KESTERITE AS WORKING BODY FOR EMERGING PHOTOVOLTAICS

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Abstract

Several studies have been published regarding kesterite and its application in photovoltaic solar cells. However, solar cells with n- and p-type layers made of kesterite have not been presented in the literature. In this paper, a model of kesterite as the working body of a solar cell is reported. Based on this, the solar-to-electricity conversion efficiency was built using the concepts of photons as the working body of the solar cell and bandgap. The assumptions made, as well as the advantages, limitations, and potential pitfalls, are discussed. Here, we propose a novel structure for kesterite solar cells, and the main condition underlying this work is that the absorption surface of the incident energy is kesterite. Additionally, the mathematical model developed by the combination of electrical and quantum parameters allowed to create a direct relationship between the electrical parameters V_{oc}, I_{sc}, FF and the quantum parameters N_e and E_g. This approach provides an introduction for researchers in photovoltaics and closely related fields on future perspectives of how to further boost research on kesterite applied in photovoltaic.

Keywords: kesterite, photovoltaic, solar cell, model, bandgap

1. Introduction

The search for renewable energy sources and ways to utilize them is one of the topics that has attracted the attention of researchers. Among the types of renewable energy, there is photovoltaic solar energy. Photovoltaic conversion is the direct conversion of sunlight into electricity without the use of a thermal engine (Goswami, 2015). The photovoltaic solar cell is the device used for this purpose. Different strategies have been explored to increase the understanding of the photovoltaic response of solar cells under different conditions.

The simulation is a fast, economic and efficient method to reveal the complex physic process that creates energy in photovoltaic devices (Ma et al., 2025). The approach using numerical simulation includes the use of different mathematical models to characterize the behavior of photovoltaic devices and thus help understand which potential conditions can result in high-performance cells.

Although many ways have been approached to understand the performance of photovoltaic solar cells, the effect of illumination on the photovoltaic response of these devices is the key point. The photovoltaic response of a photovoltaic device under illumination can be analyzed from the perspective of electrical parameters, quantum parameters and others. The mathematical model described in equation 1 helps to understand how the photovoltaic response can occur from the perspective of electrical behavior, while equation 2 is a model for studying the performance of the photovoltaic device based on quantum behavior. Although parameters such as mobility, recombination coefficients, layer thickness, absorptivity and others physical parameters not directly included in the mathematical expressions described in equations 1 and 2, these physical parameters tend to affect the electrical and quantum behavior of the photovoltaic solar cell.

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$$\eta = \frac{FF \times V_{oc} \times I_{sc}}{I(t) \times A} \quad \text{(eq.1)}$$

where efficiency (η) in the maximum output power, I(t) is the light amount that can be defined as the irradiance, that is, the power of the electromagnetic radiation incident on the cell surface by area, cell surface area (A), fill factor (FF), open circuit voltage (Voc) and short circuit current (Isc).

$$\eta^* = \frac{N_e \times E_g}{N_{ph} \times E_p} \quad \text{(eq.2)}$$

where Nph (photons/s) are the incident photons rate in the cell, Ep (J) is the photon energy, Ne (electrons/s) are the photogenerated electrons rate in the solar cells and Eg (J) is the band energy gap (Goswami, 2015). Ep can be described as in Equation 3, where h is Planck constant about 6.625 x 10-34 J s, c is the light speed about 3 x 108 m s-1, and λ is the wavelength:

$$E_p = \frac{h \times c}{\lambda} \quad \text{(eq.3)}$$

The efficiency as described by equation 2 is an overall efficiency resulting from the product of two coefficients of performance (CoPs). Ne/Nph ratio is CoP associated directly with the capacity of the photovoltaic solar cell to convert incident photons into electrons. This way, Eg/Ep ratio is associated with the relationship between energies. Eg/Ep relates the energy required for photoelectron generation to the photon energy that reaches the cell. Ne/Nph can be interpreted as an efficiency of conversion of photons to electrons. The behavior described by Ne/Nph is similar to that described by External Quantum Efficiency (EQE). EQE provides an analysis of the photovoltaic response of a photovoltaic device to each wavelength of sunlight or artificial, because EQE measures the efficiency with which the photovoltaic device converts incident photons into collected electrons at a specific wavelength.

