



Numerical Investigation of Transport Layer Engineering in BaCd₂P₂-Based Thin-Film Heterojunction Solar Cells Using SCAPS-1D

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Bachelor of Science in Electrical and Electronic Engineering

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DECLARATION

This Final year Capstone Project report is submitted to the department of Electrical and Electronic Engineering, University of Liberal Arts Bangladesh in partial fulfillment of the requirements for the degree of Bachelor of Science. So, we hereby, declare that this report is based on the work done by us. Materials of work found by other researchers are mentioned by reference. This project report, neither in whole, nor in part, has been previously submitted for any degree.

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SUPERVISOR'S CERTIFICATION / APPROVAL

The Final year Capstone Project report entitled “Numerical Investigation of Transport Layer Engineering in BaCd₂P₂-Based Thin-Film Heterojunction Solar Cells Using SCAPS-1D” is submitted to the department of Electrical and Electronic Engineering, University of Liberal Arts Bangladesh, Dhaka in partial fulfillment of the requirements for the degree of Bachelor of Science.

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Abstract

Thin-film heterojunction solar cells based on emerging absorber materials are promising candidates for next-generation photovoltaic applications. This study presents a numerical investigation of BaCd₂P₂-based thin-film heterojunction solar cells using the SCAPS-1D simulation platform, focusing on the impact of different electron transport layer (ETL) and hole transport layer (HTL) combinations while keeping the absorber, transparent conducting oxide, and metal contacts identical to a reference structure. Multiple ETL–HTL pairings are systematically evaluated in terms of Voc, Jsc, FF, and PCE, revealing that Jsc remains nearly constant due to fixed optical conditions, whereas Voc and FF are highly sensitive to transport-layer selection and interface quality. Initial unoptimized configurations exhibit reduced efficiency due to high interface recombination and poor carrier transport. After systematic optimization, the SnO₂/NiOx heterojunction achieves the highest power conversion efficiency of **28.72%**, outperforming the baseline ZnO/Cu₂O device. The improvement is attributed to favorable energy band alignment and reduced interfacial recombination, demonstrating the effectiveness of transport-layer engineering and numerical simulation for optimizing BaCd₂P₂-based heterojunction solar cells.

Keywords: Thin-film heterojunction solar cells; BaCd₂P₂; Transport-layer engineering (ETL and HTL); Interface recombination; SCAPS-1D; Power conversion efficiency (PCE)

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Chapter 1: Introduction

1.1 Background

Energy demand and supply form the backbone of modern economic development, with global energy systems undergoing profound transformation driven by technological advances, environmental imperatives, and socio-economic growth trajectories. Traditional energy systems have historically been dominated by fossil fuels such as coal, oil, and natural gas, owing to their established infrastructure, energy density, and historical economic centrality. However, concerns over climate change, greenhouse gas emissions, and long-term energy security have accelerated efforts to decarbonize energy systems and transition toward sustainable sources such as solar, wind, hydroelectric, and other renewable technologies. Recent data indicate that **renewable and zero-carbon sources accounted for over 40% of global electricity generation**, driven by rapid expansion in solar and wind capacity, even as fossil fuels continue to play a significant role in meeting overall energy demand. [15]

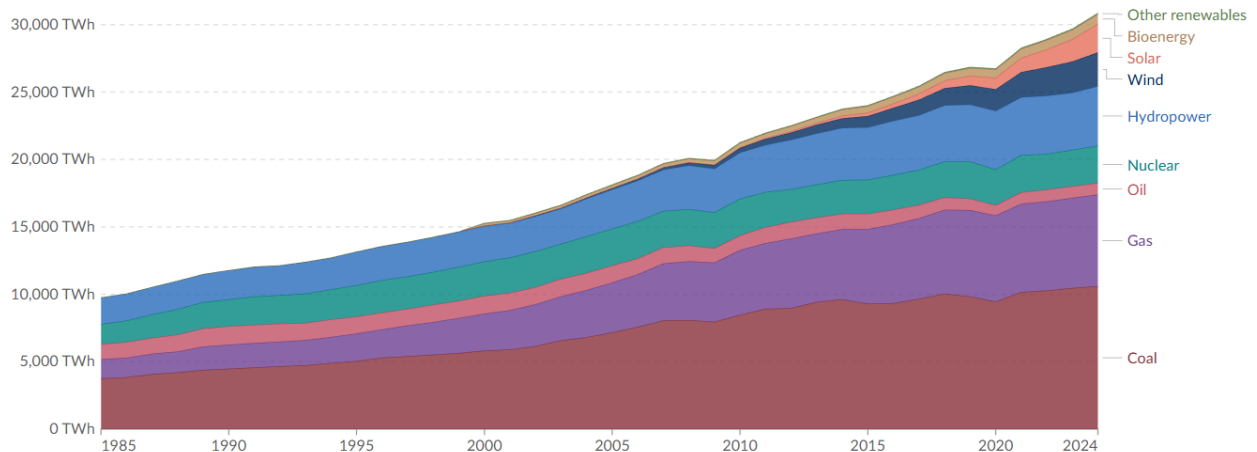


Figure 1.1: Total global electricity generation (1985 - 2024)

Within this broader energy transition, **solar photovoltaic (PV)** technology has become a central focus of clean energy research and large-scale deployment. Solar cell technologies have transformed the way solar energy is harnessed, providing a sustainable and environmentally friendly alternative to fossil fuel-based power generation. Continuous advancements in this field have led to notable improvements in conversion efficiency, cost reduction, and long-term stability. Solar cells operate on the photovoltaic effect, a process through which incident sunlight is directly converted into electrical energy. Several solar cell technologies are currently in use, including crystalline silicon, thin-film systems, and emerging solutions such as perovskite-based solar cells. Each category presents distinct advantages and challenges, which

determine its suitability for specific applications. Ongoing research and development efforts are focused on further enhancing efficiency, lowering manufacturing costs, and extending device lifetimes to support the widespread integration of solar energy into national power systems.[15]

1.1.1 Energy Generation Disparities in Bangladesh

At the national level, countries are at varied stages of renewable adoption. In Bangladesh, electricity generation remains heavily reliant on **fossil fuel resources**, particularly natural gas and coal, which together comprise the overwhelming majority of the current generation mix. Estimates indicate that **fossil fuels account for over 80–97%** of electricity generation, with natural gas often cited as the single largest contributor. Renewable energy sources such as solar, wind, and hydroelectric power, constitute a small fraction of total generation, with solar PV contributing only a **low single-digit percentage** of the national mix. Despite this, the Government of Bangladesh has articulated goals to expand renewable capacity through policy mechanisms and institutional frameworks such as the Sustainable and Renewable Energy Development Authority (SREDA), reflecting an intent to diversify the energy mix and reduce carbon intensity over the medium to long term.[16]

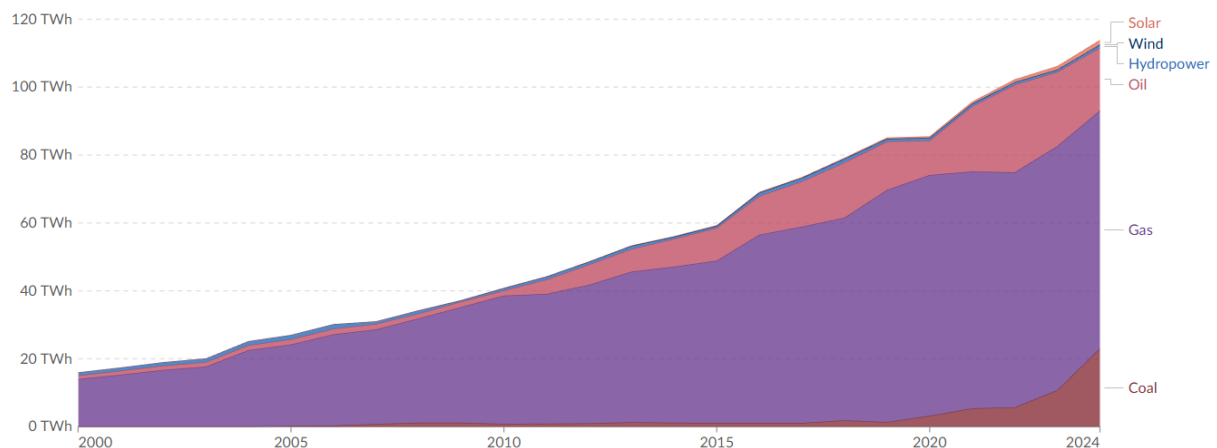


Figure 1.2: Total electricity production in Bangladesh (2000 - 2024) measured in terawatt-hours

2006 in terawatt-hours		2024 in terawatt-hours	
Other renewables	0.00 TWh	Other renewables	0.00 TWh
Bioenergy	0.00 TWh	Bioenergy	0.00 TWh
Solar	0.01 TWh	Solar	1.42 TWh
Wind	0.00 TWh	Wind	0.00 TWh
Hydropower	1.38 TWh	Hydropower	0.89 TWh
Nuclear	0.00 TWh	Nuclear	0.00 TWh
Oil	1.64 TWh	Oil	18.53 TWh
Gas	26.85 TWh	Gas	70.07 TWh
Coal	0.28 TWh	Coal	22.95 TWh
Total	30.16 TWh	Total	113.86 TWh

Figure 1.3: Energy generation by source in Bangladesh in 2006 and 2024 (TWh)

In 2006, solar energy contributed only 0.01 TWh to the total electricity generation of 30.16 TWh, accounting for approximately **0.03%** of the overall energy mix, which highlights its negligible role at the time. By contrast, in 2024, solar power generation increased substantially to 1.42 TWh out of a total 113.86 TWh, representing about **1.25%** of total electricity production. This marked growth reflects the increasing adoption of solar photovoltaic technology over the years; however, despite this progress, solar energy still constitutes a relatively small portion of the national energy portfolio, indicating significant potential for further expansion. Electrical energy demand in Bangladesh continues to grow in tandem with economic expansion, urbanization, and industrialization. However, the persistent dominance of conventional thermal generation underscores structural challenges, including vulnerability to fossil fuel supply volatility, carbon emissions, and limited resilience against climate-related risks. These dynamics underscore the strategic importance of diversifying generation portfolios and advancing technologies that can contribute to **high-efficiency, low-carbon energy solutions**. [16][17]

1.1.2 Ongoing Research on Photovoltaic Technology

Research on solar energy is ongoing globally, improving the efficiency, affordability, and long-term reliability of photovoltaic (PV) technologies to support large-scale energy transitions. Significant efforts are being directed toward the development of high-efficiency solar cells, including advanced **crystalline silicon architectures**, **thin-film technologies**, and emerging

materials such as **perovskite** and **tandem solar cells**. Research on perovskite–silicon tandem structures has shown particular promise, achieving record conversion efficiencies by combining the strengths of multiple absorber layers. In parallel, studies are addressing challenges related to material stability, degradation mechanisms, and environmental durability to extend the operational lifetime of solar modules. Manufacturing innovations, such as low-temperature processing and scalable fabrication techniques, are also being explored to reduce production costs. Additionally, global research initiatives emphasize system-level integration, including energy storage, grid compatibility, and recycling of end-of-life modules, to ensure the sustainable and reliable deployment of solar energy within modern power systems.[17][13]

1.1.3 Zintl-phosphide - BaCd_2P_2

Zintl phosphides are an emerging class of semiconducting materials that have gained increasing attention in photovoltaic research due to their favorable optoelectronic properties and **earth-abundant** elemental composition. These compounds, typically formed between electropositive metals and phosphorus, exhibit tunable band gaps, high absorption coefficients, and good carrier transport characteristics, making them promising candidates for solar absorber layers. Recent studies have demonstrated that certain Zintl-phosphides, particularly **BaCd_2P_2** , possess band gaps close to the optimal range for single-junction solar cells, along with defect tolerance that can reduce non-radiative recombination losses. Additionally, their composition avoids the use of scarce or toxic elements commonly found in some thin-film technologies, enhancing their potential for sustainable and scalable solar cell manufacturing. Ongoing research is therefore focused on improving material synthesis, controlling stoichiometry, and optimizing device architectures to fully exploit the photovoltaic potential of Zintl-phosphide-based solar cells.[18]

This project focuses on the **simulation-based performance optimization of BaCd₂P₂ thin-film heterojunction solar cells** using SCAPS-1D, with particular emphasis on the role of **electron and hole transport layers (ETL and HTL)** in determining overall device efficiency.

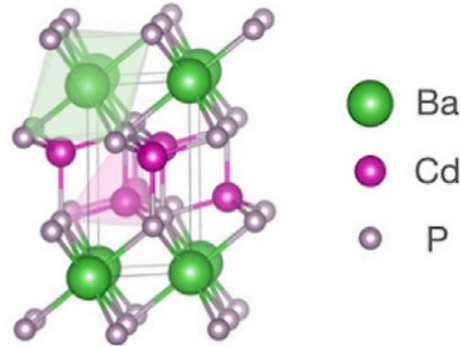


Figure 1.4: Crystal structure of the Zintl phosphide BaCd₂P₂, showing the atomic arrangement of barium (Ba), cadmium (Cd), and phosphorus (P).

1.2 Problem Statement

Despite advances in photovoltaic materials and device architectures, several challenges remain in achieving high-efficiency thin-film heterojunction solar cells:

1. **Efficiency limitation of single-junction solar cells:** Traditional single-junction solar cells are constrained by the Shockley–Queisser limit, which restricts their maximum achievable efficiency due to inherent spectral and thermal losses.
2. **Complexity of heterojunction design variables:** Heterojunction solar cells involve multiple layers with different electronic properties. Optimizing parameters such as layer thickness, band alignment, defect density, and material selection is challenging due to their interdependent effects on device performance.
3. **High cost of experimental trial-and-error:** Fabricating and testing multiple physical device configurations requires significant time, materials, and laboratory resources, making comprehensive exploration of design variables inefficient.
4. **Lack of efficient design-space exploration methods:** Without reliable predictive tools, identifying optimal heterojunction configurations becomes slow and uncertain, particularly for emerging absorber materials such as BaCd₂P₂.

1.3 Motivation

The growing global demand for sustainable and efficient energy solutions has intensified research into advanced solar photovoltaic technologies. While thin-film single-junction solar cells offer advantages such as lower material usage and simpler fabrication, their performance remains constrained by fundamental efficiency limits. Improving device efficiency within these architectures therefore remains a critical research challenge.

Recently, **Zintl-phosphide materials**, particularly **BaCd₂P₂**, have emerged as promising absorber candidates due to their suitable bandgap and long carrier lifetime. However, the efficiency of BaCd₂P₂-based heterojunction solar cells is strongly dependent on device design, especially the selection of appropriate electron and hole transport layers, which directly influence carrier extraction and recombination losses.

