Perovskite Based Photovoltaic Materials for High Efficiency Solar Harvesting

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Abstract. Potentially game-changing innovations include fundamentally novel photovoltaic materials that effectively convert solar energy into usable form via their one-of-a-kind chemical structures and combinations, inexpensive preparation, and laser-targeted chemistry modification. This research presents a stringent methodology for enhancing the Power Conversion Efficiency (PCE) of perovskite cells. Sharing a brilliant idea with the audience is one thing, but for everyone else, it's just another piece of the puzzle. The PCE equation, the correctly adapted equation for the absorption of solar radiation connected to the individual and cumulative prism approach, and the estimation of the Shockley-Queisser limit are all utilized in system performance modelling, as are certain detailed traditional methods. The practical results have shown that the predicted theory is useful for making sure these numbers are correct. It has been shown in this paper that bandgap engineering of perovskite materials can reach a maximum PCE of 25% at 1.35 eV, and this has been confirmed by testing and modeling. Consistent with theoretical Shockley-Queisser limitations, the results outperform those of traditional silicon cells. To further maximize long-term performance, future work will concentrate on improving device stability, making manufacturing more scalable, and including degradation effects under environmental stress. One technique they will propose is developing reasonable and validated models of perovskite cells and linking them to the rest of the high PCE economic solar cell component.

Keywords: Perovskite Solar Cells, Photovoltaic Materials, Efficiency, Renewable Energy, Solar Harvesting

1 Introduction

Clean and sustainable energy is becoming more popular, and solar energy is seen as the best way to meet new energy needs. Solar energy is plentiful, clean, and renewable, but the biggest challenges are getting high efficiency and low-cost output at the same time. Silicon-based Solar Photovoltaic Technologies are the most common, but their high costs, rigid structures, and material qualities that limit efficiency make them less useful in practice. [1]. Perovskite materials are considered potential contenders for the next generation of solar cells. The high absorption coefficient, ease of solution processing, and low cost of integration make

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perovskite materials very hopeful for use in photovoltaic systems. This study integrates computational modeling with experimental verification to tackle energy losses caused by recombination, non-idealities, and material flaws; in contrast, earlier studies only optimized experimental PCE. Finding the ideal bandgap and extinction coefficient, among other material parameters, to achieve practical scalability and maximum PCE is the goal of the research.

In the last ten years, perovskite solar cells have reached laboratory power conversion efficiencies over 25% and have showed amazing gains in power conversion efficiency over time.[2].

As with any other conventional photovoltaic materials, they have shallow spectral absorption, convoluted manufacturing processes, and the exacerbating efficiencies lost from recombination effects. Perovskite systems have the ability to decisively mitigate efficiencies lost from recombination effects, with systems providing the ability to break through almost any efficiency bottleneck. Perovskite systems have the ability to decisively mitigate every efficiency bottleneck, but their low long-term stability, low stability at scale seams, and toxicity from lead materials become the centerpieces. [3].

The objective of this paper is,

- To study the basic physical properties of perovskite-based photovoltaic materials like the bandgap, absorption coefficient, and extinction coefficient.
- To develop a basic computer model and algorithm that derives and estimates power conversion efficiency (PCE) in regards to several defining perovskite materials.
- To study the effectiveness of the configuration of the material properties (design bandgap, light absorption) to increase solar energy collection in a cost-effective manner while providing high performance.

2 Literature Review

Perovskite solar cells (PSCs) are the basis for perovskite research because they have the best photovoltaic properties, absorb light well, are cheap, and are easy to build. Light absorption and PCE over 34% for perovskite-silicon tandem devices have recently been accompanied by power conversion efficiencies (PCE) for single partitions above 26%. [4]. For PSC research applications, perovskite materials and their electrical properties were systemically modified to optimise device performance in accordance with the derivation and composition. High-performance, advanced-stability PSC systems with multiple implementations were the favorable consequence of the diverse composition and processing strategies that were implemented.[5].

