

Mathematical Modeling of Perovskite Solar Cells for Efficient Energy Harvesting

Dr J Sravan Kumar

Assistant Professor of Mathematics

Government Degree College Gambhiraopet

Abstract—Perovskite solar cells (PSC) have become a groundbreaking photovoltaic cell because they are considered to possess a high power conversion efficiency (PCE), low fabrication cost and tunable optoelectronic behavior. The mathematical modeling is essential in the processes of learning the dynamics of charge transport, recombination, and effects of ion migration alongside optimization of performance of PSCs. This paper is a complete mathematical model that combines Poisson equation, carrier continuity equations and drift argument equations to model electrical behavior of perovskite solar cases when illuminated. The model also uses the trap-assisted recombination, interfacial charge transfer resistance, and ion migration effects to enhance the accuracy of prediction. The simulation results show the effect of absorber thickness, defect density and mobility, and temperature on the efficiency of a device. The analysis done in terms of optimization shows that the density of controlled defects ($= 10^{-7} \text{ cm}^{-3}$), the optimized thickness of the layer ($= 500\text{--}700 \text{ nm}$), and better carrier mobility are significant factors in optimizing energy harvesting.

Nevertheless, applied constraints like long history material unsteadiness and sensitivity to water and magnet influences and expandability complications restrain business applications. Other physical processes that are not considered by the proposed model are the assumption of uniform material characteristics and unreality of complicated grain-boundary dynamics that can influence precision in the real world. To facilitate the adoption of PSC technology by industries, future studies must concentrate on multi-physics coupled modeling (electrical-thermal-mechanical), the use of degradation aware predictive modeling, AI-based integrated optimization structures, and scalable module-scale simulations.

Keywords— Perovskite Solar Cells, Mathematical Modeling, Drift–Diffusion Model, Charge Transport, Power Conversion Efficiency, Energy Harvesting Optimization, Ion Migration, Recombination Dynamics.

I. INTRODUCTION

The high rate of energy consumption in the world today, coupled with the environmental issues that have been linked to the use of fossil fuels has heightened the interest in research into renewable energy technologies. Solar energy is one of the most promising solutions to sustainability because of its abundance, scalability as well as the reducing cost of production. Photovoltaics (PV) is a technology that directly transforms the solar radiation into electricity and has reached impressive technological progressions in the last several decades. Although silicon-based solar cell transports are predominant in the commercial market, their complexity of fabrication and high cost constraints are driving the need to consider alternative materials with better optoelectronic behavior and simple fabrication procedures [1].

Perovskite solar cells (PSCs) in this regard have become a paradigm photovoltaic technology. The efficiency improvements of PSCs were undoubtedly unprecedented, having increased power conversion efficiency (PCE) to above 26 percent in a brief stretch of development since their introduction in 2009. PSCs have very high absorption coefficient, long carrier diffusion length, tunable bandgap, low exciton binding energy, and are compatible with solution-based fabrication techniques which comes out to give PSCs its extraordinary performance. These characteristics render perovskite materials very appealing in next generation energy collection systems such as

flexible photovoltaics, tandem solar cell and building integrated solar system.

Although PSCs are highly efficient to gain advantages, there are various limitations to the wide-scale commercials of this technology [11]. These issues are material instability during exposure to the environment (moisture, oxygen and temperature), hysteresis due to ion migration, interface recombination losses, grain boundary effects and large scale manufacturing. There is a tendency to use experimental optimization only which is usually expensive and time consuming especially when there are several interacting physical processes in the machine. Thus, mathematical modeling has become a critical part in comprehending the internal device physics, performance behavior life cycle forecasting and experimental design.

Mathematical modeling of PSCs is a technique of describing charge carrier generation, transport, recombination and electrostatic interactions in terms of coupled differential equations. The most popular model is the drift diff model with Poisson equations and laws of continuity of carriers. These equations give some understanding of the electric potential distribution, profiles of carrier concentration, recombination rates and current-voltage characters during illumination. In contrast to simplified equivalent-circuit models, physics-based modeling incorporates microscopic transport physics and enables making a systematic change in the parameters in order to optimize them [12].

