Maximizing Conversion Efficiency of Solar Cell

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***Abstract*—This project aims to study the current-voltage (I-V) characteristics of solar cell to maximize its conversion efficiency η.**

***Index Terms*—solar cell, conversion efficiency.**

I. Introduction

Increasing conversion efficiency of solar cell is vital to improve the energy utilization. This study aims to maximize the conversion efficiency of solar cell.

A. Problem Statement and Solution

The primary purpose of this study is to investigate and present methodologies to maximize the conversion efficiency of solar cells.

The solution to this problem is controlling the constraints as constants and vary the value of each design choice, such as the doping concentration, to find the best set of parameters for the semiconductor device under given conditions.

By enhancing the efficiency with which solar cells convert sunlight into electrical energy, we can significantly increase the viability and attractiveness of solar energy as a major component of the global energy mix. This not only aids in reducing greenhouse gas emissions but also contributes to the development of a sustainable energy infrastructure capable of meeting future energy needs.

B. Objectives and Functionalities

There are several objectives for the project:

1) Understand the impact of each design choice on conversion efficiency.
2) Identify the optimal design settings for maximizing conversion efficiency.
3) Analyze the errors introduced by the simulation.

What this project tries to achieve is the following functionalities:

1) Conduct a comprehensive analysis of the importance and effects of various design choices for PN junction solar cells.
2) Develop an optimized design that maximizes conversion efficiency.
3) Evaluate the limitations and effects of the simulation using the Synamus package [1].

C. System Overview

The system designed to maximize the conversion efficiency of solar cells employs a structured workflow involving parameter tuning, simulation, and analysis. Initially, the system sets parameters such as temperature, doping concentrations (N_a, N_d), carrier mobilities (μ_n, μ_p), depletion region position (x_{pn}), dielectric constant (ϵ_r), and bandgap energy (E_g). These parameters are fed into the SynNumSeS simulation tool, which models the solar cell's I-V characteristics and power density. The workflow includes defining parameters, solving the system without bias, applying generation rates, performing voltage sweeps, and calculating the maximum power density. This iterative process helps identify the optimal parameter set for maximizing efficiency. The system's design emphasizes the complexity of achieving an analytical solution, thus leveraging simulation for precise optimization. It addresses challenges such as high computational latency by initially performing single-variable tuning to identify key influences before conducting comprehensive multi-variable tuning to ensure the highest possible efficiency.

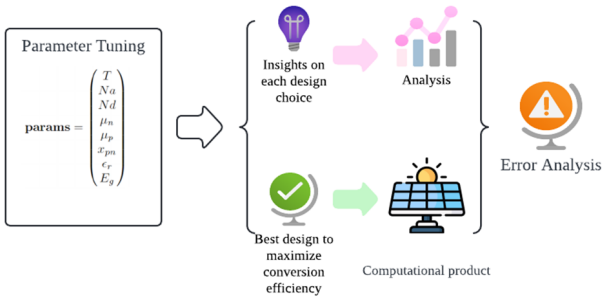


Fig. 1: System Workflow

II. Design

A. Design Motivation and Design Alternatives

***Motivation 1: Difficulty of Analytical Solution**:* The easiest design starts with a purely analytical method. In the following analysis, we will show such design is hard to achieve.

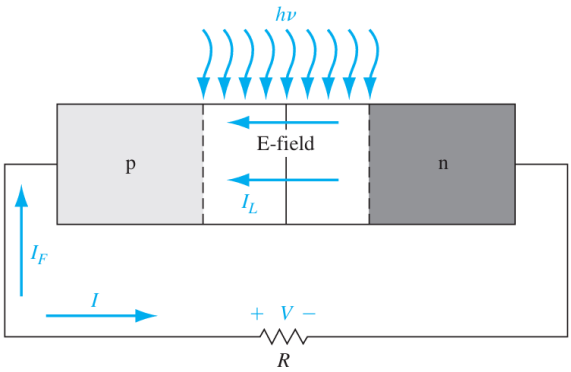


Figure 14.6 | A pn junction solar cell with resistive load.

