"Improving CZTSSe Solar Cell Efficiency: A Theoretical Study of Cadmium-Free Buffer Layers and BSF Layer Variations"

A project report submitted in partial fulfilment of the requirements for the Award of Degree of

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in

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DECLARATION OF CERTIFICATE

This is to certify that the work presented in the thesis entitled. **"Improving CZTSSe Solar Cell Efficiency: A Theoretical Study of Cadmium-Free Buffer Layers and BSF Layer Variations"** which is being submitted by ……. in partial fulfillment of the requirement for the award of Degree of **Bachelor of Technology in Electronics and Communication Engineering** to Government Engineering College, Sheoharis an authentic work carried out under my supervision and guidance.

To the best of my knowledge, the content of this project report does not form a basis for the award of any previous Degree to anyone else.

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CERTIFICATE OF APPROVAL

The forgoing thesis entitled **"Improving CZTSSe Solar Cell Efficiency: A Theoretical Study of Cadmium-Free Buffer Layers and BSF Layer Variations"**, is hereby approved as a creditable study of research topic and has been presented in satisfactory manner to warrant its acceptance as prerequisite to the degree for which it has been submitted.

It is understood that by this approval, the undersigned do not necessarily endorse any conclusion drawn or opinion expressed therein, but approve the project for the purpose for which it is submitted.

(Internal Examiner) **(External Examiner)**

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We, the members of project titled **"Improving CZTSSe Solar Cell Efficiency: A Theoretical Study of Cadmium-Free Buffer Layers and BSF Layer Variations"**, would like to extend our deepest gratitude to everyone who contributed to the success of this project. This journey has been one of collaboration, learning, and mutual support, culminating in a project that we are proud to present.

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Lastly, we extend our gratitude to each other, the members of this project group. This project was a collaborative effort that required dedication, compromise, and teamwork. We have grown individually and collectively through this experience, gaining not just knowledge but also friendships that we treasure. This project report is not only a reflection of our hard work but also a testament to the support and guidance we received from all those mentioned above. Thank you for making this journey memorable and our project a success.

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ABSTRACT

Copper Zinc Tin Sulfur Selenide (CZTSSe) solar cells have emerged as a promising alternative to traditional silicon-based solar cells due to their high absorption coefficient, suitable bandgap, and earth-abundant elements. However, CZTSSe solar cells still face challenges in achieving high efficiency due to interface defects, recombination losses, and limited understanding of buffer layer and back surface field (BSF) layer optimization.

This study presents a comprehensive numerical and theoretical investigation of cadmium-free buffer layers and BSF layer variations to enhance CZTSSe solar cell efficiency. We employ SCAPS-1D simulations to model the solar cell performance and explore the impact of different buffer layers (ZnS, ZnO, and In2S3) and BSF layer variations (thickness, doping, and material) on the device efficiency.

Our results shows that:

ZnS buffer layer yields higher efficiency compared to ZnO and In_2S_3 due to reduced interface recombination and improved band alignment.

Optimizing BSF layer thickness and doping concentration significantly enhances the solar cell performance by reducing back surface recombination and improving carrier collection.

Introduction of a thin, heavily doped BSF layer with a high bandgap material (e.g., Cd-free $Zn_{1-x}Mg_xS$) further boosts efficiency by reducing interface recombination and enhancing carrier confinement.

This study provides valuable insights into the optimization of buffer and BSF layers for high-efficiency CZTSSe solar cells, paving the way for the development of cadmium-free, high-performance solar cells. Our findings can guide experimental efforts and accelerate the commercialization of CZTSSe solar cells.

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CHAPTER – 1

1. INTRODUCTION OF THE PROJECT

Thin film solar cell technologies have made remarkable progress in efficiency, reliability and production over the last few years. Various semiconducting material such as elemental, III-V, II-VI, ternary, quaternary compound based solar cell are still under research for performance improvement.

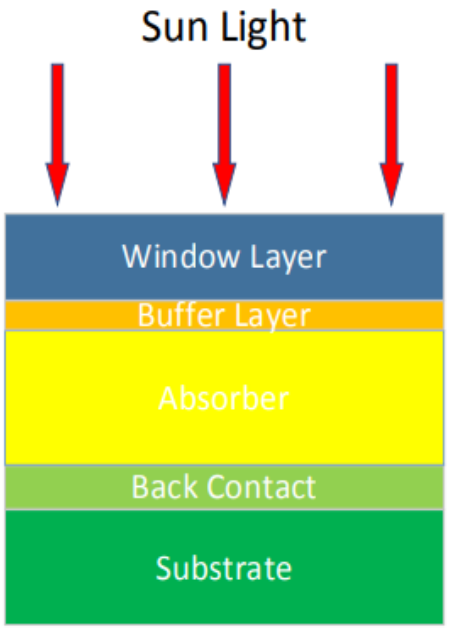


Fig.1.1[1]. Thin Film Solar Structure

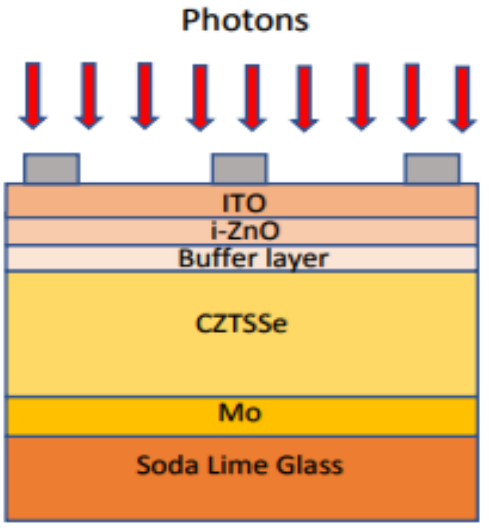


Fig. 1 Basic structure of CZTSSe solar cell

A typical thin film solar cell has the structure shown in Fig.1.1 [1]. Various layers are used in the solar cell based on the requirement to convert incident radiation into electronic carriers and then to transport them reliably to the external circuit.

a) Absorber layer:
It determines the performance of hetero junction thin film solar cell. An optimum material is required so that large number of photons are absorbed and correspondingly large number of electron-hole pairs are generated. Band gap of the absorber material must be small such that it absorbs larger portion of solar spectrum. Materials having a direct band gap of (1.1-1.7 eV) and a high absorption coefficient are used.

b) Window layer:
It is primarily used to form a p-n junction with the absorber layer in a heterojunction thin-film solar cell. Typically this layer is made very thin with high bandgap to catch low wavelength photons.

c) Buffer layer:
It is an intermediate/interface layer whose bandgap is between the window and the absorber. This reduces the conduction band offset (CBO) significantly, thereby reducing the carrier recombination, hence improving the performance of the solar cell.

d) Transparent Conducting:
Oxide (TCO) layer is the top most layer which is transparent for most of the incident radiation. Materials with bandgap more than about 3.3 eV are used as this layer.

1.1. CHARACTERISTICS

The main parameters that are used to evaluate the performance of solar cells are the short-circuit current density Jsc, the open circuit voltage Voc, the peak power Pmax, and the fill factor FF [2]. These parameters are determined from the illuminated J-V characteristic as illustrated in Fig.1.2.[3].

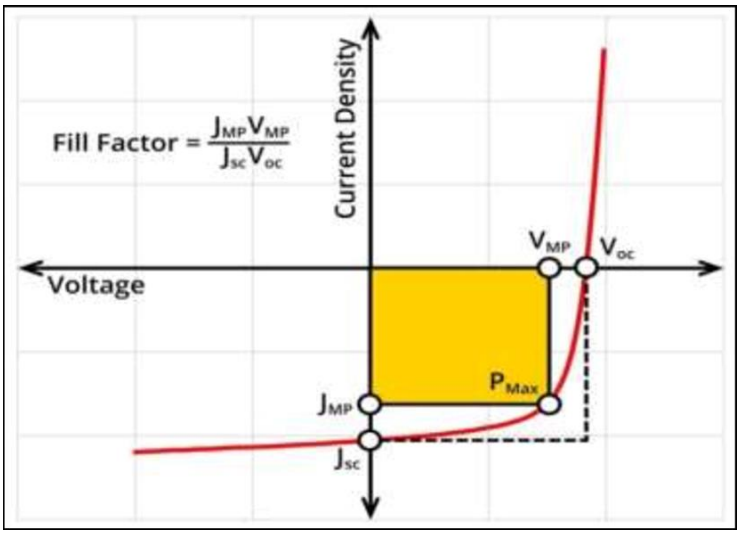


Fig. 1.2. J-V characteristics of a solar cell

a) Open circuit voltage (Voc):
This is the voltage measured when there is no current flow in the external circuit or when the external circuit is in an open condition. Some of the parameters which decide Voc are: bandgap of absorber material, amount doping of the doped layers, barrier height between the metal contact and the semiconductor, light generated current density and temperature.

b) Short circuit current density (Jsc):
This is the current density produced when the two contacts are short circuited, or when there is zero voltage across the two contacts. Some of the factors which decide Jsc are: incident light intensity, spectrum of the incident light, optical properties of the layers.

c) Fill factor (FF):
This is a parameter used to define fraction of electric power that can be extracted from the solar cell. Therefore, the FF is defined as

$$FF = VmpImp \,/\, VocIsc \,,$$

where Vmp and Imp are the voltage and current corresponding to the maximum power point Pmax. Fill factor primarily depends on solar cell series resistance (Rs) and shunt resistance (Rsh) which are a result of quality, thickness, type of semiconducting layers and its interfaces with other layers. To maximize value of FF, Rs and Rsh should be ideally zero and infinite respectively.

d) Power Conversion efficiency (η):
Light to electric power conversion efficiency is defined as

$$\eta = output\ power \,/\, input\ power = VOC * JSC * FF \,/\, PIN$$

where PIN is the solar power incident on a unit area. So to maximize efficiency, improvement in the open circuit voltage and the short circuit current density is needed.

1.2. MOTIVATION

The quaternary compound I-II-IV-VI CZTSSe (Cu2ZnSn(SSe)4) as an absorber material has gained a lot of attention in the field of thin film solar cell technology, primarily because it has a tunable direct band gap (1eV - 1.5 eV) and an absorption coefficient more than 104 cm-1 . However, champion CZTSSe solar cell has an efficiency of 12.6%.

So, improving the efficiency of CZTSSe solar cell beyond 12.6% remains a challenge.

- Cadmium Sulphide (CdS) is first choice for the buffer layer in thin film solar cells primarily because it forms an optimal spike band bending at the absorber – buffer interface.

- Because the Cadmium is toxic, replacing CdS with other efficient buffer layers is also gaining considerable attention.

- Lot of work has been reported where materials like Zinc Tin oxide ($Zn_{0.82}Sn_{0.18}O$), Zinc sulphide (ZnS) and Zinc Selenide (ZnSe), Aluminium doped Zinc Oxide (AZO) are used as alternate Buffer layers.

- To improve the performance of CZTSSe solar cells, it is important to minimize losses in performance parameters such as open circuit voltage and short circuit current density.

- In this regard, a proper growth mechanism of absorber layer need to be identified which reduces unwanted formation of secondary phases and intrinsic defects – vacancy, interstitial and anti-sites.

- Proper selection of materials for buffer and window layers is very much critical.

- Reduction of recombination at the back contact and absorber interface can be reduced by introducing the interfacial layer.

- Various interfacial layers such as Silver, Bismuth, ZnO, Carbon, TiN, Al_2O_3, TiB_2 have been reported in the literature.

CHAPTER – 2

2. ABOUT THE SOFTWARES USED

The **"Improving CZTSSe Solar Cell Efficiency: A Theoretical Study of Cadmium-Free Buffer Layers and BSF Layer Variations"** typically involves using various software tools for simulations, modeling, and data analysis.

