Parameter variation analysis of Perovskite (KGeCl₃) based solar cell using SCAPS-1D simulations

RAJ KUMAR¹, SHASHI BALA^{2,*}, REKHA DEVI³, BALWINDER SINGH⁴, PARVEEN KUMAR⁵

¹Department of Electronics and Communication Engineering, Manav Rachna International Institute of Research and Studies, Faridabad, India

²School of Engineering and Sciences, GD Goenka University, Gurgaon, Haryana, India

³Department of Electronics and Communication Engineering, Chandigarh University, Mohali, India

⁴AĈSD, C-DAC Mohali, Punjab, India

⁵Department of Electronics and Communication Engineering, Galgotias College of Engineering and Technology, Knowledge Park-II, Greater Noida, 201310, India

Potassium germanide chloride (KGeCl₃) Perovskite material has emerged as a most attractive alternative of lead-free perovskite based solar cells with tremendous power conversions efficiency for various applications. In this paper, KGeCl₃ perovskite material as active absorber layer active absorber layer and ZnO as electron transport layer (ETL) have been considered to design perovskite solar cell (PSC). In addition, hole transport material layer (HTL) of different material such as P3HT, NiO and Cu₂O have also been explored to optimize performance of PV cell using SCAPS-1D simulator under AM1.5G spectrum. The performance of existing KGeCl₃ based solar cell has also been compared with proposed KGeCl₃ PSC with different ETM and HTM. The performance parameter such as Power conversion efficiency (PCE), fill factor (FF), open-circuit voltage (V_{oc}) and short-circuit current density (J_{sc}) of the proposed KGeCl₃ based PSC has been analyzed by considering different values of the thickness, and density of interfacial defects in (KGeCl₃) absorber layer, temperature range and recombination rate of carriers. The proposed KGeCl₃ based lead free PSC with NiO as HTM and ZnO as ETM has shown 22.53 % power conversion efficiencies (PCEs) at affordable cost. Therefore, KGeCl₃-PSC with appropriate HTM and ETL can be a most suitable and attractive way to get maximum PCEs for different applications.

(Received January 16, 2025; accepted October 10, 2025)

Keywords: Perovskite, Solar cell, PCE, Current density, KGeCl₃

1. Introduction

The consumption of energy has been increasing rapidly in the era of electronics and advanced electric appliances. Thereby, conventional energy resources cannot be relied on to fulfill the huge power requirement. Solar energy is one of the attractive solutions owing to its huge availability and nature friendly. Therefore, Solar cells are considered as the potential candidate to fulfill the demand of electricity by producing maximum electric power from solar energy [1, 2].

Over the years, numerous semiconducting materials have been employed to design the effective solar cell [3]. However, perovskite materials have emerged as one of the most promising candidates attributed to their tremendous optoelectronic properties, tunable bandgaps, scalability and superb absorption coefficient as compared to silicon solar cells [4]. Tunable bandgap of perovskite material make it capable to use as top and bottom cells in case of tandem solar [5–6]. Moreover, perovskite solar cells (PSCs) have also shown their capability in terms of high efficiency, Fill factor and stability for single junction solar cells [7, 8]. Researchers have been continuously exploring more perovskite materials to enhance the PCE as well as stability of PSCs. Therefore, the different design parameters of perovskite materials such as thickness,

interface engineering, defect density, and bulk doping, have been explored to optimize and enhance the performance of PV cells [9–12]. Among the different perovskites materials, lead based Perovskite materials have been found to be very toxic and dangerous for the environment as well as humankind. Thereby, researchers have started exploring the lead-free perovskite materials for safe environment with appropriate PCE [13, 14]. Sn and Ge are considered as replacement of lead-based perovskite due to its ability to perform equivalent to lead based PSCs. Ge-based perovskite was originated in 2013 by Stompous et al., and further, in 2015 by Krishnamoorthy [15, 16].