Fig. 2: solar cell architecture

For a solar cell, we have [2]

$$I = I_L - I_F = I_L - I_S\left[\exp\left(\frac{eV}{kT}\right) - 1\right] \tag{1}$$

Several factors can impact the conversion efficiency (η) of a semiconductor device. These factors include:

- The material of the semiconductor, represented by its permittivity (ϵ_r).
- The physical layout of the semiconductor device, such as the position of the depletion region (x_{np}).
- The doping concentrations (N_D for donors and N_A for acceptors).
- Minority carrier lifetime and diffusion constants, which are influenced by carrier mobility (μ_n for electrons and μ_p for holes).
- Temperature (T).

Our goal is to identify the optimal settings to maximize η by tuning these parameters.

$$\textbf{params} = \begin{pmatrix} T \\ Na \\ Nd \\ \mu_n \\ \mu_p \\ x_{pn} \\ \epsilon_r \\ E_g \end{pmatrix} \tag{2}$$

$$\eta = \frac{P_m}{P_{in}} \times 100\% = \frac{I_m * V_m}{P_{in}} \times 100\% \tag{3}$$

In this equation, I_m, V_m are the current and voltage to produce maximum power output P_m. With P_{in} assumed to be given, we rewrite P_m with parameters [2]

$$P_m = I_m * V_m = \left(I_L - I_S\left[\exp\left(\frac{eV_m}{kT}\right) - 1\right]\right)V_m \tag{4}$$

Also, we have [2]

$$I_S = J_S * A = A\left(\frac{eD_n n_{p0}}{L_n} + \frac{eD_p p_{n0}}{L_p}\right) \tag{5}$$

where A is the cross-sectional area for the semi-conductor device.

We can also express I_S in the following format [2]

$$I_s = eAn_i^2\left(\frac{D_n}{L_n N_A} + \frac{D_p}{L_p N_D}\right) \tag{6}$$

Given the formula:

$$P_m = I_m \cdot V_m = \left(I_L - I_S\left[\exp\left(\frac{eV_m}{kT}\right) - 1\right]\right)V_m \tag{7}$$

First, we differentiate P_m with respect to V_m:

$$\frac{dP_m}{dV_m} = \frac{d}{dV_m}\left(V_m\left(I_L - I_S\left[\exp\left(\frac{eV_m}{kT}\right) - 1\right]\right)\right) \tag{8}$$

Using the product rule of differentiation, we get:

$$\frac{dP_m}{dV_m} = \left(I_L - I_S\left[\exp\left(\frac{eV_m}{kT}\right) - 1\right]\right) \tag{9}$$

$$+V_m \cdot \frac{d}{dV_m}\left(I_L - I_S\left[\exp\left(\frac{eV_m}{kT}\right) - 1\right]\right) \tag{10}$$

Simplifying the expression inside the derivative:

$$\frac{d}{dV_m}\left(I_L - I_S\left[\exp\left(\frac{eV_m}{kT}\right) - 1\right]\right) \tag{11}$$

$$= -I_S \cdot \frac{d}{dV_m}\left(\exp\left(\frac{eV_m}{kT}\right) - 1\right) \tag{12}$$

$$= -I_S \cdot \frac{d}{dV_m}\left(\exp\left(\frac{eV_m}{kT}\right)\right) \tag{13}$$

Using the chain rule:

$$= -I_S \cdot \exp\left(\frac{eV_m}{kT}\right) \cdot \frac{e}{kT} \tag{14}$$

Substituting this result back into the derivative of P_m:

$$\frac{dP_m}{dV_m} = \left(I_L - I_S\left[\exp\left(\frac{eV_m}{kT}\right) - 1\right]\right) + V_m\left(-I_S \cdot \exp\left(\frac{eV_m}{kT}\right) \cdot \frac{e}{kT}\right) \tag{15}$$

$$= I_L - I_S\left[\exp\left(\frac{eV_m}{kT}\right) - 1\right] - V_m \cdot I_S \cdot \exp\left(\frac{eV_m}{kT}\right) \cdot \frac{e}{kT} \tag{16}$$

