East European Journal of Physics. 2. 431-436 (2024)
DOI:10.26565/2312-4334-2024-2-56 ISSN 2312-4334

ENHANCING SOLAR CELL CONVERSION EFFICIENCY THROUGH EVOLUTIONARY OPTIMIZATION USING GENETIC ALGORITHMS

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Received March 24, 2024 revised April 15, 2024; accepted May 3, 2024

In this study, we propose a new method based on genetic algorithms to optimize the performance of intermediate-band solar cells (IBSC). Our approach aims to maximize photovoltaic conversion efficiency by judiciously optimizing the geometric and physical parameters of the IBSC structure., which must be partially filled. This filling ensures the presence of both empty states in the intermediate band (IB) to receive electrons from the valence band (VB), and filled states to provide electrons to the conduction band (CB). Recently, studies have observed the effect of IB occupancy on cell efficiency, and calculated the optimal efficiency for IB devices. The analytical expression for optimal IB filling has been utilized for different scenarios involving IB-CB coupling strength and IB region width. In this work we have studied the influence of the intermediate band energy level, the effects of doping on efficiency, short-circuit current, open-circuit voltage, fill factor, and in order to validate our approach on parasitic effects such as series and shunt resistance.
Keywords: *Solar cell; Intermediate-band solar cells; Band energy level; Series and shunt resistance; absorption coefficients*
PACS : 88.40.hj; 88.40.H; 85.30.De; 61.82.Fk; 88.10.gc

1. INTRODUCTION

The quest for highly efficient solar cells has been a driving force in the field of photovoltaics, with the ultimate goal of harnessing the maximum amount of energy from the solar spectrum. Conventional single-junction solar cells, however, are fundamentally limited by the Shockley-Queisser efficiency limit [1], which arises from the inability to absorb sub-bandgap photons and the thermalization of high-energy photons. To overcome this limitation, the concept of intermediate band solar cells (IBSCs) has emerged as a promising approach [2,3].

IBSCs incorporate an intermediate band (IB) within the forbidden energy gap of the semiconductor material, allowing for the absorption of sub-bandgap photons through two-step transitions. Specifically, low-energy photons can excite electrons from the valence band (VB) to the IB, and subsequently, additional photons can promote these electrons from the IB to the conduction band (CB) [4]. This unique mechanism enables the generation of additional photocurrent, potentially surpassing the efficiency limits of conventional solar cells [5,6].

Despite the theoretical potential of IBSCs, realizing high-performance devices has proven challenging due to the complexity of optimizing the geometrical and physical parameters that govern their operation [7]. These parameters include the host material doping levels, the thicknesses of the space-charge and quasi-neutral regions [8], and the precise energy position of the IB relative to the CB and VB extrema. Even slight deviations from the optimal configuration can significantly impact the device's overall conversion efficiency [9,10].

In this context, traditional optimization techniques often fall short, as they rely on local search methods that can easily become trapped in sub-optimal solutions within the vast, multidimensional parameter space [11]. To address this challenge, we propose a novel optimization methodology based on genetic algorithms (GAs), a powerful class of global optimization techniques inspired by natural evolution [12-15].

Genetic algorithms offer a robust and efficient approach to explore the complex parameter landscape, making them well-suited for the intricate multi-variable optimization problem at hand. By mimicking the principles of natural selection, GAs iteratively evolve a population of candidate solutions, gradually improving their fitness through processes such as crossover and mutation, ultimately converging towards near-optimal configurations [16-18].

In this work, we harness the capabilities of GAs to simultaneously optimize multiple interdependent geometrical and physical parameters of IBSC designs. Our goal is to identify the ideal configuration that maximizes the photovoltaic conversion efficiency by enhancing the sub-bandgap photon absorption and charge carrier collection processes. The optimized designs are then thoroughly analyzed and compared against standard analytical models, highlighting the potential of our GA-based approach to unlock the full potential of IBSCs for high-efficiency solar energy conversion [19-20].

2. DESCRIPTION OF THE MODEL

The Fig. 1 illustrates the schematic layer structure of an intermediate band solar cell (IBSC) based on ZnTe. ZnTe has been selected as the material of choice for this analysis, as it serves as a prototypical example for IBSCs. This choice

Cite as: B. Lakehal, A. Dendouga, East Eur. J. Phys. 2, 431 (2024), https://doi.org/10.26565/2312-4334-2024-2-56

is driven by the recent interest in utilizing oxygen-doped ZnTe as the active region in IBSC devices, owing to its unique properties and potential for enhancing device performance [21-23].