In search of lead free perovskite materials, latest perovskite $KGeCl_3$ has been explored and optimized to achieve reasonable efficiency and high stability for PV cells [17–19]. The $KGeCl_3$ perovskite absorber layer in PSCs has outperformed the conventional perovskite materials in terms of optical, electrical properties, and stability [20–24]. The performance parameters of PV cell such as power conversion efficiency (PCE), open-circuit voltage (V_{OC}), fill factor (FF) and short-circuit current density (J_{SC}) have been explored by varying the design parameters of the absorbing materials for optimization [25–28].

In PSC, apart from the perovskite layer hole transport layer (HTL) and electron transport layer (ETL) play very vital role to enhance the performance of PV cell. The fabrication of the PSC is quite an expensive and long process. Therefore, performance of PSCs can be analyzed by computational modelling and simulation studies rather than following the expensive fabrication process.

The performance of PSCs can be improved by considering appropriate material for ETL and HTL. TiO₂, ZnO, and SnO₂ can be used as ETLs [29–32] and CuI, CuO, Cu₂O, P3HT, NiO and Spiro-OMeTAD materials are suitable for HTLs [33–35]. However, TiO₂ is generally not preferred as ETM due to its high annealing temperature requirements for processing. Similarly, PEDOT:PSS and Spiro-OMeTAD are restricted material owing to high cost and less stability. Cu₂O and NiO Layers at interface of KGeCl₃ are also used to mitigate the oxidation effects of Ge-based perovskites. Hence, HTMs and ETMs are also being explored to have efficient PV cell.

In this paper, KGeCl₃ has been taken as active absorber layer and ZnO as ETL of Perovskite solar cell. In addition, different HTMs such as P3HT, NiO and Cu₂O have been explored for optimized performance of PV cell using SCAPS-1D simulator under AM1.5G spectrum. The performance of existing KGeCl₃ based solar cell has been compared with proposed KGeCl₃ PV cell with different ETM and HTMs. The performance parameters like PCE, FF, J_{sc} and V_{oc} of the proposed KGeCl₃ based cell have been analyzed at different values of thickness and defect density of the KGeCl₃ layer. Further, performance has also been analyzed by varying diffusion length of charge carriers as well as temperature range. The proposed KGeCl₃ based lead free PSC with NiO as HTM and ZnO as ETM has shown more than 22.53% PCE.

2. Simulation setup

This paper demonstrates the design of KGeCl₃-based perovskite solar cell (KGeCl₃-PSC) with potassium germanide chloride (KGeCl₃), nickel oxide (NiO), and zinc oxide (ZnO) as active absorber layer, HTL and ETL respectively. The structure of proposed KGeCl₃-PSC comprised of transparent conducting oxide (ITO/ETL/KGeCl₃ (active absorber layer)/HTL/back contact, has been shown in Fig. 1. The anode of silver (Ag) has been used in proposed PSC.

The proposed PSC was also simulated independently using different HTMs such as P3HT, NiO and Cu₂O. It has been observed from that different simulation results that PSC with NiO as HTL shows remarkable efficiency near to 23%. By incorporating the properties of ETL and HTL, the performance parameters of PV cell such as carrier mobility, losses due to recombination and stability get enhanced under different environment. Table 1 describes the design parameter of all layers considered in KGeCl₃-PSC.

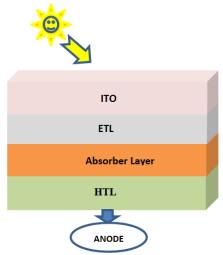


Fig. 1. Structure of proposed KGeCl₃–PSC (colour online)

The proposed KGeCl₃ based PSC simulated by using SCAPS 1D simulator at a room temperature. SCAPS 1D simulator was designed at University of Gent of Belgium by M. Burgelman and his associates. It basically incorporates the Poisson's equations along with hole and electron continuity equations [2, 37].

$$Dn\frac{\partial^2 n(x)}{\partial x^2} + \mu E_n \frac{\partial n(x)}{\partial x} + G_n(x) - R_n(x) = 0 \quad (1)$$

$$Dp\frac{\partial^2 p(x)}{\partial x^2} + \mu E_p \frac{\partial p(x)}{\partial x} + G_p(x) - R_p(x) = 0 \quad (2)$$

Here, p(x) and n(x) signifies the positive and negative charge carriers concentration respectively. In addition to that, $G_n(x)$ and $G_p(x)$ representing the photo generation rate; $R_p(x)$ and $R_n(x)$ representing amount of recombination of charge carriers occur. Whereas, E(x), μ and D signifies the electric field originated, carrier mobility and diffusion constant in the perovskite layer, respectively [38–39].

