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Numerical Study Exploring of Inorganic $KGeCI_3$-Based Perovskite Solar Cells Using SCAPS-1D Software

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Abstract: In this study, potassium germanium trichloride ($KGeCI_3$) is investigated as a promising absorber layer for perovskite solar cell applications due to its favourable photovoltaic properties. Graphene Oxide (GO) is employed as the electron transport layer (ETL), whereas P3HT serves as the hole transport layer (HTL). A thin-film solar cell architecture incorporating germanium (Ge) is designed and analyzed as a potential lead-free alternative. To enhance device stability and minimize the adverse effects associated with germanium-based perovskites, the material parameters were carefully optimized, resulting in performance characteristics comparable to those of lead-based thin-film solar cells. The simulation outcomes reveal that the $KGeCI_3$-based device delivers a power conversion efficiency (PCE) of 29.57%, an open-circuit voltage (V_{oc}) of 1.25 V, short-circuit current density (J_{sc}) of 28.77 mA/cm², and fill factor (FF) of 81.63%. The results suggest that $KGeCI_3$ is a viable absorber material for next-generation solar cells and holds considerable potential for the fabrication of low-cost, environmentally friendly, and high-efficiency thin-film photovoltaic devices.

Keywords: *Perovskite Solar Cell, Photovoltaic Effects, Organic Solar Cells.*

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I. INTRODUCTION

The utilization of solar power has proven to be one of the most promising options for renewable energy resources due to its availability and eco-friendliness. Utilizing solar power to generate electricity through the process of photovoltaics using solar cells has become one of the most important achievements in the field of PV. Thus, this technology is revolutionizing the whole industry. In recent decades, there has been a search for various semiconducting materials that would prove useful for photovoltaic applications. In this regard, perovskites have appeared to be one of the most promising semiconducting materials because of their unique optoelectronic properties [1,2]. The most significant benefit offered by perovskite materials is that of tenable bandgap which allows perovskites to be employed for top and bottom sub-cells in tandem and multijunction solar cells. Furthermore, PSCs exhibit outstanding performance in terms of PCE and other photovoltaic properties when they are used in single junction designs. Hence, a lot of research is currently being conducted on perovskites in order to develop more efficient devices. To optimize PSC performance, researchers have explored various material and device engineering strategies, including absorber layer thickness optimization, interface modification, defect passivation, and bulk doping. Owing to their broad solar-spectrum absorption, low-cost fabrication potential, scalability, and compatibility with next-generation photovoltaic technologies, perovskite materials are considered promising candidates for large-scale commercial deployment [3,4].

The general chemical formula of perovskite materials is ABX_3, where A and B represent cations and X denotes a halide anion. Traditionally, lead (Pb)-based compounds have been widely employed in perovskite solar cells because of their favourable electronic and structural properties. However, the toxicity and environmental concerns associated with lead have motivated significant research toward the development of environmentally friendly and lead-free perovskite alternatives [5,6]. The substantial improvements that have been made in first-principal Density Functional Theory (DFT) calculations have led several research teams to perform their studies using lead-free inorganic perovskites such as $KGeX_3$ (X=Cl, Br, I) perovskite. The M. Namisi et al. investigated the properties of $KGeCl_3$ perovskite in various crystal structures using DFT analysis. Hamideddine et al. performed a calculation for the electrical, optical, and thermoelectric properties of $KGeI_{3-x}Br_x$ perovskite through the DFT technique [7].

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In this research work, we examine the simulated Ge-thin film solar cell. The results found from previous studies confirm the suitability of the Ge-perovskite solar cell as an alternative, which motivates us for further studies. In this study, a thin film solar cell device model has been developed with three active layers. In the proposed thin film device, Poly(3-hexylthiophene) (P3HT) is used as the HTL, while graphene oxide (GO) is chosen for ETL. $KGeCl_3$ is considered for the photoactive absorber layer. FTO works as a transparent front contact that helps to transmit light onto the photoactive layer of the device. We systematically investigated the effects of the photoactive layer thickness and defect density, as well as the operating temperature, together with work function of back contact, on the performance of PSC. For numerical simulation studies of the device parameters like J_{sc}, V_{oc}, FF, and PCE, SCAPS-1D software tool has been used.