2.1. Scaps1 D

- SCAPS is a one dimensional solar cell simulation program developed at the department of Electronics and Information Systems (ELIS) of the University of Gent, Belgium.
- SCAPS is originally developed for cell structures of the CuInSe2 and the CdTe family. Several extensions however have improved its capabilities so that it is also applicable to crystalline solar cells (Si and GaAs family) and amorphous cells (a-Si and micromorphous Si). An overview of its main features is given below:
- up to 7 semiconductor layers
- almost all parameters can be graded (i.e. dependent on the ocal composition or on the depth in the cell): Eg, χ, ε, NC, NV, vthn, vthp, μn, μp, NA, ND, all traps (defects) Nt
- recombination mechanisms: band-to-band (direct), Auger, SRH-type
- defect levels: in bulk or at interface; their charge state and recombination is accounted for
- defect levels, charge type: no charge (idealisation), monovalent (single donor, acceptor), divalent (double donor, double acceptor, amphoteric), multivalent (user defined)
- defect levels, energetic distributions: single level, uniform, Gauss, tail, or combinations
- defect levels, optical property: direct excitation with light possible (impurity photovoltaic effect, IPV)
- defect levels, metastable transitions between defects
- contacts: work function or flat-band; optical property (reflection of transmission filter) filter
- tunneling: intra-band tunneling (within a conduction band or within a valence band); tunneling to and from interface states
- generation: either from internal calculation or from user supplied g(x) file
- illumination: a variety of standard and other spectra included (AM0, $AM_{1.5}D$, $AM_{1.5}G$, $AM_{1.5}Gedition_2$, monochromatic.
- illumination: from either the p-side or the n-side; spectrum cut-off and attenuation
- working point for calculations: voltage, frequency, temperature

- the program calculates energy bands, concentrations and currents at a given working point, J-V characteristics, ac characteristics (C and G as function of V and/or f), spectral response (also with bias light or voltage)

- batch calculations possible; presentation of results and settings as a function of batch parameters

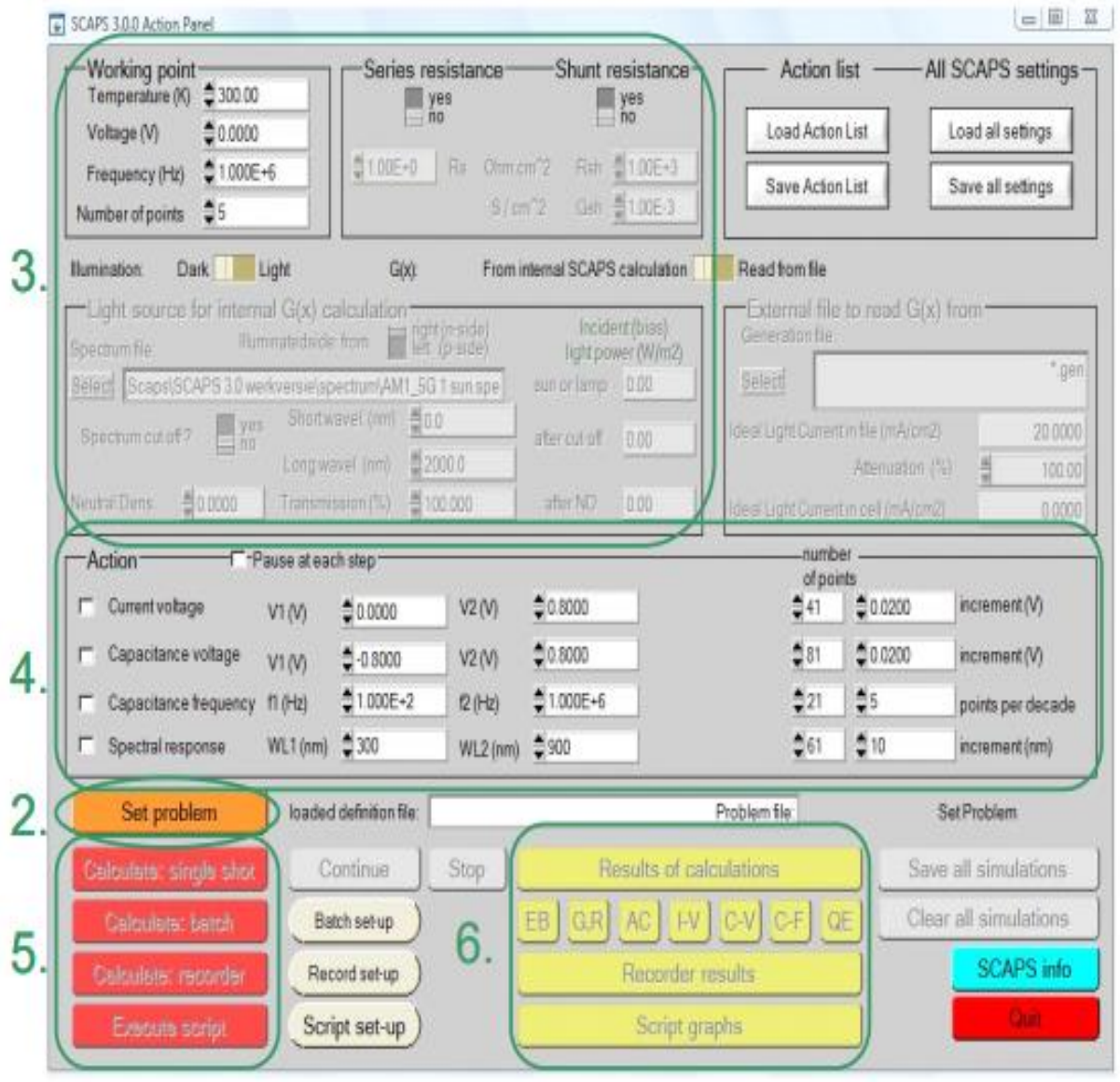
- loading and saving of all settings; start-up of SCAPS in a personalised configuration; a script language including a free user function

- very intuitive user interface

- a script language facility to run SCAPS from a ‘script file’; all internal variables can be accessed and plotted via the script.

- a built-in curve fitting facility

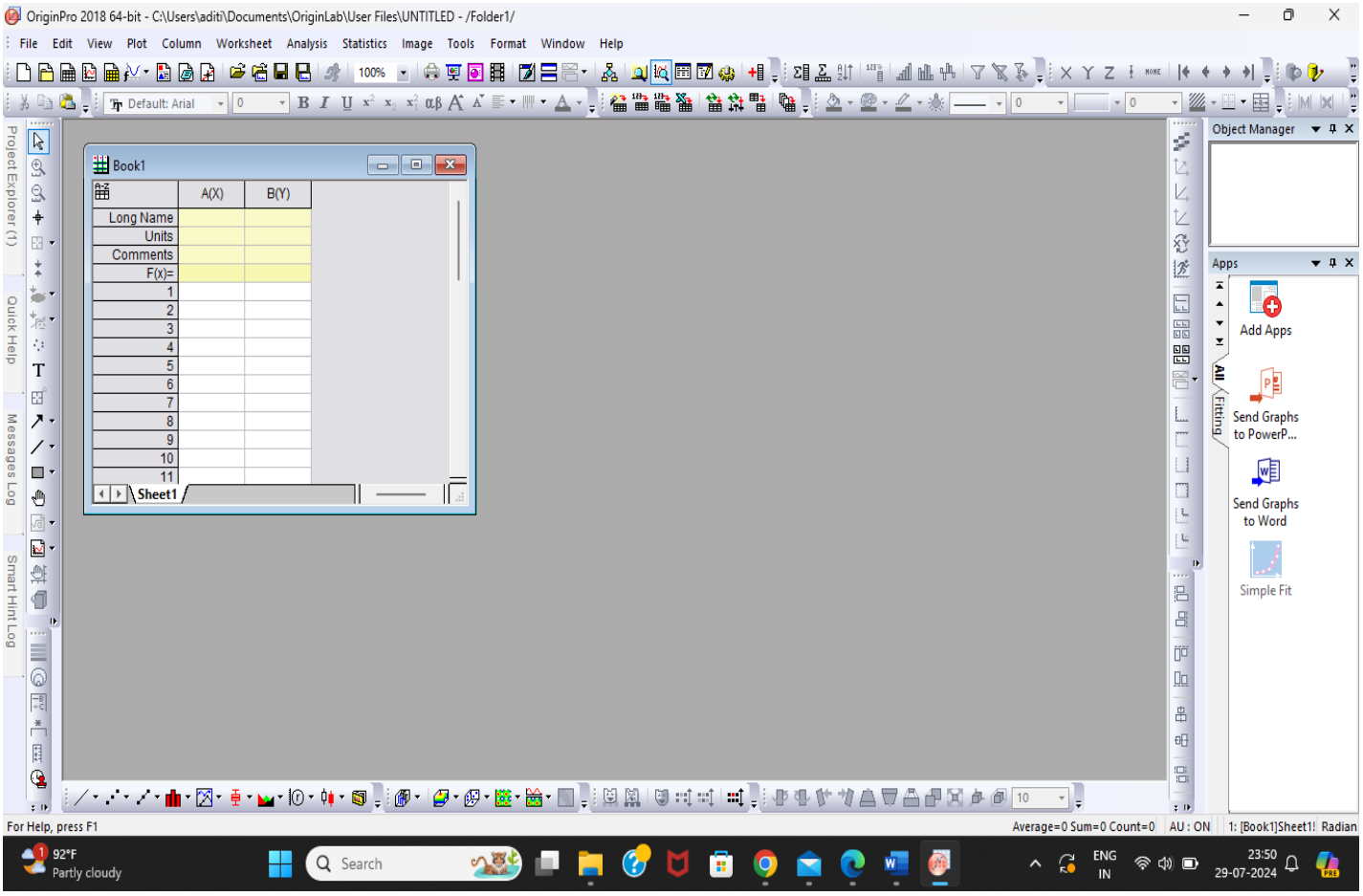
- a panel for the interpretation of admittance measurements.



2.2. ORIGIN 2018

- Origin is a powerful data analysis and publication-quality graphing software, tailored to the needs of scientists and engineers. What sets Origin apart from other applications is the ease with which you can customize and automate your data import, analysis, graphing and reporting tasks

- Origin graphs and analysis results can automatically update on data or parameter change, allowing you to create templates for repetitive tasks or to perform batch operations from the user interface, without the need for programming.



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CHAPTER – 3

3. SIMULATION

- **Table 1: Baseline parameters of different layers used in the simulation**

Parameter	CZTSSe [19], [20]	i-ZnO [21]	CdS [22]	ITO [23], [24]
Thickness (um)	2	0.01	0.04	0.05
E_g (eV)	0.96 - 1.5	3.25	2.43	3.3
χ_e (eV)	4.505 - 4.155	4.55	4.4	4.4
ε_r	13.6	9	10	8.9
N_C (cm^{-3})	2.2 E+18	2.2 E+18	2.2 E+18	5.2 E+18
N_V (cm^{-3})	1.8 E+19	1.75 E+19	1.8 E+19	1.0 E+18
$V_{th,e}$ (cm/s)	1.0 E+7	1.0 E+7	1.0 E+7	1.0 E+7
$V_{th,h}$ (cm/s)	1.0 E+7	1.0 E+7	1.0 E+7	1.0 E+7
μ_e(cm^2/Vs)	100	25	100	10
μ_h (cm^2/Vs)	25	5	25	10
Doping(cm^{-3})	1.0 E+16 (A)	1.0 E+18 (D)	1.0 E+18 (D)	1.0 E+20 (D)
Abs. const. ($cm^{-1}eV^{(½)}$)	4.0 E+4	1.5 E+5	1.9 E+5	1.0 E+6
Defect type	Single (A), Single (D)	Single (D)		
σ_e (cm^2)	1.0 E-13, 1.0 E-14	1.0 E-15		
σ_h (cm^2)	1.0 E-12, 1.0 E-17	1.0 E-13		
Reference	E_v, E_v	E_v		
Et (eV)	0.185, 0.85	1.650		
N_t($1/cm^3$)	2.27 E+16, 9.7 E+16	5.0 E+14		
Electrodes	Bottom Contact (Mo)	Top Contact (grid)		
Alignment / ϕ_m (eV)	5	Flat		
S_e (cm/s)	1.0 E+5	1.0 E+7		
S_h (cm/s)	1.0 E+7	1.0 E+5		
Tunnelling	No	No		

Symbols:
electrons e, holes h, acceptors A, donors D, bandgap Eg, electron affinity χe, conduction band C, valence band V, effective band states density N, dielectric permittivity(relative) εr, charge carrier mobility μ, thermal velocity Vth, trap position Et, capture cross-section σ, surface recombination velocity S and trap density Nt.

