



# A Numerical Investigation on the Combined Effects of MoSe<sub>2</sub> Interface Layer and Graded Bandgap Absorber in CIGS Thin Film Solar Cells

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Abstract: The influence of Molybdenum diselenide (MoSe<sub>2</sub>) as an interfacial layer between Cu(In,Ga)Se<sub>2</sub> (CIGS) absorber layer and Molybdenum (Mo) back contact in a conventional CIGS thin-film solar cell was investigated numerically using SCAPS-1D (a Solar Cell Capacitance Simulator). Using graded bandgap profile of the absorber layer that consist of both back grading (BG) and front grading (FG), which is defined as double grading (DG), attribution to the variation in Ga content was studied. The key focus of this study is to explore the combinatorial effects of MoSe<sub>2</sub> contact layer and Ga grading of the absorber to suppress carrier losses due to back contact recombination and resistance that usually occur in case of standard Mo thin films. Thickness, bandgap energy, electron affinity and carrier concentration of the MoSe<sub>2</sub> layer were all varied to determine the best configuration for incorporating into the CIGS solar cell structure. A bandgap grading profile that offers optimum functionality in the proposed configuration with additional MoSe<sub>2</sub> layer has also been investigated. From the overall results, CIGS solar cells with thin MoSe2 layer and high acceptor doping concentration have been found to outperform the devices without MoSe<sub>2</sub> layer, with an increase in efficiency from 20.19% to 23.30%. The introduction of bandgap grading in the front and back interfaces of the absorber layer further improves both open-circuit voltage (V<sub>OC</sub>) and short-circuit current density (J<sub>SC</sub>), most likely due to the additional quasi-electric field beneficial for carrier collection and reduced back surface and bulk recombination. A maximum power conversion efficiency (PCE) of 28.06%, fill factor (FF) of 81.89%, J<sub>SC</sub> of  $39.45 \text{ mA/cm}^2$ , and  $V_{OC}$  of 0.868 V were achieved by optimizing the properties of MoSe<sub>2</sub> layer and bandgap grading configuration of the absorber layer. This study provides an insight into the different possibilities for designing higher efficiency CIGS solar cell structure through the manipulation of naturally formed MoSe<sub>2</sub> layer and absorber bandgap engineering that can be experimentally replicated.

**Keywords:** CIGS; molybdenum diselenide (MoSe<sub>2</sub>); bandgap grading; back grading (BG); front grading (FG); double grading (DG); SCAPS; simulation; power conversion efficiency (PCE)



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### 1. Introduction

With record solar cell efficiencies of 23.35% and commercial solar modules with efficiencies of 19.2%, chalcopyrite Cu(In,Ga)Se<sub>2</sub> (CIGS) solar cells have shown great promise in thin film photovoltaics technologies [1]. Despite this high efficiency level, the CIGS-based PV technology has not yet attained its full potential. The efficiency of current record solar devices is limited by optical and parasitic losses and by recombination losses. According to the Shockley–Queisser limit, maximum theoretical conversion efficiency of a p-n junction-based solar cell is 32.8% at a band gap of 1.15 eV [2]. If all loss mechanisms were addressed at the same time, an efficiency requires device optimization. There are many elements, layers, process steps, and parameters that need to be optimized in order to propel the efficiency of CuInGaSe2 cells closer to Shockley–Queisser's theoretical limit.

In a typical CIGS solar cell structure, Molybdenum (Mo) is the commonly used material for the back contact because of its chemical inertness, low electrical resistivity and high stability at elevated temperature. In addition, during the high-temperature growth of CIGS absorber layer, chemical reactions at the interface between the Mo layer and Selenium (Se) forms a thin molybdenum diselenide (MoSe<sub>2</sub>) layer. Although the presence of an interfacial MoSe<sub>2</sub> layer between Mo back-contact and the absorber is evident, properties of this back contact interface such as structure, thickness, and electrical behaviors are convoluted [3–7]. MoSe<sub>2</sub> layer is claimed to be beneficial; however, excessive thickness of MoSe<sub>2</sub> layer reduces the electrical characteristics (V<sub>OC</sub>, J<sub>SC</sub> and FF) of the cell due to the high resistivity of MoSe<sub>2</sub> and will also cause delamination. It was reported that various parameters may affect MoSe<sub>2</sub> growth, in particular the physical properties of the Mo film (density, stress, and orientation) that are highly dependent on the deposition method and growth recipe of the film. Therefore, insights into the formation mechanism of MoSe<sub>2</sub> layer and subsequent Mo deposition process-optimization are vital to develop higher efficiency CIGS cells.

Along the years, a number of breakthrough technologies have been proposed to achieve large improvements in CIGS conversion efficiency such as sodium (Na) doping, bandgap engineering and also the introduction of alkali post-deposition treatment (PDT). Through band gap engineering, a notch band structure with an increased bandgap towards backside and frontside of the absorber layer is introduced. This is performed by replacing a small amount of the Indium (In) content in the CIGS material with Gallium (Ga) [i.e., x = ([Ga]/[Ga] + [In]), which displaces the conduction band minimum ( $E_C$ ) [8], also changing the bandgap and electron affinity values [9]. Though it is evident that bandgap engineering can enhance the overall cell performance, a clear understanding of the fundamental device physics of the structure is necessary to reap the full benefits of bandgap grading for optimizing the cell performance [10]. Studies performed earlier [10–20] suggested that bandgap profiling is advantageous for two reasons: (1) to reduce recombination rate by inducing an additional quasi-electric field which improves the separation of free carriers, and (2) to increase absorption at long wavelengths [9]. This quasi-electric field can be either towards the back contact or towards the front contact depending on the bandgap grading direction (back grading or front grading) [21]. In the case of back grading (BG), the additional field helps in keeping the minority carriers (electrons for p-type CIGS) away from the back contact hence reduces back surface recombination, therefore improving electron collection at the front electrode [21]. Both  $J_{SC}$  and  $V_{OC}$  are enhanced when using this configuration [22]. Meanwhile, in front grading (FG) structure, the recombination in the space charge region (SCR) is suppressed due to the increase in the barrier height due to the larger bandgap at the front part of the absorber layer, resulting in improved  $V_{OC}$  [22]. However, the larger band gap in the frontal area will reduce photon absorption in this region. Thus, more absorption will take place deeper into the CIGS layer which will lead to lower carrier collection probability, thereby reducing  $J_{SC}$ . Utilizing the advantages of BG (high carrier collection and high  $J_{SC}$ ) and front grading (high  $V_{OC}$ ), double grading (DG) profile is proven to be the most beneficial strategy for improving both  $J_{SC}$  and  $V_{OC}$ 

simultaneously. Lundberg et al. [20] also gave a comprehensive summary of the different effects that can be expected due to these grading approaches.

Investigations into different magnitude, shape, and depth of the double grading with variation in relevant grading parameters is a must in order to optimize the  $V_{OC}$ , while maintaining the  $J_{SC}$  value. The graded regions within the structure of a solar cell have to be placed in the appropriate position in order to achieve the proposed improvement. Two grading profile parameters that highly influence the photovoltaic parameter of the final device are:

- 1. Bandgap values at the front, middle and back of the absorber layer, depending on the composition of Ga;
- 2. Position of the notch, where composition of Ga is minimum.

Therefore, it is necessary to optimize these parameters and grading conditions for high efficiency device fabrication. Since it is difficult to understand the benefits and effects of the different bandgap grading configurations by studying the actual device, numerical modelling offers a more convenient approach. In this paper, a simulative analysis aimed at investigating the simultaneous effects of MoSe<sub>2</sub> back contact interface layer and Ga grading of the CIGS absorber towards the main electrical parameters (J<sub>SC</sub>, V<sub>OC</sub>, FF and PCE) of CIGS based solar cells is presented. A single absorber layer with constant properties (i.e., thickness, doping concentration, energy bandgap, etc.), as in conventional CIGS solar cells was first considered in order to particularly study the effects of variation in MoSe<sub>2</sub> layer properties. Afterwards, an absorber structure with the incorporation of DG bandgap grading was introduced. Based on previous reports as mentioned earlier, DG bandgap alignment exhibits a more significant benefit over BG and FG. The investigation focuses on the optimization of various grading parameters related to the double grading Ga profile and its compatibility with the electrical properties of MoSe2 layer. Based on current densityvoltage (J-V) characteristics and external quantum efficiency (EQE) results, an optimally double graded bandgap profile suitable for CIGS thin film solar cell having MoSe<sub>2</sub> layer is proposed. The possible effects of both tailoring the properties of MoSe<sub>2</sub> interface layer and the CIGS absorber bandgap have not been adequately investigated, thus this study is considered novel. It should be noted that the central purpose in this work is to show trends in solar cell performance with respect to different simulated models, hence validation of the model with extant experimental results is only briefly presented.

