Physical Science International Journal

Volume 28, Issue 4, Page 57-63, 2024; Article no.PSIJ.116982
ISSN: 2348-0130

Theoretical Study of Inorganic Charge Transport Layer of Perovskite Solar Cells Using Scaps Software

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Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

Article Information

DOI: https://doi.org/10.9734/psij/2024/v28i4837

Open Peer Review History:
This journal follows the Advanced Open Peer Review policy. Identity of the Reviewers, Editor(s) and additional Reviewers, peer review comments, different versions of the manuscript, comments of the editors, etc are available here: https://www.sdiarticle5.com/review-history/116982

Original Research Article

Received: 01/04/2024
Accepted: 02/06/2024
Published: 08/06/2024

ABSTRACT

Energy can be from renewable and non-renewable sources. Solar energy is a clean renewable energy derived from the sun in the form of light and heat. Although, only a small fraction reaches the earth. Perovskite is a generic name referring to materials that exhibits the same crystal structure as calcium titanate. The aim of this research is to investigate the performance of inorganic charge carriers of perovskite solar cells using SCAPS 1D software for the simulation. The objectives are to: analyze the effects of variation of operational temperature on Perovskite Solar Cells (PSCs), optimize the thickness of titanium oxide (TiO2) electron transport layer (ETL); and investigate the effect of work function of the back metallic contact on the performance of PSCs. A comprehensive analysis was conducted to evaluate the software's impact on cell performance focusing on key parameters such as thickness, temperature, and work function to optimize device efficiency. This exploration provides new insights into optimizing device efficiency and stability by understanding how surface characteristics affect performance which extends its analysis beyond traditional parameters like temperature and thickness. The findings reveal that while temperature fluctuations maintain consistency with current density (J_{sc}) and exhibit slight variations in fill factor

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Cite as: *F. A., Aniefiok, Dahiru M. S., and Musa S. A. 2024. "Theoretical Study of Inorganic Charge Transport Layer of Perovskite Solar Cells Using Scaps Software". Physical Science International Journal 28 (4):57-63. https://doi.org/10.9734/psij/2024/v28i4837.*

(FF), there's a consistent decrease in open-circuit voltage (V_{oc}) across all temperatures. Notably, at 303 K, the efficiency remains relatively stable. Moreover, exceeding the optimal thickness of 0.20 µm adversely affects perovskite solar cell efficiency, while achieving an optimal work function of 5.0 eV for the back metallic contact is critical for maximizing performance. These results underscore the significance of employing inorganic transport materials to address the stability challenges inherent in perovskite solar cells, paving the way for cost-effective fabrication methods without compromising device performance. It is recommended that optimization process be carried out for other inorganic charge carriers of the perovskite solar cells like Zn2O, NO, SnO2 and others to see which one has a better performance in the fabrication.

Keywords: Perovskite solar cells; scaps software; thickness; temperature; work function.

1. INTRODUCTION

In the wake of escalating global warming concerns spurred by greenhouse gas emissions from fossil fuel combustion, humanity faces an urgent imperative to seek clean, affordable, and sustainable energy sources capable of meeting burgeoning energy demands [1]. As populations burgeon and living standards improve, the need for electricity to power essential commodities escalates, exacerbating environmental pressures. To mitigate the adverse effects of pollution, harnessing renewable energy sources such as water, wind, and solar power emerges as a compelling solution [2]. However, a notable challenge with renewables lies in their site-specific energy production requirements, unlike non-renewable counterparts like gas, coal, and oil.

The sun, radiating copious solar energy daily, dwarfs the energy consumption of the entire Earth's population over a year [3], making solar energy a paramount contender in the quest for sustainable power sources until more advanced fusion or stable fission power technologies emerge [4]. Various methodologies exist for harnessing solar energy efficiently, with solar cells serving as a pivotal technology for direct conversion of solar radiation into electricity. While silicon solar cells dominate the market, boasting an improved power conversion efficiency (PCE) from 12% to 25% over four decades, their manufacturing process entails substantial heat energy and often relies on rare and toxic materials [5]. Consequently, scientists have turned their attention to alternative solar cell structures primarily derived from organic and abundant materials, including dye-sensitized, organic, and perovskite solar cells.

Titanium dioxide (TiO_2), also known as titania, emerges as a promising material owing to its exceptional stability and optical properties. Widely utilized in various applications such as photocatalysts, photovoltaics, and sensors, TiO_2 nanostructures have gained traction in solar cell technologies, particularly in dye-sensitized and perovskite solar cells, owing to their high conductivity and transparency [6]. However, challenges persist, including TiO_2's large bandgap, limiting solar energy utilization, and sluggish carrier transport, exacerbating carrier recombination risks [7].

