

# Enhancing Strategy CIGS Solar Cell Performance Through a New ZnSe Buffer Layer

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**Abstract** In this paper, we use the SCAPS-1D software for the numerical simulation of the Cu(In, Ga)Se<sub>2</sub> (CIGS) solar cell with a ZnSe-based buffer layer. The study focuses on the influence of the ZnSe buffer layer on the performance of the CIGS solar cell. In this study, the analysis of the effect of the ZnSe buffer layer thickness revealed that optimum performance is obtained with a thickness of 0.020  $\mu\text{m}$ . A study of the ZnSe/CIGS interface showed that optimum performance is obtained for a conduction band offset included between -0.2 eV and 0.2 eV and interface defects of less than  $10^{12} \text{cm}^{-2}$ . By introducing an electron reflector layer at the absorber/molybdenum interface of this solar cell, it emerges that the performance of the ZnSe/CIGS/Mo solar cell is superior to that of the CdS/CIGS/Mo solar cell.

**Keywords:** Numerical simulation, SCAPS-1D software, electron reflector, ZnSe buffer layer, ZnSe/CIGS interface

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## 1. Introduction

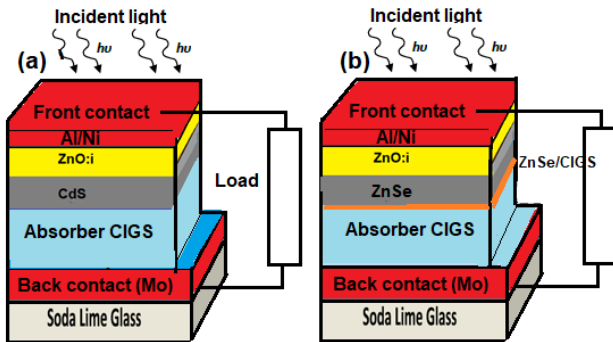
In the field of solar photovoltaics (PV), CIGS-based thin-film solar cells occupy a prominent place thanks to their low production cost and excellent conversion efficiency reaching 23.35% published in 2019 [1]. In the operation of these solar cells, the main role of the n-type conductivity buffer layer is to form the p-n heterojunction with the p-type conductivity CIGS absorber. Currently, in the PV solar field, CdS cadmium sulfide is the best buffer layer about CIGS-based thin-film solar cells in terms of efficiency [2,3]. The low-gap cadmium sulfide (CdS) buffer layer ( $E_g=2.4\text{eV}$ ) presents a handicap in terms of absorption of short-wavelength photons [4]. Indeed, the CdS buffer layer does not allow short-wavelength photons to reach the CIGS absorber, yet these photons contribute significantly to the photocurrent of the solar cell. Although present in very small quantities in the CdS buffer layer, cadmium (Cd) is a highly carcinogenic and toxic chemical element, posing serious threats to the environment [5]. For environmental reasons, its replacement by cadmium (Cd)-free material is one of the current challenges facing the scientific community [6]. The substitution of cadmium sulfide (CdS) by a zinc chalcogenide-based buffer layer such as ZnS, ZnSe, and ZnO seems to be a viable option. The advantage of zinc chalcogenide-based buffer layers lies in the fact that they

have a wide gap [7] and are therefore able to absorb short-length photons. Another advantage of zinc chalcogenide-based buffer layers is the quality of the interface with the CIGS absorber, which enables defect diffusion to be controlled [5,8]. The major motivation for using zinc chalcogenide-based buffer layers is the accessibility of the raw material zinc. Zinc chalcogenides are semiconductors in the II-VI group of compounds [4,9,10]. Several studies conducted on alternative buffer layers, including those by Hahn-Mitner, have shown that the efficiency of the solar cell with a ZnSe buffer layer of bandgap ( $E_g=2.67\text{eV}$ ) [11,12] is close to that of the solar cell with the reference CdS buffer layer of bandgap ( $E_g=2.4\text{eV}$ ). Buffer layers (ZnSe) appear to be a serious candidate for replacing CdS [13]. We also note that the ZnSe buffer can be deposited by chemical bath deposition (CBD), atomic layer deposition (ALD), co-evaporation, or vapor-phase epitaxy with organometallics [24]. However, what strategies can we implement to improve the performance of the CIGS solar cell with a new ZnSe buffer layer? In this article, we will begin with a comparative study of the current-voltage density (J-V) and quantum efficiency (Q-E) characteristics of CIGS solar cells with a CdS buffer layer and a ZnSe buffer layer. Next, we will study the influence of ZnSe buffer layer thickness and CIGS absorber on CIGS solar cell performance. A study of conduction band discontinuity and interface defects at the ZnSe/CIGS interface will also be carried out. Finally, we will implement a strategy to improve the performance of the

CIGS solar cell with a ZnSe buffer layer. This strategy will involve introducing an electron-reflector layer (EBR) at the ZnSe/CIGS interface.