Set the derivative equal to zero to find V_m:

$$I_L - I_S\left[\exp\left(\frac{eV_m}{kT}\right) - 1\right] - V_m \cdot I_S \cdot \exp\left(\frac{eV_m}{kT}\right) \cdot \frac{e}{kT} = 0 \tag{17}$$

Simplify this equation to isolate V_m:

$$I_L = I_S\left[\exp\left(\frac{eV_m}{kT}\right) - 1\right] + V_m \cdot I_S \cdot \exp\left(\frac{eV_m}{kT}\right) \cdot \frac{e}{kT} \tag{18}$$

$$I_L = I_S \exp\left(\frac{eV_m}{kT}\right) - I_S + V_m \cdot I_S \cdot \exp\left(\frac{eV_m}{kT}\right) \cdot \frac{e}{kT} \tag{19}$$

Factor out $I_S \exp\left(\frac{eV_m}{kT}\right)$:

$$I_L = I_S\left(\exp\left(\frac{eV_m}{kT}\right)\left(1 + V_m \cdot \frac{e}{kT}\right) - 1\right) \tag{20}$$

Finally, solve for V_m:

$$\frac{I_L + I_S}{I_S} = \exp\left(\frac{eV_m}{kT}\right)\left(1 + V_m \cdot \frac{e}{kT}\right) \tag{21}$$

$$\frac{I_L + I_S}{I_S\left(1 + V_m \cdot \frac{e}{kT}\right)} = \exp\left(\frac{eV_m}{kT}\right) \tag{22}$$

Taking the natural logarithm of both sides:

$$\ln\left(\frac{I_L + I_S}{I_S\left(1 + V_m \cdot \frac{e}{kT}\right)}\right) = \frac{eV_m}{kT} \tag{23}$$

$$V_m = \frac{kT}{e}\ln\left(\frac{I_L + I_S}{I_S\left(1 + V_m \cdot \frac{e}{kT}\right)}\right) \tag{24}$$

However, we didn't explicitly solve for V_m as it appears on both sides of the equation. This motivates us to use a black-boxed simulation tool, such as Synumses [1] to better compute η given any sets of parameters.

Motivation 2: High Computation Latency of the Emulation with Huge Possible Domain: It is straightforward to redesign the previous analytical continuous method into a full enumeration discrete method. Specifically, we enumerate each possible setting of the semiconductor device and use a Python simulation to calculate the corresponding conversion efficiency (η). In the following analysis, we will demonstrate the difficulty of obtaining the maximum η using this method due to time constraints.

For each simulation, the Python program takes approximately 10 seconds to run on an I-9 processor with a 24-core CPU. For a brute force enumeration of the parameter set, the time required to complete the computation is as follows.

$$t = 6^8 \times 10 \approx 194.4 \text{ days} \tag{25}$$

which is impossible for our project schedule. There must be ways to reduce this time complexity by using some assumptions of independence between each parameter and the power density by observing the initial trials conducted. It will be introduced with more details in design section.

Motivation 3: Errors Existing on Simulation: Unlike analytical result, simulation bases on converging discrete sequences, so once we pinpoint a setting that maximizes the efficiency, it is necessary to investigate the **reproducibility** and the **fault tolorence** near such settings.

B. Design Details

We first need to set up the unchanged variables for the experiment. We fix the incident light intensity 1000 W/m² (AM1.5G spectrum).

Since the P_{in} is fixed, the only thing that needs to be maximized is the output power density P_{out}. Maximizing output power density will give us the largest η.

We will split the experiment into 2 parts:

- Single Variable Tuning: tune the variable independently
- Multiple Variable Tuning: tune the variable in groups.

We assumed that the variables that are not tuned in groups independent of each other in terms of their inluence to the η. The assumptions will be obtained by single variable tuning analysis.

We will use the black-boxed method shown below to investigate both parts of the experiments.