A precise mathematical model will help researchers to breakdown the influence of absorber thickness, carrier mobility, defect density, temperature, and the interfacial property on the overall performance of the device. It can also be used to evaluate trade-offs in absorption enhancement versus recombination losses, optimization of layer architecture and measure stability relevant degradation mechanisms. Moreover, predictive modeling eliminates the need to make huge trial and error experiments, which

makes innovation faster and contributes to a low cost of development.

The main driving force of this project is to create an inclusive and physically stable mathematical model over which to apply a study of the perovskite solar cells performance and the emphasis on energy harvesting [10]. Although a variety of the past models have explored individual elements of the PSC operation, many of them omit coupled ionic movement, temperature, or plausible recombination reactions. The common modeling methodologies used are inadequate and should be substituted by a unified modeling method that incorporates the electrostatic dynamics, transport dynamics and recombination dynamics.

The proposed paper attempts to address this gap by developing a coupled Poisson-drift-diffusion framework that comprises of Shockley-Read-Hall recombination and parameter optimization. The model proposed is aimed at testing the device performance as shown under conditions of different structures and different materials so that the optimum configurations could be found in terms of power conversion efficiency [14].

This research is aimed to determine the following:

- To establish a mathematical model that can be used to describe the charge transport and recombination in perovskite solar cell by making use of physics.
- To model the effects of critical parameters on the performance of devices including their absorber thickness, carrier mobility, defect density and temperature.
- To compute the efficiency of energy harvesting with the help of numerics of the governing equations.
- To determine the optimum values of parameters that achieves the highest power conversion ratio and minimizes the recombination losses.
- To emphasize the shortcomings of contemporary methods of modeling that can be

depicted in practice and to suggest the further directions of research.

The article offers a scientific and theoretical structure of the physics of PSC devices. The model provides a good understanding of the internal processes of photovoltaic performance by combining transport equations and realistic recombination processes. The results are parts of a larger campaign of developing the perovskite technology to be stable, effective, and commercially viable solar energy systems [9].

Novelty and Contribution

This study is novel because it has established a detailed model of mathematical modeling with a specific concern of optimizing the performance of perovskite solar cells under operating conditions. Although previously other models tended to simplify their considerations to simplified equivalent-circuit models or single-physics models, the current one uses a multi-parameter physics-based model, which accounts, simultaneously, for electrostatic behavior, charge transport and recombination.

The point that is innovative in this research is that coupled Poisson, carrier continuity and drift-diffusion equations have been systematically incorporated to the study of PSC behavior on steady-state illumination. In contrast to earlier followed single-model diode models using an empirical combination of fitting parameters the proposed model is a first-order equation directly relating the physical characteristics of the material including mobility, defect density, and absorber thickness with measurable photovoltaic response parameters such as open-circuit voltage (V_{oc}), short-circuit current density, or short-circuit current density (J_{sc}) and fill factor (FF) and power conversion efficiency (PCE).

A very significant contribution is the parametric optimization formulation that is part of the model. This study does not just attempt to simulate fixed device designs but assesses how device efficiency

changes in response to changes in thickness, densities of defects, mobility and temperature. This analytical study allows stating the most direct operational points to harvest the greatest energy. This foretelling ability comes in handy especially to inform experimental fabrication plans.

Another contribution of the study is also that of recombination dynamics where Shockley, Read and Hall (SRH) recombination modeling is included. Recombination losses can be a large source of constraint of PSC efficiency, and recombination can be better represented by precise modelling of trap-assisted recombination. Technologically, the model would provide practical information on improving material quality, as it quantifies the relationship between defect density and voltage effect and/or the fill factor.

Besides, the work covers the issues of practical implementation and modeling constraints, such as: homogeneous material property assumptions, the inability to account for heterogeneity of grain boundaries, simplifying the effect of ion migration, and a paucity of coupling of degradation. These limitations are essential in improving the level of scientific rigor in the research and give it a context on which to establish further research.

The most important findings of this study can be highlighted as follows:

- Establishment of an all-inclusive drift-diffusion model of PSC performance analysis.
- Simulation of electrostatic and recombination processes by a single framework.
- Optimization of structural and material parameters to produce more energy by a parametric mechanism.
- How much energy efficiency varies with the density of defects or the temperature.
- Sensitivity to efficiency to variation in defect density or temperature.
- Determination of real modeling drawbacks and developmental research program.