II. SIMULATION METHODOLOGY

SCAPS-1D Software is a one-dimensional photovoltaic simulation tool developed by Mac Burgelman and his team for modelling multilayer solar cell structures. It requires precise electrical and optical input parameters to ensure accurate device simulations under defined operating conditions [8]. The software allows users to extensively analyse solar cell performance by adjusting key parameters such as: Interface defect density, carrier concentration, electron affinity, bandgap energy, layer thickness. donor and acceptor densities. Numerous studies have demonstrated that SCAPS-generated simulation results closely align with experimental data, confirming the software's reliability [9–11]. The SCAPS algorithm is specifically designed to solve the Poisson equation (Eq. 1) and the continuity equations for both electrons (Eq. 2) and holes (Eq. 3).

$$\frac{d}{dx}\left(-\varepsilon(x)\frac{d\psi}{dx}\right) = q\langle N_d^+(x) - N_a^-(x) + p_t(x) - n(x) - n_t(x) + p(x)\rangle \quad (1)$$

$$\frac{\partial n(x,t)}{\partial t} - G_n(x,t) + R_n(x,t) - \left(1/q\right)\frac{\partial J_n}{\partial x} = 0 \quad (2)$$

$$\frac{\partial p(x,t)}{\partial t} - G_p(x,t) + R_p(x,t) + \left(1/q\right)\frac{\partial J_n}{\partial x} = 0 \quad (3)$$

Where, V = electrostatic potential, p_t (n_t) = hole (electron) distribution, q = electron charge, $R_{n(p)}$ = electron(hole) recombination rate, ε is permittivity, $N_{d(a)}$ = donor (acceptor) concentration. $G_{p\ (n)}$ = generation rate of hole(electron), Jn(p) = electron (hole) current density, n(p) = electron(hole) concentration. Fig.1(a,b) illustrates the proposed device structure and the corresponding energy band alignment diagram, respectively.

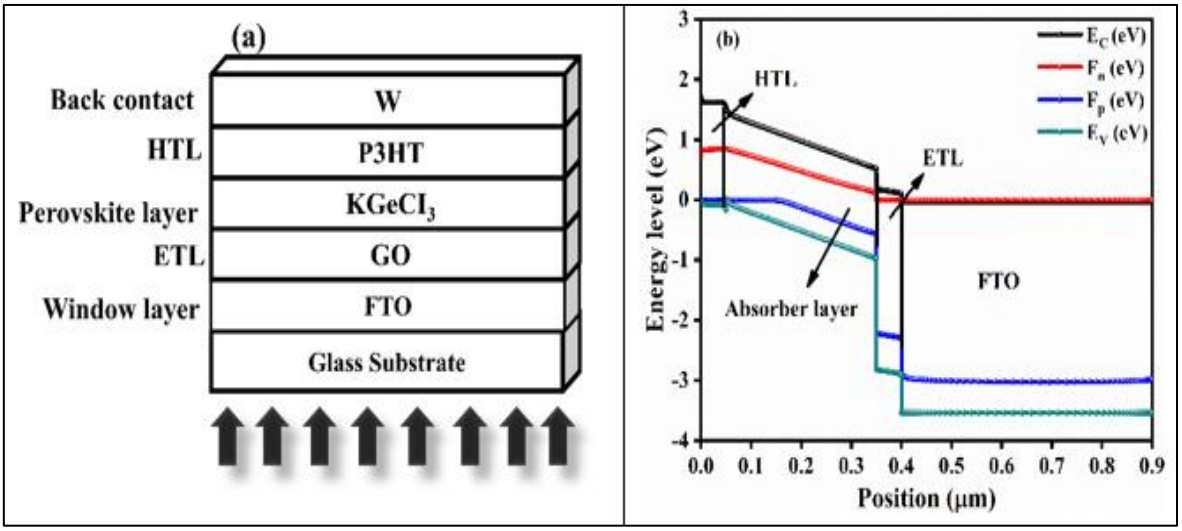

Fig 1 (a) Device Structure (b) Energy Band Diagram.

Table 1 The Simulation Input Parameters for Proposed PSC Device [12,13].