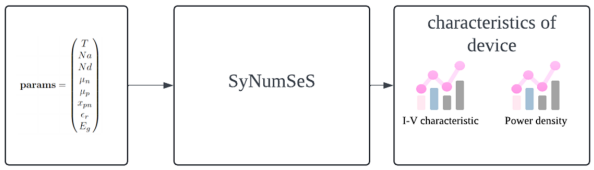


Fig. 3: Experiment Method

The steps of the algorithm used for simulating the maximum power density of a solar cell is shown below. The workflow consists of the following steps: defining parameters, solving without bias, putting generation, voltage sweep, and getting the maximum power density.

C. Steps of the Algorithm

1. Defining Parameters: The first step involves setting up the necessary parameters for the simulation. This includes initializing the geometry of the solar cell and defining material properties such as the bandgap energy and dielectric constant. Additionally, the doping concentrations for different regions of the solar cell are specified. These parameters form the foundation for all subsequent calculations.

2. Solving Without Bias: In the second step, the system's equations are solved without any external bias applied. This step is crucial for determining the equilibrium state of the solar cell, where the distribution of charge carriers and electric fields are calculated under no applied voltage.

3. Setting Generation Rate: The third step involves simulating the effect of illumination on the solar cell. The generation rate, which represents the rate at which electron-hole pairs are created due to the absorption of photons, is set. This step models how the solar cell responds to light and how it affects the carrier concentrations and currents.

4. Performing Voltage Sweep: In the fourth step, a voltage sweep is performed. This involves applying a range of bias voltages to the solar cell and calculating the resulting current density for each voltage. This step is essential for understanding the current-voltage characteristics of the solar cell and for determining its performance under different operating conditions.

5. Calculating Maximum Power Density: The final step is to calculate the maximum power density. Using the current density and voltage data obtained from the voltage sweep, the power density (which is the product of current density and voltage) is calculated. The maximum power density is then identified, which indicates the optimal operating point of the solar cell where it generates the most power.

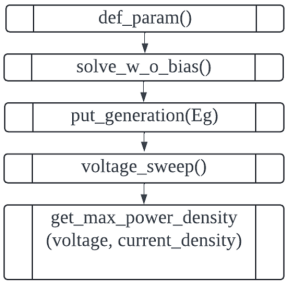


Fig. 4: Algorithm supporting SyNumSeS

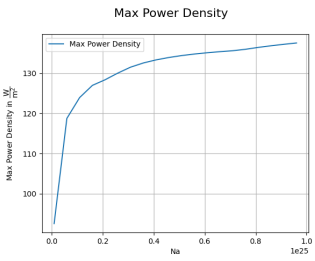
D. Result and Analysis: Single Variable Tuning

First, we will tune each parameters in the parameter set.

$$\mathbf{params_{default}} = \begin{pmatrix} T \\ Na \\ Nd \\ \mu_n \\ \mu_p \\ x_{pn} \\ \epsilon_r \\ E_g \end{pmatrix} = \begin{pmatrix} 300\,\mathrm{K} \\ 1.0 \times 10^{24}\,\mathrm{cm}^{-3} \\ 2.0 \times 10^{23}\,\mathrm{cm}^{-3} \\ 0.05\,\mathrm{cm}^2/\mathrm{Vs} \\ 0.039\,\mathrm{cm}^2/\mathrm{Vs} \\ 40\,\mathrm{nm} \\ 11.7 \\ 1.12\,\mathrm{eV} \end{pmatrix} \tag{26}$$

Each time we investigate in one parameter, we set the other parameters to their default values shown above. We tune the Na in the range of 10^{13} to 10^{25} cm^{-3} . We tune the Nd in the range of $2 * 10^{21}$ to $2 * 10^{23}$ cm^{-3}. We tune the range of the position of the depletion region between 40 nm to 500 nm. We tune the range of Eg, given that it is homogeneous across the solar cell. We tune the range of permitivity of the device. We finally tune the range of temperature.

We first obtain the Power density versus Na and Nd doping concentration, as well as power density versus depletion region position diagram.



