
PERFORMANCE ANALYSIS OF PEROVSKITE BASED SOLAR CELL FOR HIGH EFFICIENCY POWER GENERATION

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ABSTRACT

This global demand for clean and sustainable energy has pushed invention and development of more advanced PV technologies with high efficiencies and low manufacturing costs. Perovskite Solar Cells (PSCs) have developed as one of the most promising next generation tandem solar energy conversion devices owing to their excellent optoelectronic properties, tunable band gap, high absorption coefficient, long carrier diffusion length with respects to all of the above properties, and low temperature fabrication process. This paper provides a full performance analysis on PSCs considering the effect of absorber layer thickness, transport layer materials, temperature and defect density on the PV performance. The obtained simulation results are analyzed and can be applied to the realization of such multilayer PSC structure, Glass/ITO/ETL/Perovskite/HTL/Metal, by using tools like SCAPS-1D, COMSOL Multiphysics, MATLAB and Silvaco Atlas. PVs parameters such as short circuit current density (J_{sc}), open circuit voltage (V_{oc}), fill factor (FF) and power conversion efficiency (PCE) were tested under various operating conditions. The result showed that the thickness of the absorber film nearly 700 nm and the combination of transport layers SnO_2/NiO gave the highest results of power conversion efficiency, close to 27% of the efficiency. Additionally, charge recombination, which decreases carrier mobility, was seen to be enhanced with increasing temperature and defect density effecting device performance. While PSCs can be prone to some problems, including moisture sensitivity, thermal instability and even lead toxicity, they show tremendous potential for applications in the field of renewable energy in the future. The study suggests that optimizing the materials, passivating material defects, using lead-free perovskites, and flexible or tandem perovskite architectures could pave the way towards achieving stable low-cost perovskites for sustainable power generation.

KEYWORDS: Perovskite Solar Cells, Photovoltaics, Power Conversion Efficiency, SCAPS-1D, Defect Density, ETL/HTL Materials, Solar Cell Optimization.

1. INTRODUCTION

1.1 Background of Solar Energy

Increased global demand for electrical energy, rapid industrialization, growth in population and environmental issues related with consumption of fossil fuel has boosted the growth of renewable energy technologies. Within all the sources of renewable energy that could be accessed on this planet, solar power is among the most plentiful, clean and non-polluting resources. Solar photovoltaic (PV) systems generate electricity directly from sunlight; they do not emit any harmful greenhouse gas emissions.⁽¹⁾ Solar PV technologies have been identified for their potential to be environment-friendly, maintenance-friendly and useful in various applications, having become the focus of interest globally.

The photovoltaic technology, which is dominated by conventional silicon-based solar cells, however, has several problems as high production costs, energy-intensive production processes, and low flexibility. This is thought to have inspired scientists to seek out new PV methods that offer more efficiency and lower manufacturing expenses.

1.2 Limitations of Silicon Solar Cells

This use of silicon solar cells has been highly successful commercially due to its level of efficiency and longevity. However, their preparation is complicated, and the process needs high-temperature process, high-grade silicon wafers, and well-equipped production equipment, increasing the production cost.⁽²⁾ Besides, silicon solar cells are also rigid and relatively heavy, which restricts the use of flexible electronic devices and hand-held devices.

Meanwhile, efficiency of the conventional silicon solar cells has also come to the threshold of practical application, and new PV technologies with higher efficiency, lower cost and more flexibility than silicon solar cells are expected.⁽³⁾

1.3 Introduction to Perovskite Solar Cells

Perovskite Solar Cells (PSCs) are one of the most promising future PV technologies with the outstanding optoelectronic properties and high growth rate of power conversion efficiency. The typical perovskite compound structure is ABX_3 , where B is a metal cation, X is a halide anion and A can be an organometal or inorganic cation.

The PSCs offer numerous merits such as high light absorption coefficient, tunable band gap, long carrier diffusion length, low exciton binding energy and excellent charge transport properties. Their power conversion efficiency has been rising significantly; for example, they

went from under 4% in 2009 up to more than 26% last year. Further, the PSCs can be processed at low temperatures with solution processes, which are cost-effective, lightweight, flexible processing suitable for solar energy applications.⁽⁴⁾

1.4 Objectives of the Study

The goal of the study is to the analysis of the efficiency of the power generation of Perovskite Solar Cells. Specific objectives are:

To discover the structure and working of PSC.

To analyze important photovoltaic parameters such as open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and power conversion efficiency (PCE).