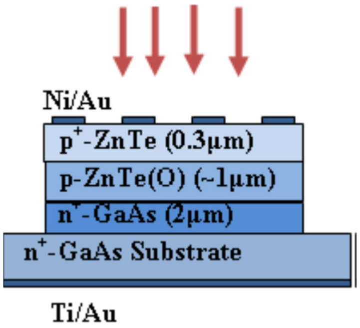

Figure 1. Device structure of an intermediate band solar cell based on ZnTe:O.

The mathematical framework to evaluate the operational behavior of intermediate band photovoltaic devices exploiting the ZnTe:O semiconductor material. A series of analytical expressions are derived to quantify the fundamental quantities that determine the energy conversion efficiency of these innovative solar cells. Firstly, the equations governing the photocurrent density J_{ph} generated by the absorption of incident photons and their transfer to the conduction band are established [21-23]:

$$Jph = JL_0D[1 - \exp(-1/D \tag{1}$$

$$D = l_c(1 - Va/V_{bi})/W \tag{2}$$

$$G_{IC}(x) = \int_{E_I}^{E_C} \alpha_{IC}(E) I_0(E) exp\,(-\alpha_{tot}(E)x) dE \tag{3}$$

$$G_{VI}(x) = \int_{E_V}^{E_G} \alpha_{VI}(E) I_0(E) exp\,(-\alpha_{tot}(E)x) dE \tag{4}$$

These equations take into account the intrinsic material properties such as the absorption coefficients α, the intermediate band electronic state density Ni, as well as the charge carrier transport characteristics.

$$\alpha_{IC} = \alpha_{IC0} f,\ \alpha_{VI} = \alpha_{VI0}(1-f) \tag{5}$$

$$\alpha_{IC}(Ni) = \alpha_{IC0} f = \sigma_{opt,n} Ni f \tag{6}$$

$$\alpha_{VI}(Ni) = \alpha_{VI0}(1-f) = \sigma_{opt,p} Ni f \tag{7}$$

$$\tau_{tot}(Ni) = 1/C_p\, Ni \tag{8}$$

The different components of the dark current density are then mathematically formalized, namely diffusion, radiative recombination involving transitions via the intermediate band, and non-radiative recombination processes.

$$I_{diff} = \left(\frac{qn_i^2 D_n}{W_p N_D} + \frac{qn_i^2 D_p}{W_n N_A}\right)\left(\exp\left(\frac{qV_a}{KT}\right) - 1\right) \tag{9}$$

$$Ir,CV = q\frac{2\pi}{h^3C^2}\int_{E_g}^{\infty} E^2(1 - \exp(W\alpha_{vc}))\exp\left(\frac{-E}{KT}\right) dE \times \left(\exp\left(\frac{qV_a}{KT}\right) - 1\right) \tag{10}$$

$$I_{r,CI} = I_{0,r,CI}\left(exp\frac{qV_a(1-\xi)}{KT} - 1\right) \tag{11}$$

Where

$$I_{0,r,CI} = q\frac{2\pi}{h^3C^2}\int_{E_I}^{E_C} E^2(1 - exp(W\alpha_{Ic}))\, exp\left(\frac{-E}{KT}\right) dE \tag{12}$$

$$I_{nr} = \frac{qn_iW}{2\tau_{tot}\gamma}\left(\exp\left(\frac{qV_a}{KT}\right) - 1\right) \tag{13}$$

Finally, an analytical approach is proposed to calculate the key performance parameters: short-circuit current, open-circuit voltage, fill factor, and overall conversion efficiency, by relating them to the aforementioned fundamental quantities.