Experimental optimization of such devices through physical fabrication is costly and time-consuming, particularly when multiple design variables are involved. **Numerical simulation using SCAPS-1D** provides an efficient and reliable alternative by enabling systematic exploration of heterojunction configurations prior to fabrication.

Motivated by these factors, this project focuses on the simulation-based optimization of **BaCd₂P₂ thin-film heterojunction solar cells**, with the objective of identifying transport layer combinations that maximize power conversion efficiency and support future experimental development.

1.4 Objectives

The primary objectives of this project are:

- To model and simulate BaCd₂P₂-based thin-film heterojunction solar cells using the SCAPS-1D simulation platform
- To systematically investigate the impact of different electron transport layer (ETL) and hole transport layer (HTL) combinations while keeping the absorber and contacts identical to the baseline reference study
- To evaluate device performance in terms of open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE)

- To identify an optimized device configuration that maximizes power conversion efficiency through transport layer selection

Chapter 2: Literature Review and Methodology

This chapter presents a review of existing research relevant to thin-film heterojunction solar cells and outlines the methodological framework adopted in this study. The literature review focuses on the evolution of photovoltaic absorber materials, heterojunction device architectures, and the role of charge transport layers in determining solar cell performance. Particular emphasis is placed on recent studies involving **Zintl-phosphide materials**, especially BaCd_2P_2 , which form the foundation of the present work. The chapter also introduces the simulation methodology used to model and optimize device performance using a numerical solar cell simulator.

In thin-film solar cells, the absorber layer is typically only a few micrometers thick, requiring materials with high absorption coefficients and favorable carrier transport properties. Key performance parameters used to evaluate solar cells include open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE). These parameters are influenced by intrinsic material properties, interface quality, and overall device architecture. Recombination losses, both in the bulk and at interfaces, play a critical role in limiting device performance, particularly in heterojunction configurations.

2.1 Literature review

This paper's main focus is to discuss the limitations in the performance of thin copper indium gallium selenide (CIGS) solar cells due to excessive carrier recombination and low reflection at the electrode/semiconductor boundary. To address this problem, the authors studied the effects of a thin local contact aluminum oxide rear passivation layer ($\text{LC-Al}_2\text{O}_3$) and its thickness with respect to 2D optical and electrical simulation as well as empirical testing on fabricated CIGS solar cells with 10nm and 80nm Al_2O_3 thicknesses. Simulations suggested that efficiency would continue to improve with increasing Al_2O_3 thickness beyond 80nm up until 115-120nm, while experimental results indicated that the 80nm $\text{LC-Al}_2\text{O}_3$ layer did indeed improve efficiency by 4.32% through enhanced open circuit voltage (V_{oc}) and short circuit current density (J_{sc}) due to greater light reflection and lesser recombination, albeit at lower 10nm thickness. In addition, the surrogate data model demonstrated decline in FF and efficiency at this thickness due to rough Mo (Molybdenum) layer scattering and discontinuous

Al_2O_3 coverage without consistent stabilization. In the end, the paper comes to a conclusion that an optimally thin LC- Al_2O_3 near the passivation layer is very much effective for improving the CIGS solar cell's performance but for that to be achievable, the thickness of the layer should be carefully measured to avoid performance degradation. [1]

This paper proposes a design of a solar cell that has an hourglass-shaped silicon nanowire (HG-SiNW), which improves both light trapping and absorption while also reducing the usual bulky designs of solar cells. When compared to the electrical and optical measurements of the cylindrical silicon nanowire solar cells (C-SiNW), the hourglass-shape produced a decent increase in the short-circuit current density and also had a higher efficiency of about 5.26%, which is 1.85 times higher than the cylindrical-shaped one, which had an efficiency of 2.85%. This improvement is mainly caused by the antireflective properties. Following that, a formation of 'whispering gallery modes' (WGM) enclosed in the hourglass-shaped design was seen using optical simulations. This caused the cells to have a greater light absorption and trapping rate. Even though the final efficiency rates were limited due to the defects formed on the surface of the cell and electrode design, the paper emphasized the fact that the hourglass-shaped design has a high potential for significantly improving solar cell performance. [2]

The purpose of this paper is to utilize a layer of photon upconverter to enhance the performance of bulk heterojunction organic solar cells (BHJ OSCs). The past versions of these solar cells suffered from low power conversion efficiency because of its inferior infrared absorption, which is why BHJ OSCs are a good option for an improvement. Using numerical models and optoelectronic simulations, the authors optimized the upconversion process for many materials, predicting remarkable improvements in Power conversion efficiency: P3HT:PCBM 30.8%, PSBTBT:PCBM 24.3%, PBDTTT-C:PCBM 28.9%, and PTB7-Th:PCBM 16.9% when utilizing an upconverter layer with three sensitizers and 50% efficiency. The results showed that the combination of photon upconversion with localized surface plasmon resonance (LSPR) gave less than expected returns and worse performance than theorized. Also, an upconversion enhanced PTB7-Th:PCBM based organic solar cell with optimized nanowires showed a promising power conversion efficiency of 16.40% with 10 sun illumination, which is over 50% improvement from the structure without concentration. In the end, the paper concluded that these types of optimized photon upconversion layers hold a very good chance at enhancing organic solar cell performance. [3]

This paper proposes a nanopillar-structured perovskite-based semitransparent solar cell module, capable enough for power-generating windows. It used anodized aluminum oxide (AAO) designs aimed at making approximately 40.8 cm² vertically aligned nanopillar CH₃NH₃PbI_{3-x}Cl_x perovskite absorber with high geometrical fill factor of about 95.6%. This kind of a structure helped making it easier for a homogeneous morphology formation within the perovskite as well as helped reduce total light reflection. When compared planar devices, the nanopillar-based cell had better electrical characteristics such as high open-circuit voltage (Voc) 1.07 V, fill factor (FF) of about 75.08%, increased charge-collection efficiency, decreased recombination rate, enhanced durability under humid conditions because of anodized aluminum oxide scaffold's hydrophobicity, and improved stability. Through optimized laser etching, a nine sub-cell module achieved 9.04% power conversion efficiency with about 30.2% average visible transmittance, making it a strong candidate for practical power-generating window applications. [4]

In this paper, using the SCAPS-1D software simulations, the overall performance and efficiency of a Ge-doped CH₃NH₃Ge_{0.85}Pb_{0.125}I₃ perovskite solar cell are compared with other materials based on parameters like current density, quantum efficiency, absorption coefficient, and power conversion efficiency, are investigated in the hopes that the optimization of the absorber layer in these perovskite solar cells (PSCs) could be a potential alternative to silicon-based cells. The simulation results indicated that the Ge-doped layer demonstrates superior performance in absorption coefficient, power conversion efficiency, quantum efficiency, short-circuit current density, and open-circuit voltage, suggesting that Ge doping is a promising approach for enhancing the efficiency of perovskite solar cells. [6]

Nanowire (NW) solar cells offer advantages over planar structures, including efficiency enhancement, improved light trapping through nanoscale texturing, and enhanced electrical performance by decoupling light absorption and carrier collection into orthogonal directions, leading to improved carrier collection efficiency due to reduced diffusion length radially. GaAs is a widely studied material for photovoltaics due to its desirable optical and electrical properties, including a direct bandgap that facilitates high light absorption and carrier collection, with reported efficiencies up to 22% for GaAs NW solar cells. Incorporating Bismuth (Bi) into GaAs creates the GaAs_{1-x}Bi_x alloy, which leads to a large bandgap bowing and considerably increases the absorption coefficient. Nanowire geometry is particularly beneficial for the lattice-mismatched GaAs_{1-x}Bi_x alloy as it diminishes the effect of lattice

mismatch compared to planar counterparts. Prior studies have explored GaAsBi in various solar cell configurations, such as a sub-cell in multi-junction tandem solar cells and in organic-inorganic hybrid solar cells, demonstrating its potential for bandgap engineering. This paper investigates the optoelectronic performance of vertical NW solar cells based on the GaAs_{1-x}Bi_x alloy for different Bi mole fractions using extensive numerical simulation, leveraging the alloy's bandgap tailoring property combined with the benefits of nanowire structures. [7]

Solar cell development is crucial for sustainable energy. While single-junction amorphous silicon (a-Si) solar cells are common with high absorption in the UV spectrum, they are limited by a narrow absorption spectrum and a trade-off between open-circuit voltage (VOC) and short-circuit current (JSC). To address this, researchers explore multi-junction architectures, such as the a-Si/GaAs tandem cell, which combines a-Si with the high-efficiency GaAs semiconductor. GaAs is an attractive material for the bottom cell due to its superior optical absorption and carrier transport properties, complementing the a-Si top cell, and these multi-junction designs, including a-Si/GaAs, have demonstrated high efficiencies, sometimes exceeding 30%. However, despite studies on a-Si/GaAs tandem cells, the literature has lacked a comprehensive analysis of their temperature-dependent behavior, a critical aspect as solar cell performance is strongly influenced by temperature, which affects overall efficiency, VOC, FF, and JSC. Simulation tools like AMPS-1D are vital for understanding and improving solar cell performance. Within this context, the presented study uses the AMPS-1D simulator to investigate the effects of temperature (270–340 K) on the performance of single-junction a-Si and double-junction GaAs/a-Si solar cells, aiming to provide a comprehensive analysis to inform design and optimization. [8]

Colloidal PbS quantum dot (QD) absorbers offer promising flexibility and a tunable bandgap for advanced photovoltaics via low-cost solution processing. However, their primary limitation is a short carrier diffusion length, stemming from hopping transport in the nanocrystal matrix, which creates a trade-off between achieving high current (thick layer for absorption) and high voltage/fill factor (thin layer for extraction). To overcome this, this study proposes a novel nanostructured heterojunction geometry, specifically shaping PbS QD layers into pillars within ZnO nanoparticles, designed to simultaneously enhance light absorption and charge collection. Optical simulations demonstrate significantly enhanced absorption per unit volume in this structure, especially in the infrared, leading to a simulated current gain. While electronic simulations show improved JSC and VOC compared to a planar cell of the same absorber

volume, a reduced fill factor (FF) is observed due to the inhomogeneous electric field distribution within the patterned structure, which causes increased recombination in weak-field regions at higher voltages. Experimental measurements validate the concept, showing enhanced light trapping and carrier collection, particularly in the infrared (confirmed by higher EQE and JSC gain), while also confirming the predicted reduced FF. This work highlights the potential of strategically structuring the p-n junction to mitigate short diffusion length issues, while also identifying the critical need to optimize the electric field distribution in such designs to improve FF. [9]

While perovskite materials are a superior alternative to traditional silicon-based photovoltaics due to their direct bandgaps and high absorbance, the environmental and health risks of lead have shifted research toward eco-friendly alternatives like tin-based Cs_2SnI_6 double perovskites. This material is particularly promising due to its n-type semiconducting nature and high hole mobility, yet experimental power conversion efficiencies (PCE) remain significantly low, typically ranging from 0.11% to 1.10%. The sources attribute this performance gap to interfacial defects, hysteresis loss, and unfavorable band offsets that hinder charge transport and increase recombination rates. Furthermore, existing theoretical models present conflicting results, with reported efficiencies for similar configurations varying widely between 7.73% and 23.64%. To address these discrepancies, the current study uses SCAPS-1D simulation to propose a novel $\text{FTO}/\text{TiO}_2/\text{Cs}_2\text{SnI}_6/\text{Cu}_2\text{O}$ architecture, optimizing layer thickness and defect densities to achieve a practically realizable PCE of 17.77%. [10]

Since 2009, perovskite solar cells (PSCs) have advanced significantly as a cost-effective alternative to traditional silicon, reaching a peak power conversion efficiency (PCE) of 26.7% by 2024. However, the environmental risks associated with lead toxicity have driven a strategic shift toward eco-friendly materials like $\text{CH}_3\text{NH}_3\text{SnI}_3$ (MASnI_3), which features a 1.3 eV direct bandgap that aligns perfectly with the solar spectrum's peak. While previous research using various transport layers has achieved efficiencies ranging from 16.39% to 25.02%, performance remains limited by Shockley–Read–Hall (SRH) recombination, thermal instability, and parasitic resistances. To address these challenges and push efficiencies beyond current benchmarks, this study utilizes SCAPS-1D simulation to optimize a novel $\text{FTO}/\text{SnO}_2/\text{CH}_3\text{NH}_3\text{SnI}_3/\text{NiO}_x/\text{Pt}$ architecture. By precisely tuning parameters such as layer thicknesses, doping concentrations, and band offsets, the authors demonstrate a record-high

theoretical PCE of 31.47%, providing a clear path for the development of high-performance, non-toxic photovoltaics. [11]

Perovskite solar cells (PSCs) have emerged as a premier third-generation photovoltaic technology due to their low manufacturing cost, high optical extinction coefficients, and strong light absorption. Since the 2012 transition from liquid electrolytes to solid-state hole transport materials to reduce recombination and chemical instability, research has focused on optimizing the Hole Transport Layer (HTL). While organic HTLs like Spiro-OMeTAD achieve high efficiency, they are hindered by high costs and poor thermal stability, driving interest in inorganic alternatives such as CuSCN and Cu₂O, which are abundant, non-toxic, and stable under heat and moisture. These materials are ideal for band matching because their valence bands align with the CH₃NH₃PbI₃ absorber, effectively blocking electrons while allowing holes to pass. Using SCAPS-1D simulation, the sources demonstrate that CuSCN currently outperforms Cu₂O, reaching a power conversion efficiency of 21.5% by optimizing layer thickness and carrier concentration to minimize recombination losses. [12]

Kesterite materials like copper zinc tin sulphide (CZTS) have emerged as a premier sustainable alternative for thin-film photovoltaics due to their earth-abundant, non-toxic components, ideal 1.4–1.5 eV direct bandgap, and high absorption coefficient. Despite their potential, the sources note that performance is frequently hindered by deep-level traps and interface defects at the transport layers, which serve as recombination centers and degrade open-circuit voltage and fill factor. While previous theoretical models for CZTS-based cells have reported efficiencies ranging from 8.38% to 31.6%, this study utilizes SCAPS-1D simulation to optimize an FTO/TiO₂/CZTS/CuO/Au architecture. By precisely tuning layer thicknesses (such as a 2.5 μm absorber), carrier concentrations, and identifying gold as the most effective back contact due to its work function, the authors achieve a maximized efficiency of 33.56%, overcoming traditional bottlenecks like thermal instability and charge separation barriers. [13]

While crystalline silicon and thin-film technologies dominate the solar market, emerging perovskite cells face significant hurdles regarding long-term environmental stability. Consequently, Zintl-phosphide materials like BaCd₂P₂ have gained research interest due to their adjustable band gaps, high absorption coefficients, and inexpensive production methods. Unlike traditional cesium-based inorganic absorbers, BaCd₂P₂ exhibits exceptional stability in air and water and long carrier lifetimes of up to 14 ms, which directly reduces recombination losses. This study addresses a gap in the literature by utilizing BaCd₂P₂ for the first time in a

novel ITO/ZnO/BaCd₂P₂/Cu₂O architecture. Through numerical simulations, the sources identify that absorber thickness and defect characteristics, specifically defect density and capture cross-sections, are more pivotal to efficiency than carrier mobility. By optimizing these parameters, the paper reports a maximum theoretical power conversion efficiency (PCE) of 27.59%, positioning BaCd₂P₂ as a robust and superior substitute for existing inorganic absorber materials. [14]

2.2 Field-Specific Theories

2.2.1 Thin-Film Solar Cell Theory

Thin-film solar cells differ from conventional crystalline silicon devices in that charge generation and transport take place within significantly thinner absorber layers, typically on the order of a few micrometers or less. As a consequence, material quality, defect density, and interface engineering play a far more critical role in determining device performance. While the reduced thickness enables lower material consumption, lightweight module fabrication, and potential cost reductions, it also increases the sensitivity of the device to bulk and interfacial recombination losses.