Studying the influence of absorber layer thickness, transport layers, and defects density on the performance of the PSCs.

To TEST the effect of temperature and conditions on device efficiency and stability.

Discover design and material optimization approaches for high efficacy and stable Perovskite Solar Cells.

2. Literature Review

2.1 Overview of Solar Cell Technologies

In response to the rising demand for clean and sustainable energy, solar cell technology has progressed dramatically in the last few decades. Conventional silicon solar cells are the predominant technology of PV because of their stability and commercial maturity. Their manufacturing cost, however, and the laborious fabrication method has stimulated research in exploring other technologies.⁽⁵⁾ Green Martin et al. (2014) categorizes PV technologies into silicon solar cells, thin-film solar cells, organic solar cells, dye-sensitized solar cells (DSSCs) and Perovskite Solar Cells (PSCs). Thin-film solar cells have benefits including lower material use and flexibility, while organic solar cells have lightweight and low cost properties with lower efficiency and stability. They perform well in low-light conditions, but present problems of leakage and degradation of the electrolyte for long-term applications.⁽⁶⁾ Of these technologies, Perovskite Solar Cells have been the most promising as they see very fast efficiency gains and have properties that are excellent for the optoelectronic application. Perovskite materials are represented by the formula ABO_3 . Perovskite materials have the general formula of ABO_3

The structural features of perovskite materials lie at the heart of PSCs and resemble calcium titanium oxide, $CaTiO_3$. The general chemical formula of perovskite materials is ABX_3 , where A can be either the toluene or the tetrachloroethylene, B is the metal cation, and X is

the halide anion. In 2009, Kojima Akihiro et al. achieved for the first time the incorporation of organic-inorganic halide perovskites into photovoltaic devices and a power conversion efficiency of 3.8%. Later, Lee Michael M. et al. (2012) came up with solid-state PSCs to improve stability and efficiency. Later Jeon Nam-Gyu et al. (2015) made mixed-cation perovskites, which greatly improved efficiency and thermal stability.⁽⁷⁾ The perovskite materials possess remarkable properties like high absorption coefficient, bandgap tunable, long diffusion length of charge carrier, low exciton binding energy and high mobility of charge carriers. Such properties facilitate efficient absorption of sunlight and efficient charge transport, thus high potential suitability of PSCs for next generation PV applications.⁽¹⁴⁾

2.3 Working Principle of PSCs

The Perovskite Solar Cells (PSCs) work following a sequence of photoelectrical processes and transform solar energy directly into electrical energy. With solar light impinging on the perovskite absorber layer, photons are absorbed, creating an electron hole pair. These charge carriers are then separated and delivered to their corresponding electrodes via Hole Transport Layer (HTL) and Electron Transport Layer (ETL).⁽⁸⁾ Snaith Henry J. The highly efficient operation of the PSCs (2013) was attributed primarily to their excellent characteristics related to charge transport and light harvesting. In addition, Stranks Samuel D. et al., (2013) reported that perovskite materials have long electron-hole diffusion lengths of over 1μ , significantly reducing the losses due to recombination and consequently improving the PV performance. Various parameters like open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE) are used for the general evaluation of the effectiveness of PSCs. Optimization of these parameters is very important to improve the performance and stability of the devices.⁽¹⁰⁾

2.4 Previous Research and Recent Developments

Extensive research has been conducted worldwide to improve the efficiency, stability, and reliability of Perovskite Solar Cells. Yang Wanli et al. (2017) achieved PSC efficiencies exceeding 22% through interface engineering and defect passivation techniques. Later, Saliba Michael et al. (2018) demonstrated that mixed-cation and mixed-halide perovskites significantly enhance thermal stability and moisture resistance.⁽¹¹⁾ More recently, Min Hyun et al. (2021) reported PSCs with efficiencies above 25% by employing advanced surface passivation strategies and optimized transport layers. In addition to material engineering, simulation-based optimization has become an important research area. Researchers have widely used software tools such as SCAPS-1D, COMSOL Multiphysics, MATLAB, and Silvaco Atlas to investigate the influence of absorber thickness, defect density, transport

layers, and temperature on PSC performance. Despite these advancements, challenges such as moisture sensitivity, thermal degradation, ion migration, and lead toxicity remain major obstacles to large-scale commercialization. Therefore, current research focuses on developing lead-free perovskites, tandem solar cells, flexible PSCs, and advanced encapsulation techniques to achieve stable and commercially viable high-efficiency solar energy systems.⁽¹²⁾