Parameters	Units	FTO	P3HT	GO	$KGeCl_3$
Electron affinity	χ {E_v}	4.0	3.5	3.86	4.0
Donor concentration	N_D {cm^{-3}}	2.0×10^{19}	0	1.0×10^{18}	0
VB effective DOS	N_V {cm^{-3}}	1.80×10^{19}	1.0×10^{18}	2.20×10^{18}	1.0×10^{18}
Electron mobility	μ_e {cm^2/Vs}	20	1.8×10^{-3}	100	9.292×10^{1}
Defect density	N_t {cm^{-3}}	1.0×10^{18}	1.0×10^{14}	1.0×10^{15}	1.0×10^{15}
Bandgap	E_g{eV}	3.5	1.7	3.0	1.10
CB effective DOS	N_C {cm^{-3}}	2.20×10^{18}	2.0×10^{18}	2.20×10^{19}	1.0×10^{18}
Hole mobility	μ_h {cm^2/Vs}	20	1.8×10^{-2}	25	6.859×10^{1}
Acceptor density	N_A {cm^{-3}}	0	1.00×10^{18}	0	1.0×10^{15}
Thickness	{nm}	500	50	50	300
Dielectric permittivity	ε	9.0	3.0	9.0	23.01

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III. RESULT & DISCUSSION

➢ *Working Effect of Temperature*

Figure 2 (a,b) show how operating temperature affects the electrical performance of PSC. To see how this works, researchers changed the device temperature from 300 K to 510 K and checked how it impacted the PV performance. They found out that the PSCs overall performance went downfall as the temperature went up. This is mainly because the series resistance (Rs) grew, while the minority carrier diffusion length shrink. As a result, charge carrier recombination got worse, making the device less efficient. While the J_{sc} saw a tiny boost due to more charge carriers being thermally generated, the V_{oc} slightly decreases. The drop in V_{oc} was way more than the increase in J_{sc}, leading to a lower PCE overall [14–16].

According to the temperature dependent results, it can be clearly seen that the PV characteristics of the system have a great dependence on the operating temperature of the cell. The maximum PCE, FF, and V_{oc} values can be achieved at 300 K. As the operating temperature of the device increases above 300 K, a steady decrease in all three parameters occurs, due to the increase in recombination processes and heat loss. Therefore, 300 K is identified as the optimum operating temperature for the proposed PSC.