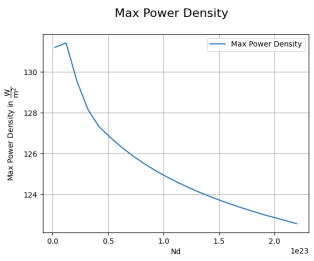


Fig. 5: Na doping concentrationFig. 6: Nd doping concentration

To better illustrate some insights of the Na vs power density diagram, I add the slope for smaller Na and larger Na. The plot and the following computation is based on a default parameter setting. I also compute the corresponding η at the large Na area, which is $\eta \approx 13.8\%$

When the value of Na increases, the slope decrease drastically, making it unnecessary to experiment with larger Na values. This will be shown in the multiple variable experiment, where we also only experiment with Na lower than 10^{25} cm^{-3}, effectively reduce the experiment cost. The analysis for Nd is quite similar to the analysis of Na, so we will omit the discussion of Nd.

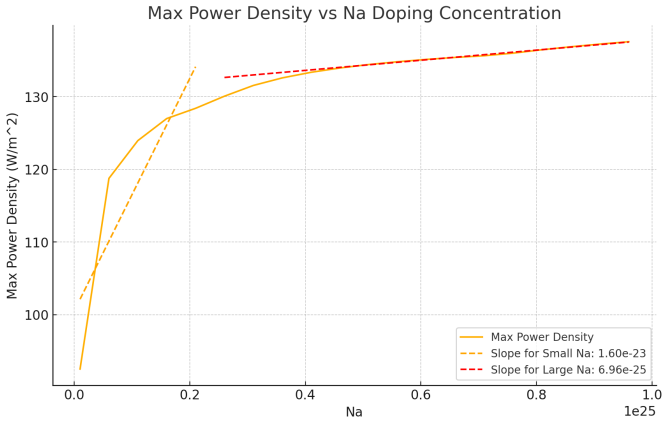


Fig. 7: Power density versus Na doping concentration

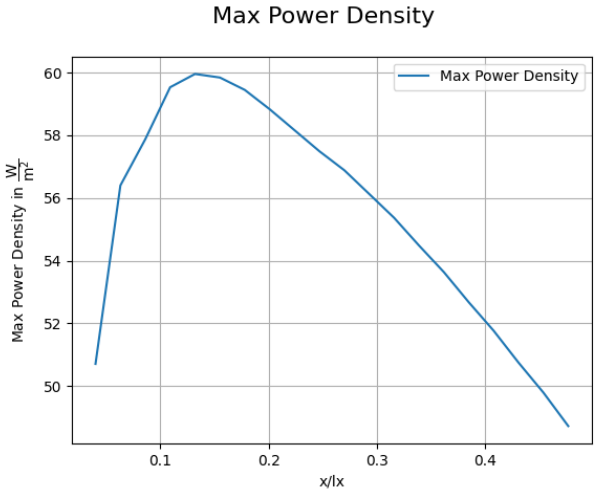


Fig. 8: Power density versus depletion region position

For the position of depletion region, we can see that the trend is not monotonous, and after further analysis, we find that the distribution of power density against Na, Nd, and position of depletion region is connected, this motivates us to investigate it further in the multiple variable analysis.

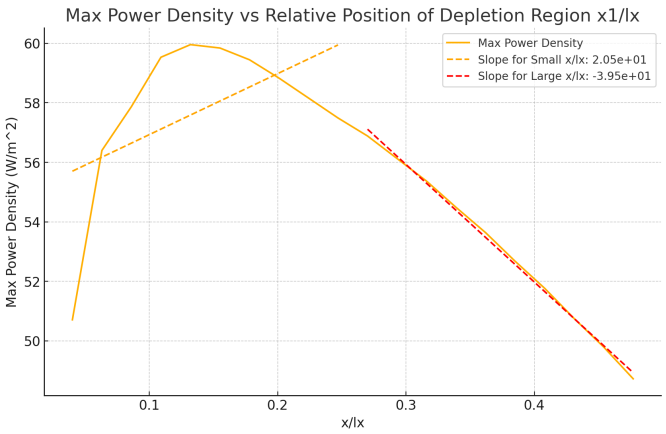


Fig. 9: Power density versus depletion region position

The energy gap can only generates valid simulation between $0.2eV$ to $1.12eV$ and its impact to power density is almost linear in a continuous scope. After tuning several other parameters, we observed that the energy gap influences the power density independent of other parameters.