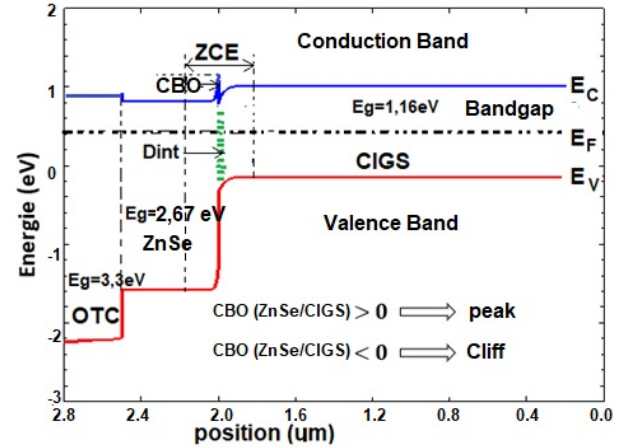
## 2. Materials and Methods

Numerical simulation is the process of optimizing the performance of solar PV devices using modeling and characterization techniques. Numerical simulation is therefore an effective tool for reproducing solar cell behavior without carrying out experiments, enabling us to predict strategies for improving conversion efficiencies. In this study, we use the SCAPS-1D software for numerical simulation. SCAPS-1D, like other PV solar cell simulation software, uses the finite-difference method with well-defined boundary conditions to solve the basic charge-carrier transport equations in semiconductors: the fish equation, and the electron and hole continuity equations [14,15]. The choice of this software is motivated by the fact that there is good agreement between the numerical simulation performed with SCAPS-1D and experimentation [16,17]. CIGS-based thin-film solar cells are chalcopyrite heterojunction cells in which the p-type electrically conductive CIGS is the cell's absorber. On top of this absorber, a CdS buffer layer with n-type electrical conductivity forms the p-n junction. A layer of highly conductive transparent oxide OTC is deposited on the buffer layer. The whole assembly is deposited on a substrate, which acts as the mechanical support. Soda-lime glass is the most widely used substrate in high-efficiency CIGS cells, due to its properties compatible with the CIGS absorber [4,18]. A front Ni/Al ohmic contact and a rear Mo ohmic contact are added to collect photo-generated electrons and holes respectively. The structure of such a solar cell is shown with the buffer layer in Figure 1.a and with the ZnSe buffer layer in Figure 1.b.



**Figure 1.** Structure of solar cell with CdS buffer layer (a) and with ZnSe buffer layer (b) used for numerical simulation.

The equivalent band diagram of the solar cell with the ZnSe/CIGS/Mo layer is shown in Figure 2. The conduction band offset (CBO) is represented by the difference in electronic affinity between the absorber (CIGS) and the buffer layer (ZnSe). To carry out our simulations, we will keep the electronic affinity of the absorber constant  $\chi(\text{CIGS}) = 4.5 \text{ eV}$  by varying that of the buffer layer  $\chi(\text{ZnSe})$  from 4 eV to 5 eV, thus resulting in a variation of the conduction band offset from -0.5 eV to 0.5 eV.



**Figure 2.** Energy band diagram with ZnSe buffer layer

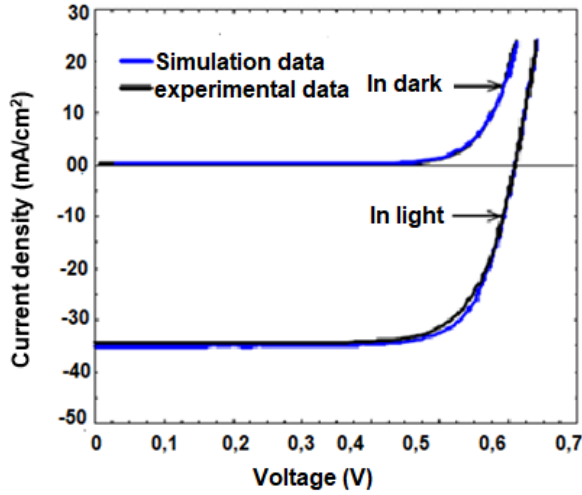
**Table 1.** Parameters used to simulate the CIGS solar cell