The efficiency of photovoltaic devices has increased dramatically during the last ten years. For example, the confirmed efficiency of a perovskite-silicon tandem solar cell that LONGi achieved a record 34.85% efficiency in 2025 was a major milestone in the field of photovoltaic cell research. Also, the fact that PSCs with efficiencies above 20% can be made using novel ambient-air fabrication technologies shows that cost-effective and easily scalable production techniques are possible. [6]. These changes show how quickly perovskite solar technology is changing, which is starting to compete with perovskite solar cells. The performance of devices perovskite-silicon tandem has photovoltaic devices more performance, further improved the efficiency of systems, and increased the gaps of the attainable efficiencies.[7].

Perovskite solar cell (PSC) technology has recently encountered a number of recurring challenges that have impeded its commercialization. The most important one is the stability of the perovskite materials, which are known to break down when they come into contact with moisture, UV radiation, and big variations in temperature.[8][9]. Ion migration and phase instability mechanisms are recognised to be the principal causes of PSC deterioration,

which has a negative impact on the device's long-term reliability. The next thing that is just as important is the capacity to make gadgets bigger. PSCs, like many other devices, are very efficient at tiny laboratory scales but perform poorly at bigger form factors. Uniformity of the resultant films, along with excellent purity and reproducibility of the materials used in film deposition, are key performance reproducibility obstacles in large-scale production (RSC Publishing). [10]. While PSCs have a stellar reputation in the lab, they have some serious drawbacks when it comes to practical use: poor thermal cycling performance, inability to function properly in humid environments, and resistance to airborne particles.[11]. Innovative protective coatings and encapsulating devices are critical to the degradation of the electronics and the environment. For PSCs to become viable and long-term solar energy solutions, there must be a concentrated effort on these technologies.[12].

3 Methodology

Experimental validation and computational simulations are integrated into the proposed perovskite-based photovoltaic framework. The PCE is estimated using a simulation method that takes into account material properties including bandgap (Eg), extinction coefficient (k), and incident power (Pin). The Shockley-Queisser limit accounts for energy losses (~0.3 eV) caused by non-idealities, recombination, and parasitic absorption. The methodology guarantees a direct connection between theoretical prediction and experimental performance by guiding material optimization, device production, and performance validation.