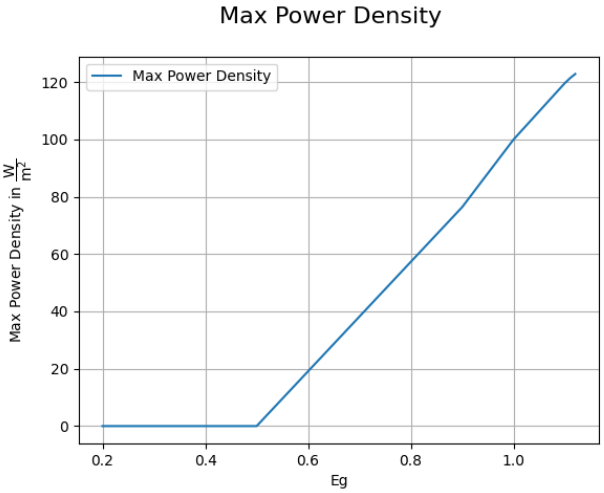


Fig. 10: Power density versus Energy band gap

The analysis of the following four diagrams provides valuable insights for maximizing the conversion efficiency (η), given a fixed input power (P_{in}), where the power density directly determines η.

- **Figure 11:** This figure shows that the power density increases with the semiconductor permittivity (ϵ_r). This suggests that using materials with higher permittivity enhances power density due to their ability to store more electric energy. However, the sudden drop at the low permittivity end indicates potential instability or inefficiencies that need to be considered.
- **Figure 12:** This figure illustrates a linear decrease in power density with increasing working temperature (T). Higher temperatures increase thermal agitation, negatively impacting power density. Thus, effective thermal management and cooling solutions are crucial for maintaining lower operating temperatures to maximize η.
- **Figure 13:** This figure shows that the power density decreases with increasing electron mobility (μ_n). This trend indicates that higher mobilities lead to increased recombination rates, reducing power density. Therefore, optimizing electron mobility to ensure efficient charge transport while minimizing recombination losses is essential.
- **Figure 14:** This figure depicts a similar decrease in power density with increasing hole mobility (μ_p). Like electron mobility, optimizing hole mobility is necessary to balance efficient charge transport and minimize recombination losses.

Overall, to maximize η, it is important to select materials with high permittivity, implement effective thermal management, and optimize the charge carrier properties by balancing electron and hole mobilities. Additionally, addressing any potential instabilities at low permittivity levels is necessary to avoid sudden drops in power density. We will cover the error analysis for the permittivity of semiconductor devices later.

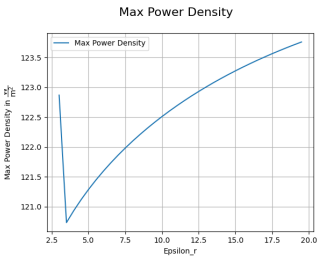


Fig. 11: Power density versus semiconductor permittivity

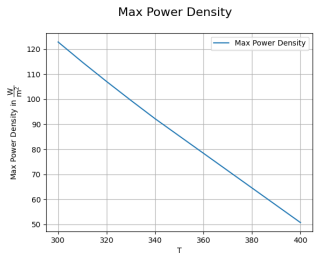


Fig. 12: Power density versus working temperature

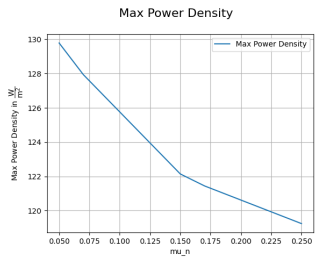


Fig. 13: Power density versus electron mobility

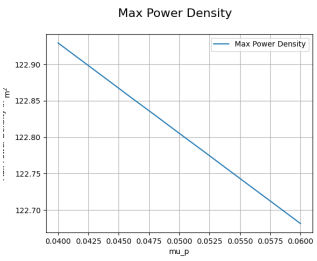


Fig. 14: Power density versus hole mobility

E. Result and Analysis: Multiple Variable Tuning

x_{np}	Na	Nd	η
4.00e-08	8.35e+24	1.67e+23	0.14347
4.00e-08	8.35e+24	1.34e+23	0.14331
4.00e-08	6.70e+24	1.67e+23	0.14285
4.00e-08	8.35e+24	1.01e+23	0.14282
4.00e-08	6.70e+24	1.34e+23	0.14270

These are the top 5 parameter sets for η. As we can see, the position of x_{np} is fixed at $40\ nm$. This is because the enumeration step being too large. To accurately pinpoint the optimized design, we should fine-tune the value of x_{np} near $40nm$.