| Layers properties                                     |                        |                        |                      |                        |
|-------------------------------------------------------|------------------------|------------------------|----------------------|------------------------|
| Layers                                                | Zno :i                 | CdS                    | ZnSe                 | CIGS                   |
| Thickness (nm)                                        | 300                    | Variable               | Variable             | 2500                   |
| Bandgap (eV)                                          | 3.3                    | 2.4                    | 2.67                 | 1.25                   |
| Electron affinity (eV)                                | 4.55                   | Variable               | Variable             | Variable               |
| Diélectric relative Permittivity                      | 9.00                   | 10                     | 9.1                  | 13.6                   |
| Effective density of state in BC ( $\text{cm}^{-3}$ ) | $3.1 \times 10^{18}$   | $3.1 \times 10^{18}$   | $2.2 \times 10^{18}$ | $2 \times 10^{18}$     |
| Effective density of state in BV ( $\text{cm}^{-3}$ ) | $1.8 \times 10^{19}$   | $3.1 \times 10^{18}$   | $1.8 \times 10^{19}$ | $1.5 \times 10^{19}$   |
| Electrons thermal velocity (cm/s)                     | $2.4 \times 10^7$      | $3.1 \times 10^7$      | $10^6$               | $3.9 \times 10^7$      |
| Holes thermal velocity (cm/s)                         | $1.3 \times 10^7$      | $1.6 \times 10^7$      | $10^6$               | $1.4 \times 10^7$      |
| Electrons Mobility ( $\text{cm}^2/\text{Vs}$ )        | 100                    | 72                     | 100                  | 100                    |
| Holes mobility ( $\text{cm}^2/\text{Vs}$ )            | 31                     | 20                     | 25                   | 12.5                   |
| Doping ( $\text{cm}^{-3}$ )                           | $1 \times 10^{17}$ (D) | $5 \times 10^{17}$ (D) | $10^{17}$ (D)        | $1 \times 10^{16}$ (A) |
| Bulk defects properties                               |                        |                        |                      |                        |
| Defects density ( $\text{cm}^{-3}$ )                  | $1 \times 10^{16}$     | $5 \times 10^{16}$     | $1 \times 10^{18}$   | $1 \times 10^{14}$     |
| Capture cross-section electron ( $\text{cm}^2$ )      | $1 \times 10^{-15}$    | $1 \times 10^{-15}$    | $5 \times 10^{-12}$  | Variable               |
| Capture cross-section holes ( $\text{cm}^2$ )         | $5 \times 10^{-13}$    | $5 \times 10^{-13}$    | $5 \times 10^{-12}$  | $5 \times 10^{-15}$    |
| Interfaces properties                                 |                        |                        |                      |                        |
|                                                       | CdS/CIGS               |                        | ZnSe/CIGS            |                        |
| Interfaces defect density ( $\text{cm}^{-2}$ )        | $1 \times 10^{-10}$    |                        | Variable             |                        |
| Capture cross-section electrons ( $\text{cm}^2$ )     | $1 \times 10^{-15}$    |                        | $1 \times 10^{-15}$  |                        |
| Capture cross-section holes ( $\text{cm}^2$ )         | $1 \times 10^{-15}$    |                        | $1 \times 10^{-15}$  |                        |

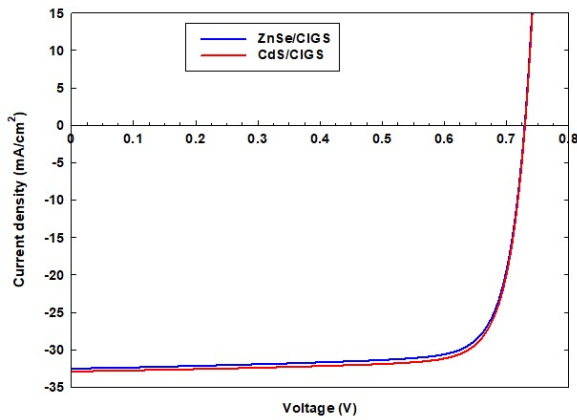
In our numerical simulation, we assume that the series resistance  $R_s$  is null and the shunt resistance  $R_{sh}$  is infinite in our model. The temperature of the ZnSe/CIGS/CdS solar cell is maintained at 300K and illuminated under standard conditions by a 1.5G AM spectrum that accounts for both direct and diffuse radiation [19]. The properties of the various layers

and interfaces used for the numerical simulation are summarized in Table 1. These properties were obtained from theoretical and experimental results [16,17] [20,21]

To validate our results, we compared the J-V characteristic curves of our numerical simulation with those obtained experimentally by Pettersson. We can see that there is good agreement between these two results, as shown in Figure. 4, which leads us to the results and discussion section.