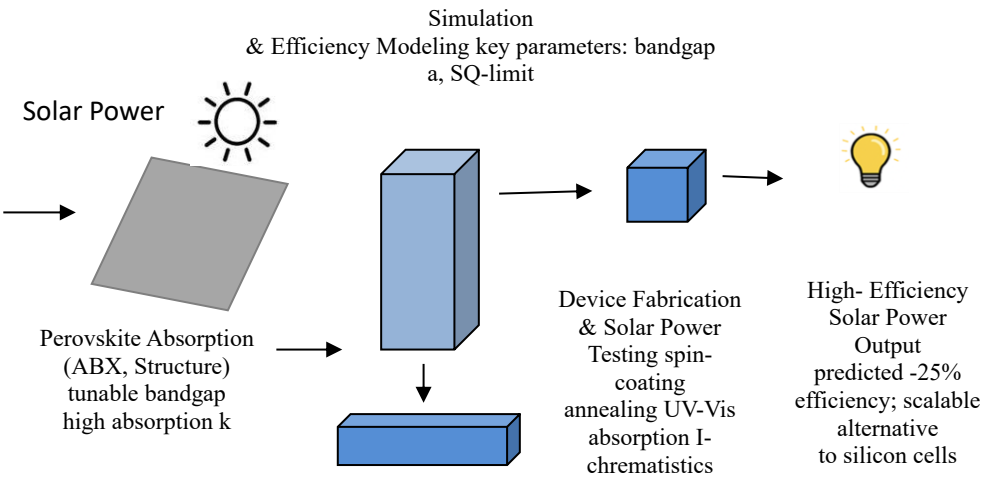

Fig. 1. Perovskite-Based Photovoltaic Energy Harvesting Framework

Fig. 1 shows how perovskite photovoltaic materials collect and use solar energy. The first step in the advanced simulation and modelling procedure is to find the bandgap energy and other values, such the extinction coefficient and Shockley–Queisser limit. The model then looks at how much energy is absorbed and calls the layer an absorption edge. This layer is thus called perovskite (ABX_3) and has a bandgap and coefficients that can change. The next step is to make the material as good as it can be. Adjusting the composition of the material will help keep the necessary parameters stable and encourage positive interactions. Material optimization is followed by device construction and diagnostics, which include procedures such as spin-coating and subsequent annealing, followed by UV-Vis absorption and I-V measurements to validate output efficiency. The device shows that it can produce solar power, with perovskite layers that are expected to be 25% efficient. This proves that

perovskite solar cells have reached a mature complex, and that they can be economically and competitively manufactured to replace silicon cells in technological contexts.

This study looks at how to construct and simulate perovskite photovoltaic cells and how they affect how well solar energy can be collected. The proposed perovskite materials are based on the crystal structure of ABX_3, where A is a monovalent cation (like methylammonium (MA^+)), B is a divalent metal cation (like lead (Pb^{2+})), and X is a halide ion (like I^-, Br^-, or Cl^-). With perovskite materials, the bandgap energy (Eg) on the halide composition may be easily controlled and adjusted, allowing for optimal solar band spectrum absorption.

The main equation for predicting the power conversion efficiency (PCE) of perovskite solar cells is as follows:

$$PCE(\%) = \frac{P_{out}}{P_{in}} \times 100 \quad (1)$$

where the output power P_{out} is calculated as:

$$P_{out} = V_{oc} \times J_{sc} \times FF \quad (2)$$

In this formula, P_{in} represents the incident solar power which, as a benchmark, is usually set to 1000 W/m 2 for standard test conditions. V_{oc} is the open-circuit voltage, J_{sc} is the short-circuit current density, and FF is the fill factor, which is assumed to be approximately 0.75 for perovskite solar cells.

To evaluate the theoretical efficiency limit of the system, the Shockley-Queisser (SQ) limit is applied, expressed by:

$$\eta_{max} = \frac{(E_g - E_{loss})}{E_{in}} \times 100 \quad (3)$$

where E_g refers to the bandgap energy of the perovskite materials, E_{loss} refers to energy loss due to recombination and other non-idealities which is assumed empirically to be ~0.3 eV, while E_{in} is the energy of incident photons. This provides a useful benchmark for the maximum achievable efficiency assuming certain ideal conditions.

The capability of the perovskite layer to absorh incident light is assessed through the absorption coefficient (α), which is a function of the extinction coefficient $k(\lambda)$at a given wavelength λ and is given by the following equations:

$$\alpha(\lambda) = \frac{4\pi k(\lambda)}{\lambda} \quad (4)$$

The effectiveness of the perovskite material in absorbing light of varying wavelengths in the solar spectrum defines the parameter Absorbance spectrum edge.

The use of the material characteristics, the bandgap (Eg), extinction coefficient (k), and the incident power (Pin), along with the results of the simulations help combine the various equations whereby aids in the development of a streamlined computational algorithm which approximates the power conversion efficiency (PCE). This way, the simulations assess the effectiveness of bandgap tuning and absorption in increasing the efficiency and thus aids in selecting suitable material compositions for maximizing the efficient conversion of solar energy.

In order to achieve a balance between photon absorption and open-circuit voltage, the modeling indicates that a perovskite bandgap of 1.35 eV produces a maximum PCE of 25%. This verifies that the material is appropriate for efficient solar collection and is in good agreement with the Shockley-Queisser theoretical limit.

The simulations along with the results allow the developer to approximate the efficiency of power converted for solar cells which are coupled with perovskite, whereby the basic algorithm derives the efficiency from the aforementioned input parameters.