3.1. PARAMETERS

- **Thickness:**
  The absorber layer, p-type CZTSSe thin film is deposited on Mo layer, having thickness in the range in micrometers. To form a p-n junction, CdS layer having thickness of 50–100 nm is coated on CZTSSe layer.

  Thicker solar cells have higher resistance, because the electrons have to travel a longer distance through the material. However, thinner solar cells also have a drawback, they have more surface area, which increases the chance of electron recombination.

- **Bandgap:**
  It is denoted by **Eg** and It's unit is **eV.**

  CZTSSe, with its significant Direct bandgap is (0.96–1.5 eV). The minimum energy needed to excite an electron from the valence band to the conduction band.

  The size of the band gap is also very important, as this affects the energy that can be harvested by the solar cell. If ($E\gamma > Eg$), then the photon will be absorbed, and any energy in excess of Eg will be used to promote the electron to an energy level above the conduction band minimum.

  If the band gap is too high, most photons will not cause photovoltaic effect. If it is too low, most photons will have more energy than necessary to excite electrons across the band gap, and the rest of energy will be wasted.

- **Electron Affinity:**
  The electron affinity of a material in the context of solar cells refers to the amount of energy released when an electron is added to the material, effectively bringing an electron from the vacuum level into the conduction band of the material.

  It's an important property in determining the band alignment at interfaces within the solar cell, such as between the absorber layer and the buffer layer or the electron transport layer.

  In solar cells, optimizing the electron affinity of the various layers is crucial for efficient charge separation and transport, minimizing energy losses and enhancing the overall efficiency of the cell. Different materials used in solar cells, such as silicon, perovskites, or various types of semiconductors, will have different electron affinities.

- **Dielectric Permittivity (Relative):**
  The dielectric permittivity of a material in the context of solar cells is a measure of the material's ability to polarize in response to an electric field, thereby affecting the electric field within the material.

  It plays a critical role in determining the capacitance of the solar cell and influences the charge separation and transport properties. In solar cells, the dielectric permittivity affects the built-in electric field across the junction, which is essential for separating and transporting the photo-generated charge carriers (electrons and holes).

  High dielectric permittivity can help in reducing recombination losses by providing better charge separation, while also influencing the optical properties of the material, such as the reflection and transmission of light.

Different materials used in solar cells, such as silicon, perovskites, organic materials, and various thin films, have distinct dielectric properties, which are tailored for optimal device performance.

- **Conduction band effective density of states:**
  The conduction band effective density of states (DOS) is a parameter that characterizes the number of available electronic states in the conduction band per unit energy and volume. It is crucial in determining the electronic properties of semiconductor materials, including those used in solar cells.

  $N_c = 6.2 \cdot 10^{15} \cdot T^{3/2}$ (cm^{-3})

  This parameter is significant in determining the carrier concentration and the position of the Fermi level within the material. In solar cells, understanding the effective DOS is essential for predicting the electrical behavior of the semiconductor, such as the generation and transport of charge carriers. It also influences the open-circuit voltage and the overall efficiency of the solar cell. Different semiconductor materials will have different effective densities of states due to variations in their band structure and electron effective mass.

- **Valence band effective density of states:**
  The valence band effective density of states (DOS) is a parameter that describes the number of available electronic states in the valence band per unit energy and volume. This concept is crucial in understanding the electronic properties of semiconductor materials, particularly in the context of hole concentration and the positioning of the Fermi level.

  $N_v = 3.5 \cdot 10^{15} \cdot T^{3/2}$ (cm^{-3})

  The effective density of states for the valence band is critical for determining the hole concentration in the semiconductor and plays a significant role in the operation of devices like solar cells. In the context of solar cells, it affects the hole transport and the overall charge carrier dynamics, which in turn influence parameters such as the open-circuit voltage, fill factor, and efficiency of the solar cell.

  The effective DOS in the valence band varies depending on the semiconductor material due to differences in the band structure and the effective mass of holes. Understanding these properties is key to optimizing the design and performance of solar cells.

- **Thermal velocity of Electrons:**
  The thermal velocity of electrons is essentially the speed at which electrons move due to thermal energy. It's related to the temperature of the material and is a result of the electrons being excited to higher energy states by thermal energy.

  The thermal velocity affects various properties of the material such as electrical conductivity, carrier mobility, and the overall efficiency of electronic devices. In photovoltaic materials like CZTSSe, understanding the thermal velocity can help in analyzing charge carrier dynamics and optimizing device performance.

  In summary, the thermal velocity of electrons in CZTSSe is a key parameter in understanding the electronic behavior of the material under thermal excitation, and it plays a crucial role in evaluating its performance in applications like solar cells.

- **Thermal velocity of Holes:**
  The thermal velocity of holes is the speed at which these holes move as a result of thermal excitation. This is similar to the thermal velocity of electrons but pertains to the behavior of the "holes" or missing electrons in the valence band.

  Understanding the thermal velocity of holes is crucial for several reasons:

  Carrier Mobility: It affects how quickly holes can move through the material, which impacts the overall electrical conductivity and the efficiency of devices like solar cells.

  Carrier Dynamics: In semiconductors, the interaction between electrons and holes (i.e., recombination and generation) is fundamental to device performance.

  Material Properties: The thermal velocity influences how the material responds to temperature changes and how it handles thermal energy.

  In summary, the thermal velocity of holes in CZTSSe is a critical parameter in analyzing and optimizing the electronic properties of the material, particularly in the context of semiconductor devices where hole mobility and dynamics play a significant role.

- **Electron and Hole mobility:** The speed at which an electron can travel in an electrical field through a solid describes the mobility of electron particles. Mathematically, the electron mobility formula is

$$vd = \mu E$$

  Where is the speed of the electron, μ is the mobility, and E is the electrical field. The same formula is not applicable to hole mobility as holes are simply the absence of electrons in a solid. Electrons are negatively charged in nature, this polarity is reversed in holes, and they are positively charged. Holes exist when an electron moves out of the outer ring of an atom due to high energy levels.

- **Doping:**

  For CZTSSe, dopants might include elements like phosphorus (P) or antimony (Sb) for n-type doping, or elements like aluminum (Al) or gallium (Ga) for p-type doping.

  Sometimes, doping with elements from the same group as the primary constituents (such as adding more zinc or tin) can help fine-tune the properties of the material.

  Overall, doping is a critical technique in materials science and semiconductor physics for tailoring the characteristics of materials to suit specific applications, such as in solar cells, where CZTSSe is used as a light-absorbing layer.

  Doping can improve the electrical conductivity of the material by increasing the number of charge carriers (electrons or holes).

  In photovoltaic materials like CZTSSe, doping can help adjust the band structure and improve the efficiency of light absorption and charge transport.

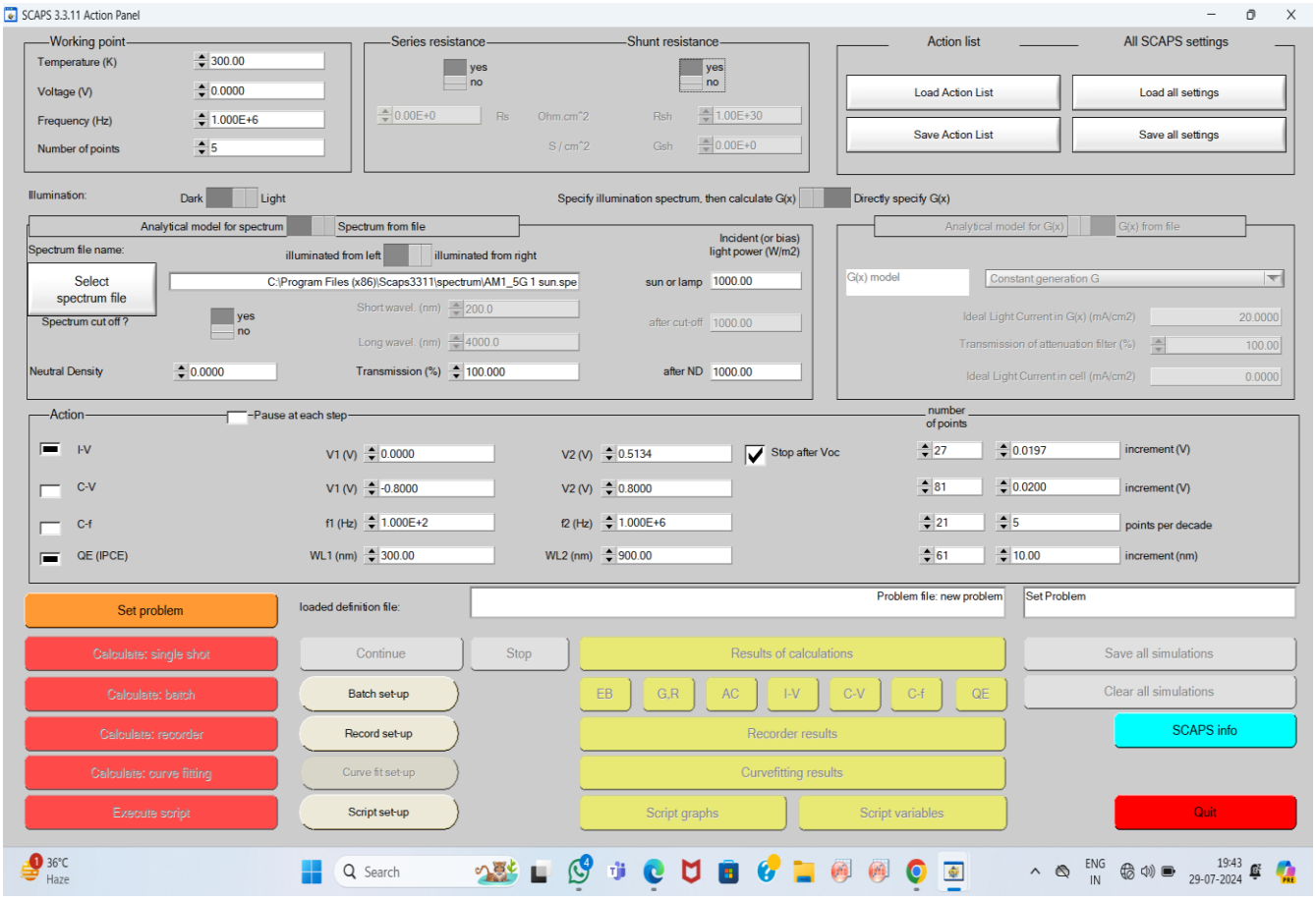
  Doping can affect the band gap of the material, which in turn influences its optical absorption and emission characteristics.