The photovoltaic solar cells have a p-n junction formed by the link between a p-type semiconductor and n-type semiconductor. The sensitivity of the p-n junction to light can be exploited to use photovoltaic devices in electrical power generation (Nijen et al., 2025; Lv et al., 2025; Čorić, Nižetić and Jurčević, 2025; Zeng et al., 2024; Zhang et al., 2024; Tepner and Lorenz, 2023; Dréon et al., 2020; Lojpur, Mitrić and Validžić, 2019; Chander et al; 2015; Khan, Singh and Husain, 2010). The use of mathematical models is one approach that has been explored to characterize the photovoltaic response of photovoltaic solar cells. Photovoltaic solar cells have attracted attention both academically and commercially because they use semiconductor materials capable of directly converting solar energy into electrical energy.

The search for renewable energy sources and ways to utilize them is one of the topics that has attracted the attention of researchers. In this context, among the materials that have been explored is kesterite, a promising material for photovoltaic devices due to its solar light absorption capacity. Kesterite is an example of a multinary semiconductor with the general chemical formula Cu2MIIMIVX4 (X = O, S, Se, Te) (Wallace et al., 2017). Some examples of kesterite, a p-type semiconductor, include Cu2ZnSnS4, Cu2FeSnS4, Cu2CdSnS4, Cu2ZnGeS4, and their selenium-based counterparts (Nazligul et al., 2020). Additionally, studies have reported that n-type kesterite can be obtained by adding silver (Ag) (Nagaoka et al, 2024), and iron (Fe) and barium (Ba) (Banu et al., 2023).

Photovoltaic conversion is the direct conversion of sunlight into electricity without the use of a thermal engine (Goswami, 2015). The photovoltaic solar cell is the device used for this purpose. The work published in 1997 by Hironori Katagiri, Nobuyuki Sasaguchi, Shima Hando, Suguru Hoshino, Jiro Ohashi e Takaharu Yokota on a photovoltaic device using a Cu_2ZnSnS_4 (CZTS) layer with an efficiency of 0.66% is attributed as the first report on a kesterite solar cell kesterite (Wallace et al., 2017). In 2013, the development of a kesterite solar cell modified with selenium (CZTSSe) was reported, achieving a record efficiency of 12.6% (Nazligul et al., 2020). In the traditional kesterite solar cell, there is a heterojunction between p-type CZTS and n-type cadmium sulfide (CdS) (CZTS/CdS), where the CZTS band gap ranges between 1.00 and 1.50 eV (Pérez et al., 2024).

Another approach in the study of kesterite in photovoltaic solar cells is the use of cell structure simulations.

From the simulation of the Mo/Mo(S,Se)2/CZTSSe/CdS/ITO/air structure, it was inferred that the defect level formed at the CZTSSe layer interfaces during the deposition of Mo(S,Se)2 or CdS layers affects the thermal stability of the cell (Hajjiah, 2023). In another study, through simulation using the Mo/Mo(S,Se)2/CZTSSe/TiO2/ITO and Mo/Mo(S,Se)2/CZTSSe/CdS/ZnO/ITO structures, it was observed that the presence of the CdS/ZnO heterojunction increases the cell efficiency, while the presence of TiO2 improves thermal stability due to its higher tolerance to heat generation and dissipation (Hajjiah, 2022).

From the simulation of kesterite solar cell with the Mo/Mo(S,Se)2/CZTSSe/CdS/ZnO/ITO/air structure, the decrease in cell conversion efficiency from 12.78% to 11.46% was attributed to energy loss influenced by thermal effects (Zandi et al., 2022). A kesterite solar cell with efficiency of 21.78% was estimated via simulation of a heterogeneous cell structure with the presence of Cu2FeSnSe2 kesterite and MoSe2 layers (Moustafa et al., 2025).