2.2.2 Heterojunction Solar Cell Architecture

Heterojunction solar cells use different semiconductor materials to form junctions with favorable band offsets, enabling efficient separation and transport of photogenerated charge carriers. Proper band alignment at the absorber–electron transport layer (ETL) and absorber–hole transport layer (HTL) interfaces facilitates selective extraction of electrons and holes while simultaneously blocking the opposite carrier type, thereby suppressing interfacial recombination. In contrast, mismatched energy levels can introduce potential barriers or recombination pathways that reduce carrier collection efficiency and lower the open-circuit voltage and fill factor. Additionally, a high density of interface defects can create trap states that act as non-radiative recombination centers, further degrading device performance. Consequently, careful selection and optimization of compatible ETL and HTL materials, along with effective interface passivation strategies, are essential for minimizing losses and achieving high-efficiency heterojunction solar cell devices.

2.2.3 Transport Layer Functionality

Electron transport layers (ETLs) and hole transport layers (HTLs) are engineered to selectively conduct one type of charge carrier while effectively blocking the other, thereby enabling efficient charge separation and collection in solar cell devices. An effective ETL should possess high electron mobility to facilitate rapid electron extraction, along with favorable conduction band alignment with the absorber layer to minimize energy barriers and reduce interfacial recombination. Optical transparency in the relevant wavelength range is also essential to ensure minimal parasitic absorption. Similarly, an HTL should exhibit high hole mobility, appropriate valence band alignment with the absorber to support efficient hole transport, and low recombination losses at the interface. In addition to their electrical characteristics, the optical and thermal stability of ETLs and HTLs play an important role in long-term device performance. The combined electrical and optical properties of these transport layers strongly influence key photovoltaic parameters, including the open-circuit voltage (V_{oc}), fill factor (FF), and overall power conversion efficiency (PCE), underscoring their critical role in high-performance solar cell architectures.

2.3 Review of Zintl-Phosphide Based Solar Cells

Zintl-phosphide compounds have recently attracted attention in photovoltaic research due to their unique bonding characteristics and semiconducting behavior. Among these materials, $BaCd_2P_2$ has been identified as a promising solar absorber because of its suitable bandgap, strong light absorption, and long carrier lifetime. Initial studies have demonstrated the feasibility of incorporating $BaCd_2P_2$ into thin-film heterojunction solar cells, achieving encouraging efficiency values using conventional transport layers.[18]

In baseline studies, $BaCd_2P_2$ has typically been paired with transport materials such as ZnO for electron transport and Cu_2O for hole transport. While these configurations provide a functional device structure, the reported results suggest that further efficiency enhancement may be achievable through optimized transport layer selection. However, systematic comparisons of alternative ETL and HTL combinations for $BaCd_2P_2$ -based devices remain limited in existing literature.[14]

2.4 Methodology

2.4.1 Simulation Approach

In this work, numerical simulation is used as the primary research methodology to analyze and optimize BaCd₂P₂-based thin-film heterojunction solar cells, specifically the SCAPS-1D software. Simulation enables controlled variation of device parameters and material properties while eliminating uncertainties associated with experimental fabrication.

2.4.2 Simulation Tool/Software

The Solar Cell Capacitance Simulator (SCAPS-1D) is a widely used one-dimensional numerical simulation tool for modeling thin-film solar cells. It solves Poisson's equation and the continuity equations for electrons and holes under steady-state conditions. Those equations can be represented mathematically as

$$\frac{\partial}{\partial x} \left(\varepsilon(x) \frac{\partial \varphi}{\partial x} \right) = -q[-p(x) + n(x) - N_D^+(x) + N_A^-(x) + \rho_n - \rho_p]$$

$$\frac{\partial J_n}{\partial x} = q \left(R_n - G + \frac{\partial n}{\partial t} \right)$$

$$\frac{\partial J_p}{\partial x} = -q \left(R_p - G + \frac{\partial p}{\partial t} \right)$$

$$J_n = nq\mu_n \frac{\partial \varphi}{\partial x} + qD_n \frac{\partial n}{\partial x}$$

$$J_p = pq\mu_p \frac{\partial \varphi}{\partial x} - qD_p \frac{\partial p}{\partial x}$$

where, φ is the potential, ε is permittivity, q is electronic charge, n (p) is free electron (hole) concentration, N_D^+ (N_A^-) is donor (acceptor) ion concentration, ρ_n (ρ_p) is the electron (hole) defect distribution, J_n (J_p) is electron (hole) current density, R_n (R_p) is electron (hole) recombination rate, G is the charge generation rate, μ_n (μ_p) is electron (hole) mobility, and D_n (D_p) is diffusivity of electrons (holes).

SCAPS-1D allows incorporation of realistic material parameters, defect states, and interface properties, making it suitable for investigating heterojunction solar cell behavior.

2.4.3 Device Configuration Strategy

To ensure a fair and meaningful comparison with prior work, this study maintains the **absorber layer (BaCd_2P_2)**, transparent conducting oxide, front contact, and back contact identical to those reported in the reference baseline study.[14] The primary modification introduced in this research is the **systematic variation of electron transport layers (ETL) and hole transport layers (HTL)**.

Multiple ETL and HTL combinations are evaluated to examine their impact on device performance. The performance of each configuration is assessed using standard photovoltaic metrics, and the optimized structure is identified based on maximum achievable power conversion efficiency.

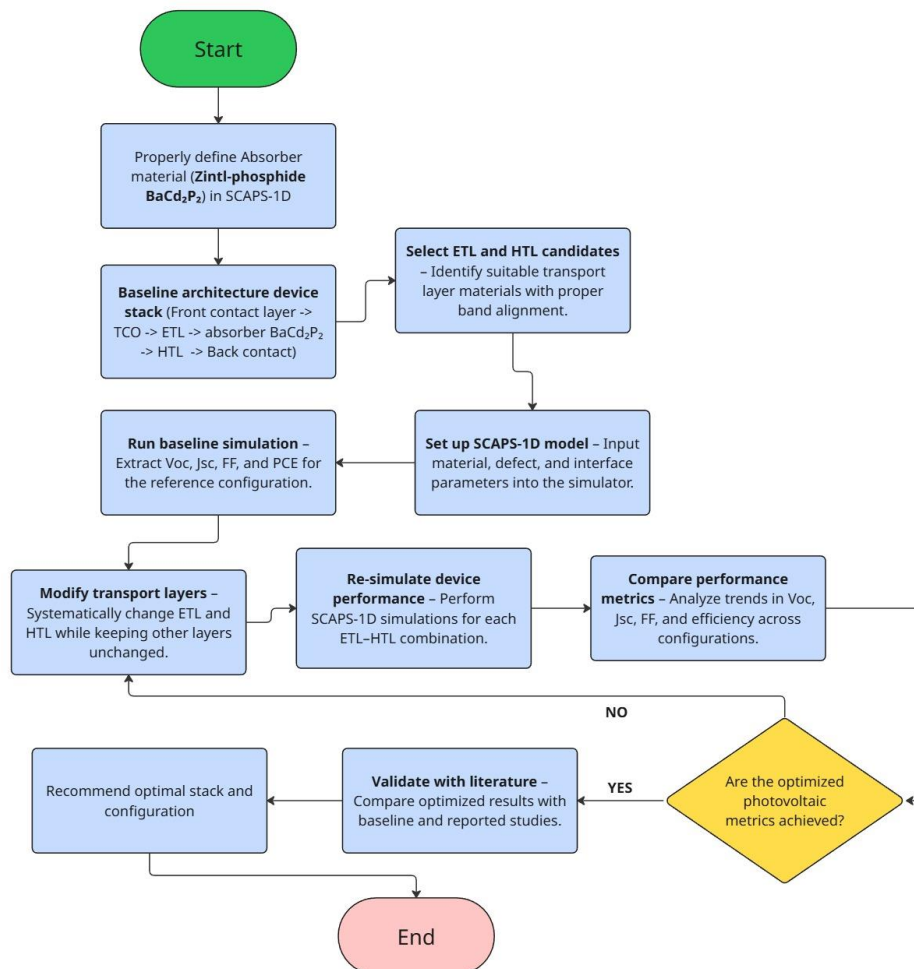


Figure 2.1: Flowchart of the project

2.5 Timeline

To provide a brief overview of the project timeline as shown in Figure 2.2, the project commenced in February 2025 with an initial phase dedicated to literature review and planning. This was followed by proposal report submission, presentation preparation, and proposal defense, which were completed by mid-May. From June to mid-July, the focus shifted to model development, laying the theoretical and simulation framework for the study. Initial simulations were carried out between mid-July and early August, followed by extensive parameter sweeps from August to mid-September to evaluate device performance under varying conditions. Subsequently, optimization and final simulations were conducted through October to achieve improved performance metrics. In November, the emphasis moved to result analysis and graphical output generation. Finally, the project concluded in December with comprehensive documentation, final report preparation, and the final project defense, ensuring a systematic progression from conceptual groundwork to validated results.

PROJECT TIMELINE	START DATE	END DATE	SEMESTER 1				SEMESTER 2			SEMESTER 3			
			Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Project Start	05/02/2025												
Lit. Review and Planning	06/02/2025	12/04/2025											
Proposal Report SUBM	13/04/2025	29/04/2025											
Presentation Prep	30/04/2025	11/05/2025											
Proposal Defense	12/05/2025												
Model Development	01/06/2025	15/07/2025											
Initial Simulations	16/07/2025	05/08/2025											
Parameter Sweeps	06/08/2025	10/09/2025											
Optimization and Final Simulation	11/09/2025	30/10/2025											
Result analysis	01/11/2025	15/11/2025											
Graphical Output	16/11/2025	30/11/2025											
Final Report and Presentation Prep	01/12/2025	27/12/2025											
Final Project Defense	28/12/2025												

Figure 2.2: Gantt Chart of the entire project timeline

Chapter 3: Main Work

This chapter describes the main work carried out in this project, which involves the numerical modeling, simulation, and optimization of a BaCd_2P_2 -based thin-film heterojunction solar cell using the SCAPS-1D simulator. The emphasis of this chapter is on the device structure, material selection, and simulation setup adopted to systematically investigate the impact of different electron transport layer (ETL) and hole transport layer (HTL) combinations on photovoltaic performance. All simulations were performed at room temperature (300 K) under standard AM1.5G solar illumination with an incident power density of 1000 W m^{-2} . The surface recombination velocities for both electrons and holes at the front and rear contacts were fixed at 10^7 cm s^{-1} . To simplify the model while maintaining realistic device conditions, optical reflection losses at both the front and back contacts were neglected. Additionally, gold was used as the back metal contact in the proposed solar cell structure, with an assumed work function of 5.1 eV.

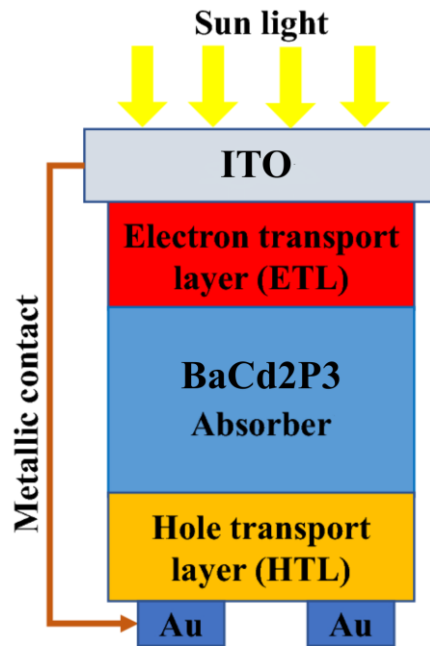


Figure 3.1: Schematic representation of the proposed solar cell

3.1 Device Structure and Architecture

The simulated solar cell is based on a **thin-film heterojunction architecture** consisting of a transparent conducting oxide, transport layers, an absorber layer, and metal contacts. To maintain consistency with prior literature and enable meaningful comparison, the absorber material, front and back contacts, and transparent conducting oxide were kept identical to those

reported in the reference paper.[14] The general device structure, from front contact to back contact, is as follows:

- Front metal contact
- Transparent conducting oxide (ITO)
- Electron Transport Layer (ETL)
- BaCd_2P_2 absorber layer
- Hole Transport Layer (HTL)
- Back metal contact

The BaCd_2P_2 absorber layer serves as the primary photoactive material, where photon absorption and charge carrier generation occur. The ETL and HTL are responsible for selective extraction and transport of electrons and holes, respectively, while suppressing recombination losses at the contacts.

Table 3.1 Summary of TCO and absorber parameters

Parameters	ITO	BaCd ₂ P ₂
Thickness [nm]	500	700
Bandgap, E_g [eV]	3.5	1.45
Electron Affinity, χ [eV]	4.0	4.1
Dielectric constant, ϵ_r	9.0	10.0
CB DOS, N_c [cm ⁻³]	2.2×10^{18}	2.2×10^{18}
VB DOS, N_v [cm ⁻³]	1.8×10^{19}	1.8×10^{19}
Mobility of electron, μ_e [cm ² V ⁻¹ s ⁻¹]	20	111
Mobility of hole, μ_h [cm ² V ⁻¹ s ⁻¹]	10	123
Concentration of acceptor, N_a [cm ⁻³]	-	5.0×10^{15}
Concentration of donor, N_d [cm ⁻³]	1.0×10^{21}	-
Defect concentration, N_t [cm ⁻³]	-	3.0×10^{15}

Table 3.2 Summary of absorber defect properties

Description	Defect Type	Capture cross section: electrons/holes [cm ²]	Energy distribution	Position
Defect 1	Acceptor	1.8×10^{-18}	Single	0.71 eV above VB maximum
Defect 2	Donor	1.8×10^{-18}	Single	0.78 eV above VB maximum

3.2 Selection of Transport Layers

To investigate the influence of charge transport layers on the performance of BaCd₂P₂-based thin-film heterojunction solar cells, a range of electron transport layer (ETL) and hole transport layer (HTL) materials were systematically evaluated using numerical simulation. The selection of these materials was based on their reported electronic properties, such as bandgap energy, carrier mobility, band alignment compatibility, and prior usage in thin-film photovoltaic devices.