The defects present in the structure of PV cell are responsible to alter its performance significantly. The Shockley Read Hall (SRH) model is also considered to manage the defect density of PV cell and expressed as [2, 38-40].

$$R = \frac{T_{n,p}^{-1}(np - n_i^2)}{n + p + 2_{ni}cosh(\frac{E_t - E_i}{kT})}$$
(3)

Here, $T_{n,p}$ denotes the relaxation time of charges. In addition to that, n and p signifies the electron and hole concentration respectively. Moreover, n_i is the intrinsic charge density, whereas E_i and E_t representing the energy level of intrinsic carriers and trap defects respectively.

The thermal velocity of charge carriers in every layer is considered as 10^7 cm/s and expresses as in relation with relaxation time

$$T_{n,p} = \frac{1}{\sigma_{n,p} \, v_{th} N_t} \tag{4}$$

 N_t and $\sigma_{n,p}$ are giving the density of defects and its cross-sectional area, respectively.

The design parameters of PV cell can be estimated by above mentioned equations. The simulation J-V characteristics of perovskite solar cell have been calibrated with experimental results demonstrated in [10], shown in Fig. 2. Further, the energy band diagram of proposed PSC has been shown in the Fig. 3. As the ETL and HTL are considered as important part of perovskite solar cells. In the absorber layer, electrons/holes pair generated when

sunlight fall on the solar cell. Then, these charge carriers move towards contacts. The valence band offsets (VBO) and conduction band offsets (CBO) at the interfaces, absorber/HTL and absorber/ETL are responsible to show the efficiency of this separation process. The valence band offset is the difference in valence band between the absorber layer and the HTL, is determined by each ETL, with KGeCl₃ as the absorbing layer and Cu₂O as the HTL. The efficiency and performance of PSCs is significantly affected by the alignment of energy levels.

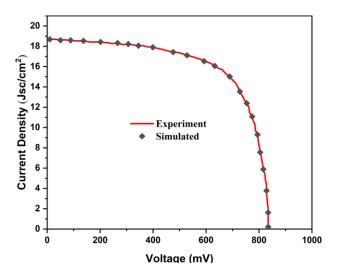


Fig. 2. J-V curve calibrated with experimental results [10] (colour online)

The absorption coefficient (α) of material is calculated by Equation (5) and A_{α} is equivalent to 10^5 .

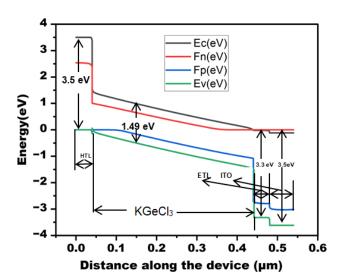


Fig. 3. Energy band diagram of KGeCl₃–PSC (colour online)

$$A=A_{\alpha}(h\vartheta-E_g)^{1/2} \tag{5}$$

Table 1. Design parameters	for simulation	of KG_0Cl .	PSC
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Parameter	Absorber material	HTMs		ETM	
	KGeCl ₃	NiO	P3HT	Cu ₂ O	ZnO
Thickness (nm)	400	40	350	350	40
Band gap (eV)	1.49	3.5	1.7	2.17	3.3
Dielectric permittivity	6.5	9	3	7.5	8.5
Effective conduction band density, N _C (cm ⁻³)					4×10^{18}
	1×10^{18}	3×10^{19}	2×10^{18}	2×10^{18}	
Effective valence band density, N _V (cm ⁻³)	1×10 ¹⁹	2×10 ¹⁹	2×10 ¹⁹	1.8×10 ¹⁹	2×10 ¹⁹
Thermal velocity of electron /hole (cms ⁻¹)	1×10^{7}	1×10 ⁷ /	1×10^{7}	1×10^{7}	1×10^{7}
	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
Electron /hole mobility, $\mu_n / \mu_p \text{ (cms}^{-1}\text{V}^{-1}\text{s}^{-1})$	1.6×10 ⁻¹ /	5×10 ⁻¹ /	1.8×10 ⁻³ /	4×10^{3}	1×10 ⁻² /
•	1.6×10 ⁻¹	5×10 ⁻¹	1.8×10 ⁻²	2×10^{2}	3×10 ⁻¹
Donor/acceptor concentration, N _D / N _A (cm ⁻³)	1×10 ¹⁵	2×10 ¹⁹	1.38×10 ¹⁸	7×10 ¹⁶	1×10 ¹⁹
Defect density, N _t (cm ⁻³)	1×10 ¹⁴	1×10 ¹⁴	1×10 ¹⁴	1×10 ¹⁴	1×10 ¹⁴

