structure exhibits strong thermal resilience, maintaining stability at temperatures above 373 K. In contrast, organic cation-based perovskites show significant vulnerability under these conditions, leading to faster degradation. In particular, $KGeCl_3$ stability persists under these environmental factors,

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indicating that $KGeCl_3$ might hold great promise in creating stable solar cell devices [5].

In this simulation, a planar nip PSC structure, FTO/GO/$KGeCl_3$/CZTS/Au, was systematically investigated in sequence to investigate the effect of defect density in the absorber layer and temperature. The main intention behind this investigation was to improve the parameters of the solar cell in order to achieve a highly efficient solar cell at a minimized cost.

2 Device structure and material parameters

These numerical simulations were made at standard test conditions with an absorption profile in accordance with the AM1.5G solar array, with an incoming power density of 100 mW/cm^2, and at an operating temperature of 300 K for an accurate performance evaluation [6,7]. Besides, the used architecture for the designed device consisted of GO as ETL, $KGeCl_3$ as absorber layers, and CZTS as HTLs. Fig.1 (a,b) illustrates the device structure and energy level.

Table 1. Device parameters of different layers [4,8,9]

Parameters	CZTS	$KGeCl_3$	FTO	GO
Thickness (nm)	50	300	500	50
Bandgap (eV)	1.5	1.10	3.5	3.0
Electron affinity (eV)	4.07	4.0	4.0	3.86
Relative Permittivity	18.1	23.01	9.0	9.0
Mobility of electron (cm^2 V s^{-1})	100	9.292×10^1	20	100
Mobility of hole (cm^2 V s^{-1})	0.10	6.859×10^1	20	25
CB effective density of states (cm^{-3})	2.2×10^{19}	1.0×10^{18}	2.20×10^{18}	2.20×10^{19}
VB effective density of states (cm^{-3})	5.5×10^{20}	1.0×10^{18}	1.80×10^{19}	2.20×10^{18}
Donor density, N_D (cm^3)	0	0	2.0×10^{19}	1.0×10^{18}
Acceptor density, N_A (cm^3)	1.00×10^{20}	1.0×10^{15}	0	0
Thermal velocity of electron (cm/S)	1.00×10^7	1.00×10^7	1.00×10^7	1.00×10^7
Thermal velocity of hole(cm/S)	1.00×10^7	1.00×10^7	1.00×10^7	1.00×10^7
Defect density, N_t (cm^3)	1.0×10^{13}	1.0×10^{15}	1.0×10^{18}	1.0×10^{15}

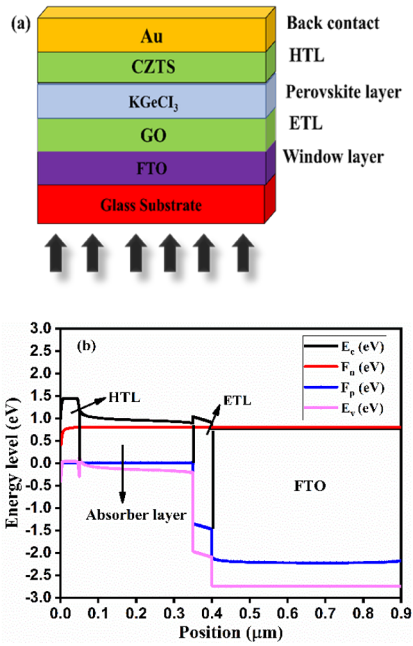


Fig. 1 (a) Device architecture **(b)** Energy level

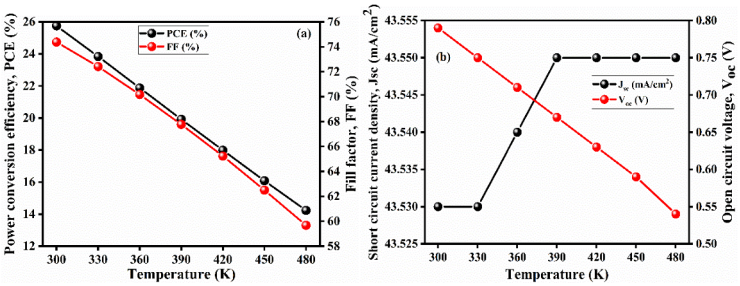
3 Result and discussion

3.1 Role of operating temperature

Solar cells generally function under operating temperatures above 300 K, and such conditions have a pronounced influence on device performance. Temperature plays a crucial role in controlling the vital parameters of PV devices, especially Voc and PCE. In order to analyze the impact of temperature on $KGeCl_3$-based PSC devices, the operating temperature has been varied as shown in Fig. 2(a,b). Rise in temperature causes a significant reduction in PCE due to a corresponding decrease in V_{oc}. This decrease in V_{oc} is associated with an increase in reverse saturation current (I_0), as labeled by the diode Eq.(1), which establishes an inverse relationship between V_{oc} and I_0.