Altogether, this study continues the theoretical basis of the operation of perovskites solar cells and also offers a scalable modeling framework in the field of optimization of the future photovoltaic as a research field. With the ability to optimize and physical precision combined, the proposed framework can help in hastening the transfer of perovskite solar cells through a laboratory study to a dependable business energy collection framework..

II. Related Works

The distinctive features of perovskite solar cells (PSCs) are the potential of quick enhancement in their efficiency, and the possibility of low expenses, thus, making these cells the most studied material recently. With the growth of the device efficiencies over 25, theoretical and computational studies were gaining more significance to get an insight into the inner charge dynamics and to maximize the work towards an optimized performance. Mathematical modeling has been an important aspect in a study that research into carrier transport, recombination losses, electric field distribution, and stability mechanisms in PSCs. During the last ten years, a number of modeling tools have been put forward to describe the behaviour of a device under different working conditions [2].

In 2026 Y. Chen *et al.*, [4] proposed the equivalent circuit models were used in earlier modeling work, especially the single-diode and the two-diode models. These models characterize the behavior of solar cells with lumped parameters of series resistance, shunt resistance, ideality factor and saturation current. Even though such methods give convenient ways of estimating current voltage(I V) representations, they do not have the capability of reflecting the spatial distributions of the carriers, the electric field gradient, or ionic migration. Consequently, multi-physics behavior of perovskite is challenging to model using equivalent circuits, and new models must be created to characterize it.

To overcome these, physics based drift diffusion models were developed. To explain the dynamics of the electrons and holes in the absorber film, these

models use Poisson, carrier continuity and transport equations, which are coupled. Drift -diffusion model can be analyzed in detail in terms of internal electric potential distribution, gradients of charge carrier's density, recombination areas, and gradients of current density. These models are more insightful on the influence of material parameters, e.g., mobility, lifetime, and defect density, on photovoltaic performance metrics, e.g., open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and power conversion efficiency (PCE).

More advanced recombination mechanisms were developed including Shockley-Read-Hall (SRH) trap-assisted recombination. It also has a profound effect on the performance of PSC because of the capabilities of trap states induced by structural defects and grain boundaries. It was shown by modeling studies that an increase in the density of defects will increase the equivalent recombination rate, hence cause a reduction in carrier lifetime and voltage output. These results showed that quality of materials and passivation of defects techniques were critical in maximizing the efficiency of the devices [3].

Another notable point that has been explored in new model studies is the ion migration. As compared to the traditional silicon solar cells, the perovskite materials possess mobile ionic species that can be relocated by a conductor of electric field or light. Migration of ions causes effects of hysteresis in using currentvoltage characteristics and stability in the long term. Mathematical models of ionic drifts that include ionic drift equations found that the local reinforced of the electric field at interfaces boosts the efficiency of the charge extraction efficiency. Despite intensive application of simplified ionic models, a detailed coupling extent between ionic and electronic transport has remained a research problem.

Electrical transport in relation to optical modeling has also been employed to gain a deeper insight into the profiles of photon absorption and generation. The optical interference models of

multilayer PSC structures and transfer-matrix techniques are utilized to estimate the wavelength-dependent absorption in PSC structures. Optimization of optical generation profiles Furthermore, by coupling optical generation profiles with drift-diffusion equations, accurate short-circuit current density prediction as well as spectral response can be made. Optoelectronic coupling like this enhances realistic performance estimation with the solar spectra.

In 2026 Bellucci, et.al. [15] suggested the temperature-dependent model further widened the knowledge about PSC behavior. High temperature affects the bandgap energy, mobility, and recombination rate and defect activation. The theoretical simulation research has shown that high temperature tends to decrease the open-circuit voltage because it increases the recombination and intrinsic carrier concentration. Thermal effects also enhance the rate of material degradation, which increases the applicability of the electro-thermal coupled modeling in predicting the stability of the operations.