3. Result and discussions

The quantum efficiency (QE) of proposed and existing [20] KGeCl₃-PSC has been compared with

respect to the wavelength of sunlight striking at PSC, as demonstrated in Fig. 4(a). The quantum efficiency (QE) shows the amount of charge collected to the number of photons absorbed by PV cell. Each and every incident

photon needs to get converted to electric charges to attain 100% QE. However, 100% QE is attained at a particular wavelength of incoming light [25]. Thereby, the QE is almost 100% for 350 nm to 500 nm wavelength of proposed device as compared to existing device and QE falls to zero around 850 nm. Thereby, proposed KGeCl₃–PSC shows tremendous QE for wide range of spectrum.

Further, J_{sc} - V_{oc} characteristics of proposed and existing $KGeCl_3\ PSC$ show their performance, as

represented in Fig. 4(b). The efficiency of proposed device is 23% Whereas, existing PSC gave 19.63% attributed to structure with appropriate ETL an HTL, capable of better utilization of incident light, can be considered as efficient and perpetual solar energy technology. The open circuit voltage, current density, efficiency and fill factor of proposed and existing device is detailed in Table 2.

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	V _{oc} (V)	J _{sc} (mA/cm ²)	FF (%)	PCE (%)
Proposed	1.181943	22.7355	82.9756	22.53
PSC				
Existing	1.13	23.47	73.34	19.47
device [20]				

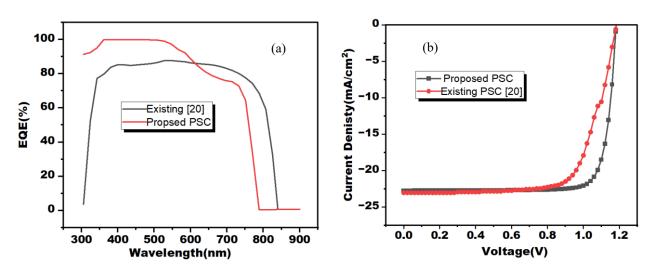


Fig. 4. Comparison of (a) quantum efficiency vs wavelength, (b) current (J) vs voltage (V) curve of proposed K (colour online)

3.1. Influence of thickness of absorber layer of PSC

In this paper, the performance of PSC with KGeCl₃ as absorber layer has been analyzed at different thickness ranging from 200 to 800 nm Fig. 5. In addition, different HTMs such as P3HT, NiO and Cu₂O have been analyzed for optimized performance of PV cell. It has been found that thin layer of KGeCl₃ perovskite gives lower current density (J_{sc}) and efficiency (η) owing to little light absorption. On the other hand, performance of PSC with high thickness of perovskite layers responsible for higher recombination. Thereby, it is required to use optimal thickness of a perovskite layer to design an efficient PSC.

The existing KGeCl₃ -PSC with different ETM and HTM exhibits PCE of 19.63% [20]. Whereas, the proposed KGeCl₃ based lead free PSC with NiO as HTM and ZnO as ETM has delivered 22.53% PCE at 500 nm thickness of perovskite. The performance of PSC reduced for thick perovskite layer owing to high recombination rate [18]. The charge particles recombine before reaching to the interface attributed to change in their diffusion length and absorption depth [2]. Therefore, V_{oc} and FF decreases as thickness of perovskite layer increases. The variation of PCE %, V_{oc}, J_{sc} and FF under the influence of thickness of perovskite of has been depicted in Figs. 5 (a)-(d).