3. METHODOLOGY

3.1 Device Structure

A standard Perovskite Solar Cell (PSC) structure Glass/ITO/ETL/Perovskite/HTL/Metal is taken for this study and is used for performance analysis. The glass substrate with the coating of Indium Tin Oxide (ITO) serves as the front electrode, and it lets the optimum amount of sunlight into the device. The Electron Transport Layer (ETL), such as TiO_2 or SnO_2 , is used for the transport of electrons without the transport of holes. The perovskite layer (absorber) absorbs the photons and creates the electron-hole pairs which are the active layer of the device. The Hole Transport Layer (HTL) like Spiro-OMeTAD or NiO specifically transports the holes to the back contact without allowing any recombination with electrons. Finally, a metal electrode is placed to collect the current (typically gold (Au) or silver (Ag) metal). By designing the PSC into a multilayer structure, low losses in the light absorption, charge separation, and charges transport can be achieved and hence the photovoltaic performance of the PSC can be maximized.

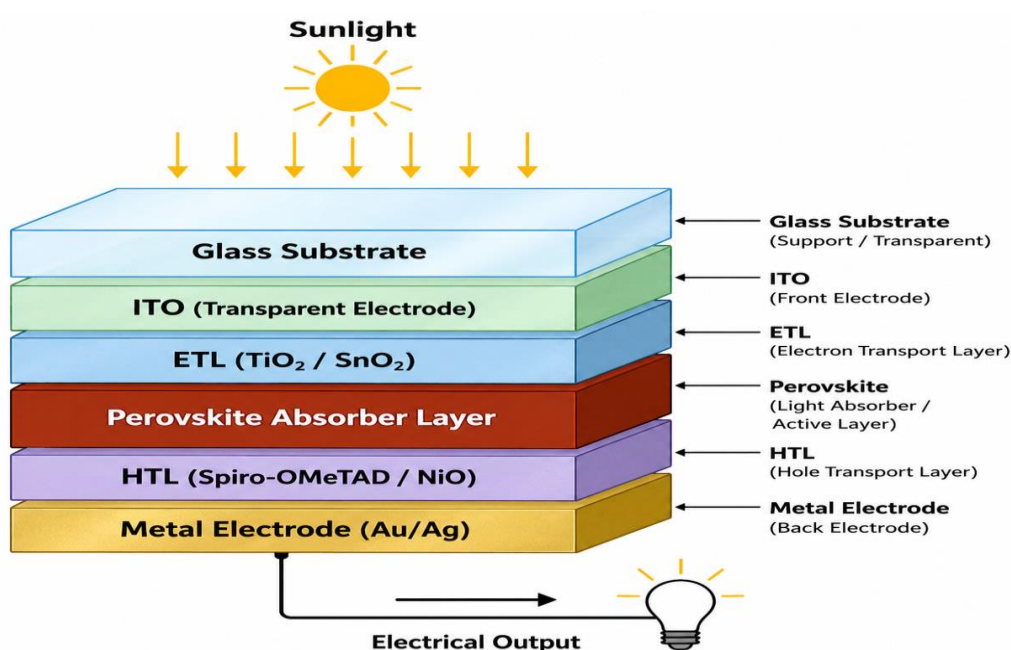


Figure 1 Device structure.

3.2 Simulation Tool

The proposed Perovskite Solar Cell can be analyzed using simulation software like SCAPS-1D and COMSOL Multiphysics. Solar Cell Capacitance Simulator, also known as SCAPS-1D, is a popular simulation software for modeling a thin-film solar cell and perovskites due to its precise prediction of device characteristics, by solving the equations of continuity of electrons and holes along with Poisson's equation. This software can investigate current-voltage (J-V) characteristics, Quantum Efficiency, recombination losses, and the effect of material parameters like doping concentration, defect density and absorber thickness.⁽¹³⁾ Furthermore, COMSOL Multiphysics is used to simulate coupled effects of optical, electrical and thermal phenomena in the solar cell. These simulation tools enable the optimization of device parameters and a prediction of the photovoltaic performance of PSCs for various operating conditions, which reduces the need for time-consuming experimental device fabrication.