Table 2: Properties of alternate buffer layers and AZO layer used in the simulation

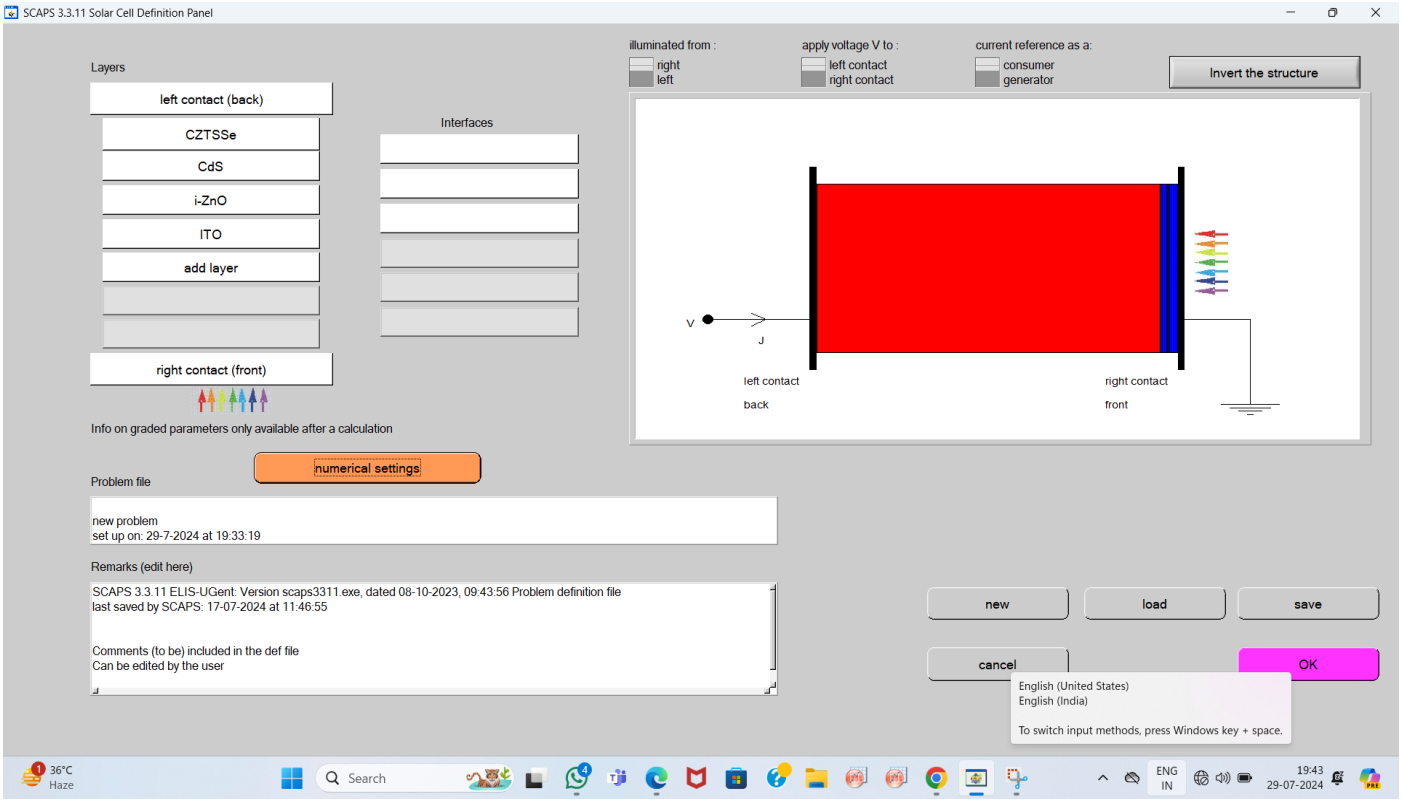
Parameter	$Zn_{0.82}Sn_{0.18}O$[25], [26]	ZnSe [27]	ZnS [28]	AZO [21]
Thickness (um)	variable	variable	variable	0.05
E_g (eV)	3	2.9	3.6	3.25
χ_e (eV)	4.1	4.02	4.5	4.5
ε_r	9	10	10	9
N_C (cm^{-3})	3.0 E+18	2.2 E+18	1.5 E+18	2.2 E+18
N_V (cm^{-3})	1.8 E+19	1.8 E+19	1.8 E+19	1.9 E+19
$V_{th,e}$ (cm/s)	2.4 E+7	1.0 E+7	1.0 E+7	1.0 E+8
$V_{th,h}$ (cm/s)	1.3 E+7	1.0 E+7	1.0 E+7	1.0 E+8
μ_e(cm^2/Vs)	100	100	250	100
μ_h (cm^2/Vs)	31	25	40	31
Doping(cm^{-3})	1.0 E+18 (D)	1.0 E+18 (D)	1.0 E+18 (D)	1.0 E+20 (D)
Abs. const. ($cm^{-1}eV^{(½)}$)	1.2 E+5	Data file	Data file	1.5 E+5

Step by step simulation of CZTSSe:

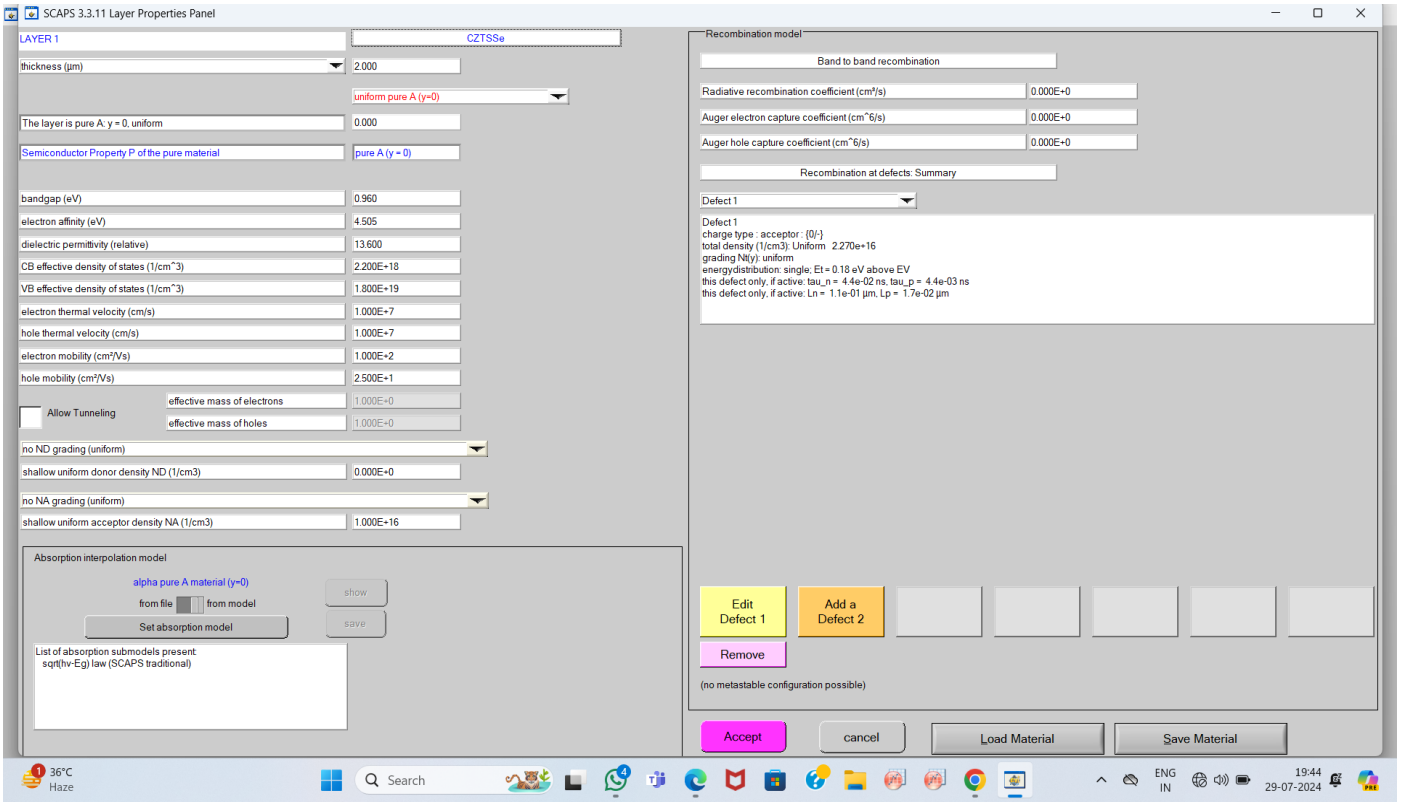
Step 1- Open SCAPS and adjust the parameters such as drag the illumination from dark zone to light zone. Change the voltage accordingly. Click on the **set problem** option.



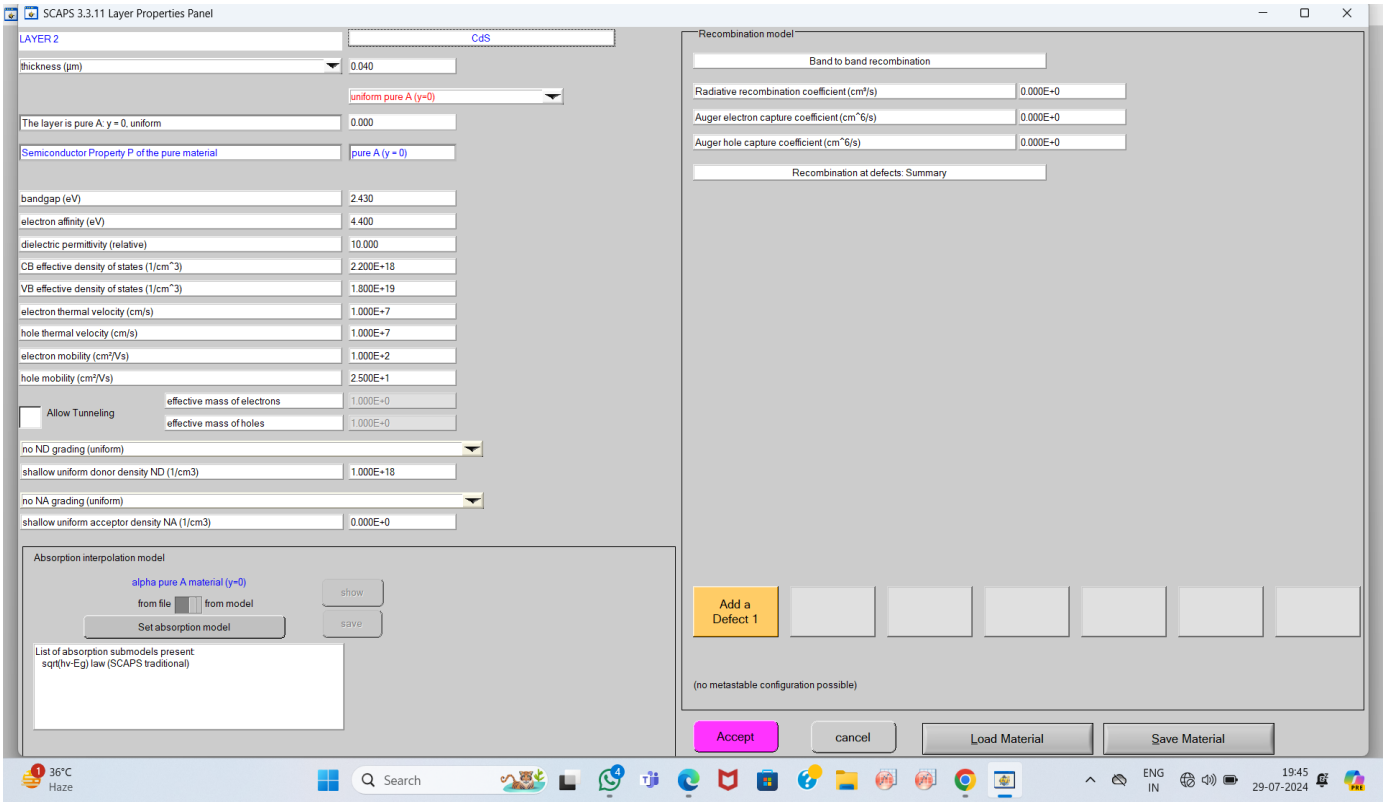
Step 2- The set problem interface gets open to grow a structure changes can be made such as direction of voltage or current preference. After developing the structure save it with the extension **.def** and then click on OK.