As we fine-tune the value of x_{np}, namely changing the position of the depletion region, we can see that η does not increase significantly. Hence, we exclude the interference of large step size when enumerating the position.

x_{np}	Na	Nd	η
5e-08	8.35e+24	1.67e+23	0.142068408622
6e-08	8.35e+24	1.67e+23	0.141150274428
7e-08	8.35e+24	1.67e+23	0.140166677177
8e-08	8.35e+24	1.67e+23	0.142068408622

F. Tolerance and Error Analysis

Based on the multiple variable analysis, we can finalize our design by carefully analyzing the error created by two factors: step size of enumeration and simulation convergence accuracy. Step size of enumeration is caused by our algorithm, as we iterate through the search space by certain quantity for each enumerated parameter. Below is a table analyzing the error introduced by the step size of enumeration of Na, Nd and x_{np}.

Data Point	1	2	3	4
$\frac{\eta_{\max}-\eta_{\min}}{\eta}$ for N_a	0.00537	0.00537	0.00539	0.00539
$\frac{\eta_{\max}-\eta_{\min}}{\eta}$ for N_d	0.00537	0.00537	0.00539	0.00539

TABLE I: Relative Change in Efficiency (η) for Different N_a and N_d Values

The relative change in efficiency (η) due to variations in acceptor concentration (N_a) and donor concentration (N_d) is approximately 0.54%, indicating that changes in N_a and N_d do not significantly affect the efficiency.

Data Point	1	2	3	4
$\frac{\eta_{\max}-\eta_{\min}}{\eta}$	0.01339	0.01347	0.01357	0.01339

TABLE II: Relative Change in Efficiency (η) for Different x_{np} Values

The relative change in efficiency (η) due to variations in x_{np} is approximately 1.35%, indicating that changes in x_{np} do not significantly affect the efficiency.

η	v_size	gen_step	η
0.143468	0.025	25	0.143
0.141326	0.025	25	0.1413
0.141352	0.025	25	0.1413
0.141405	0.02	25	0.1414
0.141406	0.02	50	0.1414

TABLE III: Summary of η, v_size, and gen_step for different trails

Explanation: The table above summarizes the efficiency η, voltage step size (v_size), generation step (gen_step), and maximum power density for five different trials.

- The first three trials, including the one with the highest efficiency of 0.143 (trial not shown here), all used a v_size of 0.025 and a gen_step of 25.
- The fourth trial used a v_size of 0.02 and a gen_step of 25.
- The fifth trial used a v_size of 0.02 and a gen_step of 50.

The efficiency η values are very close across all trials, ranging from 0.141326 to 0.143468. Despite changes in the voltage step size (v_size) and generation step (gen_step), there is no significant impact on the efficiency values.

For instance:

- Comparing trials 2 and 4, where only the v_size changed from 0.025 to 0.02, the efficiency changed slightly from 0.141352 to 0.141405.
- Similarly, comparing trials 4 and 5, where the gen_step changed from 25 to 50 while keeping the same v_size, the efficiency changed minimally from 0.141405 to 0.141406.

Thus, it can be concluded that the variations in v_size and gen_step do not significantly contribute to changes in the efficiency η. The changes in η are primarily due to other factors in the parameter set, and the minor variations observed are within the expected range of experimental or numerical simulation variability.

G. Deliverable

Below we show some characteristics of our designed solar cell.