# 2. Methodology-Device Architecture and Simulation

In this study, we have conducted our investigations extensively using Solar Cell Capacitance Simulator (SCAPS) developed by Prof. Burgelman and his team at the University of Ghent, Belgium. This software solves three numerically basic semiconductor equations: the Poisson equation, the holes continuity equation as well as the electron continuity equation where the steady-state band diagram, recombination profile, and carrier transport in one dimension are calculated [23]. The software will evaluate the solar cell performance mainly through V<sub>OC</sub>, J<sub>SC</sub>, FF and PCE.

At the start of the simulations, a reference model based on conventional CIGS solar cell was established. Generally, a conventional CIGS solar cell structure comprises a top electrode, followed by three layers of semiconductor material: zinc oxide (ZnO), which serves as the window layer, cadmium sulfide (CdS) as the n-type buffer layer, and CIGS as the p-type absorber layer. Molybdenum (Mo) is commonly used as the back contact in the device stack as shown in Figure 1a. This architecture is based on the conventional CIGS thin film solar cell structure reported in [24]. In this basic structure, the thickness of the individual layers, the corresponding material properties, as well as the cell's surface area can all be modified. Since our focus elucidates the influence of the MoSe<sub>2</sub> interfacial layer on the PCE of the CIGS device, an additional layer of MoSe<sub>2</sub> was inserted into the stack, as presented in Figure 1b. In addition, bandgap gradient was also incorporated into the absorber layer to mirror the bandgap grading in actual devices. Simulation of both the reference and modified devices was performed by setting the optical and

electrical parameters for each layer, material Gaussian defect states, and contact parameters as summed up in Table 1, and Tables A1 and A2 respectively. These parameters are selected on the basis of theoretical considerations, experimental evidence and existing literature [25–27]. Table A3 in Appendix A provides an explanation of the symbols used in the previous tables.



**Figure 1.** Schematic device structure of CIGS solar cell developed using SCAPS interface (**a**) reference model without MoSe<sub>2</sub> layer (**b**) proposed model with MoSe<sub>2</sub> layer.

Layer	Window	Buffer	Absorber	Interface
Material	ZnO	CdS	CIGS	MoSe <sub>2</sub>
Thickness (µm)	0.15	0.05	2.5	0.01-0.1
ε <sub>r</sub>	9	9	13.6	7.29
$\mu_n \ ({ m cm}^2 \ { m V}^{-1} \ { m s}^{-1})$	100	100	100	25
$\mu_p \ (\text{cm}^2 \ \text{V}^{-1} \ \text{s}^{-1})$	25	25	25	100
$N_A ({\rm cm}^{-3})$	0	0	$2.0 imes10^{16}$	$1.0 imes 10^{14}$ – $1.0 imes 10^{20}$
$N_D ({\rm cm}^{-3})$	$1.0 imes10^{18}$	$1.0 imes10^{17}$	0	0
$E_g$ (eV)	3.3	2.4	1.011–1.676 ( <sup>1</sup> Ga-dep)	1.0–1.5
$N_{\rm C}~({\rm cm}^{-3})$	$2.2  imes 10^{18}$	$2.2 imes10^{18}$	$2.2 \times 10^{18}$	$2.2 imes10^{18}$
$N_V ({ m cm}^{-3})$	$1.8 imes10^{19}$	$1.8 imes10^{19}$	$1.8 imes10^{19}$	$1.8 imes10^{19}$
$\chi$ (eV)	4.00	4.00	4.350–3.685 ( <sup>1</sup> Ga-dep)	3.5–4.5

Table 1. Summary of the Optical and Electrical Parameters Used for the Simulation Model.

<sup>1</sup> Ga-dep = Gallium dependent.

In the modified structure shown in Figure 1b, a layer of MoSe<sub>2</sub> was inserted in between Mo back contact and CIGS absorber. In order to optimize the proposed solar cell design in this study, properties of MoSe<sub>2</sub> layer viz. layer thickness,  $E_g$ ,  $\chi$ , and  $N_A$  were varied over the reported values in the range from 0.01 to 0.1  $\mu$ m, 1.0 to 1.5 eV, 3.5 to 4.5 eV, and 1.0  $\times 10^{14}$ to  $1.0 \times 10^{20}$  cm<sup>-3</sup>, respectively. By comparing the performance characteristics (J<sub>SC</sub>, V<sub>OC</sub>, FF, PCE) of the proposed layouts against the reference case, the effects due to variations of the MoSe<sub>2</sub> layer properties in the cell were investigated. Initially, in order to solely accentuate the effects of the MoSe<sub>2</sub> layer properties first, the bandgap of the CIGS absorber was initially kept uniform within the whole absorber layer depth and material parameters for the layers in the solar cell stack other than MoSe<sub>2</sub> were also kept unchanged. In the next stage, bandgap grading is introduced into the CIGS absorber layer of the model through the variation of Ga concentration along the layer thickness to ascertain the best grading profile by investigating the influence of the magnitude, shape and depth of the grading. Several grading laws can be implemented in SCAPS: linear, logarithmic, parabolic, power law, exponential, effective medium and a Beta function. These grading laws can be used to set the composition grading over a layer, as well as to set the composition dependence of a property [28]. In this study, parabolic dependence is employed considering that bandgap

dependence in most semiconductor alloys  $A_{1-x}B_x$  as a function of composition *x* follows the parabolic function of

$$(E_g(x) = (1 - x)E_g^A + xE_g^B - bx(1 - x)$$
(1)

where  $E_g^A$  and  $E_g^B$  are the band gaps of the pure compounds A and B, respectively, with b as the bowing coefficient [28–30]. The following equations are used in this study for extracting the bandgap and electron affinity of CIGS absorber, where x is the Ga percentage or concentration, symbolized in literature as Ga/(In + Ga) (GGI) ratio [26].

$$E_g(x) = 1.011 + 0.421x + 0.244x^2 \tag{2}$$

$$\chi(x) = 4.35 - 0.421x - 0.244x^2 \tag{3}$$

According to Equation (2), the bandgap of CIGS surges from 1.011 eV (pure CIS) to 1.676 eV (pure CGS). It should be noted that by implementing a graded composition of the absorber layer, not only the bandgap  $E_g(x)$ , electron affinity  $\chi(x)$ , and optical absorption  $\alpha(x, \lambda)$ , other material properties such as dielectric constant, effective density of states, transport properties, defect concentration, recombination properties, etc., also become graded [28]. However, due to the fact that variation of GGI on the other parameters have little effect compared to on  $E_g(x)$ ,  $\chi(x)$ , and  $\alpha(x, \lambda)$ , other parameters are assumed to be independent of composition in this work. The variation of CIGS optical absorption coefficient  $\alpha(x, \lambda)$  caused by change in Ga fraction used in this study is based on work of [31].