**Figure 3.** J-V characteristic curves compared with experimental results from Pettersson et al. [21]



**Figure 4.** J-V characteristics for ZnSe/CIGS/Mo and CdS/CIGS/Mo solar cells

### 3. Result and Discussion

#### 3.1. Comparative Study of the J-V and Q-E Characteristics of CIGS Solar Cells with CdS Buffer Layer and ZnSe Buffer Layer

This section compares the electrical parameters of solar cells with the CdS buffer layer and the ZnSe buffer layer. The major difference between these two solar cells is the replacement of the CdS buffer layer by the ZnSe layer. These two buffer layers have different electrical parameters, as shown in Table 1. To carry out this numerical simulation, we set the buffer layer thickness at 30 nm [11] in these two configurations. In 2018, Oubda et

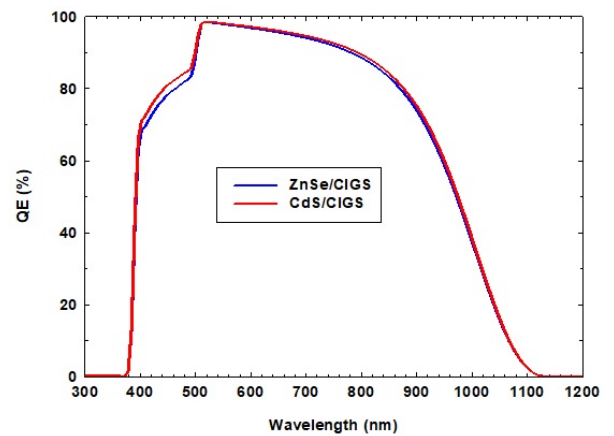
al. showed that a buffer layer thickness of 30 nm used in CIGS solar cells provides good absorber protection and is a source of better performance and photoelectric conversion efficiency [11]. The J-V characteristic curve for ZnSe/CIGS/Mo and CdS/CIGS/Mo solar cells is shown in Figure 4.

From the J-V characteristic curve, we extracted the electrical parameters of the two solar cells: open-circuit voltage  $V_{OC}$ , short-circuit current density  $J_{SC}$ , form factor (FF), and conversion efficiency ( $\eta$ ). These electrical parameters are summarized in Table 2.

**Table 2.** Electrical parameters for ZnSe/CIGS/Mo and CdS/CIGS/Mo solar cells, used to simulate the CIGS solar cell

| Electricals parameters  | $V_{OC}$ (V) | $J_{SC}$ (mA/cm <sup>2</sup> ) | FF (%) | $\eta$ (%) |
|-------------------------|--------------|--------------------------------|--------|------------|
| CdS/CIGS/Mo solar cell  | 0.7295       | 32.8964                        | 79.84  | 19.16      |
| ZnSe/CIGS/Mo solar cell | 0.7288       | 32.5247                        | 79.25  | 18.79      |

In this table, all the electrical parameters of the CdS/CIGS/Mo solar cell are superior to those of the ZnSe/CIGS/Mo solar cell. We can see that the conversion efficiency of the solar cell is 19.16% for the CdS reference buffer layer and 18.79% for the ZnSe buffer layer, i.e. a difference in conversion efficiency  $\Delta\eta = 0.37\%$ . Similarly, we note a difference in values for short-circuit current density  $\Delta J_{SC} = 0.371 \text{ mA/cm}^2$ , circuit-overt voltage  $\Delta V_{OC} = 0.007 \text{ V}$  and form factor  $\Delta(FF) = 0.007 \text{ V}$ . These differences in electrical parameter values between the CdS and ZnSe buffer layers can be explained by a decrease in the absorption of incident photons of wavelength (400 nm  $< \lambda < 900 \text{ nm}$ ) in the case of the ZnSe/CIGS/Mo solar cell compared with the CdS/CIGS/Mo cell as shown in Figure 5. It can be seen that more current is lost through absorption in ZnSe than in CdS. This may be linked to the fact that the absorption coefficient of ZnSe is higher than that of CdS. At the end of this analysis, the performance of the CIGS solar cell is better with the CdS buffer layer than with the ZnSe buffer layer. These results are in agreement with those obtained by [3,4] [11]. In the following, we will study the influence of some physical parameters of the ZnSe buffer layer and the CIGS absorber on the performance of the ZnSe/CIGS/Mo solar cell in order to determine the optimal parameters.