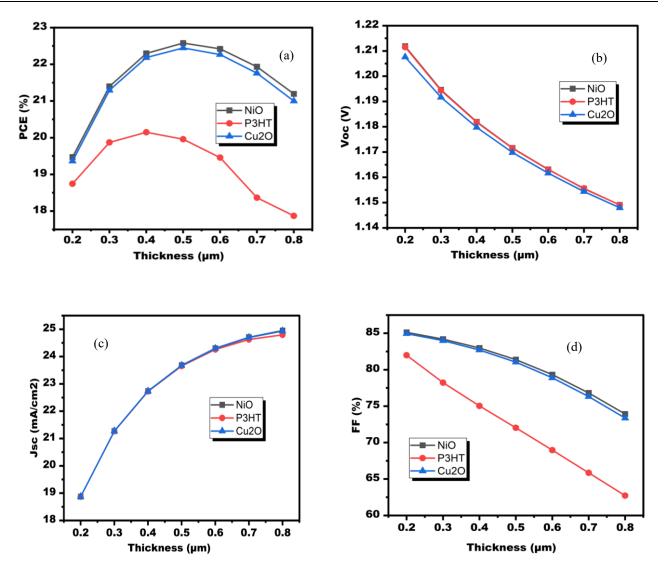


Fig. 5. Varriation of perfromace paprameters of KGeCl₃ based PSC with different ETMs on varying thickness of active layer (colour online)

3.2. Influence of total defect density in Perovskite layer

The performance of PSC can also be determined by defect density of Perovskite layers. The photo-generated charges inside the perovskite move apart attributed to electric field and travel in the direction of ETL and HTL respectively. The defects in perovskite are responsible for recombination of holes and electrons too early leading to affect the performance of the PSC. In addition to that, Gaussian defect states can be more responsible for electron

and hole trapping as compared to Urbach tail [27]. The variations of performance parameters (PCE, V_{oc} , J_{sc} and FF) versus defect density are depicted in Fig. 6 (a)-(d). From the simulation results, it has been observed that performance parameters of PSC decreases with increases in defect density the ranging from 10^{13} – 10^{17} cm⁻³. The proposed PSC is more efficient at the lowest considered value of defect density (10^{13} cm⁻³). Therefore, Perovskite layer with minimum defects can produce remarkable PSC [22, 28–30].

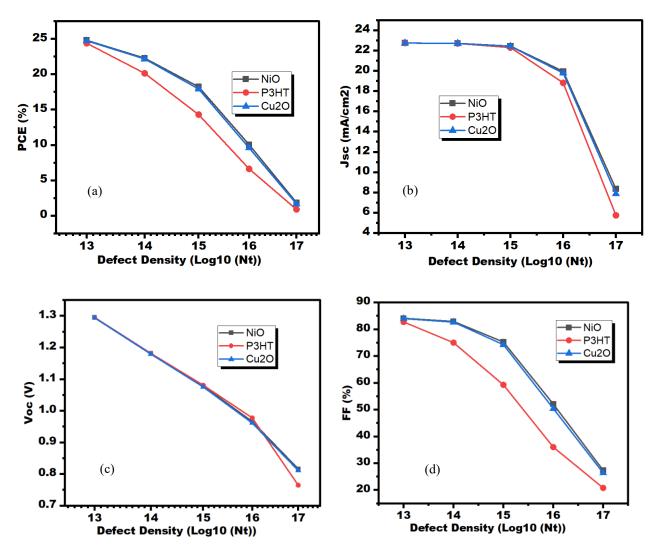


Fig. 6. Varriation of perfromace paperameters of KGeCl₃ based PSC with different ETMs on varying defect density of active layer (colour online)

3.3. Effect of temperature variation

The thermal stability can also be one of the performance factors of Perovskite solar cell (PSC). Therefore, performance of PSC has been investigated at different temperature range of 300 K-500 K. The graphs of

PCE, $V_{\rm oc}$, $J_{\rm sc}$ and FF versus temperature are depicted in Figs. 7 (a)-(d). From the simulation results, it has been seen that performance parameters of PSC decreases with increases in temperature the ranging from 300 K–500 K [19-21]. The proposed device is more efficient at the room temperature.