Based on research on kesterite photovoltaic solar cells, this work shows two models to study the photovoltaic response of this type of solar cell. The first model considers the bandgap effect to quantify the conversion of photons into electrons in a traditional kesterite photovoltaic solar cell. The second model approaches a conceptual model of (n-kesterite/p-kesterite) p-type kesterite and n-type kesterite structure. Even though different numeric models and different semiconductors have been explored in the literature to study the performance of photovoltaic solar cells, until the moment of the production of this paper, the researchers did not observe in the literature the approach using n-kesterite/p-kesterite photovoltaic solar cells. Also, the relation between electrical parameters and quantum parameters in traditional kesterite photovoltaic solar cells has not been explored. Therefore, a simplified approach for fill these gaps observed is undertaken in this work.

2. Materials and methods

First step, combine the models described in equations 1 and 2 to generate a third model that relates the electrical and quantum parameters of a photovoltaic solar cell. Second step, apply this model to analyze kesterite photovoltaic solar cells reported by Katagiri et al., 1997 and Xu et al., 2025. Third step, proposition of a conceptual model of a kesterite photovoltaic solar cell with an n-kesterite/p-kesterite structure. Fourth step, a graphical representation of the conceptual model is illustrated in this step. Fifth step, equation 2 is applied to estimate the efficiencies of the n-kesterite/p-kesterite structure under idealized conditions.

3. Results and discussion

3.1 Simplified theoretical approach on conversion of photons into electrons in a kesterite photovoltaic solar cell

The photovoltaic devices can convert visible, infrared and ultraviolet light photons into electricity (Quaschning, 2005). In photovoltaic processes, it is necessary to treat the energy transport from the quantum mechanical point of view and in this view the energy is transported by photons. The conversion of light into electricity by the photon's absorption is a complex process of interactions between electrons and vacancies, altering the production of charge due to the presence of radiative and non-radioactive interactions (Cheng and O'Carroll, 2021). A way that causes the loss of efficiency in a photovoltaic solar cell is the thermalisation of charge carriers that is associated with the absorption of photons of high energy (Richards, 2006; Shalav et al., 2007).

In the literature, to study the performance of photovoltaic solar cells different models have explored. Shockley-Queisser efficiency limit for solar cells based on possible electron hole recombination has been plotted based on the bandgap (Goswami, 2015). The analysis of the maximum possible solar cell efficiency based on the Shockley-Queisser model is complex, because it involves different phenomena such as non-absorbed sub-bandgap photons, thermalisation losses, radiative recombination and entropy losses. Others models that have been explored are external quantum efficiency (EQE), internal quantum efficiency (IQE), spectral response, diode equations for photovoltaic and equivalent electrical circuit models for photovoltaic, equations 1 and 2. More details elsewhere (Goswami, 2015; Quaschning, 2005).

The models mentioned previously helped to understand the dynamic of absorbed photons into electrons conversion that contribute to the output electrical power in a photovoltaic solar cell. Equation 1 and 2 can be seen as alternative models to the Shockley-Queisser efficiency model for photovoltaic solar cells. These simplified models help to understand how efficiently a solar cell converts absorbed photons into electrons that contribute to the output electrical power. The numerical model described by Equation 1 is associated with electrical behavior as resulted of conversion of light photons into electricity, while the numerical model described by Equation 2 is associated directly the sensitivity of photon-electrons conversion. But the efficiency described by equation 3 is not affected only by photon-to-electron ratio, because efficiency also depends on the E_p to E_g ratio. Furthermore, the behavior described by N_e/N_{ph} ratio has nature-like with EQE.