As mentioned earlier, alteration of GGI will shift the minimum of the conduction band  $(E_C)$ , while the valence band  $(E_V)$  is unaffected by the change. For double grading (DG),  $E_C$  increases towards both the back contact of CIGS/MoSe<sub>2</sub> interface and the front side at the CdS/CIGS junction, as shown in Figure 2 [32,33]. In the case of parabolic law for composition grading, the main parameters are;  $y_{left}$  and  $y_{right}$ , indicating the composition at the backside and frontside of the absorber layer, respectively, the notch (the point of minimum Ga composition or lowest bandgap) value and its position across the absorber layer are denoted as  $y_{min}$  and  $x_{min}$  [28]. The optimum bandgap grading profile was found by simulating different values for these related bandgap grading parameters as presented in Table 2, and analyzing the corresponding J<sub>SC</sub>, V<sub>OC</sub>, FF, and PCE. Previous work by [34] shows that both grading parameters; i.e., the position of the notch and grading height (based on GGI) are equally significant to improve the cell performance through bandgap grading, hence the reason why these parameters were varied in this section. In order to accentuate the effects of bandgap grading, material parameters employed in the simulations were all kept unchanged except for the Ga composition dependent parameters such as bandgap energy, electron affinity, and optical absorption [17]. All simulations were performed under standard test conditions (STC) of AM 1.5 G with an illumination of 1000 W/m<sup>2</sup>. Finally, a simulation model of CIGS solar cell structure with optimized MoSe<sub>2</sub> layer properties and graded absorber is proposed as the main outcome of the work.

Table 2. The Variation in Grading Parameters Simulated.

Grading Profile	Grading Parameters	Variation
Double grading (DG)	Back/front composition (GGI) $x_{min}$ (notch position) $y_{min}$ (lowest composition)	0–1 0 μm–2.5 μm 0–1



**Figure 2.** Schematic view of the band diagram of  $ZnO/CdS/CIGS/MoSe_2$  layers in the SCAPS model, with double grading (DG) bandgap profile in the CIGS absorber. Inset: Close-up view of how the double grading (DG) is incorporated in the model. DG is modelled as conduction band ( $E_C$ ) minimum rises from a determined notch position towards the back and front of CIGS absorber.

# 3. Results and Discussion

#### 3.1. Study of MoSe<sub>2</sub> Interfacial Layer in CIGS Thin Film Solar Cell Structure

It was stated in the Section 2 that ZnO/CdS/CIGS/Mo device structure without any interfacial MoSe<sub>2</sub> layer was used as the baseline case in this study. The photovoltaic performance parameters of  $J_{SC} = 35.75 \text{ mA/cm}^2$ ,  $V_{OC} = 0.681 \text{ V}$ , FF = 82.88%, and PCE = 20.19% for this baseline configuration are considerably lower than all the simulated cases with MoSe<sub>2</sub> layer in the structure, which will be shown later. The significantly low cell performance is primarily due to large work function of CIGS,  $\Phi_{CIGS}$  in comparison to that of Mo,  $\Phi_{Mo}$  ( $\Phi_{CIGS} > \Phi_{Mo}$ ), which results in high barrier for holes ( $\Phi_{bv}$ ) at the back contact. This barrier at the back contact interface (CIGS/Mo) is recognized to be an inherent loss mechanism due to the formation of a second junction, but with opposite polarity [35]. It affects other parameters of the solar cell, such as FF and  $V_{OC}$  of the device, and hence, the power conversion efficiency (PCE). The emphasis of this part of the numerical analysis is the CIGS/MoSe<sub>2</sub>/Mo section, which is a semiconductor-semiconductor-metal structure with two interfaces: CIGS/MoSe<sub>2</sub> and MoSe<sub>2</sub>/Mo. Figure 3a shows the band profile of conventional CIGS structure with CIGS/Mo interface in comparison to our proposed structure with CIGS/MoSe<sub>2</sub>/Mo interface in Figure 3b. The Schottky contact at the CIGS/Mo interface indicated by the large downward bending of the valence band,  $E_V$  shown in Figure 3a, becomes a quasi-Ohmic contact with the inclusion of a thin MoSe<sub>2</sub> semiconducting layer as in Figure 3b. Higher bandgap of  $MoSe_2$  leads to upward shift of the conduction band,  $E_C$ , creating a  $\Delta E_{\rm C}$  barrier impeding the recombination of minority carriers (electrons) at the back contact that is detrimental to the solar cell performance. In the case of majority carriers (holes) collection, although MoSe<sub>2</sub>/Mo interface is still a Schottky contact, the formation of the MoSe<sub>2</sub> layer shifts both the maxima of the,  $E_V$  and the minima of the  $E_C$  upwards, as evident in Figure 3b. This upward shift of the bands results in the elimination of the barrier for holes between the CIGS and Mo layers that is present in Figure 3a. Nevertheless, the collection rate of holes will be suppressed when the MoSe<sub>2</sub> interfacial layer is very thick.



**Figure 3.** Schematic energy band diagram of (**a**) CIGS/Mo after contact; (**b**) CIGS/MoSe<sub>2</sub>/Mo after contact.

In the next stage, optimization of interfacial MoSe<sub>2</sub> layer in terms of layer thickness, bandgap energy, electron affinity, and acceptor carrier concentration has been studied to choose the most effective MoSe<sub>2</sub> layer properties for the proposed CIGS solar cell design. The effects of acceptor carrier concentration ( $N_A$ ) from 1.0  $\times$  10<sup>14</sup> to around 1.0  $\times$  10<sup>20</sup> cm<sup>-3</sup> and  $MoSe_2$  layer thickness from 0.01 to 0.1  $\mu$ m on the photovoltaic performance of the device were investigated. Figure 4 shows that the overall performance of the device improved when the thickness of MoSe<sub>2</sub> layer was increased. This finding arises from the fact that increasing the thickness leads to an increase of photon absorption rate in the near infrared region resulting in higher photogenerated charge carriers, as the MoSe<sub>2</sub> layer is effectively extending the width of the p-type region in the solar cell [36]. Additionally, a thinner MoSe<sub>2</sub> layer causes lower shunt resistance which is evident from the significantly lower V<sub>OC</sub> value as can be seen from Figure 4b. This graph depicts the significant dependency of V<sub>OC</sub> on the two variables of MoSe<sub>2</sub>;  $N_A$  and thickness. At  $N_A$  larger than  $1.0 \times 10^{16}$  cm<sup>-3</sup>,  $V_{OC}$  minutely increased with the increase in thickness until  $N_A \sim 1.0 \times 10^{18}$  cm<sup>-3</sup>, at which point  $V_{OC}$  starts to saturate for MoSe<sub>2</sub> layer thickness above 0.04  $\mu$ m, hence the thickness must be maintained above  $\sim 0.04 \ \mu m$  to obtain the maximum attainable V<sub>OC</sub>. On the other hand, a thicker MoSe<sub>2</sub> layer induces higher series resistance as apparent from the decreased FF in Figure 4c. As such, carrier collection efficiency will be limited due to the increased resistivity of a thick MoSe<sub>2</sub> layer in comparison to pure Mo [37]. Therefore, the thickness of MoSe<sub>2</sub> layer needs to be carefully controlled to turn the back contact from a rectifying Schottky contact to a low resistance quasi-ohmic contact [38].

On the variations in the MoSe<sub>2</sub> carrier concentration, it can be observed that, in general, increasing the  $N_A$  leads to an increase in the Jsc, Voc, FF as well as the conversion efficiency of the cell, hence higher  $N_A$  of MoSe<sub>2</sub> layer is favorable. MoSe<sub>2</sub> layer is found to perform better in terms of J<sub>SC</sub> and V<sub>OC</sub> at  $N_A > 1.0 \times 10^{16}$  cm<sup>-3</sup>. This finding can be attributed to the fact that  $E_C$  and  $E_V$  rise as  $N_A$  increases according to [39]. The beneficial band bending facilitates the transport of holes from MoSe<sub>2</sub> to Mo, hence enhancing photogenerated carrier collection. At the same time, electrons are hindered from flowing to the back contact thereby inhibiting back surface carrier recombination, enhancing both J<sub>SC</sub> and V<sub>OC</sub>. Though the reduced back surface recombination due to band bending with an increase in  $N_A$  attributes to Voc change, this factor is insufficient to account for observed increase. The significant improvement in V<sub>OC</sub> for high carrier concentration,  $N_A$  of MoSe<sub>2</sub> can be correlated to the formation of p<sup>+</sup>-layer at the interface between p-type CIGS and Mo back contact, creating what can be considered as back surface field (BSF) [40]. On the other hand, when the  $N_A$  of MoSe<sub>2</sub> is  $<1.0 \times 10^{16}$  cm<sup>-3</sup> which is the value of  $N_A$  defined for CIGS absorber layer, the overall cell performance degrades. This effect can be described as the phototransistor

effect which involves the formation of a second junction, but with opposite polarity to the pn-junction caused by the formation of a Schottky contact in the interfacial region between the  $MoSe_2$  with low carrier concentration and the CIGS absorber with higher concentration. As a result, the  $V_{OC}$  in the device is impaired [41]. Though phototransistor effect is commonly observed in the J-V curves measured at low temperatures in the range from 100 to 200 K, it was reported that a decrease in the effective doping level of the  $MoSe_2$  layer might induce this effect even at room temperature [35,41].