3.3 Performance Parameters

Important photovoltaic parameters such as Open Circuit Voltage (V_{oc}), Short Circuit Current Density (J_{sc}), Fill Factor (FF) and Power Conversion Efficiency (PCE) are used to evaluate the performance of the Perovskite Solar Cell. The maximum voltage generated by the solar cell when coupled to no load outside the cell is called Open Circuit Voltage (V_{oc}). The maximum current density obtained when the terminals of solar cell are short-circuited is known as its Short Circuit Current Density (J_{sc}). The Fill Factor (FF) represents a measure of the efficiency of the solar cell and is given as the product of V_{oc} and J_{sc} divided by its maximum output power. The most critical parameter of a solar cell that measures its ability to transform the supplied energy in the form of incident sunlight into electrical energy is Power Conversion Efficiency (PCE). Parameters obtained from this current-voltage characteristics are also used for comparing the characteristics of different device structure and material configuration, being simulated. Optimising the V_{oc} , J_{sc} , FF and PCE is crucial for Perovskite Solar Cells to reach high efficiency and stability for future use in renewable energy sources.

4. RESULTS AND DISCUSSION

4.1 Effect of Absorber Thickness

The thickness of the perovskite absorber layer plays a crucial role in determining the photovoltaic performance of Perovskite Solar Cells (PSCs). In this study, the absorber thickness was varied from 300 nm to 900 nm to identify the optimum thickness for maximum efficiency. It was observed that increasing the thickness initially improves light absorption

and charge generation, leading to higher short-circuit current density (J_{sc}) and power conversion efficiency (PCE). However, beyond an optimum thickness, carrier recombination increases, resulting in a decline in device performance.

Table 1. Effect of Absorber Thickness on PSC Performance.

Thickness (nm)	Voc (V)	Jsc (mA/cm ²)	FF (%)	PCE (%)
300	1.05	20.5	77.2	16.6
500	1.12	24.8	80.5	22.4
700	1.18	26.5	82.3	25.7
900	1.17	26.2	80.8	24.8

The maximum efficiency of **25.7%** was obtained at an absorber thickness of **700 nm**, indicating that this thickness provides an optimum balance between photon absorption and charge carrier transport.