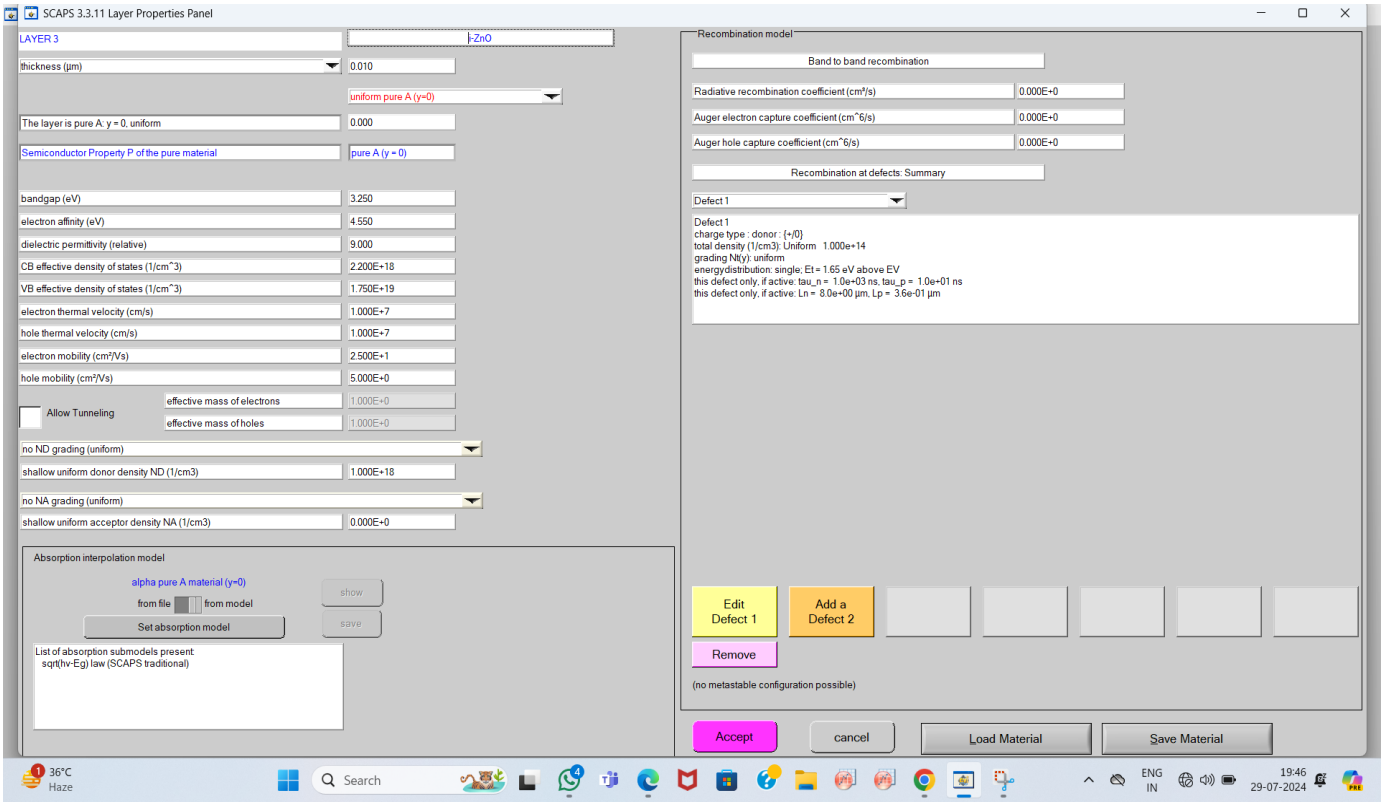


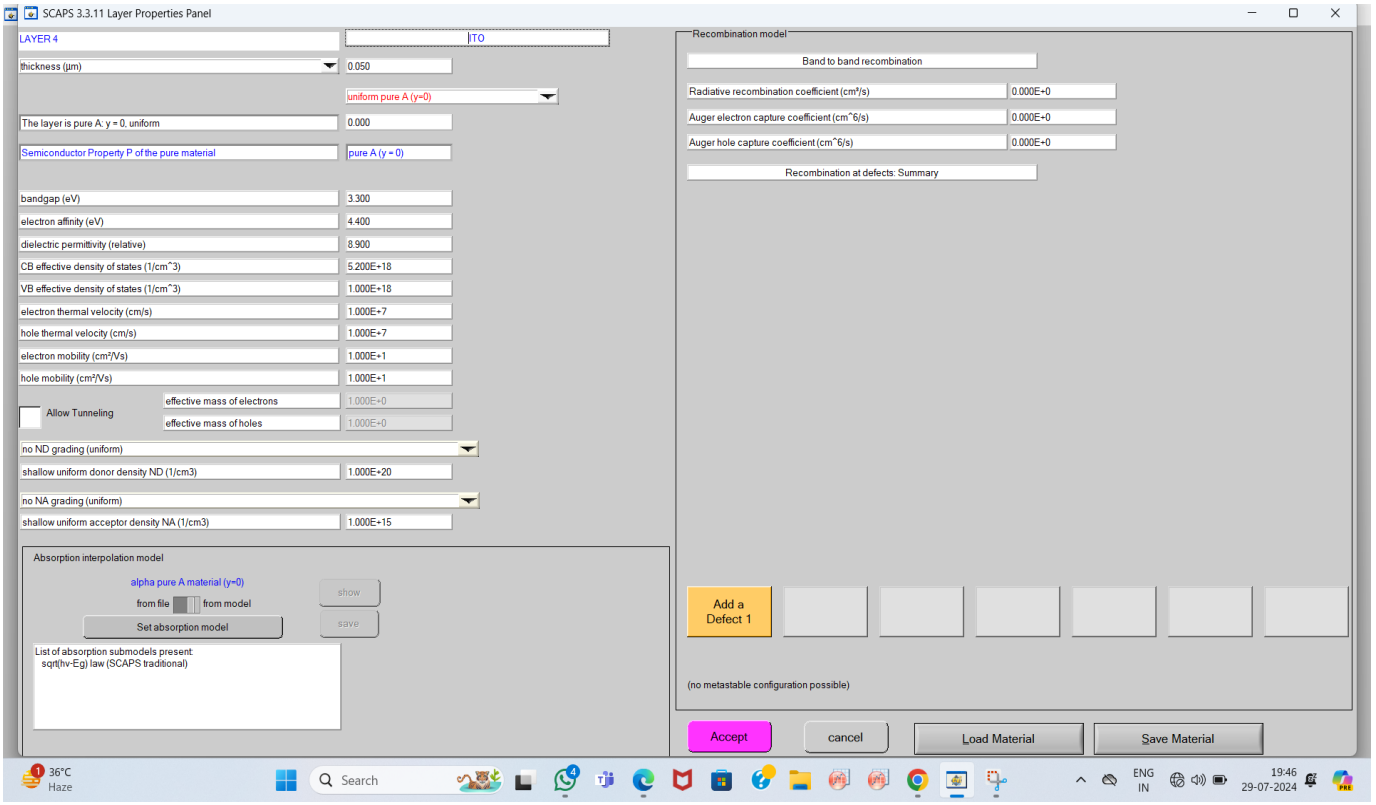
Step 3- While growing the structure we need to add different layers one by one by clicking on **Add layer**. The layer properties panel will open where we provide the values for the parameters given.



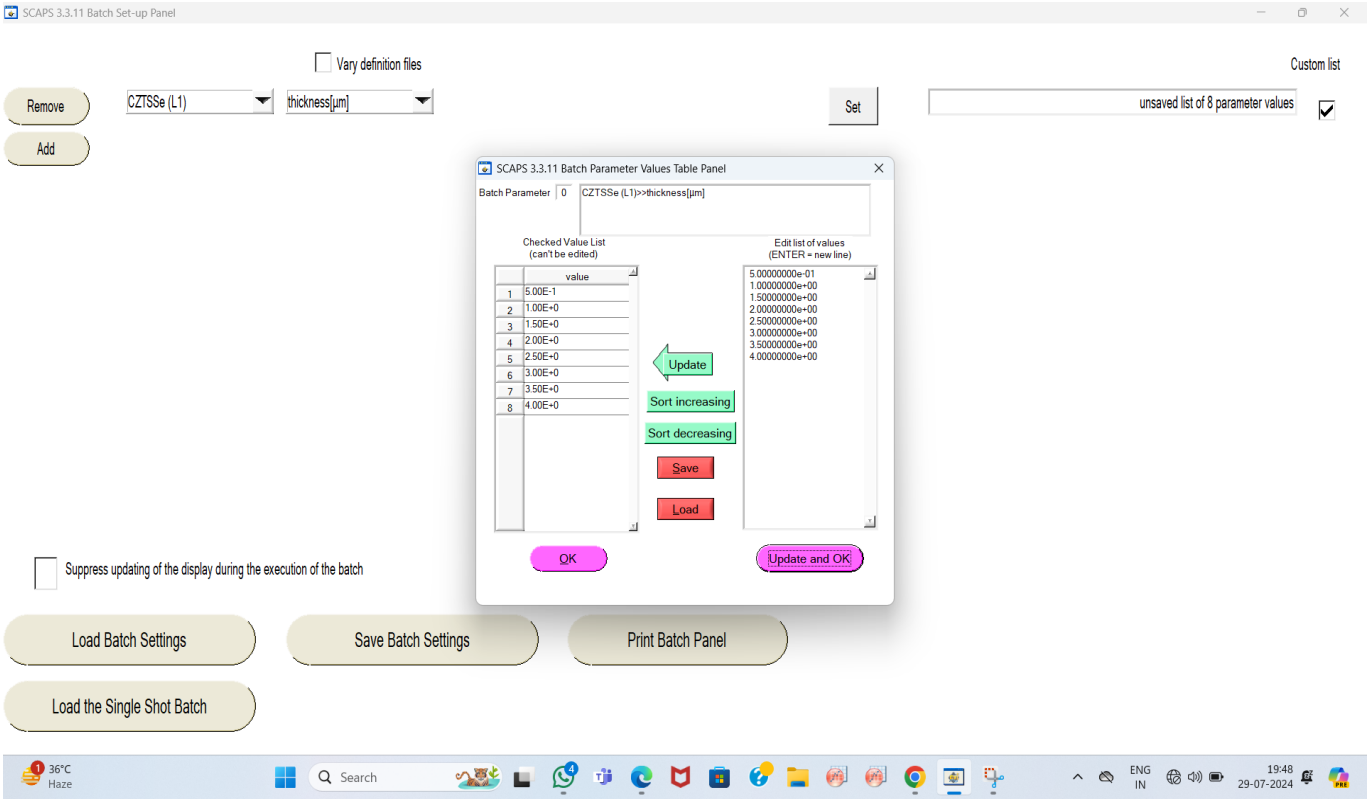
Step 4- Click on Add layer to fill the values for the buffer layers. In the right side, a the combination model box appears where we can add defects also then after adding defects click on **Accept**.