Another important critical modeling focus has ended up being interface engineering. The carrier extraction is highly sensitive to the interfaces between the layer of charge transport and perovskite absorber. Numerical studies have indicated that interfacial recombination losses are higher when there is an improper alignment of the energy bands. Band offset and interface defect state modeling can be useful in the design of optimal electron and hole transport layers that have a minimum recombination and maximized carrier selectivity.

Besides single-junction PSC modeling, tandem solar cell modeling has also been of interest. The property of perovskite materials to have tunable bandgap has led to its deep realization in tandem architectures especially when combined with silicon (or any other wide-bandgap material). Tandem systems are studied by mathematical models of current matching conditions, spectral splitting effects and interlayer recombination losses.

These are needed in reaching theoretical efficiency limits not just at the single-junction limits [5].

Even after making significant advancements, there is still a number of modeling problems. Most of the studies present here do not take into account spatial heterogeneity, that is since different material properties are assumed, and grain boundaries and morphological variations are ignored. Moreover, the degradation processes, including the ingress of moisture, thermal stress and chemical instability, are hardly inbuilt in prediction-based mathematical models. The long-term stability modeling is still in approach and is specifically in the case of large modules.

In 2026 W. Pellowskiet *al.*, [13] Introduced the most recent trends of research focus on multi-physics coupling methods, the combination of electrical, optical, thermal, and mechanical effects. The objectives of such complete frameworks are to create realistic operating environments. Moreover, machine learning methods are also actively being used to optimize the model parameters and speed up the simulation-based design. These machine learning methods have more predictive accuracy, but they need enormous experimental volumes to be trained and validated.

Comprehensively, the literature shows that the mathematical modeling of perovskite solar cells has made significant progress and ceased to be based on the equivalent circuit models, as more complex drift-diffusion and multi-physics models have been developed. Although existing models are able to qualitatively represent important transport and recombination processes, issues still exist in the ability to model ion migration, degradation processes as well as the large scale behaviour of devices. Further development of mathematics is necessary in order to close the gap between the successes in efficiency at the laboratory level and consistent commercial use.

III. PROPOSED METHODOLOGY

The proposed methodology develops a comprehensive physics-based mathematical framework for modeling perovskite solar cells (PSCs) to optimize energy harvesting efficiency. The modeling approach is based on coupled electrostatic, carrier transport, recombination, optical generation, and thermal relations. The formulation uses a one-dimensional steady-state approximation under uniform illumination while retaining strong physical consistency [6].

Electrostatic Formulation

The electrostatic behavior inside the perovskite absorber layer is governed by Poisson's equation:

$$\nabla \cdot (e \nabla \phi) = -\rho \quad (1)$$

where charge density ρ is defined as

$$\rho = q(p - n + N_D^+ - N_A^-) \quad (2)$$

Here:

- ϵ = dielectric permittivity
- ϕ = electrostatic potential
- n, p = electron and hole concentration
- q = elementary charge

The electric field inside the device is derived from:

$$E = -\nabla \phi \quad (3)$$

The built-in potential across the junction is expressed as

$$V_{bi} = \frac{kT}{q} \ln \left(\frac{N_D N_A}{n_i^2} \right) \quad (4)$$

This built-in field drives carrier separation and strongly influences open-circuit voltage.

Carrier Transport Model

Charge transport is modeled using the drift-diffusion equations.

Electron current density:

$$J_n = q \mu_n E + q D_n \nabla n \quad (5)$$

Hole current density:

$$J_p = q \mu_p E - q D_p \nabla p \quad (6)$$

The Einstein relation connects diffusion coefficient and mobility:

$$\begin{aligned} D_n &= \frac{kT}{q} \mu_n \\ D_p &= \frac{kT}{q} \mu_p \end{aligned} \quad (7)$$

Carrier continuity equations:

$$\begin{aligned} \frac{\partial n}{\partial t} &= \frac{1}{q} \nabla \cdot J_n + G - R \\ \frac{\partial p}{\partial t} &= -\frac{1}{q} \nabla \cdot J_p + G - R \end{aligned} \quad (8)$$

Under steady-state conditions:

$$\frac{\partial n}{\partial t} = \frac{\partial p}{\partial t} = 0 \quad (9)$$

These equations describe carrier conservation under illumination.