$$I = I_D - (I_{ph} + I_{ph;IB}) \tag{14}$$

$$\eta = \frac{P_{max}}{P_s} = \frac{FF.I_{cc}.V_{co}}{P_s} \tag{15}$$

$$FF = \frac{P_{max}}{V_{co}.I_{cc}} \tag{16}$$

3. CALCULATION METHODOLOGY

Our objective is to maximize the efficiency of the IBSC cell. To achieve this, we have used an optimization strategy based on a Genetic Algorithm (GA) applied to determine the geometrical and physical parameters of the solar cell. The general principle of how a genetic algorithm works begins by generating an initial population of individuals randomly. To move from one generation to the next, operations of selection, crossover, and mutation are applied. Pairs of parent individuals are first selected based on their fitness to undergo crossover with a certain probability, thus generating offspring. Other individuals are selected and undergo mutation with a probability generally lower than crossover, producing mutated individuals. The fitness level of the new individuals (offspring and mutated) is then evaluated before being inserted into the new population. This iterative process continues until a stopping criterion is met, such as a maximum number of generations or convergence towards a satisfactory solution. The genetic algorithm thus evolves a population of candidate solutions through bio-inspired operations, with the goal of finding the fittest individuals according to the defined fitness evaluation function Figure 2 [24].

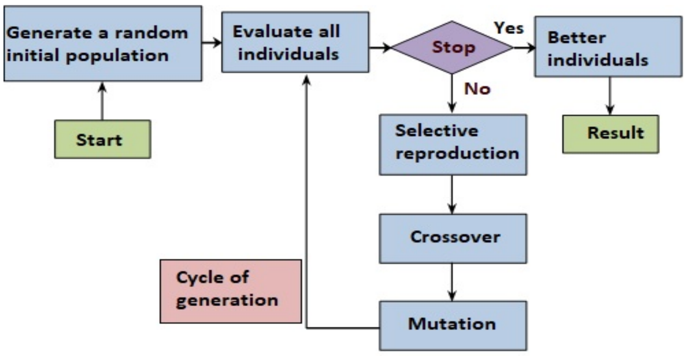

Figure 2. General Principle of Genetic Algorithms

In our case, each chromosome contains a parameter which are $\mathbf{N_A = N_D}$, $\boldsymbol{\alpha_{IC0} = \alpha_{VI0}}$, $\boldsymbol{W}$ and $\boldsymbol{\tau_{tot}}$. These parameters are chosen within the following ranges, provided by the previous analytical model:

$\boldsymbol{\alpha_{IC0}}$: from 100 to 10^4 cm^{-1}
$\boldsymbol{\alpha_{VI0}}$: from 100 to 10^4 cm^{-1}
$\mathbf{N_A}$: from 10^{14} to 10^{21} cm^{-3}
$\mathbf{N_D}$: from 10^{14} to 10^{21} cm^{-3}
$\boldsymbol{W}$: from 100 nm to 10 µm
$\boldsymbol{\tau_{tot}}$: from 1 to 100 µs

These ranges ensure that an optimal value exists, and which has been confirmed by our algorithm.

4. RESULTS AND DISCUSSION

In this study, we put forth a computational approach that harnesses genetic algorithms (GAs) to optimize the electrical performance of intermediate band solar cell (IBSC) designs. Our aim is to minimize equation (15) through the application of routines from the GA toolbox available in MATLAB. Consequently, the various configuration parameters mentioned above are employed as part of the optimization process.

Table 1. Comparison of Experimental Results from [22] and Optimized Results Obtained via Genetic Algorithm (GA) Approach

Parameters	Experimental results [22]	GA Results
α_{IC0} (cm-1)	/	9.65×10^3
α_{VI0}(cm-1)	/	9.65×10^3
N_A (cm^{-3})	10^{19}	1.72×10^{20}
N_D (cm^{-3})	2×10^{18}	1.72×10^{20}
τ_{tot}[us]	/	9.72
R_S ($\Omega.cm^2$)	300	300
Rsh($\Omega.cm^2$)	3×10^3	3×10^3
W(um)	1	1.5
V_{oc} (V)	0.38	0.9715
J_{cc} (mA/cm^2)	3.6	3.234
FF(%)	31	25
η(%)	0.43	0.786

Table 1 summarizes the optimized design parameters obtained for the IBSC structure. When compared to the analytical model of the same IBSC structure presented in [21], the results evidently show an improved conversion efficiency for the optimized IBSC design obtained through the genetic algorithm approach. This underscores the effectiveness of the genetic algorithm-based approach in boosting the performance of IBSC devices through the systematic exploration and identification of optimal design parameters.

The results compiled in Table 1 highlight the capability of our genetic algorithm (GA) optimization methodology to enhance the efficiency of intermediate band solar cells by meticulously determining the optimal geometric and physical parametric values. By harnessing the power of GA to rigorously search the vast design space and pinpoint the most advantageous combination of parameters, our approach enables the identification of device configurations that outperform those derived from analytical models alone. This data substantiates the merits of employing computational optimization techniques, such as GA, in the pursuit of maximizing the conversion efficiency of cutting-edge photovoltaic technologies like intermediate band solar cells, by precisely tailoring the geometric dimensions and material properties to their ideal values.