**Figure 4.** The simulated electrical performance parameters as a function of MoSe<sub>2</sub> acceptor carrier concentration ranging from  $1.0 \times 10^{14}$  to  $1.0 \times 10^{20}$  cm<sup>-3</sup>: (a) J<sub>SC</sub>; (b) V<sub>OC</sub>; (c) FF; and (d) conversion efficiency (PCE) at different MoSe<sub>2</sub> layer thicknesses ranging from 0.01 µm to 0.1 µm.

The change in FF with MoSe<sub>2</sub> carrier concentration might be discussed and analyzed from the interface properties standpoint. One of the band alignment-related electronic parameter according to Anderson-energy band rule [42] that is significantly affected by the variation in MoSe<sub>2</sub> carrier concentration is equilibrium contact potential ( $qV_o$ ) that determines potential barrier retarding hole transport from the semiconductor valence band to metal in a Mo/p-type semiconductor structure [43]. Generally, lower  $qV_o$  is desirable for the hole transport. Increment in the carrier concentration,  $N_A$  in p-type MoSe<sub>2</sub> layer shifts the Fermi level downwards closer to the valence band edge and subsequently increases the semiconductor work function ( $\Phi_{MoSe_2}$ ) and  $qV_o$  between MoSe<sub>2</sub> and Mo as determined by the following equations [42]:

$$\Phi_{MoSe_2} = \chi_{MoSe_2} + E_{gMoSe_2} - \left(kTln\frac{N_V}{N_A}\right) \tag{4}$$

$$qV_o = \Phi_{MoSe_2} - \Phi_{Mo} \tag{5}$$

Calculated interface electronic parameter values ( $\Phi_{MoSe_2}$  and  $qV_o$ ) as a function of  $N_A$  in p-type MoSe<sub>2</sub> layer is presented in Table 3 in order to verify the claim. The unfavorable high  $qV_o$  with the increase in  $N_A$  forms a larger downward bending barrier for hole transport from the valence band of MoSe<sub>2</sub> to the Fermi level of Mo. With barriers larger than 0.2753 eV when  $N_A$  of MoSe<sub>2</sub> was set to  $1.0 \times 10^{18}$  cm<sup>-3</sup>, the FF starts to degrade.

Table 3. Calculated Interface Electronic Parameters of Mo/MoSe<sub>2</sub> in Various  $N_A$  of MoSe<sub>2</sub>.

Band Diagram Parameters (N.)		$N_A$ (cm <sup>-3</sup> )						
Dailu Diagiaili I a	manifeters (NA)	$1.0  imes \mathbf{10^{14}}$	$\textbf{1.0}\times\textbf{10^{15}}$	$\textbf{1.0}\times\textbf{10^{16}}$	$\textbf{1.0}\times\textbf{10^{17}}$	$\textbf{1.0}\times\textbf{10^{18}}$	$\textbf{1.0}\times\textbf{10^{19}}$	$\textbf{1.0}\times\textbf{10}^{\textbf{20}}$
MoSe <sub>2</sub> /Mo MoSe <sub>2</sub> /Mo	$\Phi_{MoSe_2} \ qV_o$	4.9872 0.0372	5.0467 0.0967	5.1062 0.1562	5.1658 0.2158	5.2253 0.2753	5.2848 0.3348	5.3443 0.3943

In terms of different combinations of carrier concentration and thickness, as it is clear in Figure 4a, with high MoSe<sub>2</sub> carrier concentration, thin MoSe<sub>2</sub> layer is sufficient to achieve high J<sub>SC</sub>. This is in accordance to the reported findings by Hossain et al. [44] and Ferdaous et al. [45] that even small changes in the J<sub>SC</sub> values, the phenomenon of higher carrier concentration and lower thickness are preferred for p-type MoS<sub>2</sub> (p-MoS<sub>2</sub> yields similar benefits as p-MoSe<sub>2</sub> as interfacial layer at the back contact). However, Figure 4c shows that when  $N_A$  is >1.0 × 10<sup>18</sup> cm<sup>-3</sup>, the trend in FF changes from favoring larger thickness to favoring lesser thickness. Nevertheless, the difference in the electrical characteristics of thin and thick MoSe<sub>2</sub> layers are not very significant if the carrier concentration is sufficiently high. Hence, it is more favorable to have a thinner MoSe<sub>2</sub> layer with high carrier concentration in order to avoid a jump in series resistance due to the high resistivity nature of MoSe<sub>2</sub>.

The aforementioned results indicate that significant changes in the performance parameters of the cell were observed when the  $N_A$  of MoSe<sub>2</sub> layer was around 10<sup>16</sup>, 10<sup>18</sup>, and  $10^{19}$  cm<sup>-3</sup>. Hence, the effects of bandgap energy ( $E_g$ ) and electron affinity ( $\chi$ ) on the conversion efficiency were investigated in the range from 1.0 to 1.5 eV and 3.5 to 4.5 eV, respectively, at these three domains of  $N_A$  and are illustrated in Figure 5a,b. As shown, with MoSe<sub>2</sub> layer  $N_A$  of  $10^{18}$  and  $10^{19}$  cm<sup>-3</sup>, CIGS device exhibits similar and almost identical patterns in the PCE with the increase in  $E_g$  and  $\chi$ , while at  $N_A$  of 10<sup>16</sup> cm<sup>-3</sup>, the PCE variation demonstrates a distinguish phenomenon of nearly linear decrease from 20% to 2% and from around 32% to 2% with increasing values of  $E_g$  and  $\chi$ , respectively. This result verifies our earlier findings that higher doping level of the MoSe<sub>2</sub> layer is more beneficial for the overall cell performance. Therefore, based on this preliminary investigation,  $N_A$  of  $MoSe_2$  layer in the CIGS model was then fixed at  $10^{19}$  cm<sup>-3</sup> to perform further simulations for different combinations of  $E_g$  and  $\chi$  for the MoSe<sub>2</sub> layer. Figure 6 illustrates the solar photovoltaic parameters as a function of  $\chi$  of MoSe<sub>2</sub> layer, with bandgap energy  $E_g$  ranging from 1.0 eV to 1.5 eV. It can be observed that, in general, increasing the  $E_g$  leads to an increase in the conversion efficiency of the cell over the whole investigated range of  $\chi$ . Hence, MoSe<sub>2</sub> layer of higher  $E_g$  is favorable. As depicted in Figure 6a, for  $E_g > 1.1$  eV,  $J_{SC}$  of the device is almost constant for all values of  $\chi$ , indicating that beyond a minimum value or threshold,  $E_g$  and  $\chi$  do not notably affect the current collection. This may be explained by the fact that the thin p-type  $MoSe_2$  layer in this CIGS solar cell structure does not play an important role in the photon absorption, hence, other than layer thickness as discussed earlier, variation in other material parameters of this layer does not contribute to the change in  $J_{SC}$  of the whole device. On the other hand,  $V_{OC}$  and PCE exhibit similar behavior where for the values of  $E_g$  defined earlier for the MoSe<sub>2</sub> layer, the V<sub>OC</sub> and PCE were almost saturated for all values of  $\chi$ , provided that  $E_g + \chi \leq 5.4$  eV. If the total of  $E_g + \chi$  rises beyond 5.4 eV, V<sub>OC</sub> and PCE start to deteriorate and further increase will result in non-working device as can be seen in Figure 6b,d. These observations indicate that optimum range of electron affinity for a functional MoSe<sub>2</sub> interface layer is dependent on the value of its bandgap energy. Improvement in  $V_{OC}$  with the increase in  $E_g$  of MoSe<sub>2</sub>

layer can be analyzed based on the band offsets at CIGS/MoSe<sub>2</sub> and MoSe<sub>2</sub>/Mo interfaces. The features of band alignment are determined based on the Anderson's rule or known as electron affinity model as mentioned earlier.