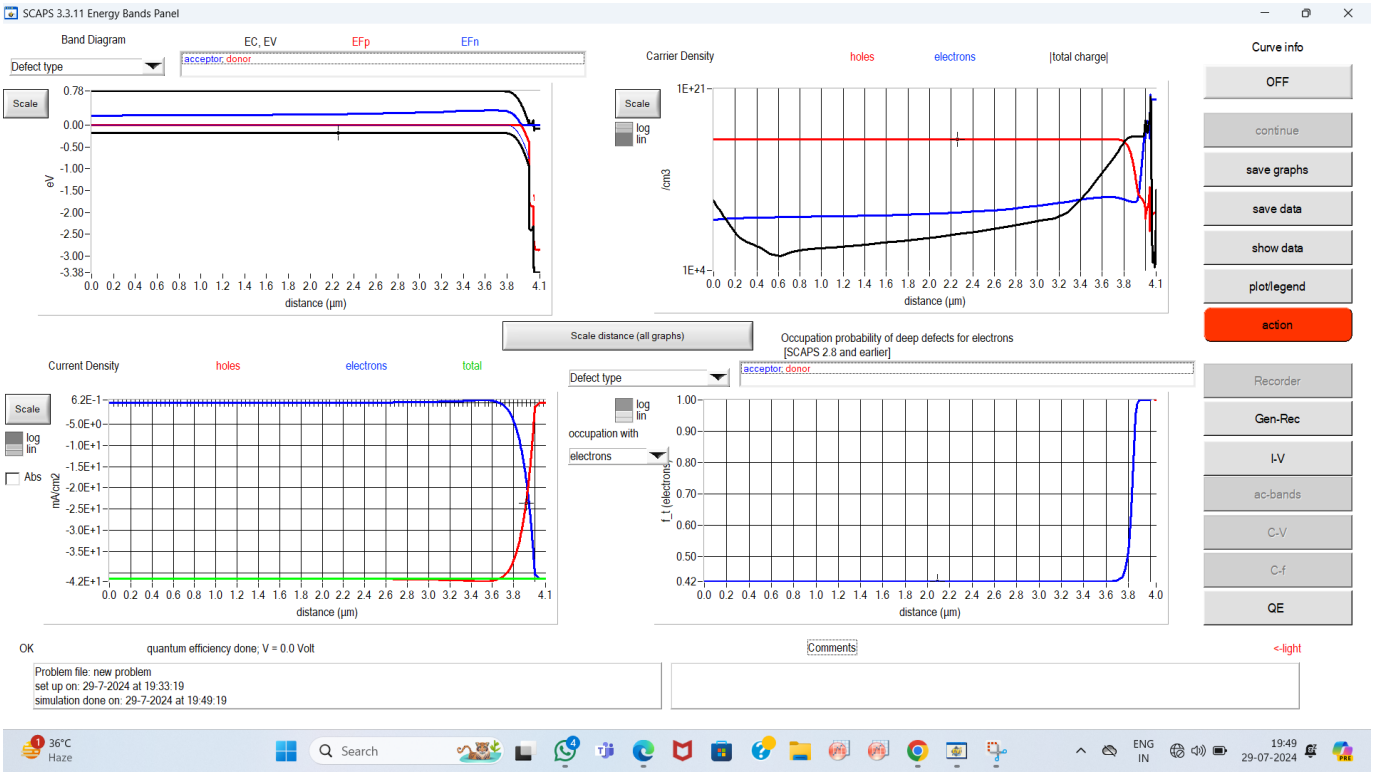




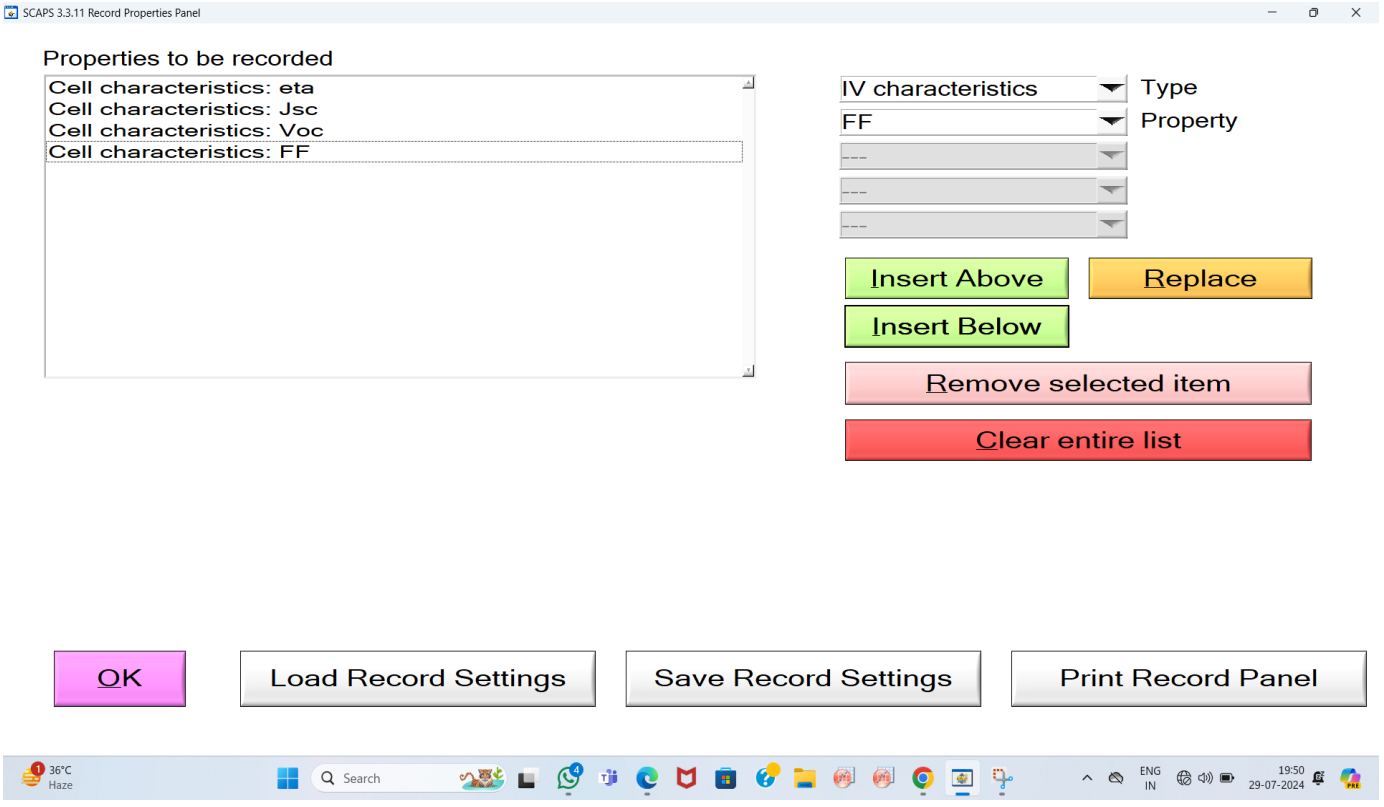
Step 5- After developing the structure click on OK. Now, the main working point will appear click on the **Batch Setup** option and enter the values that are going to be varied. Set the parameters and click on OK.



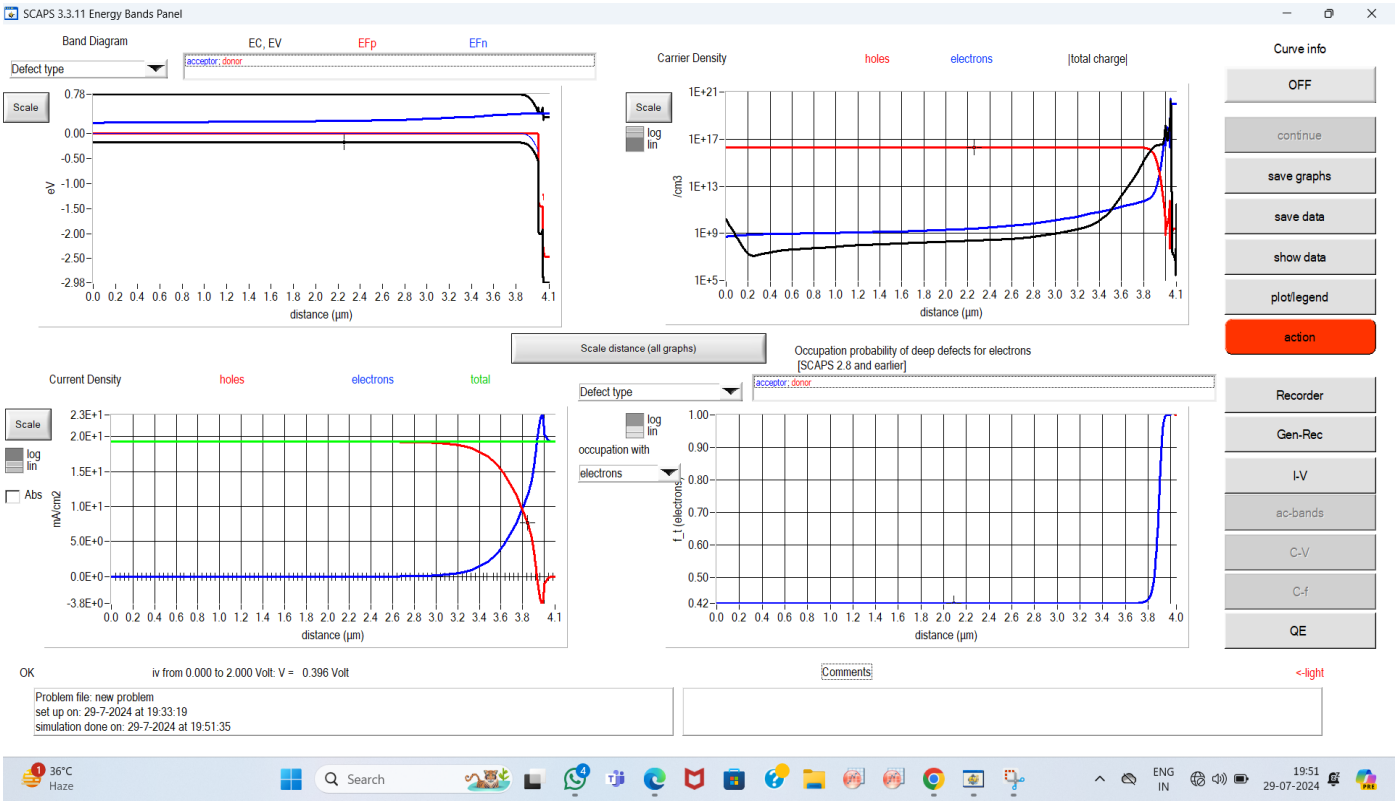
Step 6- After clicking on OK we will be back to the main interface. Now we need to tap on **Calculate: single shot** and then click on **Action** to get back to the main menu. Now click on **Calculate: Batch.** Wait until the desired steps are completed. Click on the **Show data** to get more precised details of the calculation. Again, click on **action**.



Step 7- Now, click on the **Record set-up** option. A **record properties panel** will appear. On the right hand side the drop down menu will appear for the **type** and **property** requirement. Adjust it accordingly. Multiple properties can be added the click on OK.



Step 8- Again, the main menu will appear click on the **calculate: recorder** option. Wait until the steps are completed successfully. Then click on **Recorder** option.



CHAPTER – 4

RESULTS AND DISCUSSIONS

- **Absorber layer:**

  Since the solar cell PCE mainly depends on the absorber thickness and band-alignment between the absorber and the buffer layer, optimization of these two parameters plays a critical role in deciding the performance of the solar cell. In this work, firstly, we optimize the absorber layer by considering the CdS as the buffer layer. We evaluate the suitable bandgap and electron affinity of the absorber layer by varying its composition from 0 to 1. The corresponding effect on the PCE is shown in Fig. 2 (b).

  It is clear that a 40% sulphur and 60% selenium composition in the absorber layer results in the highest PCE. This composition results in a conduction band offset (χabsorber – χbuffer) ≈ 0 eV which is well within the optimal range to reduce the photo-generated carrier recombination at the absorber-buffer interface.

  The optimized composition of the absorber has a bandgap of 1.152 eV, which is very much in agreement with the reported work[30]. Next, by keeping the parameters of different layers in the baseline structure constant, we optimise the thickness of the absorber layer.

  It is clear that an absorber thickness of 2 µm is the optimal thickness of the absorber layer. This is also very much comparable to minority carrier diffusion length resulting in optimum performance. As evident, any further increase in absorber thickness results in carrier recombination thereby saturating the PCE.