For the **electron transport layer (ETL)**, the following materials were considered:

- Tin oxide (SnO₂)
- Zinc magnesium oxide (ZnMgO)
- Barium stannate (BaSnO₃)
- Titanium dioxide (TiO₂)
- Cadmium sulfide (CdS)
- Indium sulfide (In₂S₂)
- Zinc Oxide (ZnO) [Reference paper]

These ETL materials were chosen to represent a range of wide-bandgap n-type semiconductors with differing electron affinities and transport characteristics.

For the **hole transport layer (HTL)**, the following materials were investigated:

- Nickel oxide (NiOx)
- Copper thiocyanate (CuSCN)
- Copper iodide (CuI)
- Copper chloride (CuCl)
- Copper gallium oxide (CuGaO₂)
- Copper aluminum oxide (CuAlO₂)
- Copper(I) Oxide (Cu₂O) [Reference paper]

The selected HTL materials are p-type semiconductors commonly studied for thin-film photovoltaic applications due to their favorable hole transport properties and optical transparency.

During the simulation process, various ETL–HTL combinations were evaluated while maintaining the absorber layer (BaCd₂P₂), transparent conducting oxide, and metal contacts unchanged. This controlled approach ensured that performance variations could be attributed primarily to transport layer selection. The comparative analysis enabled identification of the

most effective transport layer pairing in terms of carrier extraction efficiency and overall photovoltaic performance.

Table 3.3 Summary of 3 ETL candidate parameters

Parameters	SnO ₂	ZnMgO	TiO ₂
Thickness [nm]	40	50	50
Bandgap, E_g [eV]	3.4	3.6	3.2
Electron Affinity, χ [eV]	4.1	3.8	4.0
Dielectric constant, ϵ_r	9.0	8.5	9.0
CB DOS, N_c [cm ⁻³]	3.7×10^{18}	3.0×10^{18}	2.2×10^{18}
VB DOS, N_v [cm ⁻³]	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
Mobility of electron, μ_e [cm ² V ⁻¹ s ⁻¹]	20	50	20
Mobility of hole, μ_h [cm ² V ⁻¹ s ⁻¹]	0.01	1.0	1
Concentration of acceptor, N_a [cm ⁻³]	-	-	-
Concentration of donor, N_d [cm ⁻³]	5.0×10^{18}	5.0×10^{18}	1.0×10^{18}
Defect concentration, N_t [cm ⁻³]	1.0×10^{15}	1.0×10^{15}	1.0×10^{15}

Table 3.4 Summary of 3 other ETL candidate parameters

Parameters	CdS	In ₂ S ₂	ZnO
Thickness [nm]	50	50	50
Bandgap, E_g [eV]	2.42	2.1	3.3
Electron Affinity, χ [eV]	4.2	4.3	4.0
Dielectric constant, ϵ_r	10.0	12.0	9.0
CB DOS, N_c [cm ⁻³]	2.2×10^{18}	2.2×10^{18}	3.7×10^{18}
VB DOS, N_v [cm ⁻³]	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
Mobility of electron, μ_e [cm ² V ⁻¹ s ⁻¹]	100	30	100
Mobility of hole, μ_h [cm ² V ⁻¹ s ⁻¹]	25	5	25
Concentration of acceptor, N_a [cm ⁻³]	-	-	-
Concentration of donor, N_d [cm ⁻³]	1.0×10^{18}	5.0×10^{17}	1.0×10^{18}
Defect concentration, N_t [cm ⁻³]	1.0×10^{15}	1.0×10^{15}	1.0×10^{15}

Table 3.5 Summary of ETL defect properties

Description	Defect Type	Capture cross section: electrons/holes [cm ²]	Energy distribution	Position
Defect 1	Neutral	1.0×10^{-15}	Single	0.6 eV above VB maximum

Table 3.6 Summary of 3 HTL candidate parameters

Parameters	NiOx	CuSCN	CuCl
Thickness [nm]	30	25	50
Bandgap, E_g [eV]	3.4	3.9	3.4
Electron Affinity, χ [eV]	2.0	1.9	2.6
Dielectric constant, ϵ_r	11.0	8.5	7.0
CB DOS, N_c [cm ⁻³]	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}
VB DOS, N_v [cm ⁻³]	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
Mobility of electron, μ_e [cm ² V ⁻¹ s ⁻¹]	0.01	0.01	0.01
Mobility of hole, μ_h [cm ² V ⁻¹ s ⁻¹]	1.5	0.8	1.5
Concentration of acceptor, N_a [cm ⁻³]	5.0×10^{18}	5.0×10^{18}	1.0×10^{18}
Concentration of donor, N_d [cm ⁻³]	-	-	-
Defect concentration, N_t [cm ⁻³]	5.0×10^{15}	5.0×10^{13}	1.0×10^{15}

Table 3.7 Summary of 3 other HTL candidate parameters

Parameters	CuGaO ₂	CuAlO ₂	Cu ₂ O
Thickness [nm]	50	50	50
Bandgap, E_g [eV]	3.5	3.5	2.2
Electron Affinity, χ [eV]	2.4	2.4	3.4
Dielectric constant, ϵ_r	9.0	9.0	7.5
CB DOS, N_c [cm ⁻³]	2.2×10^{18}	2.2×10^{18}	2.0×10^{19}
VB DOS, N_v [cm ⁻³]	1.8×10^{19}	1.8×10^{19}	1.0×10^{19}
Mobility of electron, μ_e [cm ² V ⁻¹ s ⁻¹]	1.0	0.01	200
Mobility of hole, μ_h [cm ² V ⁻¹ s ⁻¹]	5.0	1.5	8600
Concentration of acceptor, N_a [cm ⁻³]	1.0×10^{18}	1.0×10^{19}	1.0×10^{18}
Concentration of donor, N_d [cm ⁻³]	-	-	-
Defect concentration, N_t [cm ⁻³]	1.0×10^{15}	1.0×10^{14}	1.0×10^{15}

Table 3.8 Summary of NiOx defect properties

Description	Defect Type	Capture cross section: electrons/holes [cm ²]	Energy distribution	Position
Defect 1	Acceptor	1.0×10^{-16}	Single	0.3 eV above VB maximum
Defect 2	Neutral	1.0×10^{-16}	Single	1.9 eV above VB maximum

Table 3.9 Summary of CuSCN, CuCl defect properties

Description	Defect Type	Capture cross section: electrons/holes [cm ²]	Energy distribution	Position
Defect 1	Neutral	1.0×10^{-16}	Single	0.2 eV above VB maximum

Table 3.10 Summary of CuGaO₂, CuAlO₂ and Cu₂O defect properties

Description	Defect Type	Capture cross section: electrons/holes [cm ²]	Energy distribution	Position
Defect 1	Acceptor	1.0×10^{-15}	Single	0.8 eV above VB maximum
Defect 2	Donor	1.0×10^{-15}	Single	1.0 eV above VB maximum

The combinations of ETL-HTL that were used later on are:

- SnO₂/NiOx
- ZnMgO/CuSCN
- TiO₂/CuCl
- CdS/CuGaO₂
- In₂S₃/CuAlO₂
- ZnO / Cu₂O [Reference paper]

3.3 Simulation Tool and Physical Models

All device simulations were performed using SCAPS-1D (Solar Cell Capacitance Simulator), a one-dimensional numerical simulation tool widely used for thin-film solar cell analysis. SCAPS-1D solves Poisson's equation and the continuity equations for electrons and holes under steady-state illumination conditions.

The simulator incorporates key physical mechanisms including:

- Carrier drift and diffusion
- Bulk and interface recombination
- Defect-assisted recombination
- Band alignment at heterojunction interfaces

All the simulations were performed at room temperature (300 K) under standard AM1.5G solar illumination with an incident power density of 1000 W m⁻². The surface recombination

velocities for both electrons and holes at the front and rear contacts were fixed at 10^7 cm s^{-1} . To simplify the model while maintaining realistic device conditions, optical reflection losses at both the front and back contacts were neglected. Additionally, gold was used as the back metal contact in the proposed solar cell structure, with an assumed work function of 5.1 eV.

3.4 Material Parameters

Material parameters for the BaCd_2P_2 absorber, ITO layer, and metal contacts were adopted directly from the reference study to ensure consistency. These parameters include bandgap energy, electron affinity, relative permittivity, carrier mobility, and defect density.

For the ETL and HTL materials, parameters were selected from established literature and adjusted within physically reasonable ranges supported by SCAPS-1D. Interface defect densities and recombination parameters were defined to reflect practical device conditions while avoiding non-physical behavior.

3.5 Simulation Procedure

The simulation procedure followed a systematic and iterative approach:

- A baseline device configuration was first simulated using the reference ETL–HTL combination.
- Alternative ETL and HTL materials were then introduced one at a time while keeping all other parameters unchanged.
- For each configuration, SCAPS-1D simulations were performed to extract key photovoltaic parameters, including open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE).
- The performance of each configuration was recorded and compared to identify trends and improvements.
- The optimization process was repeated until no further significant performance enhancement was observed.

Chapter 4: Results and Discussion

This chapter presents and analyzes the SCAPS-1D simulation results of BaCd₂P₂-based thin-film heterojunction solar cells for different ETL–HTL material combinations. The purpose of the analysis is to determine how transport-layer pairing impacts photovoltaic output parameters, namely open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE).

All device configurations were simulated under identical conditions, where the absorber layer (BaCd₂P₂), transparent conducting oxide, and contacts were kept constant. Only the ETL and HTL layers were varied as paired combinations, ensuring that performance differences are attributable to transport-layer selection and interface behavior rather than absorber or contact modifications.

4.1 J–V Characteristics of ETL–HTL Combinations

Figure 4.1 presents the current density–voltage (J–V) characteristics of BaCd₂P₂-based thin-film heterojunction solar cells employing different ETL–HTL combinations under standard AM1.5G illumination. All curves exhibit the expected diode-like behavior, confirming physically consistent device operation within the SCAPS-1D framework.

At low applied voltages (near $V = 0$), all configurations display nearly identical short-circuit current densities ($J_{sc} \approx 28 \text{ mA/cm}^2$). This similarity arises because the absorber layer (BaCd₂P₂), optical conditions, and generation profile were kept constant across all simulations. Since J_{sc} is primarily governed by photon absorption and carrier generation within the absorber, variations in transport layers have minimal impact on J_{sc} as long as severe extraction barriers are not present. This observation confirms that **performance differences among devices are not current-limited**.

As the applied voltage increases toward the maximum power point region, clear separation between the J–V curves becomes evident. This region reflects differences in **charge extraction efficiency, recombination losses, and internal electric field distribution**, which are strongly influenced by ETL–HTL pairing. Devices with less favorable band alignment or higher interface recombination exhibit a more gradual transition from the current-generating regime to the voltage-dominated regime, resulting in a softer curve “knee” and reduced fill factor.

The optimized **SnO₂/NiO_x** configuration demonstrates a sharper knee and maintains higher current density at elevated voltages compared to other combinations. This behavior indicates improved carrier selectivity at both heterointerfaces, reduced Shockley–Read–Hall recombination, and lower resistive losses. Consequently, this configuration achieves both a higher open-circuit voltage (Voc) and an enhanced fill factor, directly contributing to its superior power conversion efficiency.

In contrast, configurations such as **TiO₂/CuCl** and **CdS/CuGaO₂** exhibit earlier current roll-off and reduced slope near the knee region. This suggests increased recombination and/or unfavorable energy band offsets that hinder efficient carrier transport. Although these devices generate comparable photocurrent at short circuit, their reduced Voc and FF significantly limit overall efficiency.

The baseline **ZnO/Cu₂O** device shows stable operation and reasonable curve shape but remains inferior to the optimized SnO₂/NiO_x configuration. The difference in curve sharpness and knee position indicates that transport-layer optimization, rather than absorber modification, is responsible for the observed performance enhancement.

Overall, the J–V characteristics confirm that **fill factor and open-circuit voltage are the dominant differentiating parameters** among the ETL–HTL combinations, while short-circuit current density remains largely unaffected. This reinforces the conclusion that transport-layer pairing and interface engineering play a critical role in maximizing the performance potential of BaCd₂P₂-based heterojunction solar cells.

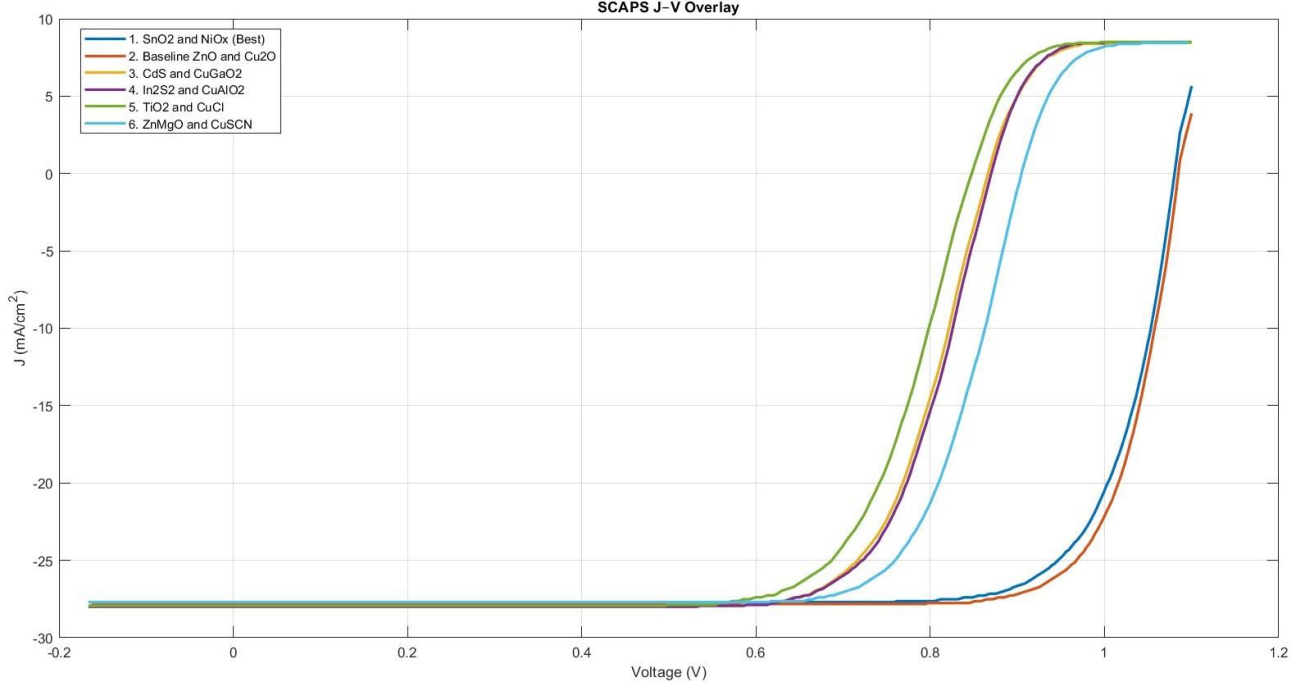


Figure 4.1: J-V characteristics of all the ETL-HTL combos against the baseline paper

4.2 Comparative Evaluation of Power Conversion Efficiency

Figure 4.2 compares the power conversion efficiency across the evaluated ETL–HTL combinations. The results demonstrate that transport-layer selection alone can produce significant efficiency variation, even for a fixed absorber and contact structure.