**Figure 5.** Quantum efficiency (Q-E) for ZnSe/CIGS/Mo and CdS/CIGS/Mo solar cells.

### 3.2. Influence of ZnSe Buffer Layer and CIGS Absorber Thicknesses and ZnSe/CIGS Interface

#### 3.2.1. Influence of ZnSe Buffer Layer and CIGS Absorber Thicknesses

In this section, we focus on the influence of the thickness of the ZnSe buffer layer and that of the CIGS

absorber on the electrical and energy performance of the Mo/CIGS/ZnSe/ZnO structure. The choice of absorber is motivated by the fact that the absorber is the most important layer of the CIGS solar cell [22,23]. Figure 6 shows the J-V characteristic curves of the solar cell for different thicknesses of the ZnSe buffer layer (Figure 6.a) and for different thicknesses of the CIGS absorber (Figure 6.b).

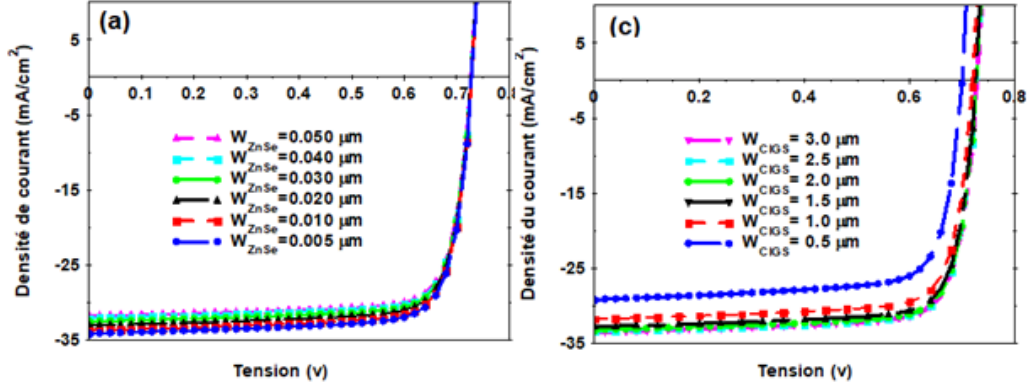


Figure 6. J-V characteristic for different ZnSe buffer layer thicknesses (a) and CIGS absorber thicknesses (b).