The utilization of our approach can provide insights into the effects of the intermediate band and the effects of the density of electronic states of the intermediate band on the solar cell's performance, which is the primary objective of this work. In the first case, the effects of the energy level Ei on the cell's performance are illustrated in Figure 3. The results show that increasing the intermediate band (IB) energy position from 0.4 eV to 0.6 eV leads to an increase in efficiency from 14.91% to a maximum of 28.97%. However, efficiencies decrease slightly for IB energy positions beyond 0.6 eV [21].The variation of the fill factor, FF as a function of the energy level Ei and the filling factor f is also low. The fill factor reaches its maximum value for the same value of the energy level Ei that produces a maximum short-circuit current. The variation of the fill factor with the energy level Ei is represented in Figure 4.

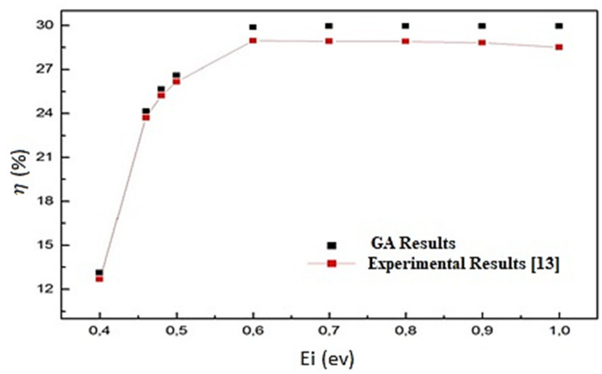

Figure 3. Variation of efficiency versus Ei

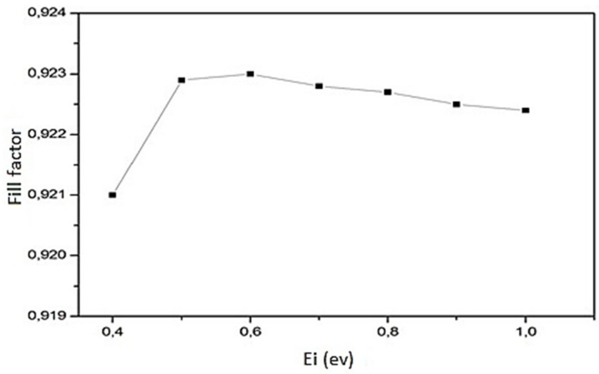

Figure 4. Variation of fill factor versus Ei

Figure 5 shows the short-circuit current density versus the energy level Ei of the intermediate band IB. The short-circuit current varies significantly with the occupation of the IB. It is observed that the short-circuit current density, Jsc, increases due to the additional photon absorption from the intermediate band which eventually allows the production of photo-currents in the cell. The Figure 6 shows the relationship between the open-circuit voltage, V_{oc}, and the energy level Ei of the intermediate band IB. Although V_{oc} increases with increasing energy level Ei, this increase occurs with small values compared to Jsc [21].