$$V_{oc} = \frac{n.T.K}{q} ln\left(\frac{J_{SC}}{I_O+1}\right) \quad (1)$$

In the above equation, k represents Boltzmann's constant, n is ideality factor, T is temperature, q is electronic charge, whereas Io represents the photocurrent. As temperature increases, the exponential growth of I_o also leads to the consequent decrease of V_{oc}. It is to be understood that this implies the thermal stability of concerned material. Also, regulation of temperature is considered as significant for achieving high PCE devices. It is also noticed that increased temperatures increase recombination rates due to higher series resistance in charge carriers, impacting efficiency as well. Temperature-induced changes in the bandgap and electrical conductivity of absorber also contribute to performance degradation [10]. Overall, these results stress the critical role of effective thermal management in achieving stable and competent PSC operation beneath realistic environmental circumstances. As the temperature increases, V_{oc} decreases significantly from 0.79 V to 0.54 V, while the FF deteriorate from 74.38% to 59.67%, and PCE drops from 25.75% to 14.23%.



(a) **(b)**

Fig:2 Temperature dependent analysis of PV characteristics in $KGeCl_3$-based PSCs.

3.2 Role of defect density of absorber layer

The performance as well as stability in terms of operation of PSCs decreases to a great extent in the presence of a large density of defects. In the present investigation, the PV parameters were extensively analyzed by varying the N_t, present in absorber layer in an extent from 10^{10} to 10^{16} cm^{-3}. For the $KeGeCl_3$-based PSC, the optimal density was found to be 10^{10} cm^{-3}, at which a PCE of 30.41% was observed, as shown in Figure 3. At densities higher than 10^{13} cm^{-3}, PCE as well as J_{sc} decreases sharply due to enhanced recombination loss due to a large density of charge traps. An increase in N_t leads to a decrease in J_{sc}, which subsequently contributes to a decrease in FF. For the FTO/GO/$KeGeCl_3$/CZTS/Au heterostructure, the PCE decreased markedly from 30.41% to 21.81% as N_t increased from 10^{10} to 10^{16} cm^{-3}. This pronounce efficiency loss is attributed to enhanced recombination within the absorber layer, consistent with previously reported studies [10,11]. The variation of key PV parameters with N_t for $KeGeCl_3$ absorber employing CZTS as HTL is illustrated in Fig. 3(a,b), where the optimized device exhibits a substantial PCE reduction of 21.81% at higher defect densities. An assessment of solar cell parameters of projected model with reported results is presented in Table 2.

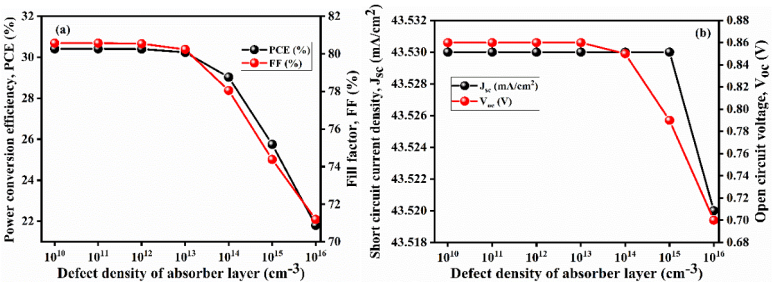


Fig. 3. Impact of defect density of absorber on PV arameters of $KGeCl_3$-based PSCs.

Table 2. Evaluation of the proposed model against recently published simulation results.

Sr. No	Device configuration	Meth.	PCE (%)	J_{sc} (mA/cm^2)	V_{oc} (V)	FF (%)	Ref.
1.	FTO/CSTO/$KGeCI_3$/PB/Au	Sim.	29.30	41.80	1.19	82.74	[4]
2.	FTO/WS_2/$KGeCI_3$/PEDOT:PSS/Au	Sim.	29.82	30.08	0.81	85.97	[5]
3.	FTO/GO/$KGeCI_3$/CZTS/Au	Sim.	30.41	43.53	1.19	82.74	Present work

4 Conclusion

In this simulation study, SCAPS-1D simulator was employed to investigate the device configuration of a Glass/FTO/GO/$KGeCl_3$/CZTS/Au PSC. The defect density of absorber layer was altered from 1.0×10^{10} cm^{-3} to 1.0×10^{16} cm^{-3}, and the optimal device performance was achieved at an absorber defect density 1.0×10^{10} cm^{-3}. To inspect the influence of operating conditions on PV performance, the device temperature was systematically adjusted from 300 K to 480 K. The lead- free based perovskite structure exhibits notable advantages, including non-toxicity, ease of fabrication, and cost-effectiveness. Based on the simulation results, CZTS emerges as a promising alternative hole transport material for achieving high-efficiency devices. Under optimized conditions specifically, an absorber thickness of 100 nm and defect density of absorber layer 1×10^{10} cm^{-3} the device attained a maximum PCE of 30.41%, with a J_{sc} of 43.53 mA/cm^2, FF of 80.57%, and Voc of 0.86 V. These findings show good agreement with recently reported studies on high-performance hole transport layers.

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