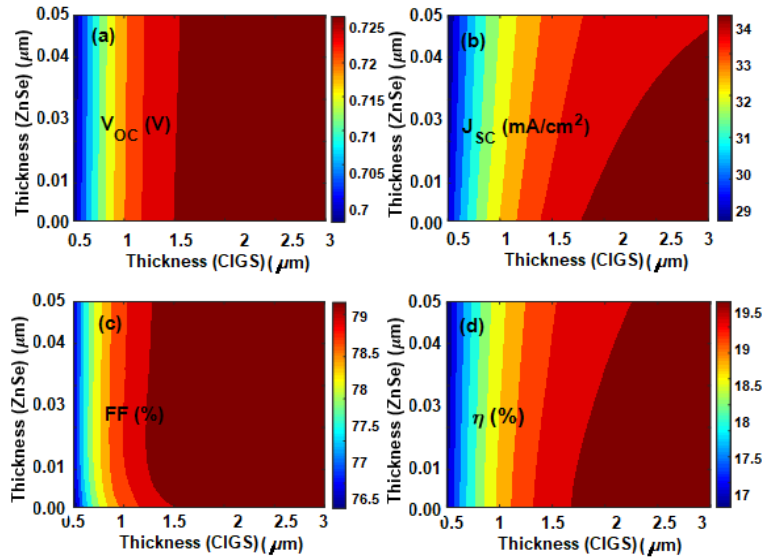


Figure 7. Influence of CIGS and ZnSe thicknesses on electrical parameters

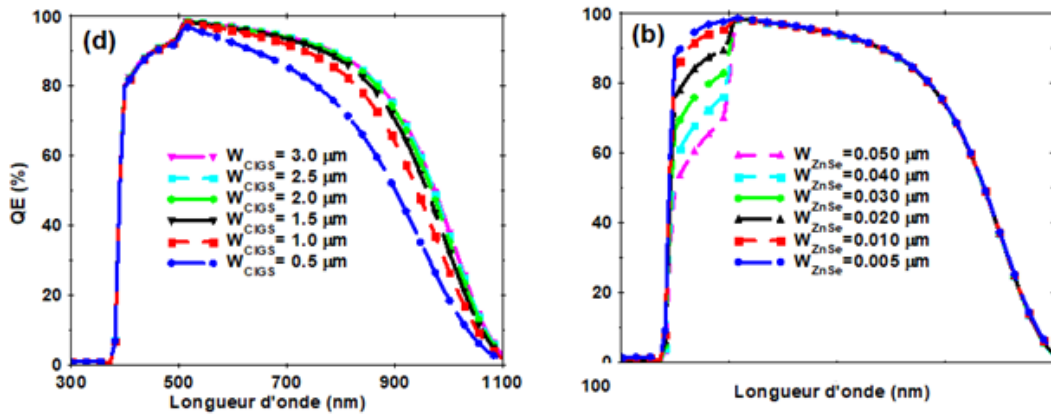
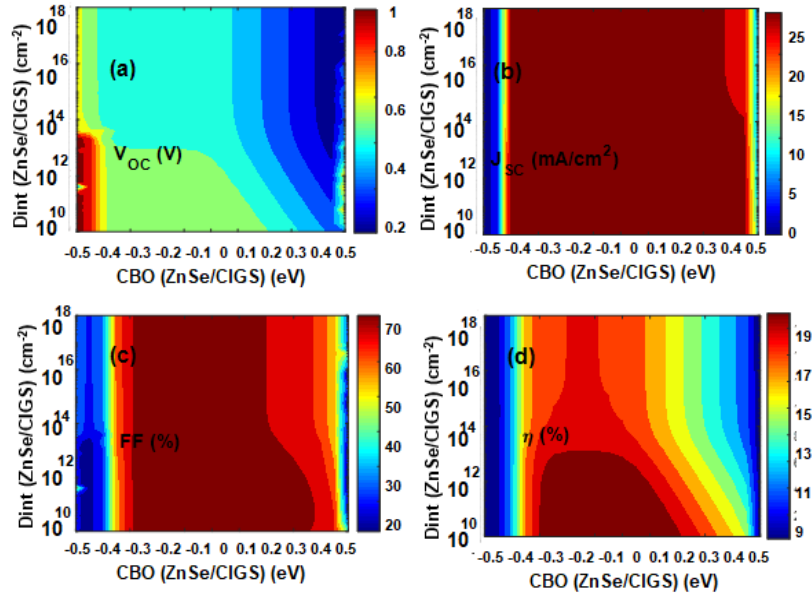


Figure 8. Q-E quantum efficiency of the solar cell for different CIGS absorber thicknesses (a) and ZnSe buffer layer thicknesses (b).





**Figure 9.** Influence of conduction band offset and defects at the ZnSe/CIGS interface on electrical parameters

A variation in the J-V characteristic is observed when the thickness of the ZnSe buffer layer and that of the CIGS absorber vary. To elucidate the J-V characteristic curves, we extracted the solar cell's electrical parameters. These parameters were used to plot Figure 7. This figure shows the influence of CIGS and ZnSe thicknesses on the electrical parameters.

Figure 8 shows the Q-E quantum efficiency curves of the solar cell for different ZnSe buffer layer thicknesses (Figure 8.a) and for different CIGS absorber thicknesses (Figure 8.b). For low absorber thicknesses ( $W_{CIGS} \leq 1.5 \mu m$ ), there is a decrease in all solar cell electrical parameters irrespective of ZnSe buffer layer thickness (Figure 7). This decrease in solar cell performance can be explained by a decrease in the absorption of incident photons with wavelengths below 500 nm ( $\lambda \geq 500 \text{ nm}$ ) when the absorber thickness is less than 1.5  $\mu m$  as shown in Figure 8.a. It can also be explained by the non-absorption of incident photons of wavelength below 500 nm ( $\lambda \leq 500 \text{ nm}$ ) when the thickness of the ZnSe buffer layer varies as shown in Figure 8.b. Beyond an absorber thickness of 1.5  $\mu m$  ( $W_{CIGS} > 1.5 \mu m$ ), good performance is obtained when  $W_{ZnSe} \leq 0.02 \mu m$ . This good solar cell performance can be explained by an increase in the absorption of incident photons of wavelength below 500 nm ( $\lambda \leq 500 \text{ nm}$ ) when the absorber thickness is greater than 1.5  $\mu m$  ( $W_{CIGS} > 1.5 \mu m$ ), as shown in Figure 8.a. It can also be explained by an increase in the absorption of incident photons of wavelengths between 400 nm and 500 nm when the buffer layer thickness ( $W_{ZnSe} \leq 0.02 \mu m$ ) as shown in Figure 8.b. We note that short-wavelength photons are absorbed in the ZnSe buffer layer and photons with wavelengths greater than 500 nm penetrate deep into the absorber before being absorbed. These photons generate electron-hole pairs near the back contact, which is a zone of high recombination, resulting in a decrease in short-circuit current density  $J_{sc}$  and conversion efficiency  $\eta$  as shown in Figure 7 b.d. The open-circuit voltage  $V_{oc}$

decreases slightly with increasing buffer layer thickness and increases with increasing absorber thickness.