From the models described by Equation 1 and 2, under $\eta = \eta^*$ condition in the maximum power point (MPP) is possible obtain the Equation 7. From model described by Equation 7 it is possible to analyze the effects of conversion of photons into electrons in a photovoltaic solar cell in the MPP condition. In the literature there are other models that can be explored in the study of the conversion of photons into electrons in photovoltaic solar cells, but these models do not consider the bandgap effect. Among these models are power conversion efficiency (PCE), external quantum efficiency (EQE) and internal quantum efficiency (IQE).

$$\eta = \frac{P_{max}}{P_{in}} = \frac{V_{max} \times I_{max}}{I(t) \times A} = \frac{FF \times V_{oc} \times I_{sc}}{I(t) \times A} = \frac{N_e \times E_g}{N_{ph} \times E_p} = \eta^* \quad \text{(eq. 4)}$$

$$P_{max} = N_e \times E_g = FF \times V_{oc} \times I_{sc} = V_{max} \times I_{max} \quad \text{(eq. 5)}$$

$$P_{in} = I(t) \times A = E \times A = N_{ph} \times E_p \quad \text{(eq. 6)}$$

$$N_e = \frac{FF \times V_{oc} \times I_{sc}}{E_g} \quad \text{(eq. 7)}$$

The model described by equation 7 is simplified model that considers the direct effect only of electrical parameters FF, V_{oc} and I_{sc} and quantum parameter E_g to analyze quantum parameter N_e. Although they are not directly included in the model, parameters such as mobility, recombination coefficients, layer thickness, absorptivity and others tend to influence electrical parameters FF, V_{oc}, I_{sc} and E_g. Furthermore, to analyze the effects of conversion of photons into electrons in a photovoltaic solar cell using Equation 7, calculus can be realized using Octave, Matlab, Python or other computational tools. Similar ways can be applied for equations 1 and 2.

Even using different parameters, the described models in equations 1 and 2 can be seen as equivalent under the perspective of efficiency in the MPP condition. This allows us a description of the cell behavior under the MPP condition from a hybrid model (equation 3) obtained by the junction of two models, which adopts an approach that the generation of electrons is influenced directly by electrical parameters and inversely by quantum parameter E_g. Adding, it is important to observe that N_e obtained from equation 7 represents only the electron rate obtained in the MPP condition.

Different models to be explored in the literature to study the performance of photovoltaic solar cells. In equation 3 there is an approach to estimate the efficiency of light conversion into electricity of the solar cell based on the quantum parameters for the cell and for the incident light, while the model used in Equation 1 is based in electrical behavior. But the relation between equations 1 e 2 described in equation 7 has not been explored in the study of kesterite photovoltaic solar cell.

Under the maximum power point (MPP) condition and when the E_g is known, from equation 7 it is possible to relate the photogenerated electrons rate (N_e) with electrical parameters FF, V_{oc} and I_{sc}. Table 1 illustrates the values of the quantum parameter N_e for traditional kesterite photovoltaic solar cells reported in literature. In the values illustrated in Table 1 estimated via equation 7, it is assumed $E_g = 1.45$ eV. This E_g is in accordance with what is cited in the literature on kesterite. The calculations are obtained using a computational tool, for example LibreOffice Calc, a free and open-source spreadsheet program.

Although many ways have been approached to understand the performance of photovoltaic solar cells, the effect of illumination on the photovoltaic response of these devices is the key point. The performance of the photovoltaic cells has been explored in the infrared region (Kapileswar et al., 2025), visible (Badea et al., 2025) and ultraviolet (Espinoza et al., 2025). Regardless of the type of radiation applied, the models described in Equations 1, 2, and 7 can be used to analyze the photovoltaic response of photovoltaic solar cells under light source. Additionally, Equation 7 can be interpreted as a new approach to analyzing the photovoltaic response. According to Equation 7, the ratio of the electrical output power (FF x V_{oc} x I_{sc}) to the bandgap (E_g) of the photovoltaic device is numerically equal to the rate of photogenerated electrons (N_e). Furthermore, the approach adopted shows a possible path to obtain a relationship between quantum parameters (N_e, E_g) and electrical parameters (FF x V_{oc} x I_{sc}).

Table 1: Photovoltaic response based in photoelectron generation.