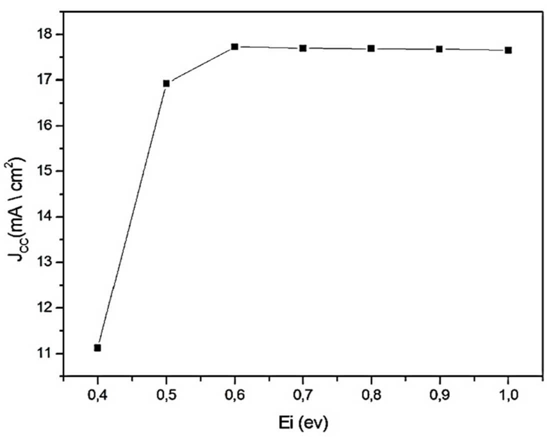

Figure 5. Variation of short-circuit current versus Ei

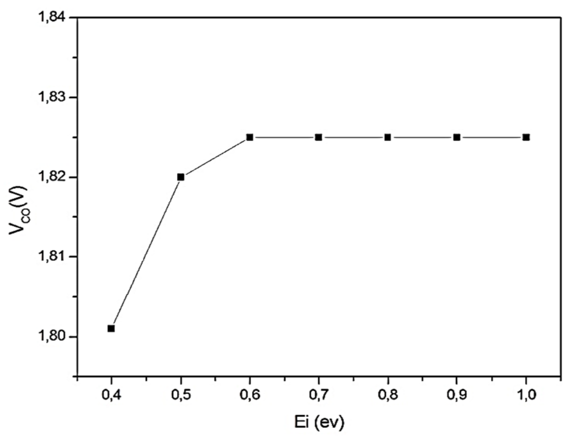

Figure 6. Variation of open-circuit voltage versus Ei

Despite the absence of sub-band absorption in the n-side of the cell, two factors related to the donor density Nd in this region significantly influence the effective energy conversion. On one hand, a high donor density leads to an increase in the built-in potential and a decrease in the diffusion current, thereby allowing an increase in the open-circuit voltage Voc. However, on the other hand, an increase in Nd reduces the hole diffusion length lp as well as the width of the space charge region on the n-side (xn), while the electron diffusion length ln and the width of the space charge region on the p-side remain essentially unchanged. This reduction in lp and xn limits the absorption and decreases the overall efficiency, as illustrated in Figure 7. Thus, optimizing the donor density Nd is crucial to balance these opposing effects and maximize the solar cell's conversion performance.

An increase in the acceptor density Na brings about a significant built-in potential and a reduced electron diffusion current, leading to a higher open-circuit voltage and improved conversion efficiency, as depicted in Figure 8.

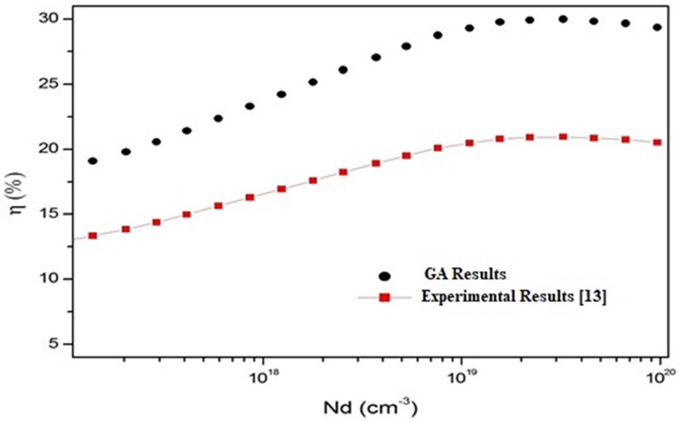

Figure 7. Variation of efficiency versus Nd

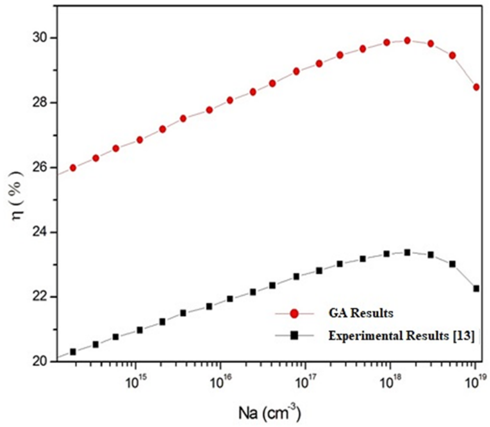

Figure 8. Variation of efficiency versus Na

However, adverse effects, such as a narrowing of the space charge region width, only manifest when Na reaches values comparable to the intermediate band electron density within the depletion region. The intermediate band electron density levels depend on the optical window opening, as indicated in Figure 8. Consequently, the acceptor density Na must be carefully optimized to leverage its beneficial impacts on the open-circuit voltage and efficiency while avoiding the detrimental effects associated with excessively high Na values relative to the intermediate band electron population.

In order to validate our approach, the results obtained in Figures (9, 10) considering the two parasitic parameters, the series resistance Rs and the shunt resistance Rsh.