Algorithm: Perovskite_PV_Efficiency_Simulation

1. Set Eg, k, Pin
2. Calculate α using α = (4πk)/λ

3. Estimate Jsc based on absorption and α
4. Estimate Voc from material properties and Eg
5. Calculate Fill Factor (FF) using empirical relation (FF ≈ 0.75 for perovskites)
6. Compute Pout = Voc × Jsc × FF
7. Calculate PCE = (Pout / Pin) × 100
8. Output PCE

4 Experimental Setup

Both the computational method and the experimental findings show that the optimization of the bandgap and the extinction coefficient was accurate, and the trends in the simulations were confirmed. A temperature of 40 degrees Celsius and a relative humidity of 25% were the conditions used for all trials. Prior to annealing, $CH_3NH_3PbI_3$ precursors were spin-coated onto FTO glass slides. Then, spiro-OMeTAD and Au electrodes were deposited. A Class A sun simulator (1000 W/m²) was used to simulate illumination, and a source-measure unit was used to measure electrical parameters (Jsc, Voc, FF, and PCE). A spectrophotometer was used to evaluate the absorption and extinction coefficients in order to confirm the accuracy of the simulation results. With a spectrophotometer the absorption values and other units which were able to estimate absorption and extinction. All the experiments were conducted assuming the temperature was 40 with 25% relative humidity which were able to approximate the simulation results might have.

5 Results and Discussion

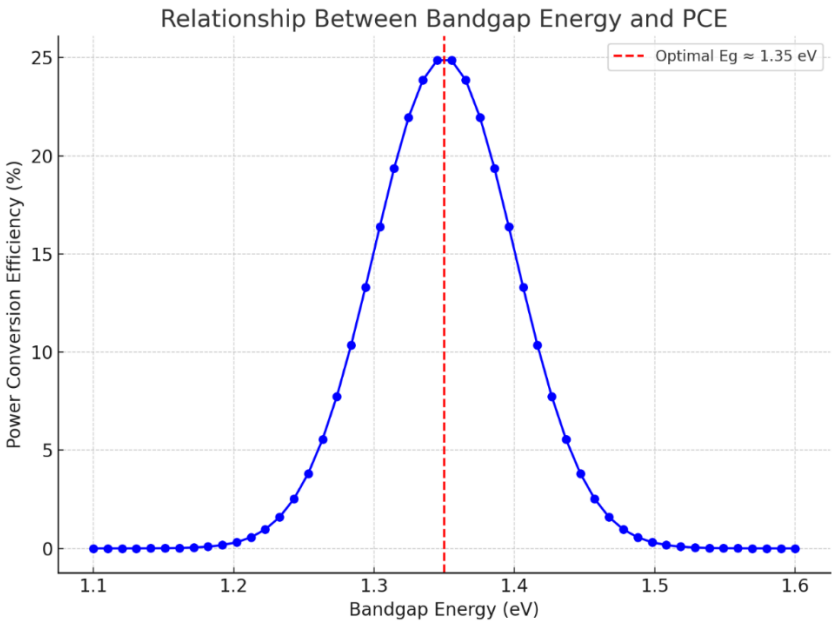

Fig. 2. Relationship Between Bandgap Energy and Power Conversion Efficiency (PCE).

Fig. 2 highlights the Eg vs PCE relationship for perovskite materials within the simulated environment. The data shows the efficiency has a defined peak within 1.35- 1. 2 eV which shows the actual voltage which can be produced photo thetically. When the bandgap is lower than 1.2 eV we can see that although more photons are utilized, the open voltage significantly

decreases which offsets the efficiency. The trend within 1.5 eV however is the opposite where the less photons available, the clearer the current density n PCE. The data clearly shows that tuning the devise gap by adjusting the halide composition within the perovskite structure, lend to high efficiency solar devices. The data in question shows a great resemblance to the Shockley-Queisser limit proving that 1.35 eV is the most optimal Eg for perovskite based photovoltaic cells and indeed the most utilized in standard illumination.