FF	**V_{oc} (V)**	**I_{sc} (mA/cm^2)**	**N_e (electrons/s cm^2)**
0.277 (Source: Katagiri et al., 1997)	0.400 (Source: Katagiri et al., 1997)	6.000 (Source: Katagiri et al., 1997)	2.862 x 10^{15} (Source: eq. 3)
0.522 (Source: Xu et al., 2025)	0.513 (Source: Xu et al., 2025)	22.300 (Source: Xu et al., 2025)	2.570 x 10^{16} (Source: eq. 3)

3.2 Simplified representation of a conceptual model of a n-kesterite/p-kesterite photovoltaic solar cell

A photovoltaic solar cell made with the junction of a semiconductor with an excess of electrons (n type) and a semiconductor with a vacancy (p type), resulting in a p-n junction, where the electrical field generated contributes to the electrical separation and vacancies induced by the light absorption (Goswami, 2015, Quaschning, 2005). To obtain the p-n junction in photovoltaic devices, different materials have been explored, such as silicon, kesterite and others. Silicon photovoltaic solar cells with n- type silicon/ p- type silicon structure have been elsewhere (Goswami, 2015). But kesterite photovoltaic solar cell with n- type kesterite/ p-type kesterite structure has not been exploited.

Kesterite is a material that can be used in photovoltaic devices, photodetectors, sensors to detect N_2, O_2, H_2 e CO_2, thermoelectric devices (Nazligul et al., 2020). Kesterite is a p- type semiconductor (Moustafa et al., 2025; Nagaoka et al, 2024; Pérez et al., 2024; Hajjiah, 2023; Hajjiah, 2022; Zandi et al., 2022; Nazligul et al., 2020; Wallace et al., 2017), but n-type kesterite also is possible (Nagaoka et al, 2024; Banu et al., 2023). Based on the literature analysis focused on the use of kesterite in photovoltaic and thermoelectric applications, p-type kestirite (p-kesterite) to n-type kestirite (n-kesterite) conversion is possible. Since synthesis of n-type kesterite is possible, and then there is potential for production of n-kesterite/p-kesterite photovoltaic solar cell, see figure 1. In the simplified conceptual model illustrated in figure 1 is inferred the potential creation of a p-n junction from n-kesterite and p-kesterite layers capable of generating electricity via the photovoltaic effect.

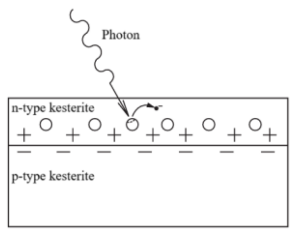

Figure 1: Visual Representation of conceptual model of a n-kesterite/p-kesterite photovoltaic solar cell.

The structure of layers as adopted in the simplified conceptual model illustrated figure 1 is like the structure of a traditional silicon solar cell. In a silicon photovoltaic solar cell, the creation of a p-n junction from p-type silicon layer and n-type silicon layer is possible, because chemical elements can be added to silicon to form n-type and p-type, and junction of n-type and p-type layers is capable of production of electricity via the photovoltaic effect (Goswami, 2015). The p-n junction of silicon photovoltaic solar cell can be represented as n-silicon/p-silicon structure, which is a homojunction.

When any photovoltaic solar cell is irradiated with light, the characteristics of the p-n junction can be explored from photovoltaic response based on models described in equation 1, equation 2, external quantum efficiency (EQE), internal quantum efficiency (IQE), Shockley-Queisser model and others. Also, photovoltaic response can be observed from electrical parameters, quantum parameters and other parameters, for example, mobility, recombination coefficients, layer thickness and absorptivity. Among models and parameters possible, table 2 illustrates the photovoltaic response potential of n-kesterite/p-kesterite photovoltaic solar cell is illustrated in model describe by equation 2. The mathematical model represented by equation 2 is simplified quantum model and this model can be used to estimate the efficiency of n-kesterite/p-kesterite cell under idealized conditions.

Table 2: Parameters and efficiencies of n-kesterite/p-kesterite cell under idealized conditions.