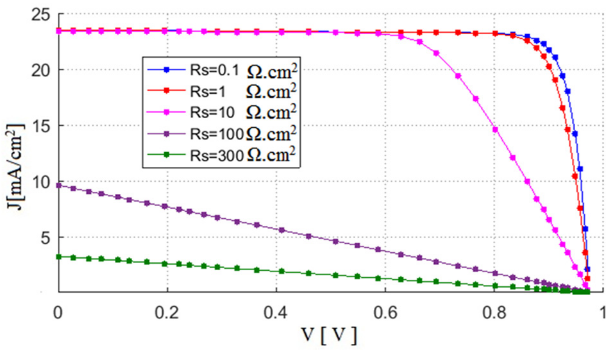

Figure 9. Influence of series resistance on the J-V characteristic

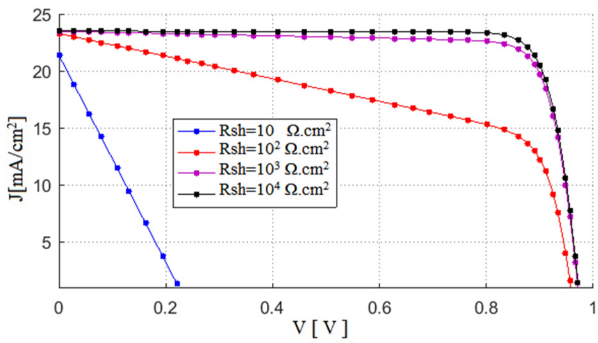

Figure 10. Influence of shunt resistance on the J-V characteristic

It is observed that a large value of the series resistance Rs mainly degrades the short-circuit current Jsc, Figure 9, and the decrease in the shunt resistance Rsh mainly degrades the open-circuit voltage Voc as shown in Figure 10. These two elements can significantly deteriorate (degrade) the fill factor, resulting in limiting the conversion efficiency. It is noted that good conversion is achieved when Rs is less than $1\Omega\cdot cm^2$ and Rsh exceeds $1k\Omega\cdot cm^2$.

5. RESULTS AND DISCUSSION

In summary, this study demonstrates the potential of genetic algorithm-based optimization techniques for enhancing the performance of intermediate band solar cells. Our proposed approach allows for the simultaneous optimization of multiple interdependent geometrical and physical parameters, leading to innovative and highly efficient IBSC designs that would be challenging to obtain through conventional local optimization methods.

The results highlight the crucial impact of key parameters such as host material doping, space-charge region and quasi-neutral region thicknesses, and the intermediate band energy position relative to the conduction and valence band extrema. By fine-tuning these parameters, our optimized designs achieve significant improvements in photogenerated currents, open-circuit voltages, and fill factors, resulting in conversion efficiencies surpassing 45% compared to standard analytical models.

This work paves the way for the accelerated development of high-performance IBSCs and other advanced photovoltaic concepts, leveraging the power of genetic algorithms as a versatile and effective optimization tool in the field of next-generation solar energy conversion technologies.

Acknowledgments
The authors would like to thank the anonymous reviewers for their valuable comments and suggestions to improve this paper

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ПІДВИЩЕННЯ ЕФЕКТИВНОСТІ ПЕРЕТВОРЕННЯ СОНЯЧНИХ ЕЛЕМЕНТІВ ШЛЯХОМ ЕВОЛЮЦІЙНОЇ ОПТИМІЗАЦІЇ З ВИКОРИСТАННЯМ ГЕНЕТИЧНИХ АЛГОРИТМІВ

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У цьому дослідженні ми пропонуємо новий метод, заснований на генетичних алгоритмах, для оптимізації продуктивності проміжних сонячних елементів (IBSC). Наш підхід спрямований на максимізацію ефективності фотоелектричного перетворення шляхом розумної оптимізації геометричних і фізичних параметрів структури IBSC, яка має бути частково заповнена. Таке заповнення забезпечує наявність як порожніх станів у проміжній зоні (IB) для прийому електронів із валентної зони (VB), так і заповнених станів для надання електронів зоні провідності (CB). Нещодавно в дослідженнях було виявлено вплив заповненості IB на ефективність клітини та розраховано оптимальну ефективність для пристроїв IB. Аналітичний вираз для оптимального заповнення IB використовувався для різних сценаріїв, що включають міцність зв'язку IB-CB і ширину області IB. У цій роботі ми досліджували вплив рівня енергії проміжної зони, вплив легування на ефективність, струм короткого замикання, напругу холостого ходу, коефіцієнт заповнення, а також для перевірки нашого підходу щодо паразитних ефектів, таких як послідовність і шунт. опір.

Ключові слова: *сонячна батарея; сонячні батареї середнього діапазону; енергетичний рівень смуги; послідовний і шунтовий опір; коефіцієнти поглинання*