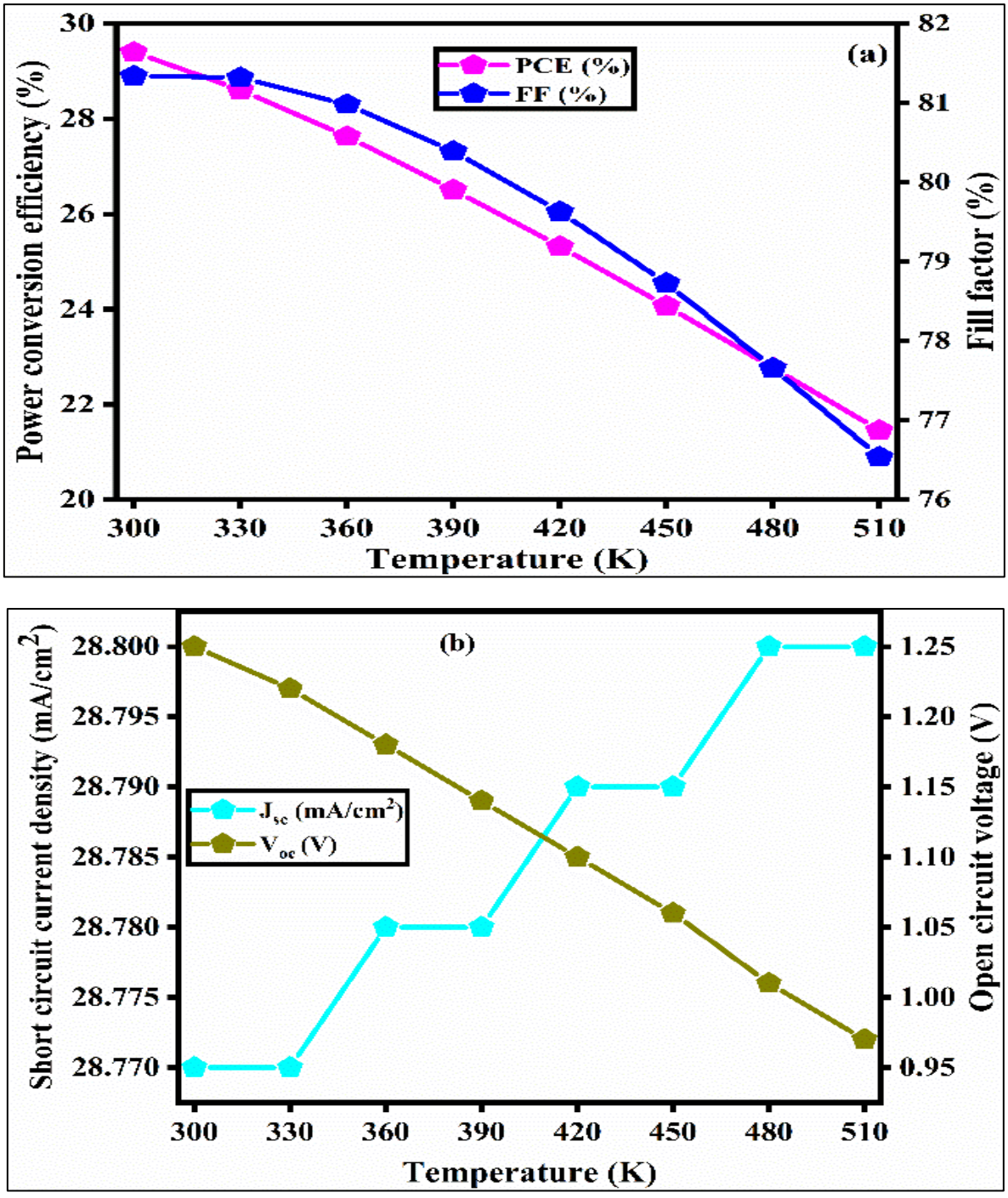

Fig 2 Effect of Operating Temperature Variations on Solar Cell Parameters.

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➢ *Working Effect of Defect Density of Absorber Layer*

Defects inherent to the $KGeCl_3$ absorber layer and interface defects are present since the beginning of fabrication. These defects occur in the form of point defects such as vacancies, interstitials, anisate defects, Frenkel defects, and Schottky defects. Other types of defects that can be found in the absorber include grain boundaries and dislocations [17]. Defect density in the absorber layer impacts the PCE of the device to a large extent. Higher defect density implies greater possibility of carrier recombination, reducing carrier lifetime and diffusion lengths [18].

In Fig. 3 (a,b), as the $KGeCl_3$ layer's defect density goes from 10^{10} to 10^{17} cm^{-3}, the performance slides. The PCE, FF, J_{sc}, and V_{oc} all drop: from 29.57% to 20.91%, 81.63% to 70.07%, 28.77 to 28.69 mA/cm^2, and 1.25 to 1.04 V, respectively.