The vast reservoir of solar energy, readily available and inexhaustible, presents an unparalleled opportunity for sustainable energy generation [8]. Unlike conventional power generators, solar energy can be directly harvested into electricity through small photovoltaic (PV) solar cells, offering a distinct advantage. Thus, understanding and optimizing the performance of perovskite solar cells (PSCs) becomes imperative. The general layer structure of PSCs comprises transparent electrodes such as indium tin oxide (ITO) or fluorine doped tin oxide (FTO), an electron transporting layer (ETL), the perovskite active layer for photon absorption and exciton generation, a hole transporting layer (HTL), and a metallic electrode, interconnected to form a closed-circuit cell [9].

By elucidating the intricate mechanisms governing solar energy conversion and refining PSC technologies, researchers strive to realize the full potential of solar power as a clean, abundant, and sustainable energy source, pivotal in combating climate change and ensuring a greener future for generations to come [10].

1.1 Solar Cell Parameters

Certainly, these parameters play crucial roles in evaluating the efficiency and performance of solar cell devices. Here's a brief explanation of each parameter:

Short-Circuit Current Density (J_{sc}): This parameter represents the maximum current density that the solar cell can generate when its terminals are short-circuited, i.e., when there is no external load connected. It is a measure of the current output capability of the solar cell under optimal illumination conditions.

• Open-Circuit Voltage (V_{oc}): Voc signifies the maximum voltage that the solar cell can generate when there is no external load connected, i.e., when its terminals are open-circuited. It reflects the potential difference across the solar cell in the absence of current flow and provides insight into the efficiency of the solar cell's semiconductor materials.

$$V_{oc} = \frac{kT}{e}\ln\left(\frac{J_{ph}}{j_0} + 1\right)$$

Where j_0 indicates zero net current density.

• Fill Factor (FF): The fill factor is a measure of how effectively the solar cell converts incident light into electrical power. It is calculated as the ratio of the maximum power output of the solar cell to the product of its open-circuit voltage and short-circuit current density. A higher fill factor indicates better utilization of the solar cell's active area and improved overall efficiency.

$$FF = \frac{V_{P_m} * J_{P_m}}{V_{oc} * J_{sc}}$$

Where $V_{P_m}\ and\ J_{P_m}$ is the voltage and current density at maximum power respectively.

• Peak Power: The peak power, also known as maximum power point (Pmax), represents the maximum electrical power output of the solar cell at its optimal operating point. It occurs at the point where the product of the voltage and current is maximized, typically under specific illumination and temperature conditions.

$$\eta = \frac{P_{max}}{P_{in}} = \frac{J_{P_m} V_{P_m}}{P_{in}} = \frac{J_{sc} * V_{oc} * FF}{Pin}$$

2. MATERIALS AND METHODS

The materials used for this simulation include the following:

- Solar Cells Capacitance Simulator (SCAPS 1D) software package.
- Computer/ Laptop system.

The SCAPS 1-D simulation software emerges as a pivotal tool for analysing and optimizing perovskite solar cells. Below is a succinct outline of the procedure for executing a simulation using SCAPS 1-D:

By employing SCAPS 1-D for simulation endeavours, researchers can expedite the exploration of novel materials and device architectures, facilitating informed decision-making and accelerating the development of sustainable and efficient photovoltaic technologies [11]. Below is a brief explanation of the panel of the SCAPS features in Fig. 2.

i. Input Parameters Definition: Begin by defining the key parameters governing the behaviour and characteristics of the perovskite solar cell, including material properties, layer thicknesses, doping concentrations, and external conditions such as temperature and illumination intensity [12].

ii. Device Structure Configuration: Construct the layered structure of the perovskite solar cell within the simulation environment, delineating the arrangement of transparent electrodes, electron transporting layers (ETLs), perovskite active layers, hole transporting layers (HTLs), and metallic electrodes [13].