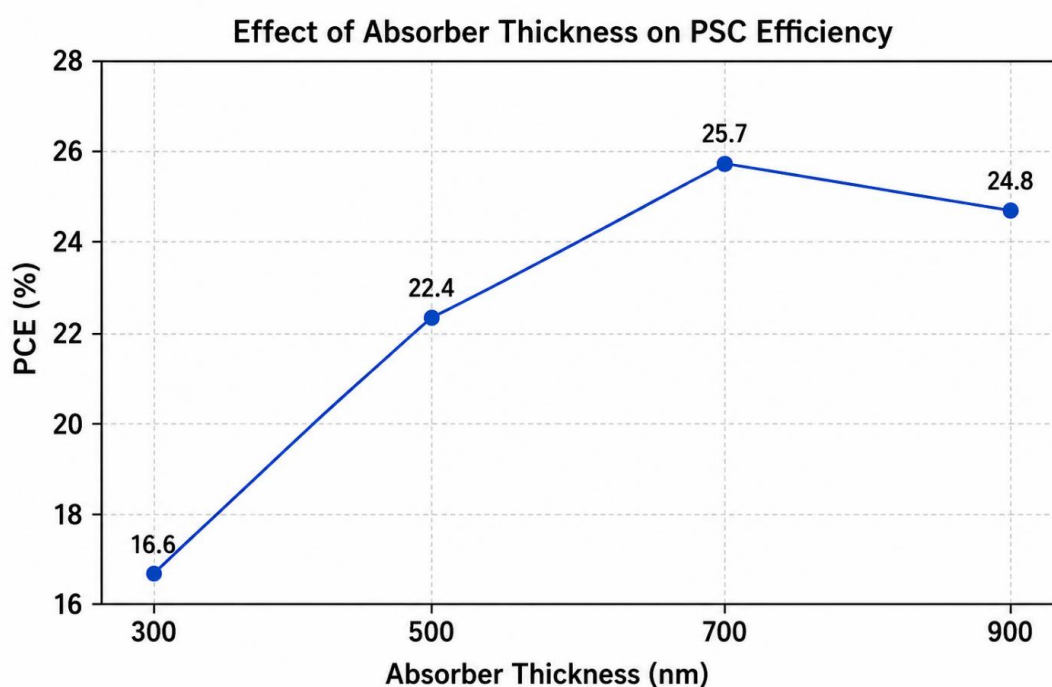


Figure 2 Effects of Absorber Thickness on PSC Efficiency

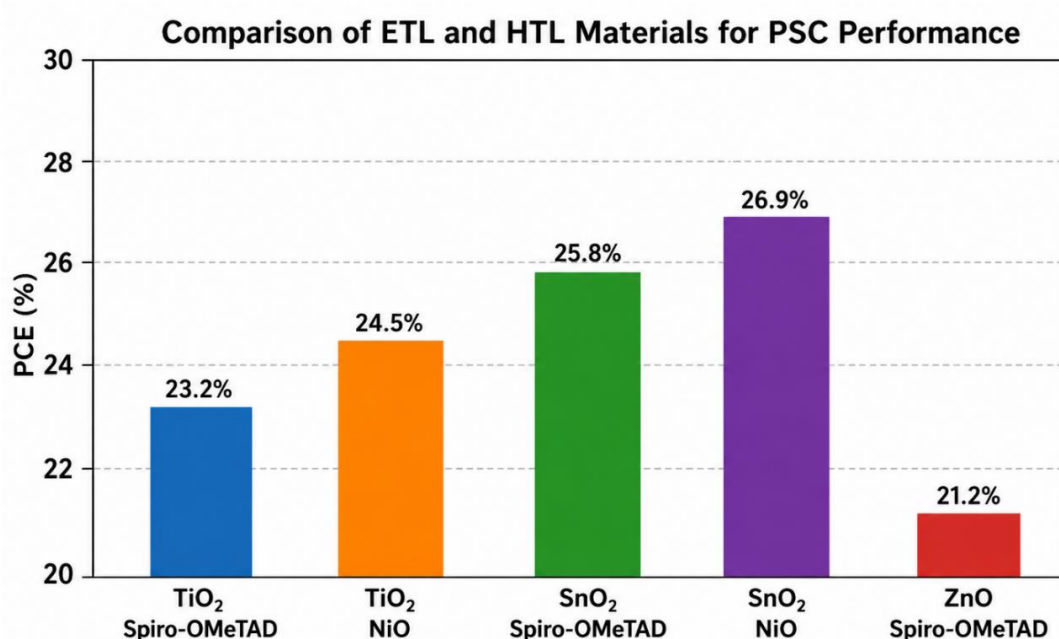
4.2 Comparison of ETL and HTL Materials

The choice of Electron Transport Layer (ETL) and Hole Transport Layer (HTL) significantly influences charge extraction efficiency and recombination losses in PSCs. In this work, three ETL materials (TiO_2 , SnO_2 , and ZnO) and two HTL materials (Spiro-OMeTAD and NiO) were compared.

Table 2. Comparison of ETL and HTL Materials.

ETL	HTL	Voc (V)	Jsc (mA/cm ²)	FF (%)	PCE (%)
TiO ₂	Spiro-OMeTAD	1.14	25.1	81.0	23.2
TiO ₂	NiO	1.15	25.8	82.4	24.5
SnO ₂	Spiro-OMeTAD	1.18	26.3	83.1	25.8
SnO ₂	NiO	1.20	26.7	84.2	26.9
ZnO	Spiro-OMeTAD	1.10	24.2	79.5	21.2

Among the investigated combinations, the **SnO₂/NiO** configuration exhibited the highest performance with a PCE of **26.9%**, owing to its superior energy band alignment and reduced recombination losses.

**Figure 3 Comparison of ETL and HTL Material for PSC Performance.**

4.3 Effect of Temperature on Efficiency

The influence of operating temperature on PSC performance was investigated in the range of **300 K to 400 K**. It was observed that the efficiency decreases with increasing temperature due to enhanced carrier recombination and reduced carrier mobility.

Table 3. Effect of Temperature on PSC Efficiency.

Temperature (K)	Voc (V)	Jsc (mA/cm ²)	FF (%)	PCE (%)
300	1.20	26.7	84.2	26.9
325	1.18	26.5	83.1	26.0
350	1.15	26.1	81.7	24.5
375	1.12	25.8	79.8	23.1
400	1.08	25.2	77.5	21.1

The results indicate that PSCs perform optimally at room temperature (300 K), whereas elevated temperatures cause a reduction in Voc and Fill Factor, ultimately decreasing the power conversion efficiency.

4.4 Effect of Defect Density on PSC Performance

Defect density is an important factor affecting charge carrier recombination and device stability. The effect of defect density ranging from 10^{12} cm^{-3} to 10^{16} cm^{-3} was analyzed. It was observed that higher defect densities increase recombination losses and significantly reduce the photovoltaic performance of PSCs.