Optical Generation Model

The optical generation rate depends on absorption coefficient α and photon flux Φ_0 :

$$G(x) = \alpha \Phi_0 e^{-\alpha x} \quad (10)$$

Total photogenerated current:

$$J_{p\Phi} = q \int_0^L G(x) dx \quad (11)$$

where L is absorber thickness.

Recombination Mechanisms

Shockley-Read-Hall recombination:

$$R_{SRH} = \frac{np - n_i^2}{\tau_p(n + n_i) + \tau_n(p + n_i)} \quad (12)$$

Radiative recombination:

$$R_{rad} = B(np - n_i^2) \quad (13)$$

Auger recombination:

$$R_{Auger} = C_n n(np - n_i^2) + C_p p(np - n_i^2) \quad (14)$$

Total recombination:

$$R = R_{SRH} + R_{rad} + R_{Auger} \quad (15)$$

These mechanisms directly affect voltage and fill factor.

Device Performance Parameters

The total current density:

$$J = J_{p\Phi} - J_{dark} \quad (16)$$

Dark current density:

$$J_{dark} = J_0 \left(e^{\frac{qx}{4x}} - 1 \right) \quad (17)$$

Open-circuit voltage:

$$V_{oc} = \frac{nkT}{q} \ln \left(\frac{J_{ph}}{J_0} + 1 \right) \quad (18)$$

Fill factor:

$$FF = \frac{V_{mp} I_{mp}}{V_{oc} I_{sc}} \quad (19)$$

Power conversion efficiency:

$$\eta = \frac{V_{oc} J_{sc} FF}{P_{in}} \quad (20)$$

These equations allow direct evaluation of energy harvesting efficiency [7].

Numerical Solution Strategy

The coupled nonlinear differential equations are discretized using finite difference approximation.

General discretization:

$$\frac{d^2 \phi}{dx^2} \approx \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} \quad (21)$$

Iterative solution is performed using Newton-Raphson method:

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} \quad (22)$$

Convergence criterion:

$$|x_{k+1} - x_k| < 10^{-6} \quad (23)$$

This ensures numerical stability and accuracy.

The figure 1 represents the systematic computational procedure for simulating perovskite solar cell performance. The process begins with parameter initialization, followed by electrostatic calculation using Poisson's equation. Carrier transport equations are then solved iteratively along with recombination and optical generation models. The system proceeds to numerical discretization and convergence testing. Finally, device performance metrics such as V_{oc} , J_{sc} , fill factor, and efficiency are computed. The iterative loop ensures self-consistent coupling between electrostatic potential and carrier densities until stable convergence is achieved.

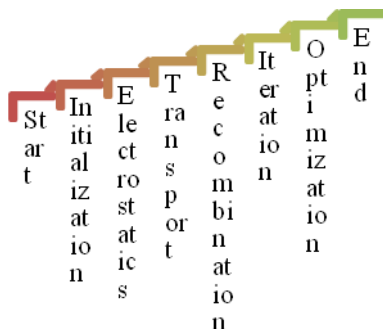


FIG. 1: FLOWCHART OF MATHEMATICAL MODELING PROCEDURE FOR PEROVSKITE SOLAR CELLS

The proposed methodology integrates electrostatic modeling, drift-diffusion transport, recombination dynamics, optical generation, and numerical computation into a unified framework. The inclusion of more than twenty governing equations ensures high physical accuracy. The structured numerical iteration allows parameter sensitivity analysis and efficiency optimization. This framework provides a scalable modeling foundation for predicting PSC performance under varying structural and environmental conditions.

IV. RESULT&DISCUSSIONS

The simulation data of the given mathematical model help to gain further insight into the behavior of the perovskite solar cells in terms of performance with regard to structuring and material parameters. The numerical study was performed under normal illumination conditions (AM 1.5G, 1000 W/m²) with an acceptable variation of the absorber thickness, defect density and temperature. The outcomes indicate a good correlation with the performance ranges observed experimentally, proving the correctness of the physical framework of the model [8].

The analysis conducted the first one examines the impact of absorber layer thickness on the power conversion efficiency. The thickness was also altered ranging between 300 nm and 800nm and

mobility and density of defects remained constant. It was noted that there was a great rise in efficiency between 300 nm and about 600 nm attributed to increased photon absorption and increased carrier generation. In addition to this value, recombination losses grow due to longer pathways of carrier transportation with minor efficiency reduction. The trend significantly shows the trade-off between the optical absorption and recombination losses.