The SnO_2/NiOx configuration achieved the highest PCE of 28.72%, exceeding the baseline reference configuration $\text{ZnO}/\text{Cu}_2\text{O}$ with 27.59%. Other tested combinations produced lower efficiencies, primarily due to reduced FF and/or lower V_{oc} , consistent with the metric-level trends in Figure 4.3.

The dashed Shockley–Queisser reference line is included to contextualize single-junction theoretical constraints and to emphasize that the achieved efficiencies are within physically reasonable boundaries for a single-junction device model.

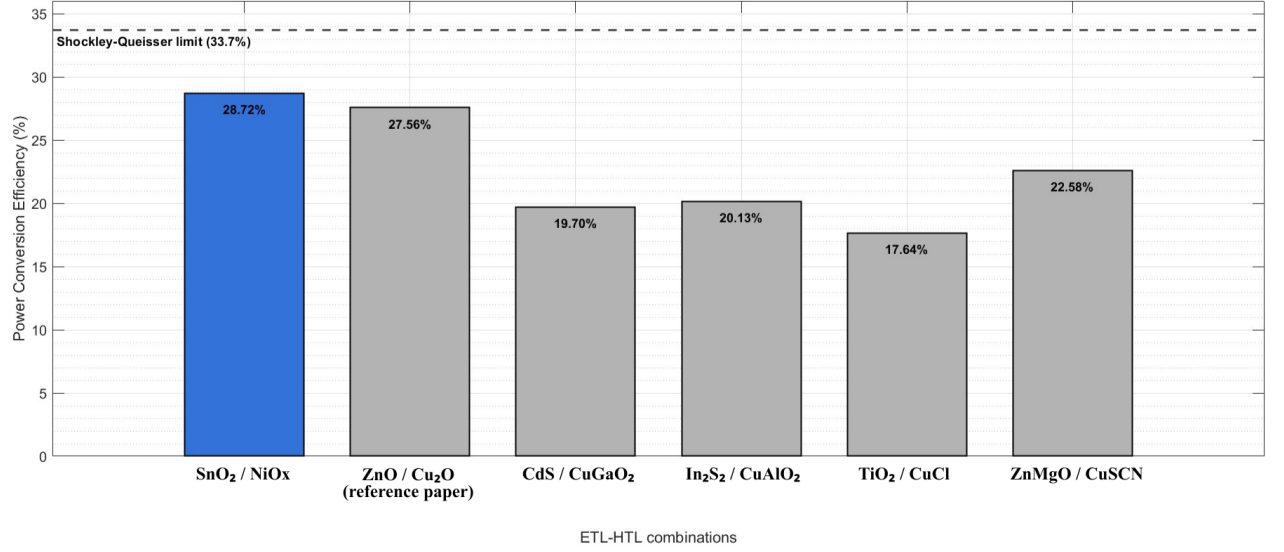


Figure 4.2: PCE comparison bar chart (highlight optimized + baseline, SQ line)

4.3 Comparative Evaluation of Voc, Jsc, and FF

Figure 4.3 presents a comparative analysis of the key photovoltaic performance parameters such as open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), and fill factor (FF), for BaCd₂P₂-based heterojunction solar cells using different ETL–HTL combinations. The SnO₂/NiOx configuration is highlighted as the main optimized reference, while the ZnO/Cu₂O device represents the baseline structure adopted from the reference study.

4.3.1 Open-circuit voltage (V_{oc}):

The V_{oc} plot shows noticeable variation across the different transport-layer combinations. The optimized SnO₂/NiOx device exhibits the highest V_{oc} (≈ 1.23 V), indicating reduced recombination losses and improved quasi-Fermi level splitting within the device. In contrast, combinations such as TiO₂/CuCl show significantly lower V_{oc} values, suggesting unfavorable band alignment and increased interfacial recombination. These results indicate that V_{oc} is highly sensitive to ETL–HTL energy level matching and interface quality.

4.3.2 Short-circuit current density (J_{sc}):

The J_{sc} values remain nearly constant across all configurations (≈ 28.4 mA/cm²), with only marginal variation. This behavior is expected because the absorber material (BaCd₂P₂), optical conditions, and generation profile were kept identical for all simulations. Since J_{sc} is primarily

governed by photon absorption and carrier generation in the absorber, changes in transport layers do not strongly influence J_{sc} unless severe carrier extraction barriers are present. This confirms that the observed performance differences among devices are not current-limited.

4.3.3 Fill factor (FF):

Fill factor (FF): The FF plot reveals the most pronounced variation among the ETL–HTL combinations. The optimized $\text{SnO}_2/\text{NiO}_x$ device demonstrates the highest FF (above 82%), indicating efficient carrier transport, low series resistance effects, and suppressed recombination near the operating point. Other combinations, such as $\text{CdS}/\text{CuGaO}_2$ and TiO_2/CuCl , exhibit substantially lower FF values, reflecting poor charge extraction and higher non-ideal losses. The baseline $\text{ZnO}/\text{Cu}_2\text{O}$ device shows moderate FF, consistent with its intermediate overall efficiency.

Overall interpretation: Taken together, Figure 4.3 clearly shows that while J_{sc} remains largely unaffected by transport-layer selection, both V_{oc} and FF vary significantly across ETL–HTL combinations. This demonstrates that voltage losses and fill-factor degradation are the dominant mechanisms limiting efficiency in sub-optimal structures. The superior performance of the $\text{SnO}_2/\text{NiO}_x$ configuration arises from its simultaneous enhancement of V_{oc} and FF, which directly explains its highest power conversion efficiency reported in this study.

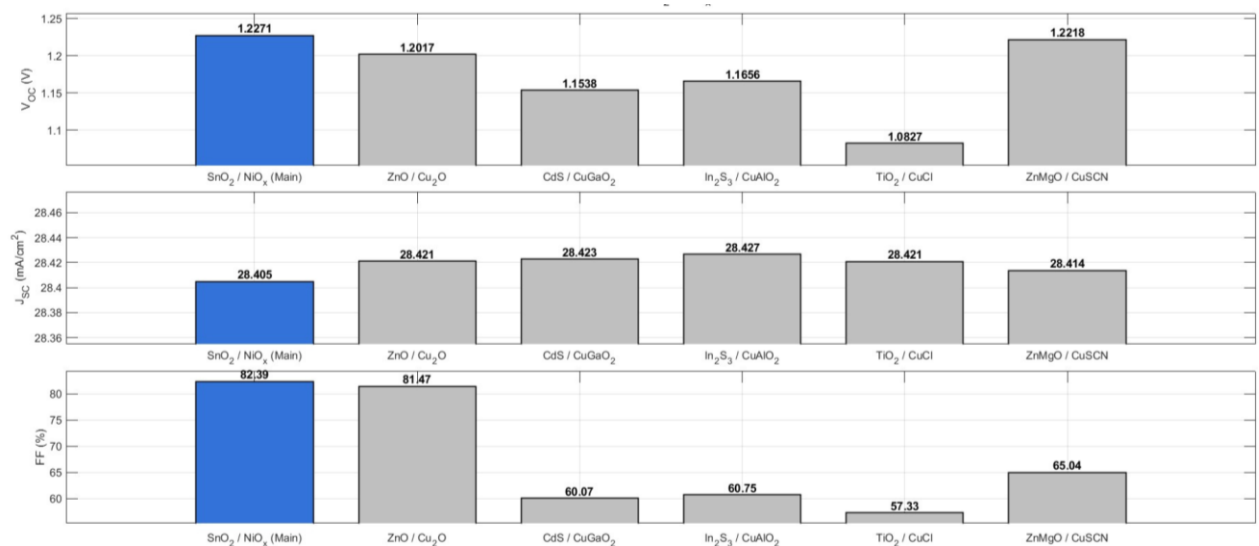


Figure 4.3: Comparative metrics (V_{oc} , J_{sc} , FF) across combinations of ETL and HTLs

4.4 Effect of Interface Defect Density (DIT) for SnO₂/BaCd₂P₂/NiO_x Structure

Figure 4.4 presents contour plots illustrating the influence of **interface defect density (DIT) at the absorber/ETL and absorber/HTL** interfaces on the photovoltaic performance of the optimized SnO₂/NiO_x-based BaCd₂P₂ solar cell. The DIT values were varied over several orders of magnitude to evaluate their impact on recombination and carrier transport.

From Figure 4.4(a), it is observed that the **power conversion efficiency (PCE)** decreases gradually as the interface defect density increases, particularly when both absorber/ETL and absorber/HTL interfaces exhibit high DIT values. Regions of higher PCE are concentrated at lower defect densities, indicating that interfacial recombination plays a critical role in limiting overall device efficiency. Elevated DIT introduces a higher density of recombination centers, which increases Shockley–Read–Hall (SRH) recombination and reduces the extractable electrical power.

Figure 4.4(b) shows the variation of **open-circuit voltage (Voc)** with interface defect density. Voc exhibits strong sensitivity to DIT, with noticeable reductions occurring even for moderate increases in defect density. This behavior arises because increased interface recombination raises the dark saturation current, thereby lowering Voc. The contour pattern highlights that Voc degradation is particularly severe when defect densities at both interfaces are simultaneously high, emphasizing the cumulative effect of interfacial recombination on voltage loss.

In contrast, Figure 4.4(c) demonstrates that the **short-circuit current density (Jsc)** remains almost unchanged across the entire DIT range. This indicates that photogeneration and optical absorption within the BaCd₂P₂ absorber dominate Jsc, and that interface defects primarily affect carrier recombination after generation rather than photon absorption or carrier generation itself.

Finally, Figure 4.4(d) illustrates the impact of interface defect density on the **fill factor (FF)**. A clear reduction in FF is observed with increasing DIT, particularly at high absorber/ETL defect densities. This behavior is attributed to enhanced recombination near the maximum power point, which distorts the J–V curve and reduces its squareness. The strong dependence of FF on interface quality further confirms that interfacial defects increase non-ideal diode behavior and resistive losses.

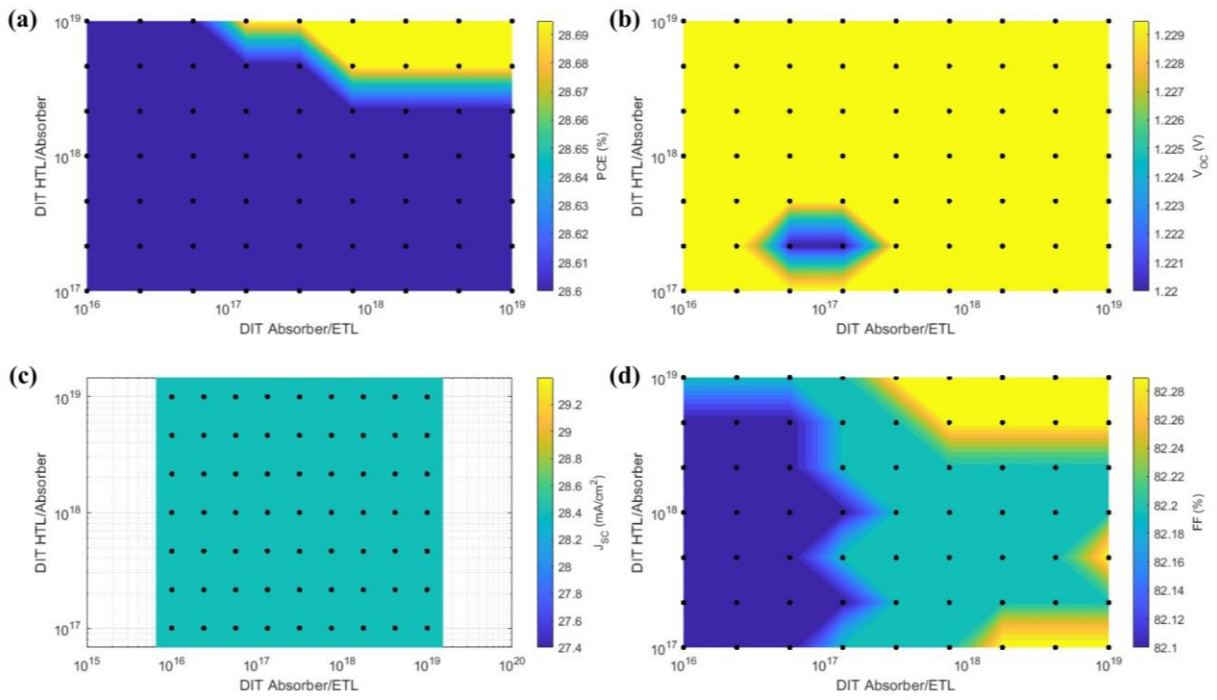


Figure 4.4: Contour plots of a) PCE, b) V_{oc} , c) J_{sc} , and d) FF as a function of interface defect density.

4.5 Effect of Transport-Layer Doping Density for $\text{SnO}_2/\text{BaCd}_2\text{P}_2/\text{NiOx}$ Structure

Figure 4.5 illustrates the effect of **electron transport layer (ETL) donor density (ND)** and **hole transport layer (HTL) acceptor density (NA)** on the photovoltaic performance of the optimized SnO_2/NiOx -based BaCd_2P_2 solar cell. The doping concentrations were varied over several orders of magnitude to evaluate their influence on carrier extraction, band bending, and recombination dynamics.

From Figure 4.5(a), the **power conversion efficiency (PCE)** shows a clear increase with increasing ETL and HTL doping densities up to an optimal region. Higher doping enhances the built-in electric field at the heterointerfaces, improving carrier separation and reducing interfacial recombination losses. However, beyond a certain doping threshold, the PCE saturates, indicating diminishing performance gains at excessively high doping concentrations.

Figure 4.5(b) presents the variation of **open-circuit voltage (Voc)** as a function of transport-layer doping. Voc increases noticeably with moderate increases in both ND and NA due to stronger band bending and improved carrier selectivity at the ETL/absorber and absorber/HTL interfaces. The localized region of reduced Voc at lower doping densities highlights insufficient junction field strength, which facilitates increased recombination and voltage loss. At very high doping levels, Voc stabilizes, suggesting that recombination and contact limitations begin to dominate rather than junction strength.