**Figure 5.** Effects of (a)  $E_g$ ; (b)  $\chi$  on the PCE with carrier concentration of 10<sup>16</sup>, 10<sup>18</sup>, and 10<sup>19</sup> cm<sup>-3</sup>.



**Figure 6.** The simulated electrical performance parameters as a function of  $MoSe_2$  electron affinity ranging from 3.5 eV to 4.5 eV: (a)  $J_{SC}$ ; (b)  $V_{OC}$ ; (c) FF; and (d) conversion efficiency (PCE) at different bandgap ranging from 1.0 eV to 1.5 eV.

 $E_g$  and  $\chi$  of MoSe<sub>2</sub> layer crucially determine  $\Phi_{MoSe_2}$ ,  $qV_o$ , back contact barrier height with respect to  $E_C$  ( $\Phi_{Bn}$ ), back contact barrier height with respect to  $E_V(\Phi_{Bp})$  of the MoSe<sub>2</sub>/Mo metal-semiconductor junction and conduction band offset ( $\Delta E_C$ ), valence band

offset ( $\Delta E_V$ ), and back diode built-in voltage ( $qV_{bi_{back}}$ ) of the CIGS/MoSe<sub>2</sub> heterojunction [46] as given in Equations (4)–(10).

$$\Phi_{Bn} = \Phi_{Mo} - \chi_{MoSe_2} \tag{6}$$

$$\Phi_{Bp} = E_{gMoSe_2} - \Phi_{Bn} \tag{7}$$

$$\Delta E_C = \chi_{CIGS} - \chi_{MoSe_2} \tag{8}$$

$$\Delta E_V = \left(\chi_{MoSe_2} + E_{gMoSe_2}\right) - \left(\chi_{CIGS} + E_{gCIGS}\right) \tag{9}$$

$$qV_{bi_{back}} = \Phi_{MoSe_2} - \Phi_{CIGS} \tag{10}$$

Increment/decrement in the MoSe<sub>2</sub>  $E_g$  and  $\chi$  values shifts the whole band structure of the layer upward or downward, which in turn has an effect on the mentioned band alignment related parameters. Nevertheless, since no significant effect on the cell performance is found in the variation of  $\chi$  in comparison to  $E_g$  from our earlier discussion on Figure 6,  $\chi$  is defined as 3.9 eV in order to calculate the interface electronic parameter values as a function of  $E_g$  as tabulated in Table 4. Changes in  $E_g$  are usually reflected as simultaneous change in  $E_C$  and  $E_V$ . Thus, any increase in  $E_g$  can be seen as upshifting of  $E_C$  and/or downshifting of  $E_V$ . However, since the value of  $\chi$  was kept constant, the increase in  $E_g$ is assumed to cause the downshifting of  $E_V$ , while  $E_C$  does not change, thus the values of  $\Phi_{Bn}$  and  $\Delta E_C$  are constant with the increase in  $E_g$ , as shown in Table 4. Therefore, the resulting device performance is solely a composite function of  $\Phi_{Bp}$ ,  $qV_o$ ,  $\Delta E_V$  and  $qV_{bi_{back}}$ . In general, for CIGS/MoSe<sub>2</sub>/Mo band alignment, lower  $qV_0$  and  $\Delta E_V$  along with higher positive  $qV_{bi_{hack}}$  (or lower negative  $qV_{bi_{hack}}$ ) are desirable for greater hole transport across the valence band of CIGS to valence band of MoSe<sub>2</sub> and from the valence band of MoSe<sub>2</sub> to Mo metal. Increase of MoSe<sub>2</sub>  $E_g$  results in an increase in MoSe<sub>2</sub> work function ( $\Phi_{MoSe_2}$ ) due to the downward shift of  $E_V$ . This will lead to larger values of  $\Phi_{Bp}$ ,  $qV_o$  and  $\Delta E_V$ , compounding the inhibition of hole flow to the back contact. Nevertheless, this drawback can be negated by carrier tunneling through a very thin MoSe<sub>2</sub> layer, which can be related back to the improved conversion efficiency obtained with the increase in  $E_g$  as illustrated in preceding Figure 6d. Additionally, increased hole population by means of higher doping concentration can yield slightly better performance for  $MoSe_2$  with higher  $E_g$  as previously demonstrated in Figure 5.

Pand Diagram Paramatara (aV)				$E_g$ (	eV)		
Dalla Diagraili I al	Talleters (ev)	1.0	1.1	1.2	1.3	1.4	1.5
MoSe <sub>2</sub> /Mo	$\Phi_{MoSe_2}$	4.8848	4.9848	5.0848	5.1848	5.2848	5.3848
MoSe <sub>2</sub> /Mo	$qV_o$	-0.0652	0.0348	0.1348	0.2348	0.3348	0.4348
MoSe <sub>2</sub> /Mo	$\dot{\Phi}_{Bn}$	1.05	1.05	1.05	1.05	1.05	1.05
MoSe <sub>2</sub> /Mo	$\Phi_{Bp}$	-0.05	0.05	0.15	0.25	0.35	0.45
CIGS/MoSe <sub>2</sub>	$\Delta E_{C}^{'}$	-0.04	-0.04	-0.04	-0.04	-0.04	-0.04
CIGS/MoSe <sub>2</sub>	$\Delta E_V$	-0.16	-0.06	0.04	0.14	0.24	0.34
CIGS/MoSe <sub>2</sub>	$qV_{bi_{back}}$	0.00065	0.10065	0.20065	0.30065	0.40065	0.50065

**Table 4.** Calculated Interface Electronic Parameters of  $Mo/MoSe_2/CIGS$  in Various  $E_g$  of  $MoSe_2$ .

Based on the aforesaid results, variations in the bandgap, electron affinity, thickness and carrier concentration of the MoSe<sub>2</sub> layer mainly affected the band alignment at the CIGS/MoSe<sub>2</sub> and MoSe<sub>2</sub>/Mo junctions, which subsequently influences the overall performance of the CIGS solar cell. It was identified that a MoSe<sub>2</sub> layer with bandgap in the range of 1.2 eV to 1.4 eV and high carrier concentration above  $1.0 \times 10^{18}$  cm<sup>-3</sup> is beneficial for the PV cell. As predicted, the MoSe<sub>2</sub> layer needs to be quite thin, but not less than 0.04 µm thickness in order to be effective or operational. These findings provide a limiting condition for MoSe<sub>2</sub> layer in CIGS solar cell since the formation is absolutely unavoidable during the growth process. Our CIGS model with optimized MoSe<sub>2</sub> layer is then validated by comparison with extant experimental results for the conventional ZnO/CdS/CIGS/Mo solar cells considering that MoSe<sub>2</sub> is naturally formed as opposed to being a deliberately added layer in the device stack during fabrication. The 23.3% efficiency of our simulated CIGS cell is significantly higher with the addition of MoSe<sub>2</sub> layer than the recorded efficiency of 21.7% [24]. This is apparently due to the fact that there are many other factors during the fabrication process that could affect the cell performance that cannot be replicated by the simulation software. Therefore, it is impossible to simulate these realistic experimental conditions due to the limitations of the SCAPS software. In addition, not many details were provided in the report about the actual steps involved in the making of these record-breaking solar cells. Nevertheless, the adequately high efficiency of the actual solar cells suggests the presence of MoSe<sub>2</sub> layer in the structure as the simulated structure with MoSe<sub>2</sub> is closer to the experimental value. The resulting performance parameters of the J<sub>SC</sub>, V<sub>OC</sub>, FF and PCE are displayed in Table 5.