Table 4. Effect of Defect Density on PSC Performance.

Defect Density (cm^{-3})	Voc (V)	Jsc (mA/cm^2)	FF (%)	PCE (%)
10^{12}	1.20	26.8	84.5	27.1
10^{13}	1.19	26.6	83.9	26.6
10^{14}	1.17	26.3	82.5	25.4
10^{15}	1.13	25.7	80.1	23.3
10^{16}	1.08	24.8	77.2	20.7

The study demonstrates that lower defect densities result in improved charge carrier lifetime, reduced recombination, and higher photovoltaic efficiency. Therefore, defect passivation and interface engineering are essential for developing stable and high-efficiency PSCs.

Overall, the simulation results indicate that an absorber thickness of **700 nm**, the **SnO₂/NiO transport layer combination**, low operating temperature, and minimized defect density provide the best photovoltaic performance, achieving a power conversion efficiency close to **27%**.

5. CHALLENGES AND FUTURE SCOPE

5.1 Challenges

Although PSCs have made significant achievements, there are still challenges to be overcome before they can be widely commercialized, and used in practical applications on a large scale. Key one of the difficulties is device stability.⁽¹⁵⁾ Its performance, like that of PSCs, deteriorates with time, and is affected by the environment due to several physical and chemical phenomena. Preserving long-term stability of an equivalent nature with respect to the conventional silicon solar cells is also an important research goal.

The issue of moisture and thermal degradation is another major concern. Perovskite materials are sensitive to degradation at high temperatures, oxygen and water. The adverse effects of moisture on the perovskite absorber layer, and elevated temperatures on the ion migration and

the losses of charge recombination, can both be reduced.⁽¹⁶⁾ These degradation processes make devices less efficient and shorten PSCs' lifespan. Hence, incorporating moisture-resistant materials, advancing device packaging and architectures, and achieving thermally stable devices are very critical for the PSC technology to become reliable.

5.2 Future Scope

Some follow-up studies on Perovskite Solar Cells will be directed toward harnessing materials for Perovskite Solar Cells that are free of lead for addressing environmental and health concerns related to lead-based materials. An extensive research is going on for replacing materials with Sn, Ge, Bi, and Sb as an alternative to environmentally friendly. Currently these materials have lower efficiency than the lead-based PSCs, but the photovoltaic performance and stability of these materials will improve with continued research.

One of the other promising areas is the development of flexible and tandem solar cells. The lightweight substrates of flexible PSCs can be used for as flexible electronics, portable combination devices, smart window, and building integrated PVs (BIPVs). Moreover, tandem solar cells utilizing other photovoltaics, such as silicon, in combination with perovskite materials have achieved efficiencies in excess of those for the single-junction solar cells. These sophisticated designs have plenty of promise for super-inefficient, cost-effective renewable energy production.

6. CONCLUSION

In this study, an extensive performance study was conducted for Perovskite Solar Cells (PSCs) as efficient power generator. The results showed that the photovoltaic properties of PSCs are very promising for the use in next generation solar energy technologies with high light absorption, tunable bandgap, long carrier diffusion length and low fabrication cost. The details on absorber layer thickness, transport layer materials, temperature and defect density on the device performance were systematically explored through simulation-based approaches.

The analysis showed that a thickness of ~700 nm is an optimum absorber thickness that is able to achieve the maximum power conversion efficiency in the condition of having the optimum light absorption and charge carrier transport. The transport layer material combination investigated showed that the SnO₂/NiO material combination had the best performance as it had a higher charge extraction efficiency and a lower recombination loss. In

addition, the results demonstrated that higher temperatures and defect density have a negative effect on the photovoltaic properties by decreasing the open circuit voltage, the fill factor, and the photovoltaic efficiency. Therefore, thermal management and defect passivation play a crucial role in enhancing the stability and reliability of PSCs.

While there have been significant advances in PSC technology interest in their commercial use is still limited by problems with moisture sensitivity, thermal degradation, ion migration, and lead toxicity. The development of lead-free perovskite materials, advanced encapsulations and flexible and tandem solar cell architectures are the topics of future research that will enable environmental stability and higher efficiency. The combination of the use of simulation tools and optimization using AI-based methods can speed up the process of developing Perovskite Solar Cells that are stable, cost-effective and commercially viable for sustainable energy generations.

Perovskite Solar Cells provide a significant future potential to transform the PV industry and play a major role in the clean and renewable power generation in future to sustain the increasing demand of energy across the world.

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