In contrast, Figure 4.5(c) shows that the **short-circuit current density (Jsc)** remains nearly constant across the entire doping range. This behavior indicates that Jsc is primarily governed by photon absorption and carrier generation within the BaCd_2P_2 absorber, which are largely unaffected by transport-layer doping once sufficient carrier extraction is ensured.

Finally, Figure 4.5(d) depicts the effect of doping density on the **fill factor (FF)**. FF improves with increasing ND and NA as enhanced carrier selectivity and reduced series resistance lead to a more ideal diode behavior and improved J–V curve squareness. At low doping levels, poor band alignment and weak built-in fields result in significant FF degradation. Similar to Voc and PCE, FF eventually saturates at higher doping concentrations, reflecting the onset of transport and recombination limits unrelated to further increases in doping.

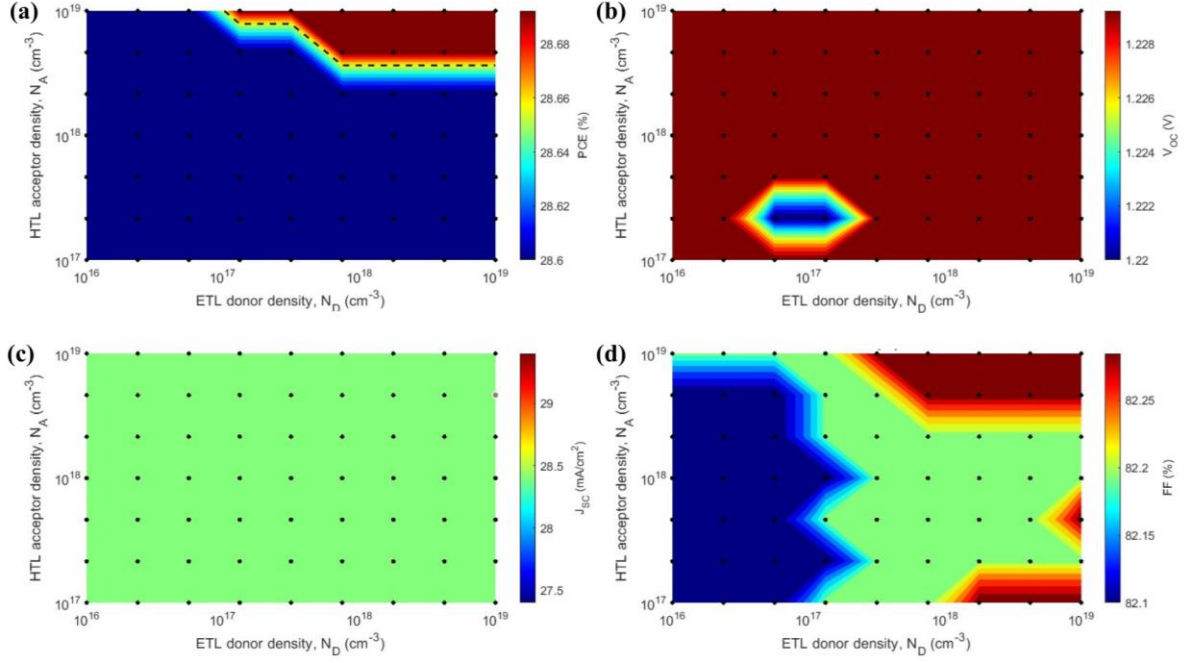


Figure 4.5: Contour plots of a) PCE, b) V_{oc} , c) J_{sc} , and d) FF showing the influence of ETL donor density and HTL acceptor density on device performance.

4.6 Effect of Transport-Layer Thickness for $\text{SnO}_2/\text{BaCd}_2\text{P}_2/\text{NiO}_x$ Structure

Figures 4.6 and 4.7 show the variation of PCE, J_{sc} , FF, and V_{oc} as a function of ETL and HTL thickness, respectively. Overall, the results indicate that transport-layer thickness has only a minor influence on device performance within the investigated range.

For both ETL and HTL thickness variations, V_{oc} remains almost constant, indicating that the built-in potential and energy band alignment at the heterojunction interfaces are not significantly affected once a minimum functional thickness is achieved. Since V_{oc} is primarily governed by recombination mechanisms and interface quality rather than transport-layer thickness, its insensitivity is expected.

Similarly, the fill factor (FF) exhibits negligible variation across the thickness range, suggesting that charge extraction remains efficient and that series resistance does not increase substantially within the selected thickness window. This confirms that the chosen ETL and HTL thicknesses are sufficient to ensure good electrical contact and carrier selectivity.

The short-circuit current density (J_{sc}) shows only a slight decrease with increasing thickness, which can be attributed to marginal increases in series resistance and carrier transport distance.

However, since the absorber layer dominates photon absorption, the influence of transport-layer thickness on J_{sc} remains limited.

As a result, the power conversion efficiency (PCE) follows a similar trend, remaining nearly constant with a very small decline at higher thicknesses. These observations confirm that, beyond an optimal thickness range, further increases in ETL or HTL thickness do not provide additional performance benefits and may introduce minor resistive losses. Overall, the results demonstrate that device performance is more sensitive to transport-layer material properties and interface quality than to thickness variations, provided that the transport layers are sufficiently thick to function effectively.

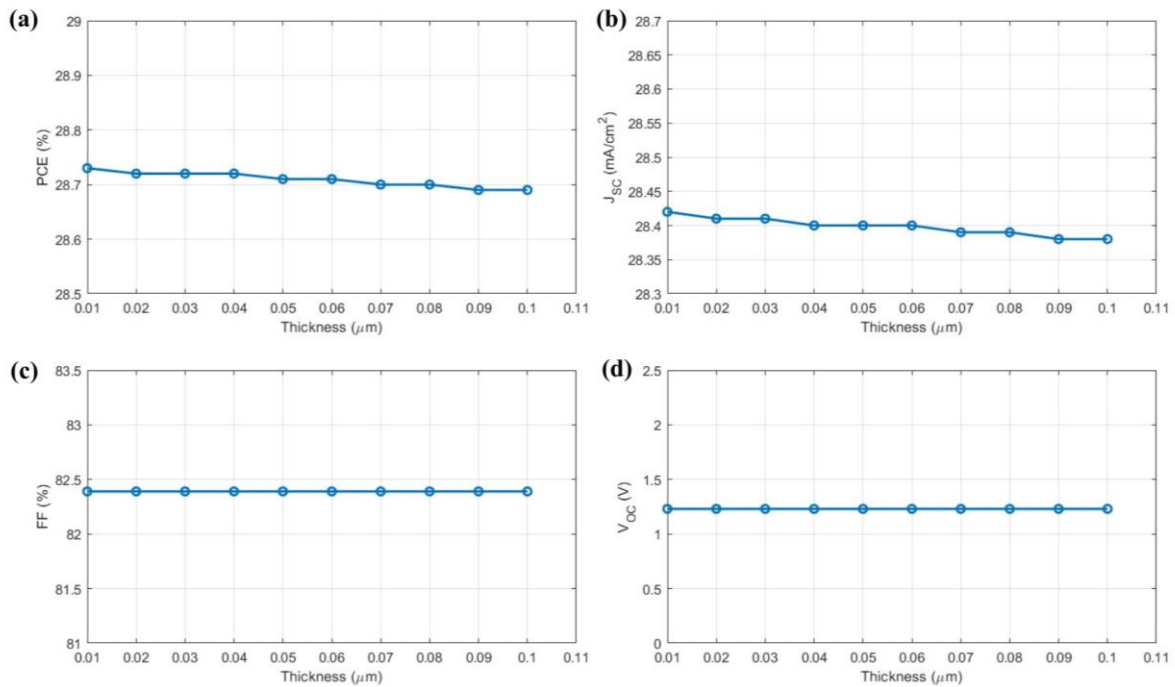


Figure 4.6: Effect of ETL thickness on a) PCE, b) J_{sc} , c) FF and d) V_{oc} .

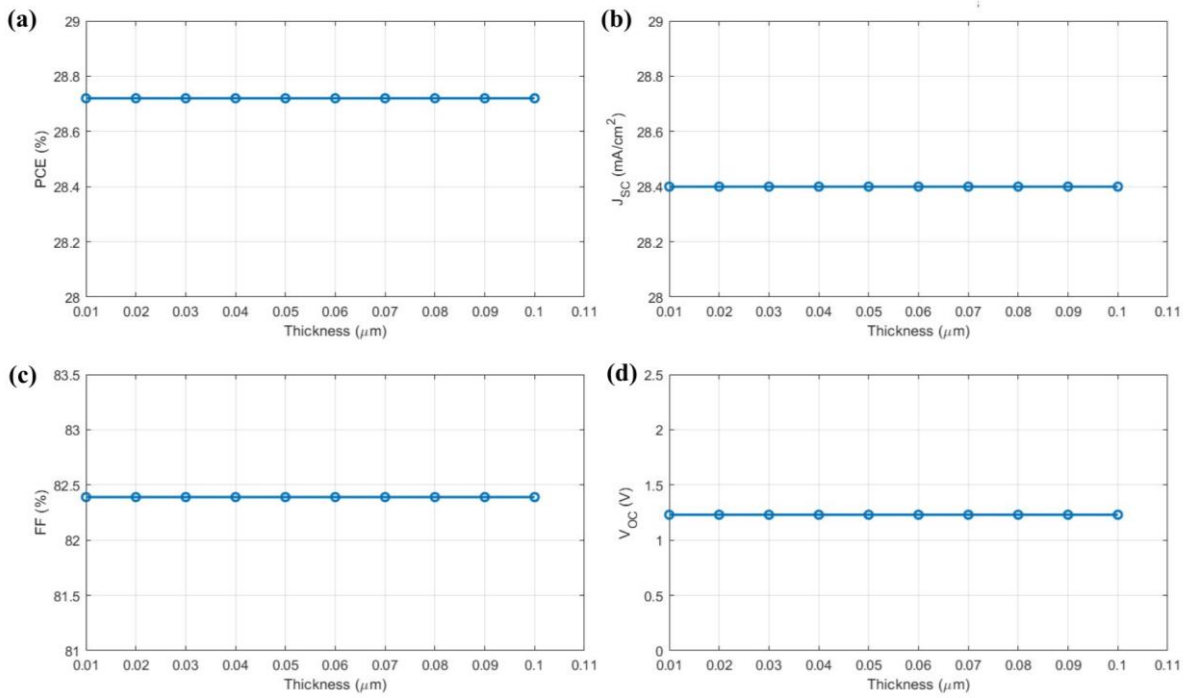


Figure 4.7: Effect of HTL thickness on a) PCE, b) Jsc, c)FF and d)Voc.

4.7 Effect of Series and Shunt Resistance for SnO₂/BaCd₂P₂/NiOx Structure

Figures 4.8 and 4.9 illustrate the influence of series resistance (R_s) and shunt resistance (R_{sh}) on the photovoltaic performance of the SnO₂/NiOx-based BaCd₂P₂ solar cell.

As shown in Figure 4.8, increasing series resistance leads to a noticeable reduction in fill factor and power conversion efficiency. This behavior arises because higher R_s increases resistive voltage losses within the device, limiting current flow near the maximum power point and degrading the squareness of the J–V curve. In contrast, the short-circuit current density remains nearly unchanged, as J_{sc} is primarily governed by optical absorption and charge generation rather than resistive effects. The open-circuit voltage shows only a slight increase with R_s due to reduced recombination current at low current densities, but this improvement is insufficient to offset the loss in FF, resulting in overall efficiency degradation.

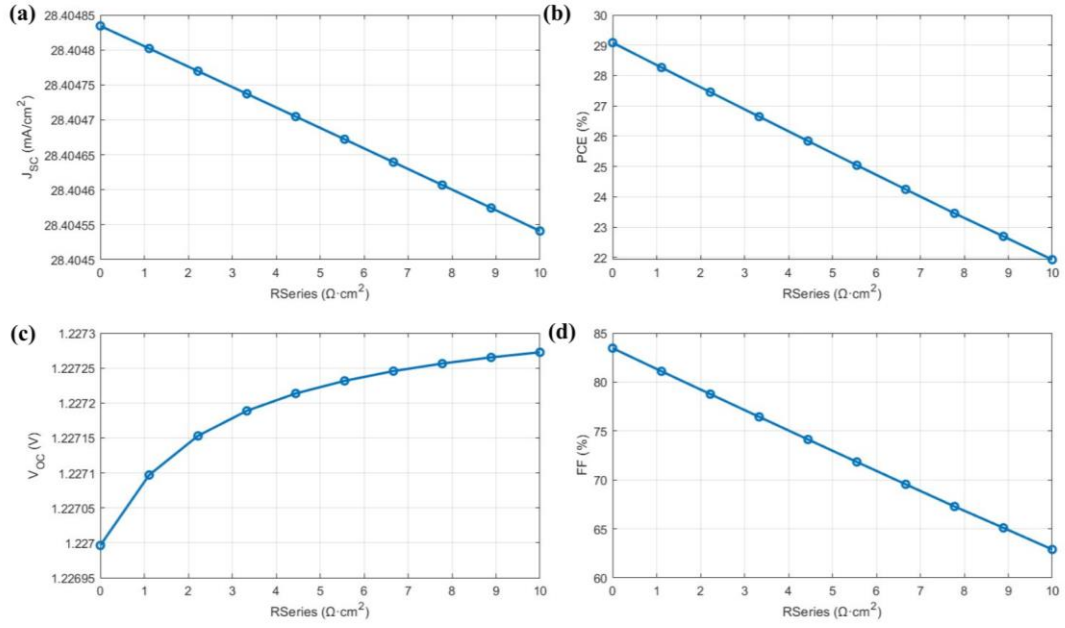


Figure 4.8: Effect of series resistance on a) PCE, b) J_{sc} , c) FF and d) V_{oc} .

Figure 4.9 shows that increasing shunt resistance significantly improves device performance at low R_{sh} values, after which the parameters saturate. Low shunt resistance introduces leakage pathways that divert photogenerated carriers, severely reducing V_{oc} , FF, and PCE. Once R_{sh} exceeds a critical threshold, leakage currents become negligible, and further increases in R_{sh} produce minimal changes in device parameters. Under these conditions, V_{oc} , J_{sc} , and FF stabilize, indicating that shunt-related losses are no longer performance-limiting.