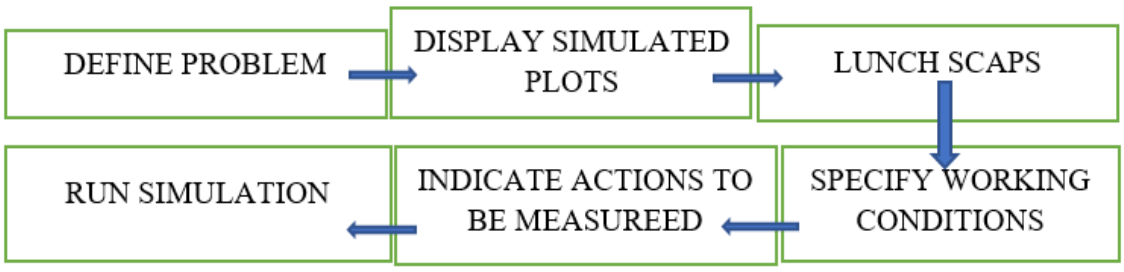

Fig. 1. Flow chart for the operation of the SCAPS 1-D

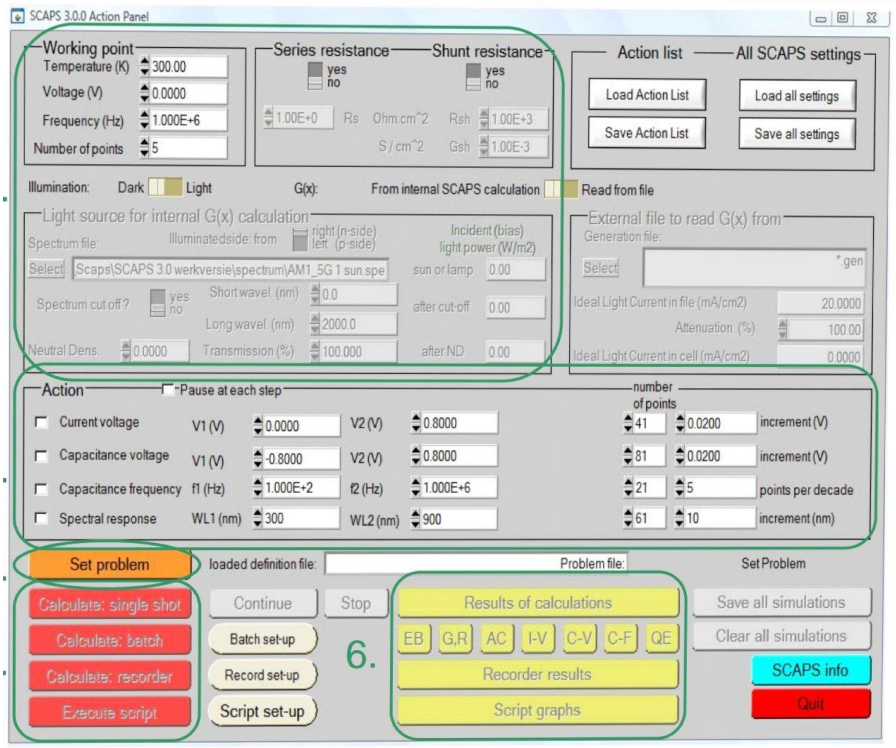

Fig. 2. Panel of the SCAPS 1-D software

iii. Numerical Solution: Utilize numerical methods to solve the coupled system of equations describing charge transport, recombination, and optical absorption phenomena within the perovskite solar cell structure. SCAPS 1-D employs sophisticated algorithms to accurately simulate the device's behaviour under varying operating conditions [14].

iv. Parameter Optimization: Iteratively adjust the input parameters to optimize the performance metrics of the perovskite solar cell, such as short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and peak power, towards achieving enhanced efficiency and stability [15].

v. Analysis and Interpretation: Analyze the simulation results to gain insights into the underlying physical mechanisms governing the operation of the perovskite solar cell [16].

3. RESULTS AND DISCUSSION

The following were obtained during the simulation:

ϖ Variation of temperature on the photovoltaic performance.

The results depicted in Fig. 3 illustrate the impact of varying operational temperatures ranging from 273 K to 313 K on the performance of the solar cell device. Notably, it is observed that temperature fluctuations have negligible effects on both the short-circuit current density (J_{sc}) and fill factor (FF). However, there is a discernible influence on the open-circuit voltage (V_{oc}), albeit slight. This underscores the nuanced interplay between temperature and the characteristics of the device, highlighting the significance of transport materials in mediating temperature effects. Generally, the operational temperature significantly affects the performance of the device, necessitating careful consideration and optimization to achieve desired outcomes.

ϖ Electron transport layer thickness

Fig. 4 elucidates the impact of varying electron transport layer (ETL) thickness on the performance of different solar cell structures. Optimal absorption layer thickness is crucial for efficient photon absorption and generation of electron-hole pairs. Increasing the optimal thickness beyond 0.20 µm reduces the efficiency of the perovskite solar cells. Hence, electron transport layer (ETL) thickness was optimize for the fabrication to be 0.20 µm. The results

indicate a direct correlation between absorber thickness and device efficiency, with efficiency increasing as the absorber thickness escalates up to a maximum point (optimum thickness). This enhancement in efficiency can be attributed to the increased absorption of photons, resulting in the generation of more electron-hole pairs. However, beyond the optimum thickness, efficiency begins to decline due to increased recombination of generated electrons and holes, stemming from the longer diffusion distances traversed by charges.