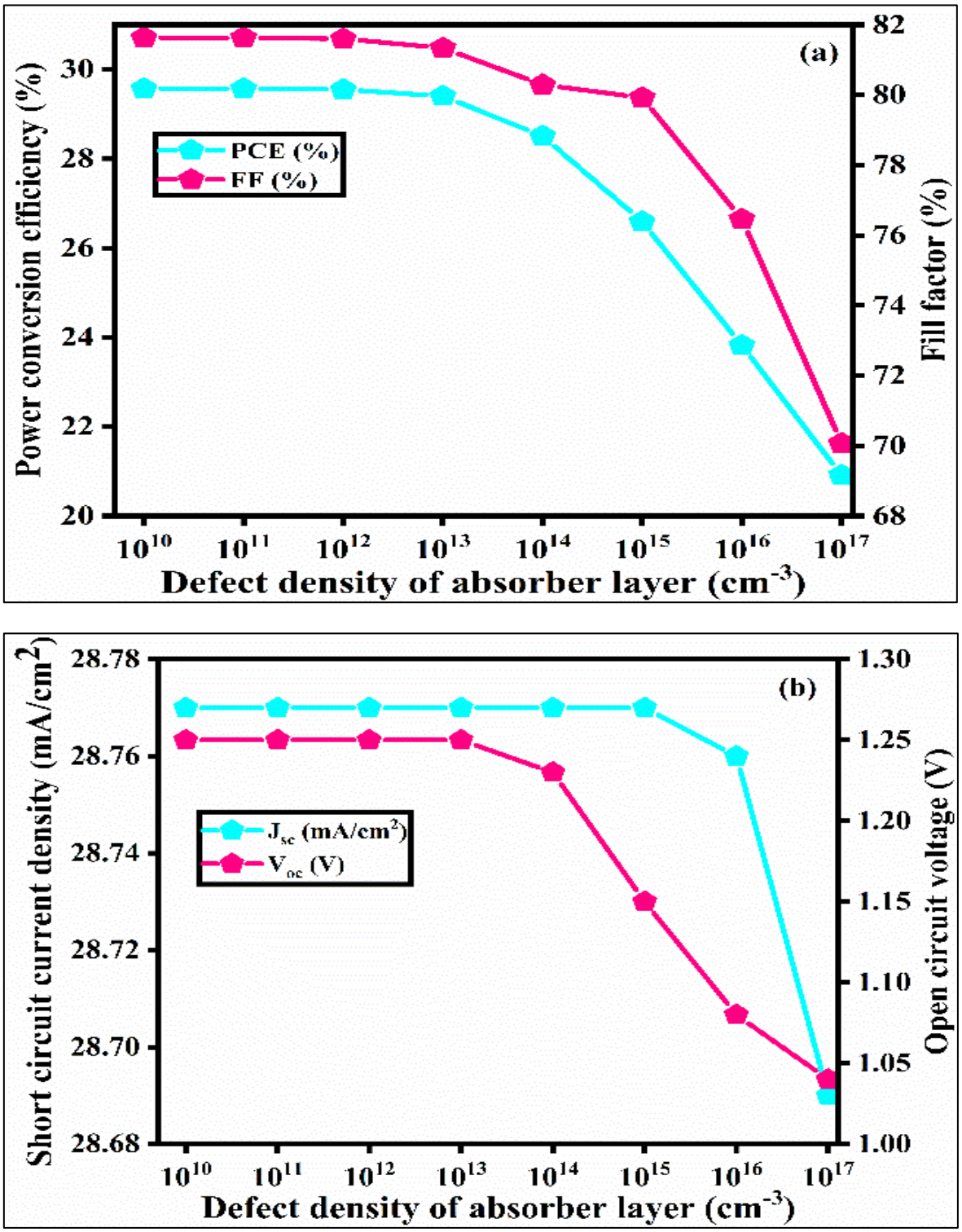

Fig 3 Impact of Absorber Layer Defect Density on Solar Cell Performance.

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➢ *Impact of Absorber Layer Thickness*

The absorber layer is key in solar cells; it catches photons and makes electron-hole pairs. To see how thickness affects performance, we changed the active layer from 200 nm to 1225 nm, keeping everything else constant. As Fig. 4(b) shows, J_{sc} goes up with thicker layers. The higher J_{sc} is due to better light absorption and more charge carriers being made. Below 410 nm, there's a fast increase in J_{sc}, but after that, it grows slower. In Fig. 4(a), the FF drops as the absorber layer gets thicker. This happens because of more internal power loss and charge carrier recombination. While thicker layers boost light absorption and carrier generation, they also hurt charge transport and device performance. A thicker absorber layer facilitates greater photon absorption and charge carrier generation, thereby improving the overall efficiency of the device [18,19]. With a 1225 nm absorber thickness, the value of PCE of 29.06%, J_{sc} of 29.14 mA/cm², FF of 79.94%, and V_{oc} of 1.24 V. These numbers prove that finding the right thickness can finely tune the balance between charge generation and recombination, making the device way more PV effective.