### 3.2.2. Influence of Conduction Band Offset and Defects at the ZnSe/CIGS Interface

This section is focused on the study of defects at the ZnSe/CIGS interface. As defects at the ZnSe/CIGS interface, we have conduction band offset denoted CBO and interface defects denoted Dint. The conduction band offset at the ZnSe/CIGS interface varies from -0.5 eV to 0.5 eV and the interface defects vary from  $10^{10} \text{ cm}^{-2}$  à  $10^{18} \text{ cm}^{-2}$ . Figure 9 shows the simultaneous impact of conduction band offset and interface defects on electrical parameters.

For low values of the conduction band discontinuity ( $CBO < -0.4 \text{ eV}$ ), a drop in electrical parameters such as short-circuit current density  $J_{sc}$ , form factor FF and conversion efficiency  $\eta$  is observed whatever the value of the interface defects. This drop in performance can be explained by a high cliff. The cliff acts as a barrier to injected electrons, encouraging the majority of charge carriers to recombine via the defects present at the ZnSe/CIGS interface. For very high values of the conduction band discontinuity ( $CBO > 0.4 \text{ eV}$ ), we also have a decrease in all electrical parameters whatever the value of the interface defects. This is probably due to a very high peak that acts as a barrier against photo-generated charge carriers in the absorber. When the conduction band discontinuity is included between -0.2 eV and 0.2 eV, the short-circuit current density  $J_{sc}$  is optimal and constant. The same applies to the FF form factor. Concerning the conversion efficiency  $\eta$ , it is optimal when interface defects are less than  $10^{12} \text{ cm}^{-2}$ . These optimum performances may be linked to good alignment of the band discontinuity at the ZnSe/CIGS interface. They may also be explained by low recombination phenomena due to the low value of defects at the ZnSe/CIGS interface.

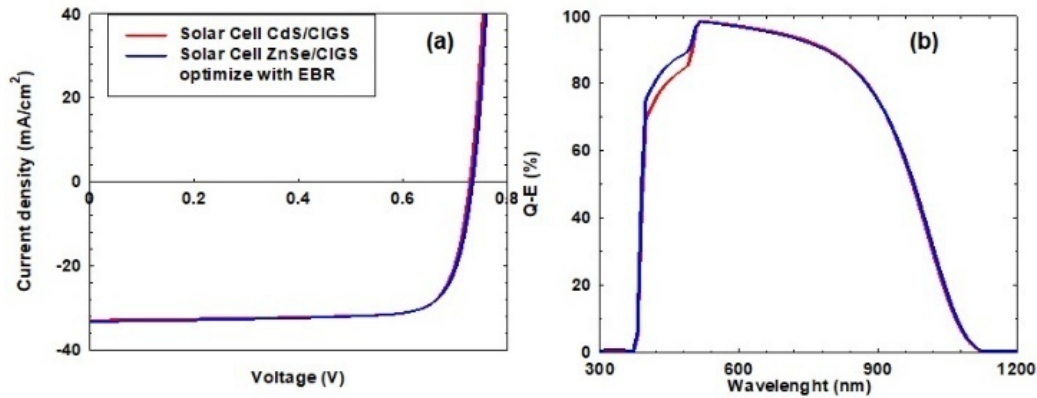


Figure 10. J-V characteristic and Q-E quantum efficiency of CdS/CIGS/Mo solar cell and ZnSe/CIGS/Mo solar cell optimized with EBR.

### 3.3. Optimization strategy for the ZnSe/CIGS/Mo Solar Cell.

In the previous section, we showed that optimum performance is obtained with a ZnSe buffer layer thickness of 0.020  $\mu\text{m}$  and a conduction band offset is included between -0.2 eV and 0.2 eV when interface defects are less than  $10^{12}\text{cm}^{-2}$  at the ZnSe/CIGS interface. The optimal electrical parameters obtained from the numerical simulations are used to improve the performance of the ZnSe/CIGS/Mo solar cell. Next, we compare the electrical performance of the ZnSe/CIGS/Mo solar cell with that of the ZnSe/CIGS/Mo solar cell with the optimum electrical parameters. Table 3 shows the electrical parameters of the two configurations.