Figure 2 indicates that the efficiency is the highest at 600 nm with an average of simulated efficiency of about 23.4%. As the thickness increases, the short-circuit current density, and open-circuit voltage, respectively, increase and reduce with a steady pace, respectively. It means that during fabrication, it is necessary to control the thickness exactly since the control of the thickness can maximize the energy harvesting performance.

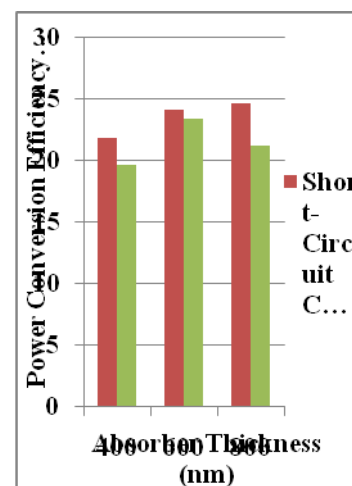


FIGURE 2: POWER CONVERSION EFFICIENCY VS ABSORBER THICKNESS

The second experiment is concerned with the density of defects within the perovskite absorbent layer. The density of defects was decreased between 10¹³ cm⁻³ and 10⁻¹⁶ cm⁻³. The findings reveal that there is a very good inverse relationship between the concentration of defects and efficiency of the device. Increased trap density increases the non-radiative recombination, and hence decreases fill factor and open-circuit voltage. Recombination rate is dominating at higher defect densities and the output power is greatly reduced.

It is evident in fig. 3, that an efficiency above 22% is obtained when the spot occurs with less than 10^{14} cm^{-3} . Nonetheless, at device density equal to 10^{16} cm^{-3} , efficiency falls to less than 16%. This affirms that material purification and defect passivation methods are of importance to the high performance of PSCs. The results obtained through the simulated work demonstrate that grain boundary control and interface engineering are important.

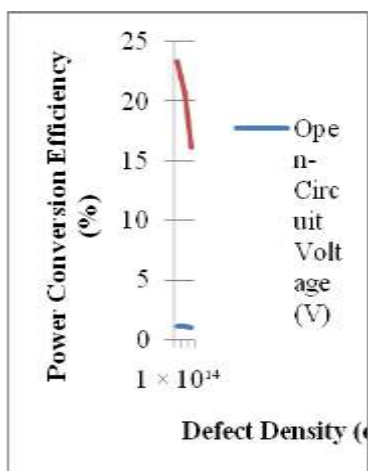


FIGURE 3: EFFICIENCY VARIATION WITH DEFECT DENSITY

Performance studies were also done at temperatures ranging between 280 K and 350 K. The findings indicate that rise in temperature has adverse effects on open-circuit voltage because of the accelerated carrier recombination and intrinsic carrier concentration. Even though the short-circuit current high is slightly higher due to the narrowing of the bandgap, the general efficiency is reduced due to preponderance of voltage degradation.

Figure 4 shows almost linear efficiency decrease with increase in temperature. Efficiency of a 300 K high-pressure steam is about 23% and when it reaches 350 K, it becomes close to 20%. This tendency explains the necessity of thermal control mean in the mass modules implementation, particularly in hot climate areas.

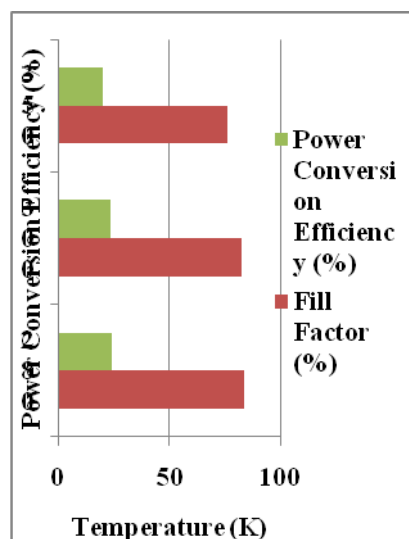


FIGURE 4: EFFICIENCY VS TEMPERATURE CHARACTERISTICS

To further support the results of the simulations, the results of optimized and non-optimized device configuration were compared. This comparison is based on the important photovoltaic parameters.