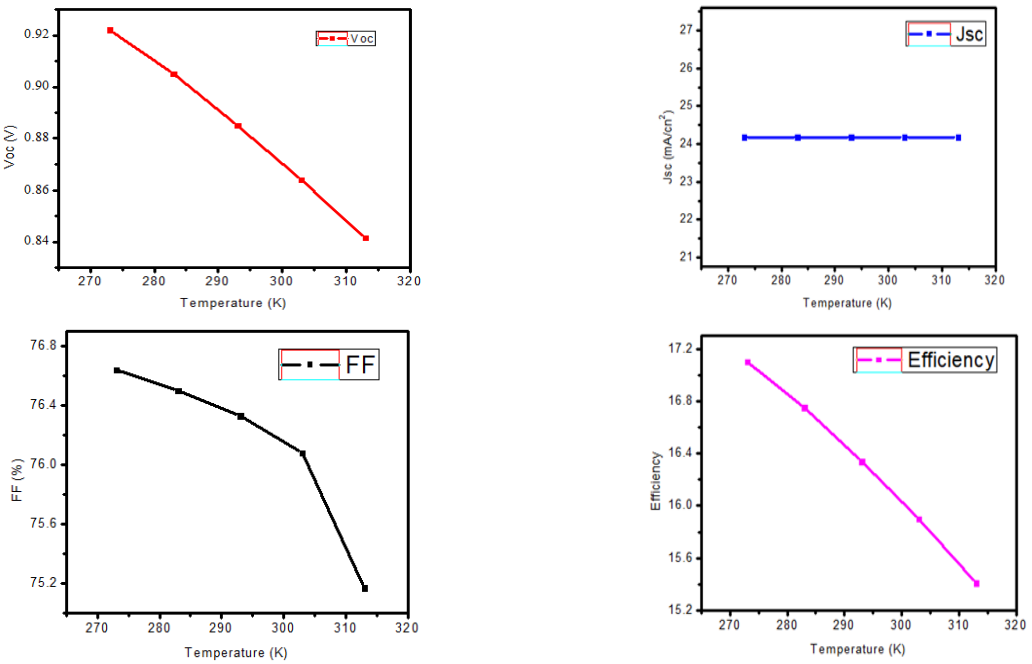

Fig. 3. Effect of temperature on the photovoltaic performance

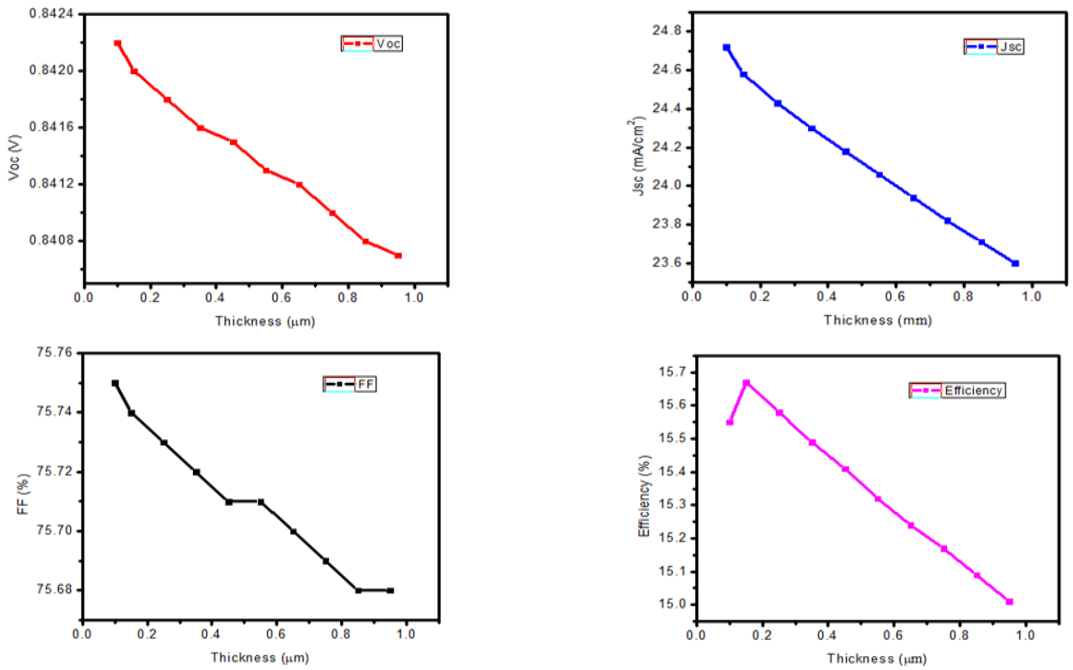

Fig. 4. Electron transport layer thickness

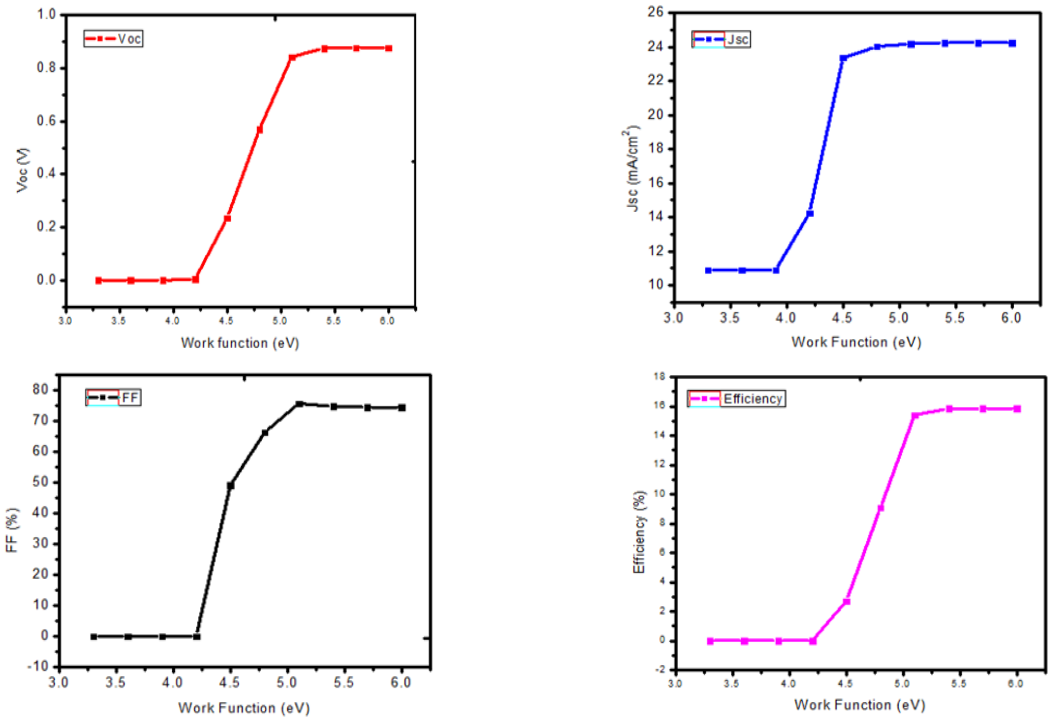

Fig. 5. Impact of work function of the back metallic contact on the photovoltaic performance

ϖ Work function on the photovoltaic performance

In Fig. 5, the variation of the work function value is explored to understand its influence on device performance. The optimal work function for the back metallic contact was obtained to be 5.0 eV, below that reduces the efficiency of the perovskite solar cells. Therefore, increment beyond 5.0 eV has no effect on the photovoltaic performance. The results underscore the dependence of the perovskite solar cell's work function on the type of charge transport materials employed and their method of combination. This highlights the critical role of optimizing the work function in enhancing device efficiency and performance, emphasizing the need for meticulous selection and integration of charge transport materials within the device architecture.

4. CONCLUSION

Rise in temperature remains constant with Jsc and slight change in the FF which revealed that there is decrease in Voc at all temperature and at 303 K the efficiency remains unchanged. Hence, temperature has no effect on Jsc. The influence of the work function of the back metallic contact on the photovoltaic performance of perovskite solar cells is significant, as it directly impacts charge extraction and recombination processes within the device. Specifically, variations in the work function can adversely affect solar cell performance by altering the charge aggregation at the depletion region, thereby influencing charge carrier transport and recombination dynamics. This strategic approach not only improves device efficiency but also contributes to the overall stability and reliability of the solar cell under varying operating conditions.

5. RECOMMENDATION

It is recommended that optimization process be carried out for other inorganic charge carriers of the perovskite solar cells like Zn2O, NO, SnO2 and others to see which one has a better performance in the fabrication.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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Peer-review history:
The peer review history for this paper can be accessed here:
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