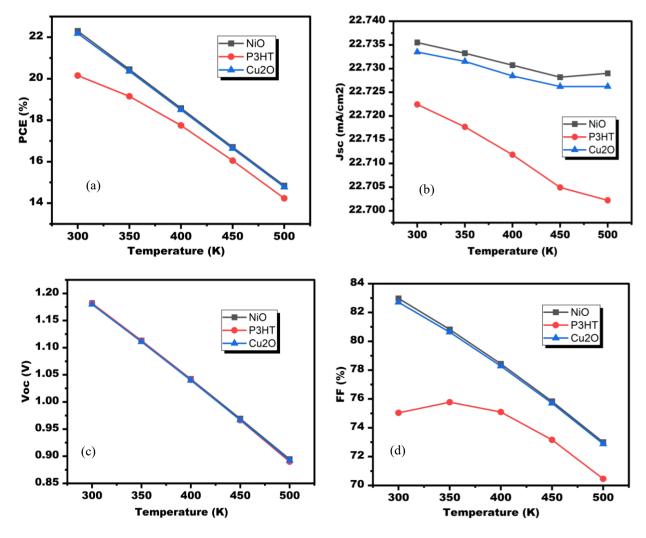


Fig. 7. Varriation of perfromace paprameters of KGeCl₃ based PSC with different ETMs on varying temperature of active layer (colour online)

3.4. Influence of defect density of the KeGl₃ layer on recombination rate

Shockley Read Hall (SRH) model can be used to obtain the performance of PSC under the influence of variation in defect density of a KeGl₃ layer by determining the recombination rate [18–21]. A recombination rate along the device at different defect densities has been represented in Fig. 8. The rate of recombination got increased as defect density increases. Thereby, the performance parameters of the PSC show degradation as density of defects increases, as depicted in Fig. 6.

The relaxation time of carriers is contrary to defect density, as given in Eq. 4. The recombination rate is also equated inverse to relaxation time of charge carriers, can be seen from Eq. 3. Thereby, it is summarized from the mathematical equations that relaxation time of charged carrier's decreases as defect density increases, leading to high recombination rate. The relaxation time of mobile charge carriers is too related to diffusion length [25]. Therefore, it is confirmed that a less recombination rate

and high diffusion length helps to obtain high efficiency of 22.53 % of proposed PSC.

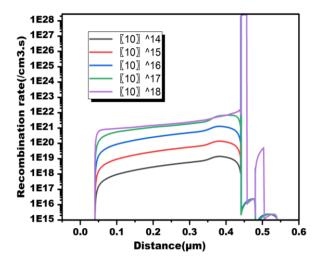


Fig. 8. Recombination rate along the PSC for different defect densities (colour online)

4. Conclusion

This work demonstrated the design of Perovskite solar cell (PSC), comprised of KGeCl₃ as active absorber layer, ZnO as ETL and NiO as HTL with optimized performance using SCAPS-1D simulator under AM1.5G spectrum. The proposed device has shown higher PCE equivalent to 22.53 % as compared to existing device with 19.63 % PCE. The performance parameters such as PCE, opencircuit voltage, short-circuit current density and fill factor of the proposed KGeCl₃-PSC degrades as the thickness of KGeCl₃ exceeds 500 nm due to high recombination. The absorber layer with high defect density and under high temperature also found to be responsible to reduce the performance of PSC. The recombination rate increases with the defect density leads to influence the PSC's performance. Therefore, the proposed KGeCl3 based lead free PSC with optimized HTM and ETM, thickness of absorber layer and defect density can be attractive candidate as solar cell for future applications.

Acknowledgements

We like to extend our gratitude to Prof. Marc Burgelman and his team from University of Gent of Belgium for providing the SCAPS 1D software tool for simulation.

Author's contribution:

All authors contributed equally.

Availability of data and material:

Data used for the results are available in the manuscript in tabular and graphical form.

Declarations:

Conflict of interest: There is no conflict of interest among the authors.

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^{*}Corresponding author: shashi.sbbs@gmail.com