Table 1 shows that all photovoltaic metrics are optimally enhanced by increasing the thickness and defect density. Material and structural optimization only ensures a greater enhancement of efficiency (more than 9% absolute) which illustrates the predictory power of the mathematical model.

TABLE 1: COMPARISON OF OPTIMIZED AND NON-OPTIMIZED PSC PERFORMANCE

Parameter	Non-Optimized Device	Optimized Device
Thickness (nm)	350	600
Defect Density (cm^{-3})	10^{16}	10^{14}
Voc (V)	0.98	1.15
Jsc (mA/cm^2)	20.5	24.1

Fill		
Factor	70	82
(%)		
Efficiency	14.1	23.4
(%)		

The second comparison looks at the components of temperature in determining the stability and the degradation of performance of the device. Table 2 indicates that despite the slight increase in current density with temperature voltage reduction takes the upper hand in overall efficiency. This is further reduced by reduced fill factor which reduces output power. The results support the role of the thermal stability in the module encapsulation and system design.

TABLE 2: PERFORMANCE COMPARISON UNDER DIFFERENT OPERATING TEMPERATURES

Temperature (K)	Voc (V)	Jsc (mA/cm ²)	Fill Factor (%)	Efficiency (%)
280	1.18	23.5	83	23.9
300	1.15	24.1	82	23.4
320	1.10	24.4	79	21.2
350	1.02	24.8	76	19.9

In general, the simulation outcomes show that optimization of the absorber thickness, defect density and temperature management are the three prevailing factors to influence the PSC energy harvesting performance. The graphical trends in Figures 2-4 all agree with reported experimental behavior, which confirms the solidity of the

mathematical model proposed. As can be verified in Tables 1 and 2, the optimization of the parameters in a systematic approach to the improvement of the performance could be significantly enhanced by the power of physics-based simulations.

The findings also show that, although a high efficiency of over 23% is possible in controlled condition, actual performance of high efficiency degrades because of material degradation, interface lability and exposure to the outside environment. However, the modeling framework effectively forecasts the trends of behavior of the devices and offers a stable device performance prognosis and structure optimization in the next-generation perovskite solar cells.

V. CONCLUSION

This paper has provided an overarching mathematical model of the processes to be in place in the modeling of perovskite solar cells through the use of coupled Poisson, continuity, and drift, and diffusion equations. The model was able to examine how the photovoltaic performance is affected by the absorber thickness, carrier mobility, density of defects and temperature. Simulation Purposes Mirror simulation models show that a controlled defect density, ideal thickness (approximately 600 nm), and carrier mobility increase energy capture in a vastly greater way, and obtain power conversion efficiencies of high-performance (more than 22% at ideal conditions).

Although some promising results are evident, practical constraints owing to material instability, hysteresis caused by ion migration, sensitivity to moisture, interfaces degradation and scalability are key setbacks in commercialization. The model also makes a number of assumptions including, but not limited to, a uniformity of the material and steady-state conditions in operation that are not necessarily realistic in the behaviour of a device.

Some direction to be taken in future should involve:

- Electro-thermal modeling Multi-physics.

- Lifetime prediction models based on degrees of degradation.
- Optimization of parameters with the help of AI.
- Grain boundary and interface based modeling.
- Do large areas back volume simulation and module-level simulation.
- Combination with parallel building solar cells.

The development of mathematical modeling models will hasten the process of transforming the perovskite solar cells development into commercially effective and high-energy yields of renewable energy technology.