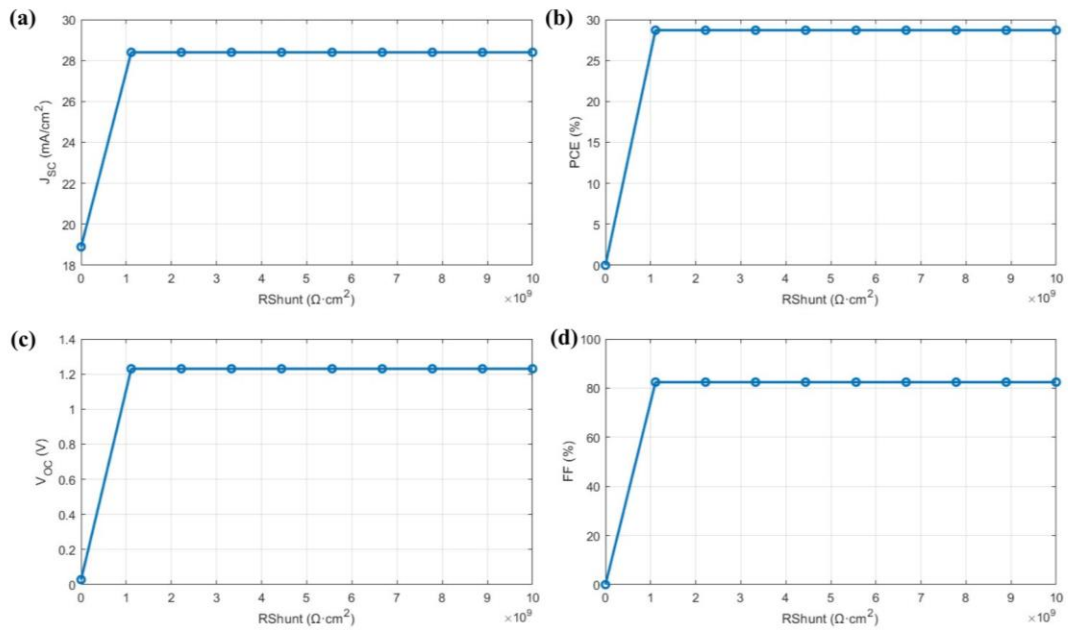


Figure 4.9: Effect of shunt resistance on a) PCE, b) J_{sc} , c) FF and d) V_{oc} .

4.8 Overall Effect of Parameter Optimization on SnO₂/NiOx Device Performance

Initial simulations of the SnO₂/NiOx heterojunction solar cell exhibited a significantly reduced power conversion efficiency despite showing relatively high fill factor and short-circuit current density. This behavior was primarily caused by **excessive interface defect densities and suboptimal transport-layer properties** in the unoptimized device configuration.

At the SnO₂/BaCd₂P₂ interface, a high interface defect density ($D_{it} \approx 1.0 \times 10^{12} \text{ cm}^{-2}$) with a defect energy level located at $E_t = 0.72 \text{ eV}$ and large electron and hole capture cross sections ($\sigma_n = \sigma_p \approx 1.0 \times 10^{-15} \text{ cm}^2$) was introduced. Similarly, the BaCd₂P₂/NiOx interface contained a defect density of approximately $5.0 \times 10^{11} \text{ cm}^{-2}$ with comparable trap energy and capture cross sections. These interface states act as strong **Shockley–Read–Hall recombination centers**, significantly increasing interfacial recombination and suppressing quasi-Fermi level splitting within the absorber, which directly limits the open-circuit voltage.

In addition to interface-related losses, the unoptimized structure was characterized by **low carrier mobility in the absorber layer** and insufficient donor and acceptor concentrations in the ETL and HTL, respectively. These factors hindered efficient carrier transport and extraction, increasing carrier residence time near the interfaces and further enhancing recombination losses. As a result, the unoptimized device exhibited a low Voc and a reduced power conversion efficiency of **18.13%**, despite maintaining a relatively high fill factor.

Figure 4.10 compares the J–V characteristics of the unoptimized and optimized SnO₂/NiOx devices. Following systematic optimization of interface defect densities, transport-layer doping levels, and carrier mobility, the device performance improved substantially. The optimized structure achieved a maximum efficiency of **28.72%**, primarily due to significant enhancements in Voc and Jsc, while maintaining a high fill factor.

Notably, the relatively high Jsc observed even in the unoptimized device indicates that photon absorption and carrier generation within the BaCd₂P₂ absorber remained effective, as optical properties and absorber thickness were unchanged. Similarly, the consistently high fill factor suggests that series resistance effects were limited and that charge extraction pathways were not severely resistive. Together, these observations confirm that the SnO₂/NiOx structure possessed strong intrinsic performance potential, which was fully realized only after careful interface and transport-layer optimization.

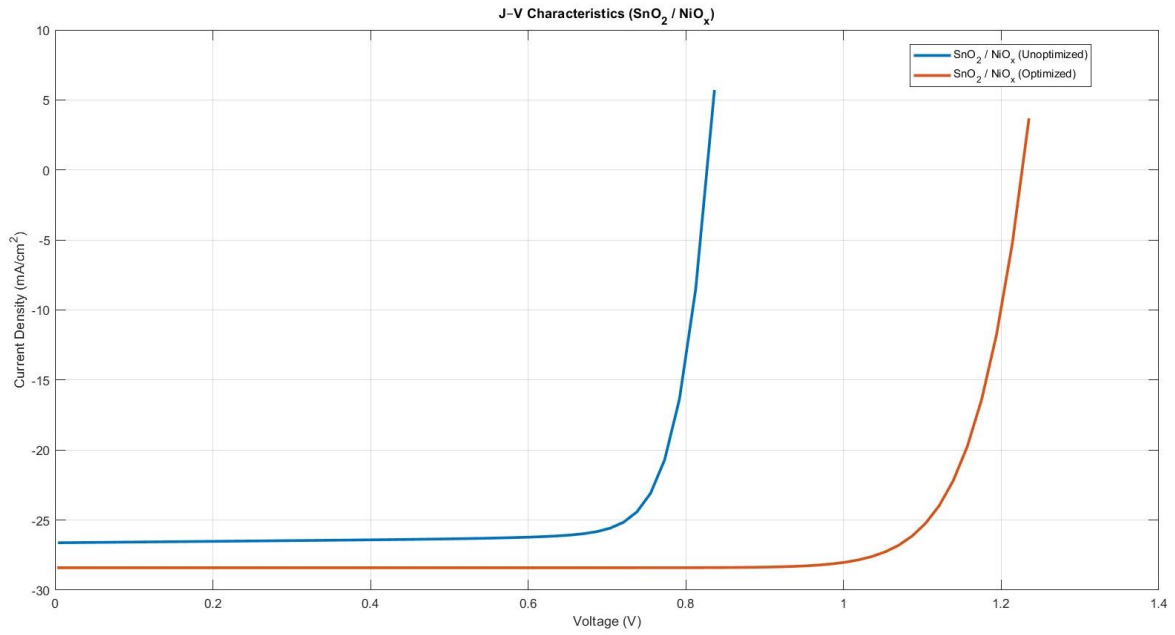


Figure 4.10: Comparison of J–V characteristics for unoptimized and optimized SnO₂/NiO_x structure

4.9 Energy Band Alignment analysis of SnO₂/NiO_x vs ZnO/Cu₂O

While J–V and metric plots confirm performance differences, the underlying cause must be supported through band alignment and interface behavior. Figure 4.5 present the SCAPS-derived energy band diagrams for the optimized and baseline devices, respectively.

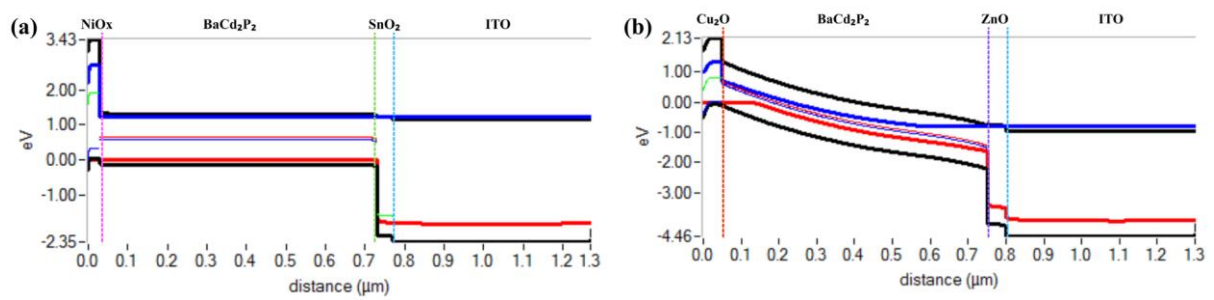


Figure 4.11: Band diagram of a) Optimized SnO₂/BaCd₂P₂/NiO_x and b) Baseline ZnO/BaCd₂P₂/Cu₂O

4.9.1 Optimized Configuration (SnO₂ / BaCd₂P₂ / NiO_x)

In the optimized SnO₂/NiO_x configuration, the conduction band alignment at the SnO₂/BaCd₂P₂ interface forms a favorable electron-selective contact with a minimal energy

barrier for electron extraction. Simultaneously, the valence band offset at the BaCd₂P₂/NiOx interface promotes efficient hole transport while suppressing electron back-injection into the HTL. This asymmetric band alignment enhances carrier selectivity at both interfaces, reducing interfacial Shockley–Read–Hall recombination and maintaining strong quasi-Fermi level splitting across the absorber. As a result, photogenerated carriers are efficiently collected before recombination, which supports higher open-circuit voltage and fill factor and contributes to improved quantum efficiency across the active absorption region.

4.9.2 Baseline Configuration (ZnO / BaCd₂P₂ / Cu₂O)

In contrast, the baseline ZnO/Cu₂O structure exhibits less favorable band alignment at one or both heterointerfaces. The conduction and valence band offsets introduce larger extraction barriers and promote carrier accumulation near the interfaces. This accumulation increases the probability of recombination, particularly under forward bias conditions. Although photon absorption and carrier generation within the BaCd₂P₂ absorber remain effective, the reduced carrier selectivity leads to partial carrier loss before collection. This behavior is consistent with the lower Voc and fill factor observed for the baseline device and explains its reduced overall efficiency compared to the optimized structure.

4.10 Quantum Efficiency Comparison: $\text{SnO}_2/\text{NiO}_x$ vs $\text{ZnO}/\text{Cu}_2\text{O}$

Figure 4.12 present the quantum efficiency (QE) spectra of the optimized $\text{SnO}_2/\text{BaCd}_2\text{P}_2/\text{NiO}_x$ device, the unoptimized $\text{SnO}_2/\text{BaCd}_2\text{P}_2/\text{NiO}_x$ device, and the baseline $\text{ZnO}/\text{BaCd}_2\text{P}_2/\text{Cu}_2\text{O}$ device. As all configurations employ the same BaCd_2P_2 absorber layer under identical optical conditions, the observed variations in QE primarily reflect differences in carrier collection efficiency rather than changes in optical absorption.

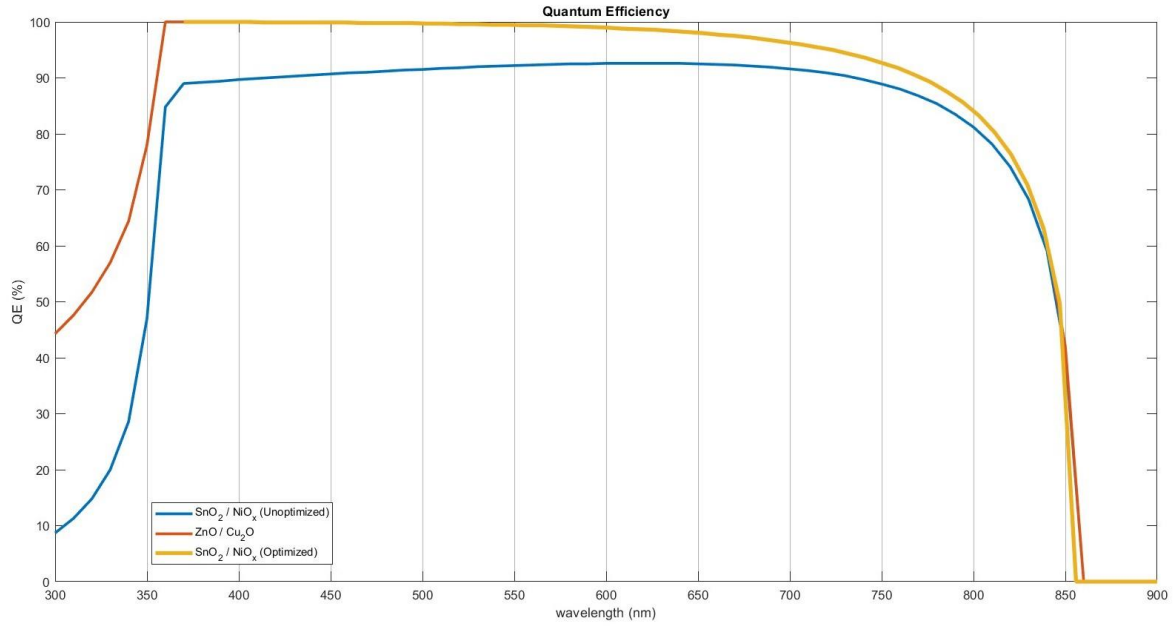


Figure 4.12: Quantum efficiency comparison of optimized and unoptimized $\text{SnO}_2/\text{NiO}_x$ devices and the reference structure.

The optimized $\text{SnO}_2/\text{NiO}_x$ device exhibits near-unity QE across most of the visible wavelength range and maintains a high response up to the absorption edge. This behavior indicates highly efficient carrier extraction throughout the absorber, enabled by favorable energy band alignment at both the ETL/absorber and absorber/HTL interfaces. Reduced interfacial recombination and improved carrier selectivity allow photogenerated electrons and holes to be collected efficiently before recombination occurs.

In contrast, the unoptimized $\text{SnO}_2/\text{NiO}_x$ device shows a noticeably reduced QE, particularly at shorter wavelengths. This reduction suggests enhanced recombination losses for carriers generated near the front interface, consistent with the presence of high interface defect densities and suboptimal transport-layer properties in the unoptimized structure. Although the absorber remains identical, inefficient interface carrier extraction limits overall collection efficiency.

The baseline ZnO/Cu₂O device also exhibits lower QE compared to the optimized SnO₂/NiOx configuration, with reduced response at shorter wavelengths and a steeper decline near the long-wavelength cutoff. These features indicate increased interfacial recombination and less effective carrier transport, particularly for carriers generated close to the heterointerfaces.

The similar long-wavelength cutoff observed in all devices confirms that the absorber bandgap remains unchanged across configurations. Therefore, the superior and more uniform QE response of the optimized SnO₂/NiOx device directly supports its enhanced Voc and fill factor, demonstrating that the observed performance improvement arises from improved transport-layer engineering and interface quality rather than optical effects.

Chapter 5: Conclusion

The project presented a numerical investigation of BaCd₂P₂-based thin-film heterojunction solar cells using the SCAPS-1D simulation framework, with a primary focus on assessing the impact of different ETL–HTL combinations on device performance. To ensure a controlled and meaningful comparison, the absorber layer, transparent conducting oxide, and metal contacts were kept identical to those reported in the reference study, while only the transport layers were varied.