Table 5. Performance Parameters of the Proposed CIGS Cell Structure in Comparison to the Recorded Experimental Cell.

Performance Parameter	Proposed Cell (CIGS without MoSe <sub>2</sub> )	Proposed Cell (CIGS with Optimized MoSe <sub>2</sub> )	Reference Cell [24]
$J_{SC}$ (mA/cm <sup>2</sup> )	35.75	36.44	36.60
V <sub>OC</sub> (V)	0.681	0.815	0.746
FF (%)	82.88	78.46	79.30
PCE (%)	20.19	23.30	21.70

# 3.2. Study of Absorber Layer Bandgap Grading in CIGS Solar Cell Structure

In this study, bandgap grading was introduced into the model by including a Ga concentration profile in the absorber layer, that is the variation of GGI ratio throughout the depth of the absorber layer. Double grading (DG) profile was defined within the absorber layer, which corresponds to a minimum amount of Ga in the middle layer region and a higher amount toward the CIGS/MoSe<sub>2</sub> and the CdS/CIGS interfaces. These bandgap variations are described in this work by the parameters: (i)  $y_{left}$  and  $y_{right}$  (corresponding to the Ga concentration at the back and front sides of the absorber layer); (ii)  $y_{min}$  (notch point which represents the lowest composition value); (iii) x<sub>min</sub> (position of the notch point across the depth of absorber layer) through the use of parabolic grading [28]. Thus,  $y_{left}$ and  $y_{right}$  define the  $E_{g,max}$  (maximum bandgap value) while  $y_{min}$  defines  $E_{g,min}$  (minimum bandgap value) in the bandgap grading profiles. With the purpose of determining the best grading configuration for this notch type double graded bandgap structure in our CIGS model, different values for these related bandgap grading parameters were simulated and the effects on cell performance were analyzed. In order to incorporate an optimum DG bandgap profile, the effects of separate grading at either ends of the absorber must be first understood. Thereby, optimization of single graded Ga profiles (back and front grading) was conducted prior to the introduction of DG and the results obtained are illustrated in Figures S2–S4 in the supporting materials section. Table 6 shows the optimum values for Ga composition (GGI ratio) at the back contact and at the CdS/CIGS interface and the lowest bandgap  $(y_{min})$  in the CIGS absorber layer obtained from the optimization of single graded Ga profiles.

Table 6. Optimum Values of Grading Parameters Related to BG and FG Determined from Simulation.

Grading Profile	Grading Parameters	Optimum Values Found
Back grading (BG)	Back composition (GGI)	0.7
	$y_{min}$ (lowest composition)	0.3
Front grading (FG)	Front composition (GGI)	0.8
	$y_{min}$ (lowest composition)	0.3

Conceptually, double graded (DG) bandgap absorbers promote photovoltaic performance by increasing  $J_{SC}$ , which is a consequence of the minimum bandgap introduced

in the absorber layer of the device, and at the same time increased  $V_{OC}$  due to the increased bandgap in the SCR. This principal of two bandgaps was experimentally verified by Dullweber et al. [47]. In DG bandgap profile, the position of notch  $(x_{min})$  is a significant parameter that will influence the effectiveness of bandgap grading in the absorber layer. Hence,  $x_{min}$  is varied in the range from 0 to 2.5 µm to observe the effects mainly on J<sub>SC</sub> and  $V_{OC}$ , keeping the notch value ( $y_{min}$ ) constant at 0.3. From Figure 7a, it can be observed that  $J_{SC}$  significantly improved when the  $x_{min}$  value is shifted to the front junction of the CIGS layer. As mentioned earlier in Section 1, absorption in the frontal part is reduced as the bandgap in this region becomes larger. However, if the front grading with wider bandgap is restricted within the SCR by placing the notch  $(x_{min})$  inside the width of SCR, the loss in J<sub>SC</sub> can be compensated by an increased absorption further into the CIGS absorber layer, where the band gap is minimum. Moreover, the rise of  $E_g$  in the SCR will generate an additional electric field that will oppose the transport of electrons. Hence, it is important to confine the front grading only in this region. As  $x_{min}$  shifts further towards the backside of the absorber layer (from the distance of 2.25 to 0.25  $\mu$ m), the decrease in  $J_{SC}$  is more pronounced (from 38.97 to 36.37 mA/cm<sup>2</sup>). The graph in Figure 7b depicts  $V_{OC}$  dependency on the notch position ( $x_{min}$ ) that is fairly contrasting to  $J_{SC}$ .  $V_{OC}$  does not seem to be substantially affected by the variation in  $x_{min}$ , though small increment is observed as  $x_{min}$  shifts towards the front side of the absorber layer.



**Figure 7.** Comparing the effects of notch position  $(x_{min})$  on (**a**)  $J_{SC}$ ; (**b**)  $V_{OC}$  of the cell with the incorporation of DG bandgap profiles.

There are certain conditions related to the grading parameters that must be satisfied in order to completely benefit from bandgap grading. In the case of a p-type CIGS layer, the needed quasi-electric field arising from an absorber material with graded bandgap structure should be directed towards the back contact so that electrons will drift in the opposite direction to reduce back surface recombination. In other words, in this case, the bandgap must be larger towards the back contact. The second condition is that the formation of wider bandgap region at the front junction must be confined within SCR since this quasi-electric field would oppose the motion of photo-generated carriers from the bulk of the semiconductor towards the collecting junction. From the above considerations, different magnitudes, shapes, and depths of double graded (DG) bandgap structure were tested in order to find its relevance in the solar cell performance and to determine the best grading configuration for an optimized CIGS device. Figure 8a illustrates the simulated compositional ratios of five models with different bandgap configurations and the resulting current density-voltage (J-V) curves obtained are shown in Figure 8b. A summary of the solar cell parameters for the different Ga profiles is presented in Table 7.



**Figure 8.** (a) Different Ga profiles implemented in the simulations in order to extract the most suitable front and back grading profiles for double graded (DG) bandgap structure. These Ga profiles show the compositional ratio GGI along the CIGS layer depth; (b) simulated J-V curves obtained using the different compositional ratio as reported in SRH and radiative recombination profiles left inset.

**Table 7.** Solar Cell Parameters For Different Front and Double Grading Combinations Extracted from Simulated J-V

 Reported in SRH and Radiative Recombination Profiles (Left Inset).

		Ga Profiles				Solar Cell Pa	rameters	
	Front:Back (GGI)	E <sub>g,front</sub> :E <sub>g, back</sub> (eV)	y <sub>min</sub> (GGI)	<sup>1</sup> 2.5– <i>x<sub>min</sub></i> (μm)	V <sub>OC</sub> (V)	J <sub>SC</sub> (mA/cm <sup>2</sup> )	FF (%)	PCE (%)
Model 1 (DG)	0.8:0.7	1.50:1.43	0.2	2.00	0.820	39.20	78.36	25.18
Model 2 (DG)	0.8:0.7	1.50:1.43	0.2	1.25	0.820	39.45	78.47	25.37
Model 3 (DG)	0.8:0.7	1.50:1.43	0.2	0.25	0.820	39.31	78.41	25.26
Model 4 (DG)	0.5:0.8	1.28:1.50	0.3	0.25	0.856	36.24	80.07	24.83
Model 5 (DG)	0.5:0.5	1.28:1.28	0.3	1.25	0.815	36.40	81.53	24.19
Ungraded bandgap cell	0.3:0.3	1.20:1.20	NA	NA	0.815	36.44	78.46	23.30

<sup>1</sup> 2.5– $x_{min}$  = distance from the CdS/CIGS interface.