Parameters	Value
1,000 ampere	6.242×10^{18} electrons s^{-1}
1,000 eV	1.600×10^{-19} J
Speed of light	3.000×10^{8} m s^{-1}
Planck's constant	6.625×10^{-34} J s
Intensity of monochromatic radiation at a wavelength of 638 nm incident on cell	1.000×10^{-3} W
Kesterite Band Gap Energy	1.45 eV
Cell efficiency under $N_e = N_{ph}$ condition	74.45 %
Cell efficiency under $N_e = 0.5N_{ph}$ condition	37.24 %
Cell efficiency under $N_e = 0.05N_{ph}$ condition	3.72 %

Table 2 illustrates the parameters and their values used to estimate the light-to-electricity conversion efficiency of n-kesterite/p-kesterite photovoltaic solar cell using equation 2. To illustrate how the n-kesterite/p-kesterite cell efficiency can be obtained from equation 2 are assumed simplified conditions: (i) monochromatic radiation at wavelength of 638 nm incident on cell with intensity about 1.000×10^{-3} W; (ii) each incident photon is capable of generating an electron-hole pair in the n-kesterite/p-kesterite homojunction, which it result in $N_e = N_{ph}$; (iii) only 50% of the incident photons generate electron-hole pairs in the n-kesterite/p-kesterite homojunction, which it result in $N_e = 0.5N_{ph}$; (iv) only 5% of the incident photons generate electron-hole pairs in the n-kesterite/p-kesterite homojunction, which it result in $N_e = 0.05N_{ph}$.

Although the mathematical values assumed in conditions (i), (ii), (iii) and (iv) are arbitrary, they can still be associated with physical parameters. The condition (i) is associated with the light source, a physical parameter. Assumptions (ii), (iii), and (iv) can be inferred as simplified views of the potential effects associated with physical parameters, such as thickness, mobility, charge carriers, absorptivity and others. The conditions (i), (ii), (iii) and (iv) can be seen as simplified assumptions that allow for a quick application of equation 2.

The study of the efficiency of n-kesterite/p-kesterite cell under simplified conditions also can help to understand the potential impacts on the cell if the device is exposed to non-ideal conditions. These non-ideal phenomena are concatenated in simplified conditions iii and iv. The conditions adopted in assumptions ii, iii and iv can be briefly interpreted as resulting from impacts caused, for example, by the defect level formed at the interfaces during layer deposition, thermal effects, layer thickness, and radiation with different wavelengths. Although the conditions assumed constitute a simplifying hypothesis, they have mathematical consistency and serve as a starting point for establishing a basic model for an initial understanding of the complex physical behavior involved in the photovoltaic cell response.

The work presents a new approach to solar cells using kesterite as the working body for photovoltaics, in which the existence of kesterite in the p layer and n layer of the solar cell is assumed. This approach differs from other experimental and simulation works cited in the literature on kesterite photovoltaic solar cells, since they only consider the existence of kesterite as a p-type semiconductor forming a heterojunction with another n-type semiconductor. Additionally, the conceptual model focuses on the types of materials that can be used, not on how this will be technically done. It serves to provide insight into research trends associated with kesterite photovoltaic solar cells. This research trend is viable since literature reports that it is possible to produce n-type kesterite. Thus, this model serves as a step towards research aimed at obtaining a kesterite cell with a p-n homojunction.

4. Conclusion

The first proposed model describes by equation 7 shows the direct relationship between electrical and quantum parameters of a photovoltaic solar cell. The model is applied to estimate the photovoltaic response based on the photogenerated electrons of a kesterite photovoltaic solar cell. Also, a conceptual model of a kesterite solar cell with an n-kesterite/p-kesterite structure is reported.

In the n-kesterite/p-kesterite cell model, idealized conditions were adopted to estimate the efficiency of the kesterite solar cell. These conditions serve as a starting point for future studies on the n-kesterite/p-kesterite homojunction in photovoltaic solar cells. Expanding the model to consider the impact of polychromatic radiation, layer thickness, thermal effects, and the presence of other layers tends to make the model more realistic in the study of kesterite solar cells.

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