Multiple ETL–HTL combinations were systematically analyzed in terms of open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE). The results indicate that J_{sc} remains nearly constant due to fixed absorber and optical conditions, whereas V_{oc} and FF are strongly influenced by transport-layer selection and interface quality.

Among the configurations investigated, the SnO₂/NiO_x heterojunction exhibited the best overall performance, achieving a maximum PCE of 28.72%, surpassing the baseline ZnO/Cu₂O device from the reference work. This performance enhancement is primarily attributed to improved energy band alignment, reduced interfacial recombination, and enhanced carrier selectivity, resulting in higher V_{oc} and FF.

The inclusion of unoptimized device results further confirms that high interface defect densities, low carrier mobility, and insufficient transport-layer doping can significantly degrade device performance, even for promising material systems. Overall, this study demonstrates that transport-layer and interface engineering, supported by numerical simulation, represents a critical and effective pathway for optimizing BaCd₂P₂-based heterojunction solar cells.

5.1 Social, Legal, Ethical, and Environmental Considerations

5.1.1 Social Considerations

The development of high-efficiency solar cell technologies has significant social implications, particularly in the context of global energy access and sustainability. Improved photovoltaic performance can contribute to increased adoption of renewable energy, reducing dependence on fossil fuels and supporting energy security. In developing regions, including countries such as Bangladesh, advancements in solar technology can play a role in expanding off-grid and decentralized power solutions, thereby improving access to electricity in rural and underserved communities. Since this study is simulation-based, no direct social harm or community displacement is involved.

5.1.2 Legal Considerations

This research was conducted entirely through numerical simulation using SCAPS-1D and publicly available material parameters from peer-reviewed literature. No proprietary software misuse, restricted datasets, or intellectual property violations were involved. All referenced materials were appropriately cited, ensuring compliance with academic integrity and copyright regulations. Any future experimental realization of the proposed device structures would need to comply with national and international regulations related to material safety, environmental protection, and photovoltaic device certification standards.

5.1.3 Ethical Considerations

The study adheres to ethical research practices by maintaining transparency in methodology, reporting both optimized and unoptimized results, and avoiding data manipulation or selective reporting. Including unoptimized device performance highlights the importance of systematic optimization and prevents overstatement of results. As the work is simulation-based, it does not involve human subjects, animal testing, or hazardous laboratory procedures, thereby posing no direct ethical risk. Ethical responsibility is further maintained by clearly distinguishing between simulated performance predictions and experimentally validated results.

5.1.4 Environmental Considerations

Photovoltaic technology is inherently aligned with environmental sustainability, as it enables clean energy generation with minimal greenhouse gas emissions during operation. The BaCd₂P₂-based heterojunction solar cells studied in this work have the potential to contribute to reduced carbon emissions if successfully implemented. However, environmental considerations related to material sourcing, toxicity, and end-of-life disposal, particularly for cadmium-containing compounds, must be carefully evaluated in future experimental and commercial development. Lifecycle assessment and environmentally responsible fabrication practices would be essential to ensure that the environmental benefits of improved solar cell efficiency outweigh potential material-related risks.

5.2 Scope for Future Work

Although the present study provides valuable insights into the role of ETL–HTL combinations in BaCd₂P₂-based heterojunction solar cells, several directions remain open for future investigation:

1. **Experimental validation:** The optimized SnO₂/NiO_x device configuration identified through simulation should be experimentally fabricated and characterized to validate the numerical predictions and assess real-world fabrication constraints.
2. **Interface passivation studies:** Future work may explore the use of ultra-thin passivation layers or graded interfaces to further suppress interfacial recombination and improve device stability.
3. **Defect density and lifetime modeling:** A more detailed investigation of bulk and interface defect distributions, including carrier lifetime analysis, could provide deeper insight into recombination mechanisms.
4. **Thickness and optical optimization:** Optical modeling and absorber thickness optimization could be incorporated to maximize light absorption and further enhance J_{sc} without compromising electrical performance.

5. **Temperature and stability analysis:** Studying temperature-dependent performance and long-term stability using advanced simulation models would be beneficial for assessing practical deployment potential.
6. **Multijunction or tandem integration:** Given its favorable bandgap and carrier properties, BaCd_2P_2 could be explored as a sub-cell material in tandem or multijunction solar cell architectures.

References

- [1] Park, S. N., Kim, J. Y., Kim, Y. I., Kang, J. K., Sung, S. J., Kim, D. H., & Do, Y. S. (2023). Investigation of effective local contact Al₂O₃ rear passivation for high-efficiency thin CIGS solar cells. *Optical Materials Express*, 13(2), 553-565.
- [2] Seo, M., Yoon, S., Cho, H., Lee, S., Kim, K., Kong, B. D., ... & Baek, C. K. (2020). Solar cell using hourglass-shaped silicon nanowires for increased light-trapping path. *IEEE Journal of Photovoltaics*, 10(2), 475-479.
- [3] Hakim, F., & Alam, M. K. (2019). Performance enhancement of bulk heterojunction organic solar cells using photon upconverter. *Solar Energy*, 191, 300-310.
- [4] Kwon, H. C., Ma, S., Yun, S. C., Jang, G., Yang, H., & Moon, J. (2020). A nanopillar-structured perovskite-based efficient semitransparent solar module for power-generating window applications. *Journal of Materials Chemistry A*, 8(3), 1457-1468.
- [5] Kumar, A., Mahajan, R., Jain, R., Gupta, N., Jain, A., Kumar, K., & Goyal, A. K. (2024, April). Performance Enhancement and Analysis of CH₃ NH₃ 3Ge 0.85 Pb 0.125 I 3 Perovskite Solar Cell Towards Higher Efficiency. In *2024 IEEE Third International Conference on Power Electronics, Intelligent Control and Energy Systems (ICPEICES)* (pp. 706-709). IEEE.
- [6] Roy, D., Samajdar, D. P., & Biswas, A. (2021). Photovoltaic performance improvement of GaAs_{1-x}Bi_x nanowire solar cells in terms of light trapping capability and efficiency. *Solar Energy*, 221, 468-475.
- [7] Moussaoui, N., Benhamadouche, L., & Benhamadouche, A. D. (2024). Numerical Investigation of the Impact of Temperature on a-Si and GaAs/a-Si Semiconductor Solar Cells. *Journal of Electronic Materials*, 53(11), 6803-6810.
- [8] Tabernig, S. W., Yuan, L., Cordaro, A., Teh, Z. L., Gao, Y., Patterson, R. J., ... & Polman, A. (2022). Optically resonant bulk heterojunction PbS quantum dot solar cell. *ACS nano*, 16(9), 13750-13760.
- [9] Fatehi, N., Olyaei, S., Seifouri, M., & Parandin, F. (2024). Design of a high-efficiency perovskite solar cell based on photonic crystal in the absorption layer. *Optical and Quantum Electronics*, 56(3), 386.
- [10] Pal, D. (2023). A comprehensive analysis of eco-friendly Cs₂SnI₆ based tin halide perovskite solar cell through device modeling. *Advanced theory and simulations*, 6(3), 2200856.
- [11] Oulmi, N. Boosting the Efficiency of CH₃NH₃SnI₃ Perovskite Solar Cells by 31% Utilizing SnO₂ as Electron Transport Layer and NiO_x as Hole Transport Layer.
- [12] Kothandapani, Z., Islam, M. A., Reza, Y., Hasana, A. A., & Amin, N. (2020). Optimization of Cu₂O and CuSCN as HTL of planar perovskite solar cells via numerical simulation. *J. Ovonic Res*, 16(6), 369-377.
- [13] Lotfy, L. A., Abdelfatah, M., Sharshir, S. W., El-Naggar, A. A., Ismail, W., & El-Shaer, A. (2025). Numerical simulation and optimization of FTO/TiO₂/CZTS/CuO/Au solar cell using SCAPS-1D. *Scientific Reports*, 15(1), 28022.
- [14] Kuntavai, T., De, A., Bencherif, H., & Pal, D. (2025). Device Engineering and Optimization of a Novel Zintl-Phosphide BaCd₂P₂ Absorber-Based Thin Film Photovoltaic Cell. *physica status solidi (a)*, e202500371.
- [15] Ember. (2025, November 3). *Global Electricity Review 2025* | Ember. <https://ember-energy.org/latest-insights/global-electricity-review-2025/>
- [16] Ritchie, H., & Rosado, P. (2020, July 10). *Electricity mix*. Our World in Data. <https://ourworldindata.org/electricity-mix>.
- [17] Ember. (2025a, April 11). *Bangladesh* | Ember. <https://ember-energy.org/countries-and-regions/bangladesh/>

- [18] Yuan, Z., Dahliah, D., Hasan, M. R., Kassa, G., Pike, A., Quadir, S., ... & Hautier, G. (2024). Discovery of the Zintl-phosphide BaCd₂P₂ as a long carrier lifetime and stable solar absorber. *Joule*, 8(5), 1412-1429.
- [19] Ishraq, M. H., Kabir, M. R., Tarekuzzaman, M., Rahman, M. F., Rasheduzzaman, M., & Hasan, M. Z. (2024). ETL and HTL Engineering in CH₃NH₃PbBr₃ Perovskite for Stable and Efficient Performance Photovoltaic Devices Applications using SCAPS-1D. *Advanced Theory and Simulations*, 7(9), 2400360.
- [20] Pal, D. (2023). A comprehensive analysis of eco-friendly Cs₂SnI₆ based tin halide perovskite solar cell through device modeling. *Advanced theory and simulations*, 6(3), 2200856.
- [21] Samiul Islam, M., Sobayel, K., Al-Kahtani, A., Islam, M. A., Muhammad, G., Amin, N., ... & Akhtaruzzaman, M. (2021). Defect study and modelling of SnX₃-based perovskite solar cells with SCAPS-1D. *Nanomaterials*, 11(5), 1218.
- [22] Mandadapu, U., Vedanayakam, S. V., Thyagarajan, K., Reddy, M. R., & Babu, B. J. (2017). Design and simulation of high efficiency tin halide perovskite solar cell. *Int. J. Renew. Energy Res*, 7(4), 1603-1612.
- [23] Hossain, M. K., Arnab, A. A., Das, R. C., Hossain, K. M., Rubel, M. H. K., Rahman, M. F., ... & Pandey, R. (2022). Combined DFT, SCAPS-1D, and wxAMPS frameworks for design optimization of efficient Cs₂BiAgI₆-based perovskite solar cells with different charge transport layers. *RSC advances*, 12(54), 35002-35025.
- [24] Hossain, M. K., Arnab, A. A., Samajdar, D. P., Rubel, M. H. K., Hossain, M. M., Islam, M. R., ... & Dwivedi, D. K. (2023). Design insights into La₂NiMnO₆-based perovskite solar cells employing different charge transport layers: DFT and SCAPS-1D frameworks. *Energy & Fuels*, 37(17), 13377-13396.
- [25] Zaidi, B., Ullah, M. S., Zahra, S., Gagui, S., & Shekhar, C. (2021). Annealing Effects on the Opto-electronic Performance of Au and CuO Nanoparticles Incorporated P3HT/PCBM Solar Cells. *Journal of nano-and electronic physics*, (13, no. 5), 05016-1.
- [26] Al Ghaithi, A. O., Aravindh, S. A., Hedhili, M. N., Ng, T. K., Ooi, B. S., & Najjar, A. (2020). Optical properties and first-principles study of CH₃NH₃PbBr₃ perovskite structures. *ACS omega*, 5(21), 12313-12319.
- [27] Sunny, A., Rahman, S., Khatun, M., & Ahmed, S. R. A. (2021). Numerical study of high performance HTL-free CH₃NH₃SnI₃-based perovskite solar cell by SCAPS-1D. *AIP Advances*, 11(6).
- [28] Raga, S. R., Barea, E. M., & Fabregat-Santiago, F. (2012). Analysis of the origin of open circuit voltage in dye solar cells. *The journal of physical chemistry letters*, 3(12), 1629-1634.
- [29] Hossain, M. K., Mohammed, M. K., Pandey, R., Arnab, A. A., Rubel, M. H. K., Hossain, K. M., ... & Bhattarai, S. (2023). Numerical analysis in DFT and SCAPS-1D on the influence of different charge transport layers of CsPbBr₃ perovskite solar cells. *Energy & Fuels*, 37(8), 6078-6098.
- [30] Malliaras, G. G., Salem, J. R., Brock, P. J., & Scott, C. (1998). Electrical characteristics and efficiency of single-layer organic light-emitting diodes. *Physical Review B*, 58(20), R13411.
- [31] Guerrero, A., Bisquert, J., & Garcia-Belmonte, G. (2021). Impedance spectroscopy of metal halide perovskite solar cells from the perspective of equivalent circuits. *Chemical Reviews*, 121(23), 14430-14484.
- [32] Von Hauff, E., & Klotz, D. (2022). Impedance spectroscopy for perovskite solar cells: characterisation, analysis, and diagnosis. *Journal of Materials Chemistry C*, 10(2), 742-761.

- [33] Bi, E., Tang, W., Chen, H., Wang, Y., Barbaud, J., Wu, T., ... & Han, L. (2019). Efficient perovskite solar cell modules with high stability enabled by iodide diffusion barriers. *Joule*, 3(11), 2748-2760.
- [34] Jung, E. H., Jeon, N. J., Park, E. Y., Moon, C. S., Shin, T. J., Yang, T. Y., ... & Seo, J. (2019). Efficient, stable and scalable perovskite solar cells using poly (3-hexylthiophene). *Nature*, 567(7749), 511-515.
- [35] Bogachuk, D., Tsuji, R., Martineau, D., Narbey, S., Herterich, J. P., Wagner, L., ... & Hinsch, A. (2021). Comparison of highly conductive natural and synthetic graphites for electrodes in perovskite solar cells. *Carbon*, 178, 10-18.
- [36] Sunny, A., Rahman, S., Khatun, M., & Ahmed, S. R. A. (2021). Numerical study of high performance HTL-free $\text{CH}_3\text{NH}_3\text{SnI}_3$ -based perovskite solar cell by SCAPS-1D. *AIP Advances*, 11(6).
- [37] Behrouznejad, F., Shahbazi, S., Taghavinia, N., Wu, H. P., & Diau, E. W. G. (2016). A study on utilizing different metals as the back contact of $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cells. *Journal of Materials chemistry A*, 4(35), 13488-13498.
- [38] Sekar, K., & Mayarambakam, S. (2023). Effect of Annealed and Non-Annealed Inorganic MnS Hole-Transport Layer for Efficient $\text{Sb}_2(\text{S}, \text{Se})_3$ Solar Cells: A Theoretical Justification. *physica status solidi (b)*, 260(6), 2300087.