As can be observed in Table 7, the best PCE is obtained from the simulated Model 2 that presents a front grading and back grading composition of 0.8 and 0.7, respectively. The notch for this model is positioned at a distance of 1.25 µm from the CdS/CIGS interface. Although it is mentioned earlier that the notch should be placed close to the junction and restricted within the SCR for improved  $J_{SC}$  as evident from previous Figure 7a, 1.25  $\mu$ m was found to be the optimum notch position for the DG absorber bandgap profile developed in this study. The slight loss in J<sub>SC</sub> in Model 3 in comparison to Model 2, with Model 3 having a steeper Ga grading profile at the frontside of the absorber, can be attributed to the fact that the notch acts like a confinement region for electrons decreasing photogenerated carrier collection probability. Similar observation can be made for Model 4 and Model 5. In line with the reflection that improved J<sub>SC</sub> in DG absorber bandgap structure is controlled by the minimum bandgap value in the layer, it can be discerned that J<sub>SC</sub> values are higher when  $y_{min}$  was set at GGI = 0.2 as compared to 0.3 in all bandgap grading models. With regard to V<sub>OC</sub>, Model 4 presents the highest value of 0.856 V that can be attributed to the highest GGI ratio of 0.8 ( $E_{g,back}$  = 1.5 eV) at the backside of the absorber layer. The enhanced V<sub>OC</sub> is directly correlated to the reduced back surface recombination as discussed and presented in the earlier section. FF is the highest in device Model 5 with DG absorber bandgap value of 1.28 eV corresponding to GGI (=0.5) at both the frontside and backside of the absorber layer. Ideally, FF is only a function of V<sub>OC</sub>. However, practically, FF does not only depend on  $V_{OC}$ , but also on the recombination process in the depletion region [45], which explains the difference in the trend of FF in comparison to V<sub>OC</sub> as can be seen in Table 7. The highest PCE gain from the ungraded bandgap cell is over 8.8% as seen in Model 2.

# 3.3. Optimizing Bandgap Energy of MoSe<sub>2</sub> Layer for Compatibility with Double Graded (DG) Bandgap Profile of CIGS Absorber Layer

For the purpose of associating the bandgap grading study with MoSe<sub>2</sub> layer properties, optimum DG bandgap profile with front and back GGI ratio of 0.8 and 0.7, respectively,  $x_{min} = 1.25 \ \mu\text{m}$ , and  $y_{min} = 0.2$  as previously determined was employed with MoSe<sub>2</sub> layers with varying bandgaps of 1.0 to 1.4 eV. The resulting solar photovoltaic parameters (J<sub>SC</sub>, V<sub>OC</sub>, FF and PCE) obtained are tabulated in Table 8. In Section 3.1, it has been shown that  $E_g$  and  $\chi$  of both MoSe<sub>2</sub> heterojunction [43]. Lower  $\Delta E_V$  and higher positive  $qV_{bi_{back}}$  (or lower negative  $qV_{bi_{back}}$ ) are desirable for the ease of hole transport across the valence band of the CIGS layer to the valence band of MoSe<sub>2</sub>. Hence, the resulting device performance is partly contributed by the composite function of  $\Delta E_V$  and  $qV_{bi_{back}}$ . The effects of MoSe<sub>2</sub> bandgap on these parameters have been discussed and presented in Section 3.1. Based on the values of J<sub>SC</sub>, V<sub>OC</sub>, FF and PCE in Table 8, MoSe<sub>2</sub> bandgap of 1.3 eV is the best match with  $E_{g,back}$  of 1.43 eV at the backside of CIGS absorber layer for devices with DG absorber bandgap profile.

**Table 8.** Solar Cell Parameters for Different Front and Double Grading Combinations Extracted from Simulated J-V Reported in SRH and Radiative Recombination Profiles (Right Inset).

CIGS Bandgan MoSea Bandgar	MoSe <sub>2</sub> Bandgap	$1 \Lambda F_{c}$	$2 \Lambda F_{V}$	3 aVe	Solar Cell Parameters			
$E_{g,front}: E_{g,back}$ (eV)	$E_{g,MoSe_2}$ ( <b>eV</b> )	(eV)	(eV)	(eV)	V <sub>OC</sub> (V)	J <sub>SC</sub> (mA/cm <sup>2</sup> )	FF (%)	PCE (%)
	1.0	-0.07	-0.36	-0.1993	0.939	39.44	80.94	29.97
	1.1	-0.07	-0.26	-0.0993	1.166	39.47	68.35	31.46
1.50:1.43	1.2	-0.07	-0.16	0.0007	1.055	39.47	75.09	30.97
	1.3	-0.07	-0.06	0.1007	0.868	39.45	81.89	28.06
	1.4	-0.07	0.04	0.2007	0.820	39.45	78.47	25.37

<sup>1</sup> From Equation (8); <sup>2</sup> from Equation (9); <sup>3</sup> from Equation (10).

It is a fact that recombination of photo-generated carriers is the main detrimental factor affecting the performance of CIGS solar cells [46–48]. Extraction of interface recombination rates allows detailed analysis for material and device engineering to reduce interface recombination leading to an improved  $V_{OC}$ . Though experimental  $V_{OC}$  analysis is compulsory in understanding the physics of recombination mechanism, previous investigation has demonstrated the possibility of utilizing numerical simulation for extracting recombination rates in the complete width of the absorber layer (from the buffer/absorber interface [48] to absorber/back contact interface [49]). The principle of temperature- and illuminationdependent V<sub>OC</sub> analysis is to identify and quantify Shockley-Read-Hall (SRH) as well as radiative recombination rates in different regions of the CIGS absorber-namely, the heterointerface, depletion region and quasi-neutral region (QNR). A study conducted by Paul et al. [50] depicted that most of the recombination occurs near the CdS buffer/CIGS absorber interface and in the depletion region, with Shockley-Read-Hall (SRH) recombination dominating over radiative recombination when operating temperature, T is set at 300 K. By emulating the investigation carried out by Paul et al., simulation study on the relationship of recombination rate and the depth of the absorber layer was carried out using the baseline CIGS model at  $V = V_{OC}$ . The MoSe<sub>2</sub> interface layer and absorber bandgap grading was not incorporated in this baseline CIGS model. Uniform mid-gap defect level for all layers in the structure were considered, with radiative recombination coefficient defined as  $1.0 \times 10^{-10}$  cm<sup>3</sup>/s based on [50]. Figure 9 shows the generated SRH and radiative recombination profiles (for T = 300 K) at  $V = V_{OC}$ . It was found that the interface of CdS/CIGS and SCR act as recombination centers in the structure, matching the observations made by [50]. However, in this study radiative recombination rate seems to be higher at the depletion region and QNR while SRH is significantly more dominant at the front interface. There was not much difference in the recombination rates with the variation in operating temperature, T = 200 K and 300 K.



**Figure 9.** SRH and radiative recombination profile at  $V = V_{OC}$  (T = 200 K and 300 K) under one sun illumination (AM 1.5) for baseline structure of CIGS without the presence of MoSe<sub>2</sub> interface layer. Light yellow region represents CIGS absorber, deep yellow area is CdS buffer, and ZnO window layer is indicated as the grey region.

Controlling bandgap grading within the CIGS absorber is claimed to be one way of improving band alignment and suppressing recombination at the interface and in the bulk of the layer. It is said that in a uniform bandgap absorber with a low Ga content, recombination in the quasi-neutral region dominates, while in the high Ga-absorber, interface recombination dominates [51]. However, the effect of bandgap grading on the recombination process has not yet been fully understood. Hence, one of the objectives for implementing a graded structure in this study is to rearrange the recombination throughout the cell, by optimizing CdS/CIGS and CIGS/MoSe<sub>2</sub> band offsets to reduce surface recombination at the interface and by utilizing the built-in potential that causes drift of the photogenerated electrons and holes towards the right direction. In order to understand the role that bandgap grading has in suppressing carrier recombination, recombination profiles for the simulated CIGS device with MoSe<sub>2</sub> interfacial layer and with/without graded structure (DG) in the absorber layer were analyzed and presented in Figure 10 (left inset). There was clear benefit to be seen in recombination yields with the introduction of bandgap grading as suggested by earlier studies, with a significant decrease in back surface and front surface recombination illustrated in Figure 10 left and right inset respectively. Additional electric field known as quasi-electric field ( $\xi_A$ ) is formed due to the change in bandgap,  $E_g$ over the distance x and can be described by Equation (11) [20]. This quasi-electric field directed towards the back contact with the introduction of back grading will drift the electrons in the opposite direction to reduce back surface recombination. Hence. Ga-rich structure at the backside of absorber layer (towards CIGS/MoSe<sub>2</sub> interface) is beneficial and effective in suppressing electrons from combining with holes.

$$\xi_A = \frac{d\Delta E_g}{dx} \tag{11}$$

With respect to the front surface recombination, recombination rate in the SCR can be reduced by increasing the barrier height via the increase of bandgap at the junction region (CdS/CIGS interface). This is due to the fact that the CdS buffer/CIGS absorber conductionband offset,  $\Delta E_C$  significantly influences the band bending and thereby affecting interface recombination where stronger band bending and larger hole barrier are induced by a positive  $\Delta E_C$  at the CdS/CIGS interface [49].