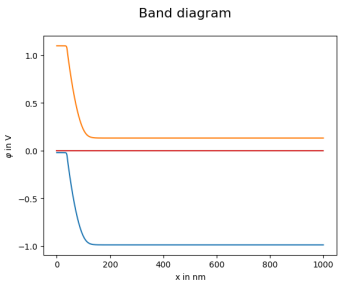


Fig. 15: Banddiagram of the designed device

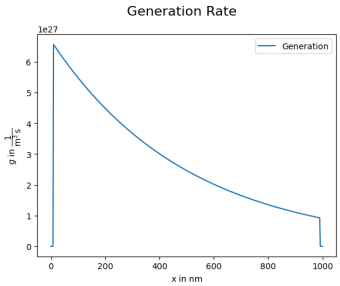


Fig. 16: generation rate over the designed device

Below we show the boost our design has over the baseline (solar cell with default parameter), our design has 10% boost on η, from 12.9% to 14.2%.

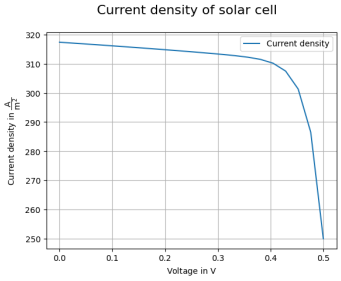


Fig. 17: IV characteristic curve of designed device

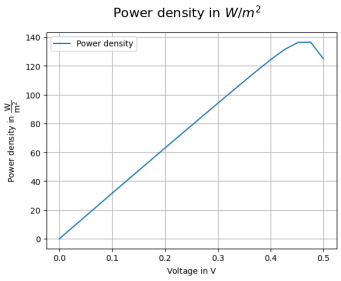


Fig. 18: power density curve of designed device

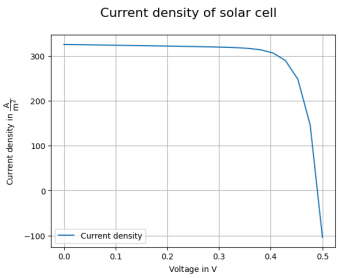


Fig. 19: IV characteristic curve of baseline device

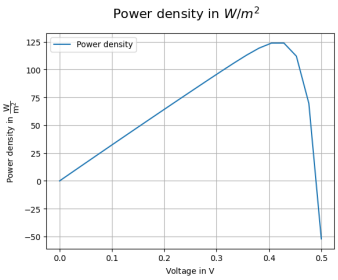


Fig. 20: power density curve of baseline device

III. Conclusion

A. Achievement

This study has successfully achieved the objectives set in previous sections. It increases the conversion efficiency from 12.9% with default parameter to 14.2% with current parameters, with a 10% boost. It explored various strategies to enhance the conversion efficiency of solar cells, using both single variable analysis and multiple variable analysis. The study explores the impact of each parameter to conversion efficiency of solar cell under a default setting, and explores the integral impact of a group of parameters to conversion efficiency of solar cell. The study also analyses the error introduced by the nature of simulation by python package.

B. Uncertainties

Despite the achievements, there are still a list of uncertainties left for future exploration. First, this study only investigate one group of variables, assuming the other parameters are independent of each other. This is a strong assumption and should be investigated further. It is uncertain under what condition this assumption is true and vice versa. Another uncertainty is the scope of design choices. This study focuses on the 8 parameters that can influence the performance of the semiconductor solar cell. However, more parameters can be crucial to improve the conversion efficiency. Another uncertainty is the intensity of the incident light. This study set the incident light constant at 1 kW/m^3. However, the output power density is not independent from the intensity of input light, as it influence the generation rate in different positions on the semiconductor device.

C. Future works

The future work could be focusing on the following aspects:

1) Investigating combination of different parameters and their impact to conversion efficiency.
2) Find more design choices of solar cell. Explore semiconductors instruments of different types
3) Explore the impact of intensity of incident light.

References

[1] P. Abele and M. Schäfer, "Synumses: A python package for numerical simulation of semiconductor devices," *HTWG Konstanz - University of Applied Sciences*, 2023.

[2] D. A. Neamen, *Semiconductor Physics and Devices: Basic Principles*, Fourth. New York, NY: McGraw-Hill Education, 2012.