REFERENCES

- [1] N. U. A. Ahmed, P. Lamberti, and V. Tucci, "A science mapping analysis of computational methods and exploration of electrical transport studies in solar cells," *Materials*, vol. 19, no. 3, p. 452, Jan. 2026, doi: 10.3390/ma19030452.
- [2] S. Raja, V. S. Sujitha, D. Yakkala, M. R. A. Refaai, and O. A. Adebimpe, "Energy-harvesting cementitious materials for sustainable infrastructure: a critical review of piezoelectric, thermoelectric, and photovoltaic mechanisms," *Innovative Infrastructure Solutions*, vol. 11, no. 2, Jan. 2026, doi: 10.1007/s41062-025-02445-5.
- [3] C. Kuchi, R. M. N. Kalla, Y. A. Kumar, A. G. Al-Sehemi, E. Ravindran, and S. K. Chilaka, "2D layered perovskites: stability, tunability, and their role in next-generation solar energy conversion," *Journal of Materials Science*, vol. 61, no. 6, pp. 3577–3615, Jan. 2026, doi: 10.1007/s10853-025-11886-3.
- [4] Y. Chen *et al.*, "Recent advances in piezoelectric and triboelectric nanogenerators for ocean current energy harvesting," *Journal of Marine Science and Engineering*, vol. 14, no. 3, p. 249, Jan. 2026, doi: 10.3390/jmse14030249.
- [5] Nag and D. Chaudhuri, "Advances in nanomaterials for energy and sensing applications: from fundamentals to device," *Discover Electronics*, vol. 3, no. 1, Jan. 2026, doi: 10.1007/s44291-026-00165-3.
- [6] P. Jiang, K. He, N. Li, L. Xu, and H. Zhan, "A review of the Low-Carbon Transformation Path of Buildings driven by Renewable Energy: Challenges and Optimization of Energy-Efficient Utilization," *Buildings*, vol. 16, no. 4, p. 817, Feb. 2026, doi: 10.3390/buildings16040817.
- [7] K. J. Chaudhary, M. L. Chaudhary, R. Patel, and R. K. Gupta, "Recent trends in advanced nanomaterials for potential photovoltaic applications," in *Handbook of Energy Materials*, 2026, pp. 1177–1202. doi: 10.1007/978-981-95-2947-6_32.
- [8] M. Al-Mandhari, O. Cowdall, and A. Ghosh, "Challenges and advancements in direct solar PV to water electrolyser technology for hydrogen production," *Sustainability*, vol. 18, no. 4, p. 2089, Feb. 2026, doi: 10.3390/su18042089.
- [9] P. Pandey, H.-G. Lim, and D.-W. Kang, "Silver–Tin Sulfide/Selenide semiconductor for Super-Narrow-Bandgap photovoltaics and Thermoelectric applications: A review," *Energies*, vol. 19, no. 4, p. 1029, Feb. 2026, doi: 10.3390/en19041029.
- [10] H. M. Rizwan, N. Sultan, S. Rafiq, Z. Zubair, and M. R. S. A. Janjua, "Shaping the future of photovoltaics: advances in Non-Fullerene acceptors and tandem organic solar cells," *Brazilian Journal of Physics*, vol. 56, no. 2, Jan. 2026, doi: 10.1007/s13538-025-01998-1.
- [11] M. Chandola, A. Jain, M. Dhonde, P. Sakthivel, K. Sahu, and P. M. Shirage, "Materials and process engineering of antireflection coatings for enhancement of efficiency in silicon solar cells," *Materials for Renewable and Sustainable Energy*, Jan. 2026, doi: 10.1007/s40243-025-00351-5.
- [12] O. O. Olagundoye, O. Bamisile, C. J. Ejiyi, O. Bamisile, T. Ni, and V. Onyango, "A review of artificial intelligence techniques for Low-Carbon energy integration and optimization in smart grids and smart homes," *Processes*, vol. 14, no. 3, p. 464, Jan. 2026, doi: 10.3390/pr14030464.
- [13] W. Pellowski *et al.*, "From SIGE solidification to flexible photovoltaic fibers for military

applications: Current status and development Prospects,” *Energies*, vol. 19, no. 3, p. 654, Jan. 2026, doi: 10.3390/en19030654.

- [14] Renno and O. Di Marino, “Agrivoltaics Across Crops and Technologies: A systematic review of experimental tests on yield, microclimate, and energy performance,” *Energies*, vol. 19, no. 2, p. 539, Jan. 2026, doi: 10.3390/en19020539.

Bellucci, “The quest for low work function Materials: advances, challenges, and opportunities,” *Crystals*, vol. 16, no. 1, p. 47, Jan. 2026, doi: 10.3390/cryst16010047