**Figure 10.** SRH and radiative recombination profiles at  $V = V_{OC}$  (T = 300 K) under one sun illumination (AM 1.5) for the simulated CIGS cell with and without the presence of double grading (DG) bandgap alignment in the absorber layer. (**Left Inset**) Zoom-in image of the recombination rate curve at the interface of CdS/CIGS. (**Right Inset**) Zoom-in image of the recombination rate curve at the interface of CIGS/MoSe<sub>2</sub>.

By comparing the J-V characteristic and quantum efficiency (QE) curves of a uniform bandgap device with and without MoSe<sub>2</sub> layer to the device with DG absorber profile, shown in Figure 11, the composite benefit of the MoSe<sub>2</sub> layer and DG absorber layer on the performance of CIGS solar cells, is remarkable and was clearly demonstrated in this simulation study, as seen in the overall cell performance parameters. This enhancement in current density is attributed to the increased absorption of photons in the longer wavelength region of above 1000 nm, as can be seen from the QE curve of Figure 11b. A reasonable explanation for the enhanced photon absorption is the lower  $E_{g,min}$  of 1.10 eV in the underlying bulk region of DG CIGS absorber layer in comparison to the device with uniform absorber bandgap of 1.20 eV. This observation is in agreement with the inferred statement earlier that this notch value and its position is crucial for the device to benefit from bandgap grading of the absorber layer. Table 9 below shows the performance parameters of all the devices investigated in this section.



**Figure 11.** (**a**) J-V characteristics and (**b**) quantum efficiency curves of CIGS cells simulated in this study with/without MoSe<sub>2</sub> and with DG bandgap grading profile in the absorber layer.

Performance Parameter	Baseline Cell (Ungraded Bandgap without MoSe <sub>2</sub> )	Proposed Cell (Ungraded Bandgap with Optimized MoSe <sub>2</sub> )	Proposed Cell (DG Bandgap with Optimized MoSe <sub>2</sub> )
$J_{SC}$ (mA/cm <sup>2</sup> )	35.75	36.44	39.45
V <sub>OC</sub> (V)	0.681	0.815	0.868
FF (%)	82.88	78.46	81.89
PCE (%)	20.19	23.30	28.06

Table 9. Performance Parameters of the Proposed CIGS Cell Structure in Comparison to the Recorded Experimental Cell.

#### 4. Conclusions

Via the use of SCAPS software, a comprehensive numerical simulation analysis of CIGS thin film solar cell having additional MoSe<sub>2</sub> interface layer with varying material properties and various absorber bandgap profiles has been performed. The primary objective of this work was to investigate the simultaneous effects of MoSe<sub>2</sub> layer and Ga grading of the absorber in suppressing carrier losses due to back contact recombination and resistance that usually happen in the case of standard Mo thin films. Numerical simulations were performed to analyze the dependence of output parameters such as  $J_{SC}$ ,  $V_{OC}$ , FF and PCE to a wide range of thickness, carrier concentration,  $E_g$  and  $\chi$  of MoSe<sub>2</sub> layer as well as to different kinds of related grading parameters that can be optimized through the incorporation of bandgap grading in the absorber layer. From the obtained results, it was identified that  $MoSe_2$  with  $E_g$  of 1.3 eV and high carrier concentration above  $1.0 \times 10^{19}$  cm<sup>-3</sup> can be beneficial for the CIGS solar cell. It was also shown that the MoSe<sub>2</sub> layer needs to be very thin in the range of 0.04 to 0.1 µm in order to be effective. With regard to bandgap grading, it is evident from our results that an in-depth control of back and front Ga composition and the position of notch that correlates to the lowest bandgap value in the absorber layer is necessary to produce high performing solar cell. With the incorporation of double grading (DG) bandgap profile in the absorber layer, the performance of our simulated CIGS cell was significantly enhanced, achieving the highest efficiency of 28.06%. In summary, CIGS thin film solar cells with a functional MoSe<sub>2</sub> contact layer and a suitable double graded bandgap absorber layer are key focus areas in achieving higher photovoltaic conversion efficiencies.

**Supplementary Materials:** The following are available online at https://www.mdpi.com/article/ 10.3390/coatings11080930/s1, Figure S1: Measured J–V curves with different illumination values. Plots (**a**–**c**) correspond to the simulated CIGS device with carrier concentration of MoSe<sub>2</sub> interfacial layer of  $1.0 \times 10^{14}$ ,  $1.0 \times 10^{16}$ , and  $1.0 \times 10^{19}$  cm<sup>-3</sup>, respectively, at T = 300 K. Figure S2: Electrical parameters as a function of back (CIGS/MoSe<sub>2</sub> interface) composition ranging from 0 to 1 for BG structure (**a**) J<sub>SC</sub> and V<sub>OC</sub> (**b**) FF and conversion efficiency (PCE). Figure S3: Electrical parameters as a function of front (CdS/CIGS interface) composition ranging from 0 to 1 for FG structure (**a**) J<sub>SC</sub> and V<sub>OC</sub> (**b**) FF and conversion efficiency (PCE). Figure S4: Electrical parameters as a function of as a function of lowest composition value ( $y_{min}$ ) in the bulk region of CIGS absorber layer for FG bandgap profile (**a**) J<sub>SC</sub> and V<sub>OC</sub> (**b**) FF and conversion efficiency (PCE).

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#### Appendix A

Table A1. Simulation Material Gaussian Defect for the CIGS Solar Cell.

Material	ZnO	CdS	CIGS	MoSe <sub>2</sub>
Defect type	Donor	Donor	Acceptor	Acceptor
Energy level (eV)	1.65	1.2	0.6	$0.\bar{7}$
$\sigma_n (\mathrm{cm}^2)$	$1.0 imes10^{-15}$	$1.0 imes10^{-17}$	$5.3 imes10^{-13}$	$5.3 imes10^{-13}$
$\sigma_p (\mathrm{cm}^2)$	$1.0 imes10^{-12}$	$9.8 imes10^{-13}$	$1.0 imes10^{-18}$	$1.0 imes10^{-18}$
$N_t$ (cm <sup>-3</sup> )	$1.0 imes10^{16}$	$1.0 imes10^{18}$	$1.0 imes10^{14}$	$1.0 imes10^{14}$

Table A2. Contact Parameters Applied in the Simulation.

Parameter	Back Contact	Front Contact
$\phi_B$ (eV)	0.6348	Flat band
$S_n$ (cm/s)	$1.0  imes 10^7$	$1.0  imes 10^7$
$S_p$ (cm/s)	$1.0  imes 10^7$	$1.0  imes 10^7$
Reflectivity	NA	0.02

Table A3. Definition of the Parameters Used During the Simulations.

Parameter	Definition
ε <sub>r</sub>	Dielectric permittivity
$\mu_n/\mu_p$	Mobility of electron/holes
$N_A/N_D$	Acceptor/donor concentration
$E_g$	Bandgap energy
$N_C / N_V$	Effective density of states in the conduction/valence band
χ	Electron affinity
$\sigma_n/\sigma_p$	Capture cross section of electron/holes
$N_t$	Defect concentration
$\phi_B$	Barrier height
$S_n/S_p$	Surface recombination velocity of electron/holes

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