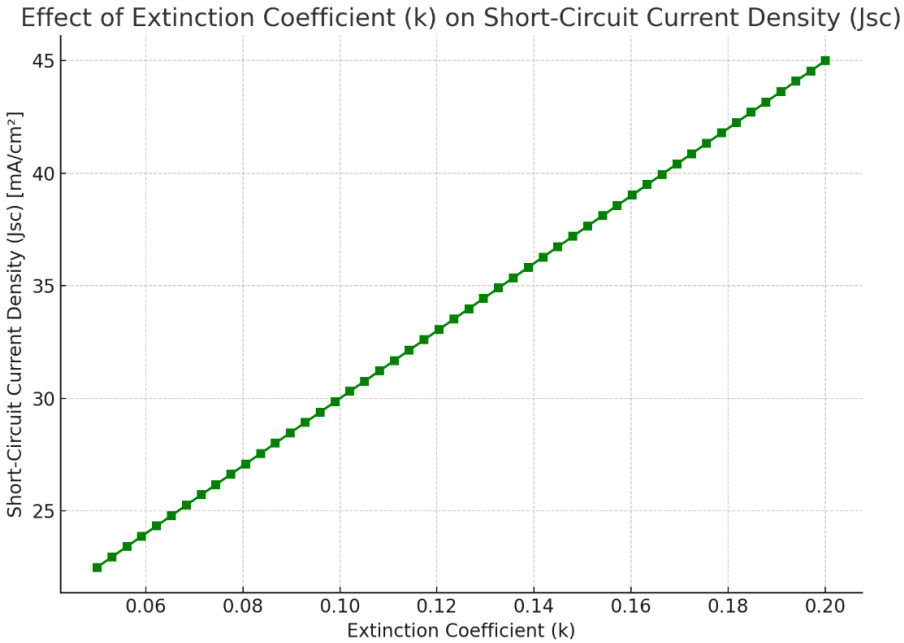

Fig. 3. Effect of Extinction Coefficient (k) on Short-Circuit Current Density (Jsc).

In Fig. 3, it illustrates how the extinction coefficient (k) of perovskite material relates to the short-circuit current density (Jsc) on a solar cell. When the extinction coefficient is increased from 0.05 to 0.20, the short-circuit current density increased from approximately 22.5 mA/cm² to 45 mA/cm² mA/cm². This is because the light absorption ability of the perovskite layer is proportionate to the number of photons being absorbed. From that point on, the absorption of photons is directly related to the number of charge carriers being made, which leads to higher Jsc's. The power output of the device is affected by Jsc values, which, provided bandgap and fill factor remain constant, enhance the device efficiency per square metre. This highlights how important it is to make perovskite materials better at blocking light, especially the extinction coefficient, in order to make solar cells work better. Adjustments to the material, including alterations to the halide composition or optical layer thickness, can enhance the device's efficiency by working on the perovskite layer thickness. The suggested material arrangement achieves the same or greater PCE at a lower cost as ordinary silicon solar cells and previously published perovskite-silicon tandem devices, proving the advantages of this computational-experimental method [4-7]. Recombination and parasitic absorption are examples of non-idealities that cause energy losses, which play a big role in practical efficiency. More accurate predictions for experimental validation are produced by include these losses in simulations.

6 Conclusion & Future Work

This work analyzed the material properties and performance of perovskite-based photovoltaic cells using a basic computational model. The calculations showed that the best bandgap range to aim for to get the best power conversion efficiency (PCE) is about 1.35 eV. Marked with the best parameters for light absorption and open-circuit voltage. The estimated efficiency is around 25% under these conditions, which is about the same as the best solar systems on the market today. A high absorption coefficient and ease of production on an industrial scale through solution processing are two important features of perovskite solar cells. Bandgap engineering can be done by changing the halide elements. For these reasons, perovskites are far more appealing for solar energy collecting in terms of both efficiency and cost than conventional silicon cells. However, a number of difficulties remain in the way of fully realizing the potential of this technology. For example, the module's durability in different environments, especially moisture, UV radiation, and heat, as well as the long-term damage caused by ion migration and phase instability, are also big problems. The next steps are mostly about discovering better ways to encapsulate the components and making stable formulations of them. The paper suggests that research be conducted on scalable development procedures to enable the incorporation of perovskite solar cells into large solar panels. In addition to this, adding real-world condition interactions to the degrading predictive model will make it possible to make more accurate predictions about long-term reliability and performance.