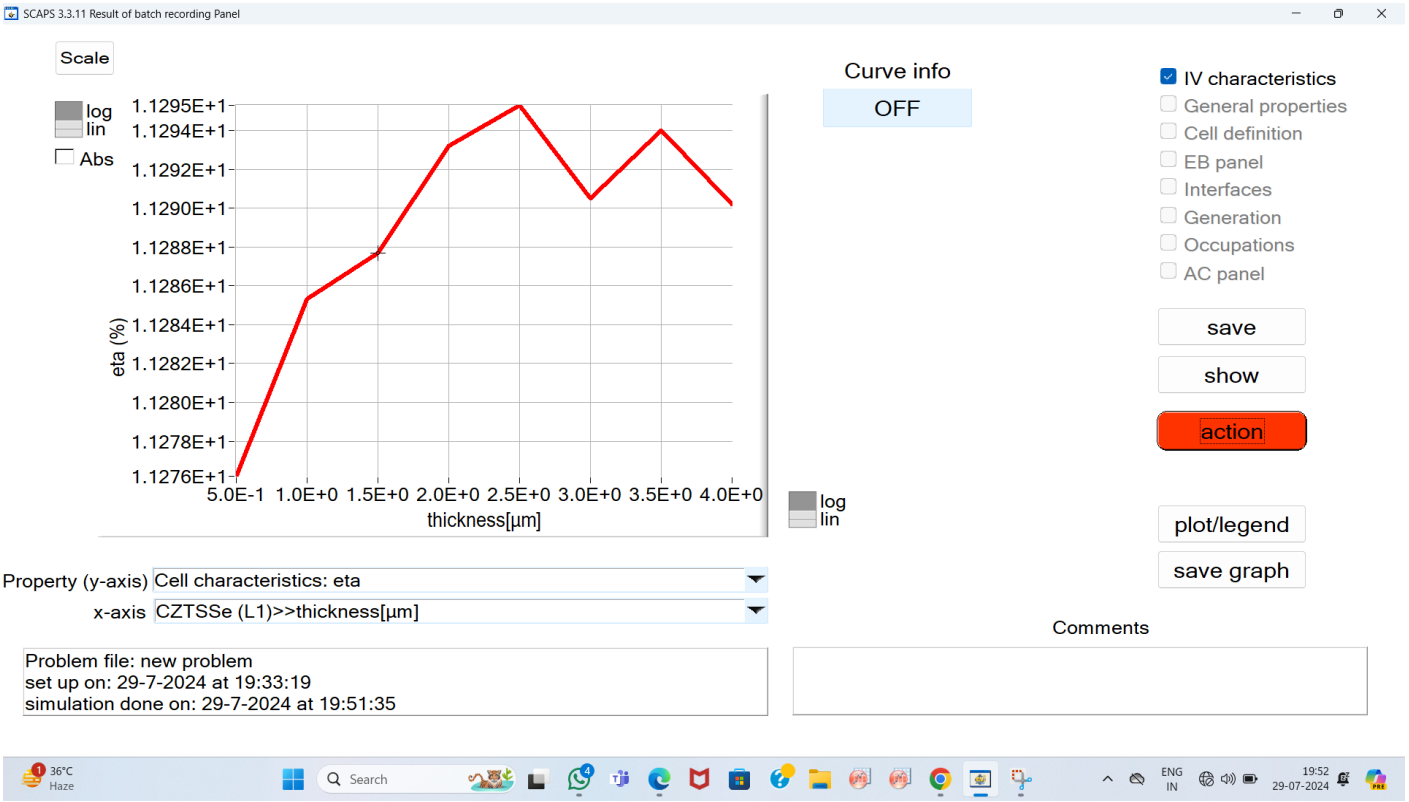


Fig: This shows the result of Batch Recording Panel

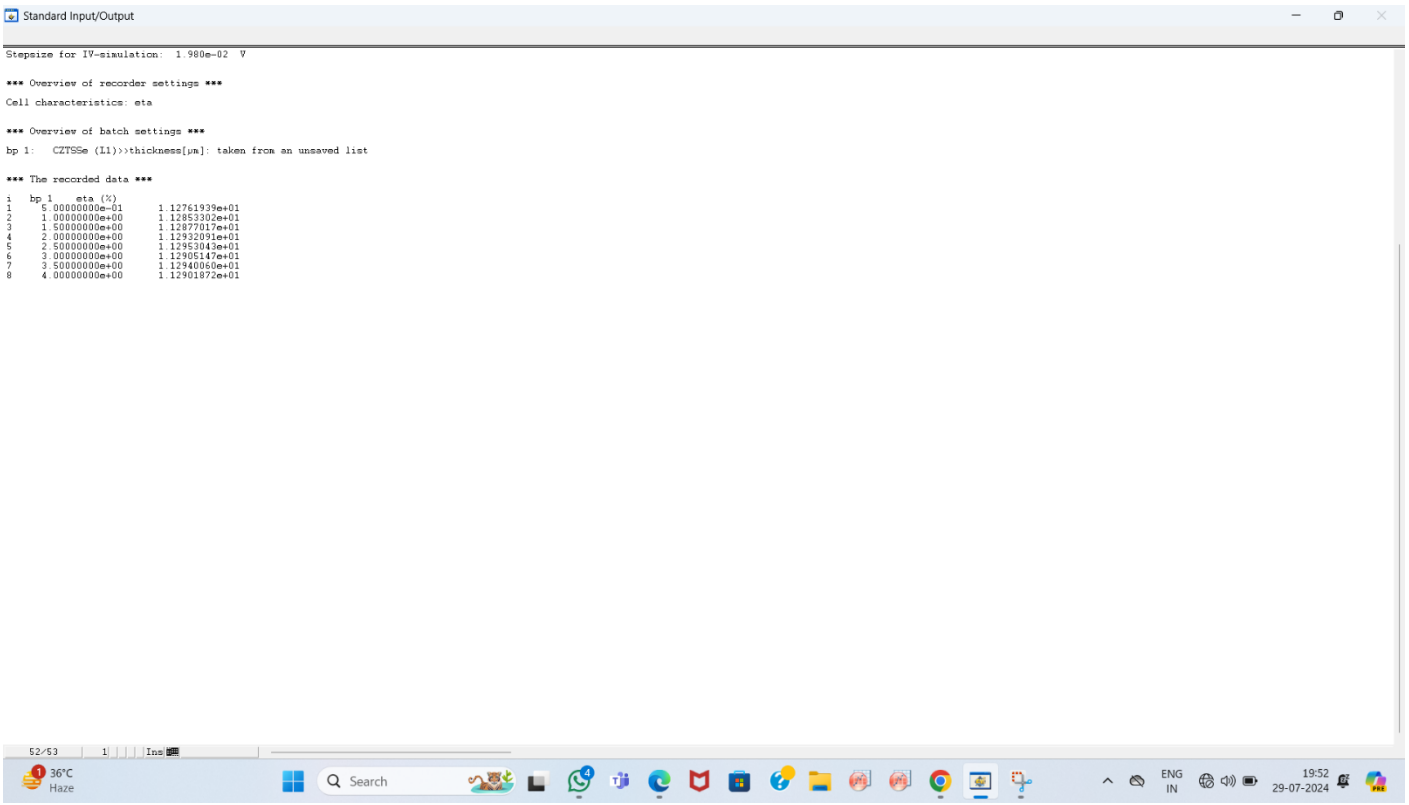


Fig: This shows the Standard Input output panel

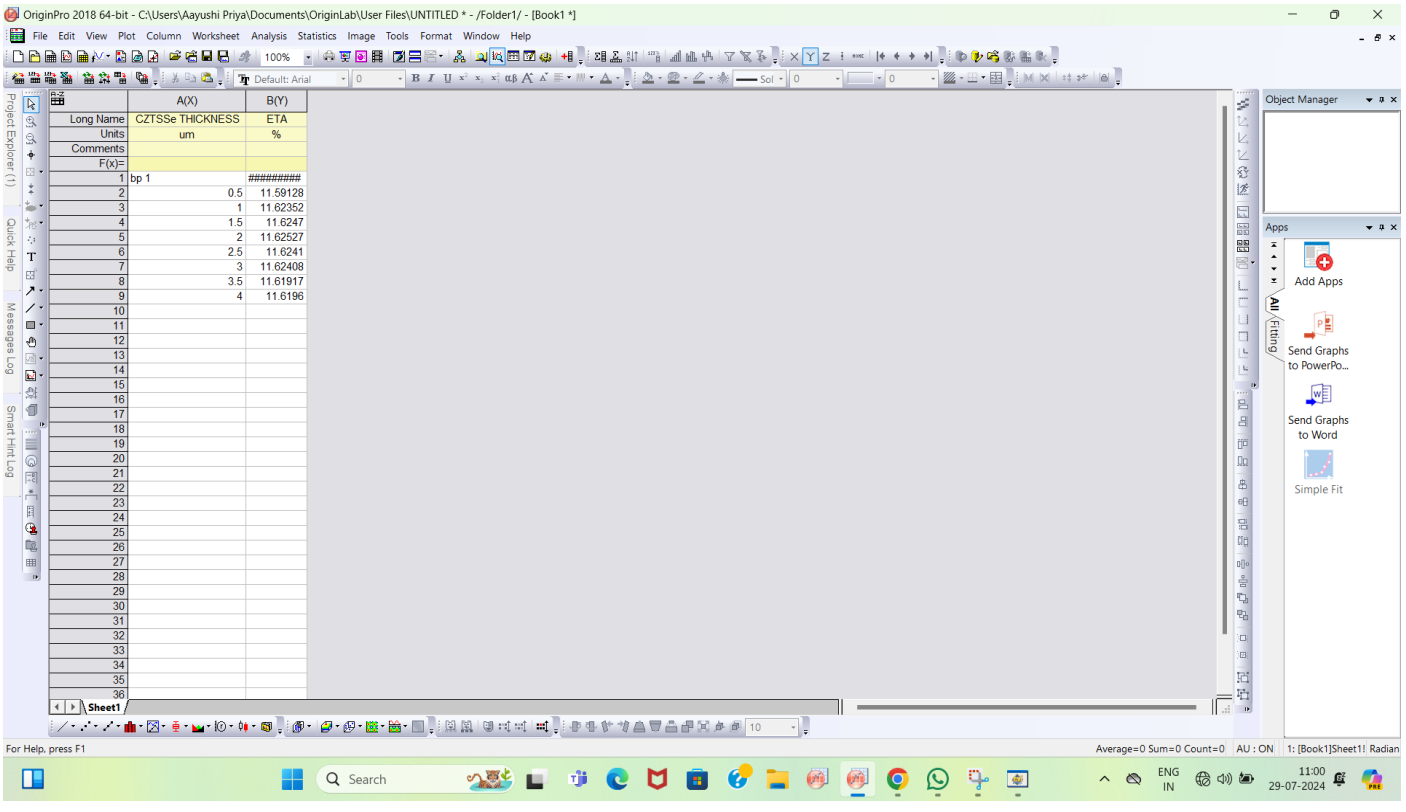


Fig: Main interface of Origin

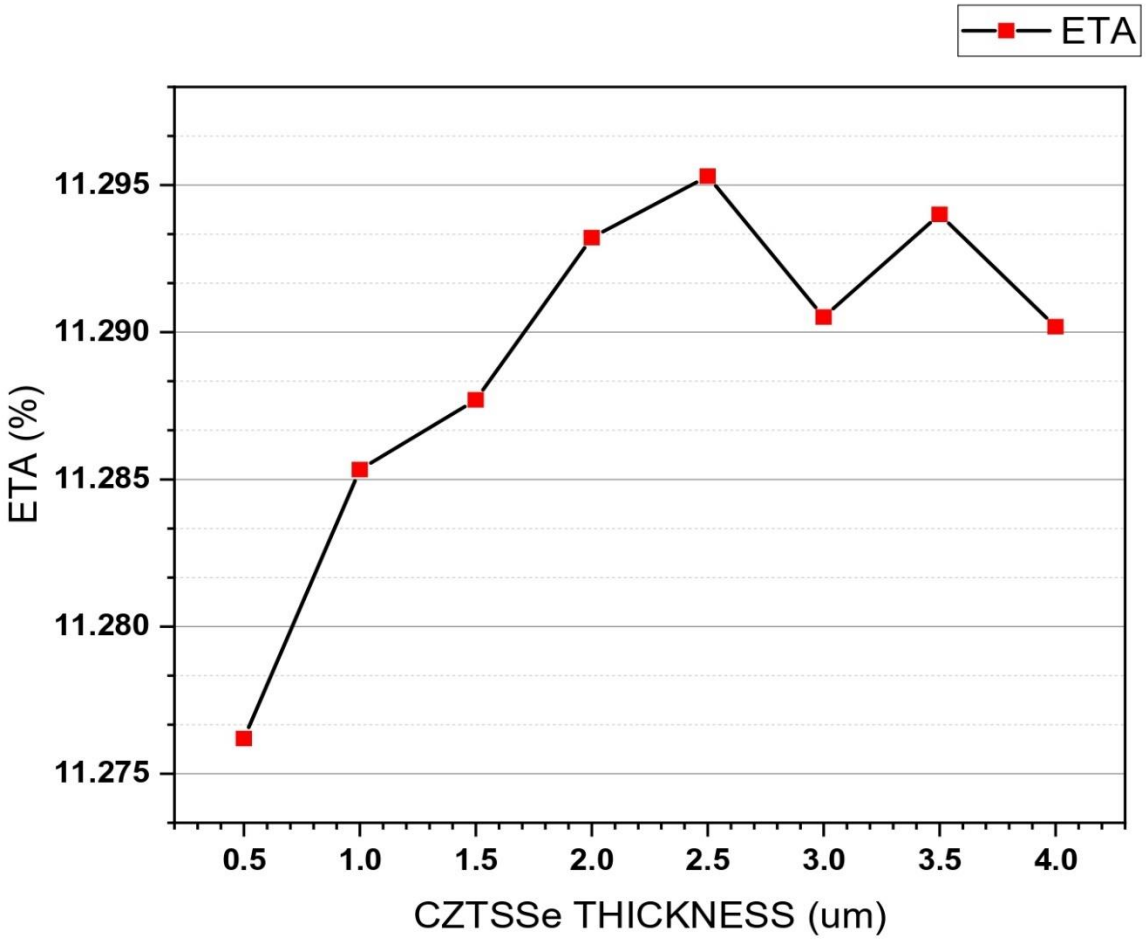
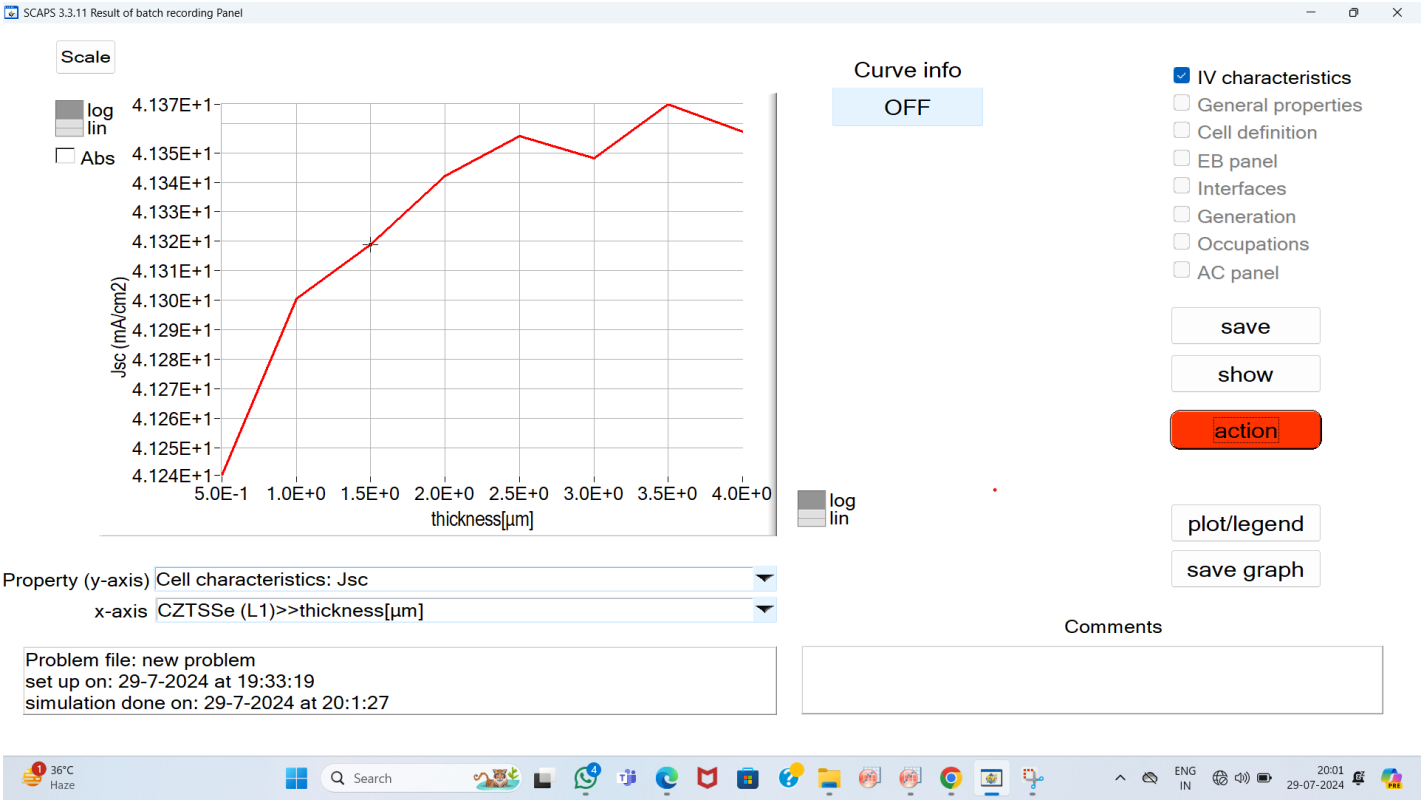


Fig: Shows the precised thickness and efficiency graph



- **Cadmium-free buffer layer:**

  In this section, we evaluate the candidature of Zn0.82Sn0.18O, ZnSe and ZnS as the alternate buffer layers. We evaluate the optimum thickness of these layers for higher performance by keeping the parameters of the previously optimized absorber layer and other layers constant.

  The various electrical and optical properties of the candidate buffer layers are taken from the literature and are listed in Table 2. In this work, we evaluate and compare the alternate buffer layer performance by optimizing its thickness. Fig. 3 shows the performance parameter variation of the solar cell with respect to the thickness of the buffer layer.

  Comparing the overall performance parameters, it is evident that Zn0.82Sn0.18O has relatively constant and better performance when compared to Cd-free ZnS and ZnSe buffer layers.

  This can be attributed to proper band alignment between the CZTSSe layer and the Zn0.82Sn0.18O layer. A spike of +0.265 eV in the band alignment between buffer and absorber is considered conducive enough for the transport of photogenerated electrons towards the front contact. Hence a comparable performance in CZTSSe solar cell is achieved when Cd-free Zn0.82Sn0.18O is used as a buffer layer.

  Further, having a higher bandgap, the use of Zn0.82Sn0.18O allows the absorber layer to absorb most of the high energy photons. This also allows using an ultra-thin buffer layer in the structure. Fig. 3 suggests that 40 nm thickness for the buffer layer is optimum for the performance of the solar cell.

- **Indium-free cheaper TCO:**

  In this section, we evaluate the candidature of AZO as the alternate for ITO as TCO. The detailed electrical and optical properties used in the simulation are shown in Table 2. Further, to compare their performance, we assume their bulks as defect-free and we assume the same thickness, carrier concentration for both the TCOs.

  Detailed performance parameters of CZTSSe solar cell with ITO and AZO used as TCO is listed in Table 3. It is clear from the table that when AZO is employed as TCO, an improvement in the performance of the CZTSSe solar cell is achieved. This is primarily due to the optimal band alignment of AZO with i-ZnO which reduces photo-generated carrier recombination and thereby increase in the Jsc and PCE.

- **Table 3: Performance comparison of CZTSSe solar cell with different TCOs**

Buffer	**TCO**	PCE (%)	Voc (V)	Jsc (mA/cm^2)	FF (%)
CdS	ITO	14.51	0.588	34.4	71.77
	AZO	14.62	0.5881	34.63	71.78
$Zn_{0.82}Sn_{0.18}O$	ITO	14.53	0.5883	34.5	71.6
	AZO	14.62	0.5901	34.72	71.4
ZnSe	ITO	14.28	0.5884	34.82	69.72
	AZO	14.38	0.5884	35.0	69.72
ZnS	ITO	13.98	0.5882	33.57	70.81
	AZO	14.12	0.5882	33.9	70.83

CHAPTER – 5

5.1. CONCLUSION

- In this study, Cd-free Zn0.82Sn0.18O, ZnSe and ZnS are considered as alternate buffer layers in the CZTSSe solar cell structure.

- Simulation results indicate that Zn0.82Sn0.18O has an overall performance comparable to the toxic CdS.

- Further, AZO when employed as TCO results in higher performance of the solar cell. Hence AZO can be a possible non-expensive alternative to the ITO.

- The investigated structure (SLG/Mo/Cu2ZnSn(S0.4Se0.6)4/Zn0.82Sn0.18O/i-ZnO/AZO) in this study is environment friendly, cheaper may lead to further interest in the photovoltaic research community.