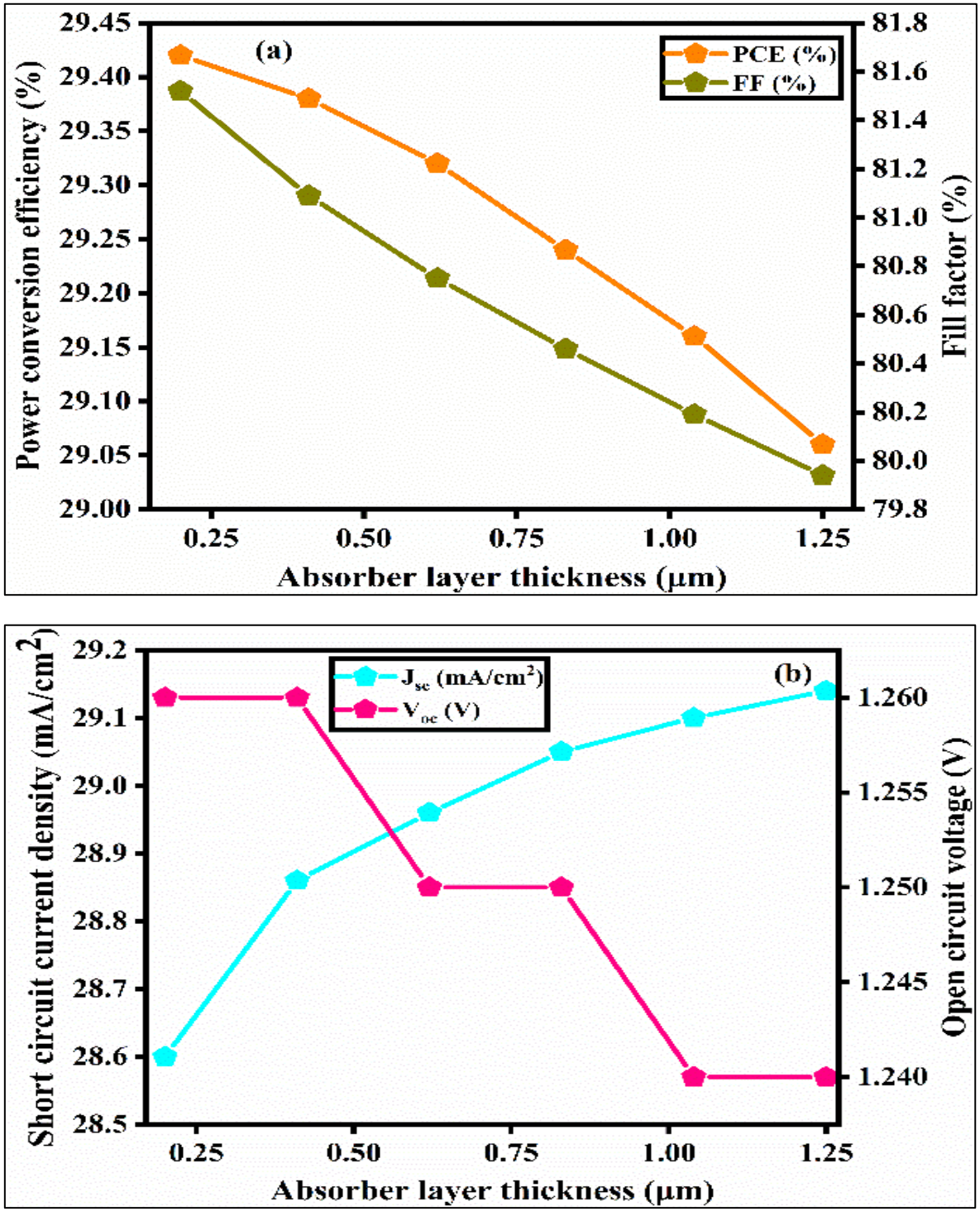

Fig 4 Effect of Absorber Thickness on the Performance Characteristics of Solar Cells.

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➢ *Impact of Work Function of Back Contact*

The performance of the SCs can be increased by altering the work function of the metal back contact as it has impact on the output characteristics of the system when GO is used as ETL while P3HT as HTL. Various metals having work functions ranging from 4.7 to 5.3 eV have been tried in this study to increase efficiency but the most suitable metal for back contact having work function of 5.1 eV is gold and hence the maximum PCE achieved using this metal back contact is 25.44 % shown in Fig. 5(a). Bending of the curve takes place due to metal semiconductor junction and leads towards ohmic contact hence decrease in barrier height of majority carriers occurs along with increase in metal work function. As per Fig. 5 (a,b) there is a slight improvement in J_{sc} and V_{oc} values, but the FF varies from 60.83 to 82.69 % as shown in Fig 5(a). Thus, this study shows that Au can be used for back metal contact [20]