Table 3. Electrical parameters of the two configurations

| Electrical parameters             | $V_{OC}$ (V) | $J_{sc}$ ( $\text{mA}/\text{cm}^2$ ) | $FF$ (%) | $\eta$ (%) |
|-----------------------------------|--------------|--------------------------------------|----------|------------|
| ZnSe/CIGS/Mo Salar cell.          | 0.7288       | 32.5247                              | 79.25    | 18.79      |
| ZnSe/CIGS/Mo Salar cell optimized | 0.7440       | 32.5378                              | 79.08    | 18.91      |

Table 4. Electrical parameters of the EBR layer [25]

| electron-reflector layer                              | Properties      |
|-------------------------------------------------------|-----------------|
| Thickness (nm)                                        | 10              |
| Bandgap (eV)                                          | 1.4             |
| Electron affinity (eV)                                | 13.6            |
| Dielectric relative Permittivity                      | 4.45            |
| Effective density of state in BC ( $\text{cm}^{-3}$ ) | $2.2 * 10^{18}$ |
| Effective density of state in BV ( $\text{cm}^{-3}$ ) | $1.8 * 10^{19}$ |
| Electrons thermal velocity (cm/s)                     | $10^7$          |
| Holes thermal velocity (cm/s)                         | $10^7$          |
| Electrons Mobility ( $\text{cm}^2/\text{Vs}$ )        | 100             |
| Holes mobility ( $\text{cm}^2/\text{Vs}$ )            | 25              |
| Doping ( $\text{cm}^{-3}$ )                           | $2.0 * 10^{19}$ |

In this table, we see that the open-circuit voltage  $V_{OC}$ , short-circuit current density and conversion efficiency  $\eta$  of the ZnSe/CIGS/Mo solar cell with optimum electrical parameters increase slightly. Although these electrical performances are improved, they remain inferior to those of the CdS/CIGS/Mo solar cell. To further improve the performance of the ZnSe/CIGS/Mo solar cell, we will implement a strategy involving the introduction of an

electron-reflector layer (EBR) at the interface between the CIGS absorber and the Mo molybdenum back contact. The electrical parameters of the EBR layer are summarized in Table 4.

The J-V characteristic and (Q-E) quantum efficiency curves for the CdS/CIGS/Mo solar cell and the ZnSe/CIGS/Mo solar cell with optimal parameters and an EBR layer are shown in Figure 10.

To compare the performance of the two solar cells, we have extracted the electrical parameters of the J-V characteristics. These electrical parameters are summarized in Table 5.

Table 5. Electrical parameters of the two solar cells

| Electrical parameters                      | $V_{OC}$ (V) | $J_{sc}$ ( $\text{mA}/\text{cm}^2$ ) | $FF$ (%) | $\eta$ (%) |
|--------------------------------------------|--------------|--------------------------------------|----------|------------|
| CdD/CIGS/Mo Salar cell.                    | 0.7295       | 32.8964                              | 79.84    | 19.16      |
| ZnSe/CIGS/Mo Salar cell optimized with EBR | 0.7338       | 33.2517                              | 78.57    | 19.18      |

With the exception of the FF form factor, all the other electrical parameters of the ZnSe/CIGS/Mo solar cell with optimum parameters and an EBR layer are superior to the electrical parameters of the CdS/CIGS/Mo solar cell. The EBR layer acts as a reflector (optical mirror) for electrons, creating a potential barrier in the conduction band, preventing them from being captured by the Mo and thus preventing their recombination. The EBR layer has ohmic behavior with the molybdenum back contact layer, which explains the improved performance of the solar cell.

## 4. Conclusion

At the end of our study, an analysis of the effect of the thickness of the ZnSe buffer layer showed that optimum performance is obtained with a thickness of 0.020  $\mu\text{m}$ . A study of the ZnSe/CIGS interface showed that optimum performance is obtained for a conduction band offset included between -0.2 eV and 0.2 eV and for interface defects are less than  $10^{12}\text{cm}^{-2}$  at the ZnSe/CIGS interface. The use of an electron-reflector layer at the back interface between the absorber and the back contact and the optimal parameters obtained improved the performance of the ZnSe/CIGS/Mo solar cell. A comparative study of J-V characteristics and quantum efficiency shows that the performance of the

ZnSe/CIGS/Mo solar cell with the EBR layer is superior to that of the CdS/CIGS/Mo solar cell.

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