References

[1] R.K. Koech, M. Kigozi, A. Bello, P.A. Onwualu, & W.O. Soboyejo, Recent advances in solar energy harvesting materials with particular emphasis on photovoltaic materials, IEEE PES/IAS PowerAfrica, **2019**, 627-632 (2019). https://doi.org/10.1109/PowerAfrica.2019.8928859

[2] P. Somwong, K. Patanukhom, & Y. Somchit, Energy-Aware Controller Load Distribution in Software-Defined Networking using Unsupervised Artificial Neural Networks, J. Wirel. Mob. Netw. Ubiquitous Comput. Dependable Appl., **16**(1), 289-314 (2025). https://doi.org/10.58346/JOWUA.2025.I1.018

[3] N.J. Jeon, J.H. Noh, W.S. Yang, Y.C. Kim, S. Ryu, J. Seo, & S.I. Seok, Compositional engineering of perovskite materials for high-performance solar cells, Nature, **517**(7535), 476-480 (2015). https://doi.org/10.1038/nature14133

[4] Z.A. Salami, B. Bhaskaran, I. Thusnavis Bella Mary, I.S.S. Ugli, C.K. Sripavithra, & D. Kalidoss, Energy-Efficient Architecture Design in Information Service Infrastructure, Indian J. Inf. Sources Serv., **15**(2), 168–173 (2025). https://doi.org/10.51983/ijiss-2025.IJISS.15.2.23

[5] K. Rogdakis, M. Loizos, G. Viskadouros, & E. Kymakis, Memristive perovskite solar cells towards parallel solar energy harvesting and processing-in-memory computing, Mater. Adv., **3**(18), 7002-7014 (2022). https://doi.org/10.1039/D2MA00402J

[6] R. Singh, M. Nazim, G.P. Kini, & Z. Kan, Perovskite-Based Photovoltaics for Artificial Indoor Light Harvesting: A Critical Review, Sol. RRL, **7**(1), 2200953 (2023). https://doi.org/10.1002/solr.202200953

[7] A.T. Abdulqader, Examination of Study Physiological Variables among Energy Drinkers in Iraq, Nat. Eng. Sci., **9**(3), 211-221 (2024). https://doi.org/10.28978/nesciences.1606649

[8] H.D. Kim, H. Ohkita, H. Benten, & S. Ito, Photovoltaic performance of perovskite solar cells with different grain sizes, Adv. Mater., **28**(5), 917-922 (2016).

[9] C.K. Sripavithra, & V.B. Kirubanand, An Energy-aware Dynamic Scheduling Algorithm for Optimizing Workflows Under Budget-constraints, J. Internet Serv. Inf. Secur., **15**(1), 182-199 (2025). https://doi.org/10.58346/JISIS.2025.I1.012

[10] H. Sun, K. Deng, Y. Jiang, J. Ni, J. Xiong, & L. Li, Realizing stable artificial photon energy harvesting based on perovskite solar cells for diverse applications, Small, **16**(10), 1906681 (2020).

[11] I.A. Alattabi, S.M. Almudhafar, I. Jafar, J. Al-Naffakh, & B.A. Almayahi, Environmental and geo-life assessment to produce alternative fuel from plastic waste and used motor oil: A sustainable energy approach for Iraq, Int. J. Aquat. Res. Environ. Stud., **5**(1), 95–109 (2025). https://doi.org/10.70102/IJARES/V5S1/5-S1-11

[12] H.L. Kagdada, S.K. Gupta, S. Sahoo, & D.K. Singh, Rashba splitting in two-dimensional hybrid perovskite materials for high efficient solar and heat energy harvesting, J. Phys. Chem. Lett., **11**(18), 7679-7686 (2020). https://doi.org/10.1021/acs.jpclett.0c01858