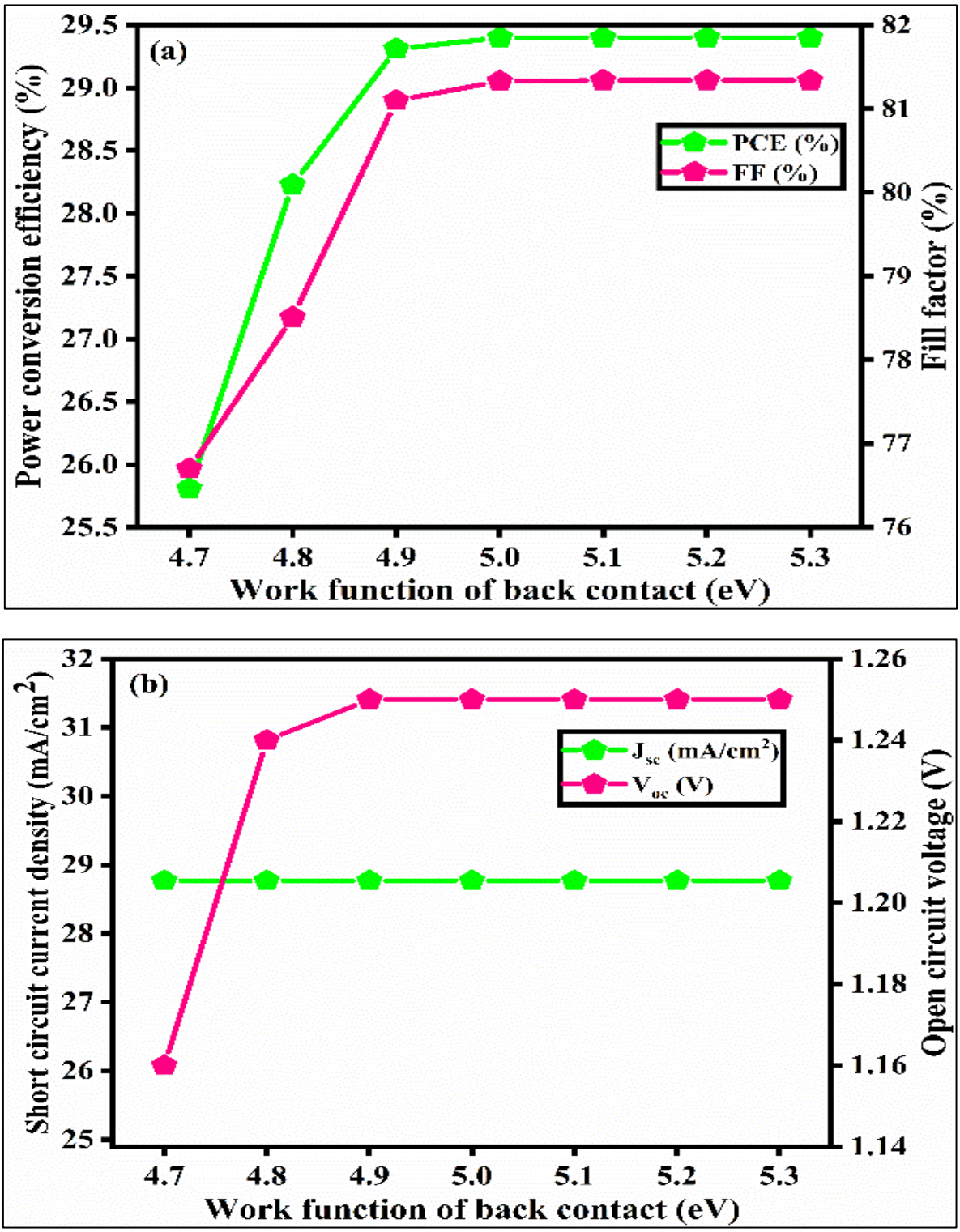

Fig 5 Effect of Back Contact Work Function on Solar Cell Parameters.

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IV. CONCLUSION

In this work, a lead-free inorganic PSC with a nip planar architecture based on $KGeCI_3$ was numerically investigated using the SCAPS-1D simulation platform. The influence of thickness and defect density of absorber layer on PV performance was systematically evaluated. Furthermore, the effects operating temperature and metal work function of back contact were examined to optimize device characteristics. Under optimized conditions, the proposed device delivered a PCE of 29.57%, V_{oc} of 1.25 V, J_{sc} of 28.77 mA/cm^2, and FF of 81.63%. The findings of this study offer valuable guidance for the development and optimization of environmentally benign germanium-based PSCs as potential alternatives to lead-containing PV technologies.

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