- In this work, ZnS, ZnSe, and Zn0.8Sn0.2O are considered as possible alternatives for CdS. Similarly, Aluminium doped Zinc Oxide(AZO) is considered as an alternative for ITO. Firstly, a cell model with CdS and ITO (Mo/CZTSSe/CdS/ZnO/ITO) is developed using SCAPS-1D software.

- To optimise the performance parameters namely open-circuit voltage(Voc), short-circuit current density(Jsc), fill factor(FF), and the power conversion efficiency (PCE) for irradiation under normal working conditions, thickness and the composition ratio of the absorber layer(CZTSSe) are evaluated through numerical simulations.

- PCE of 14.51% is achieved for a 40% of Sulphur content and 2 um of thickness Cu2ZnSn(SxSe1-x)4 when CdS is used as the buffer layer.

- For the same structure, replacing ITO with AZO results in a PCE of 14.62%. Use of Cadmium-free buffer layers ZnS, ZnSe and Zn0.82Sn0.18O with ITO as window layer result in PCE of 13.98%, 14.28%, and 14.53%, respectively.

- For the Cadmiumfree buffer layers, an improvement in PCE is achieved when ITO is replaced by AZO, with the highest being 14.62% for Zn0.82Sn0.18O. This can be attributed to the smaller conduction band offset, which reduces the recombination of photogenerated carriers and improves the carrier transport in the solar cell.

- The above results indicate that the Zn0.8Sn0.2O and AZO can be potential candidates for the buffer layer and window layer, respectively, for high-performance and cheap kesterite solar cell.

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5.2. FUTURE SCOPE

CZTSSe (Copper Zinc Tin Sulfide Selenide) solar cells are a promising technology in the field of photovoltaics. Here are some potential future directions and scope for CZTSSe solar cells:

1. **Efficiency Improvement:**
   Current CZTSSe solar cells have lower efficiencies compared to other thin-film technologies like CIGS and CdTe. Research is focused on improving the efficiency by optimizing material properties, improving interface quality, and developing better fabrication techniques.

2. **Cost Reduction:**
   One of the advantages of CZTSSe solar cells is the abundance and low cost of raw materials (Cu, Zn, Sn, S, and Se). Further reducing the production costs through scalable manufacturing processes could make CZTSSe a more competitive option in the market.

3. **Stability and Durability:**
   Improving the long-term stability and durability of CZTSSe solar cells is crucial for their commercial viability. Research is ongoing to understand and mitigate degradation mechanisms, including the effects of moisture, heat, and light.

4. **Flexible and Lightweight Applications:**
   The potential for making flexible and lightweight solar panels using CZTSSe could open up new applications, such as in portable electronics, wearable technology, and building-integrated photovoltaics (BIPV).

5. **Eco-friendliness and Sustainability:**
   CZTSSe solar cells are considered environmentally friendly due to the non-toxic and abundant nature of their constituent materials. This characteristic makes them a sustainable alternative to other thin-film technologies that may use rare or toxic elements.

6. **Integration with Other Technologies:**
   CZTSSe solar cells could be integrated with other renewable energy technologies, such as storage systems or hybrid photovoltaic-thermal systems, to enhance overall energy efficiency and reliability.

7. **Research and Development:**
   Ongoing R&D in material science, nanotechnology, and device engineering can further enhance the performance and adoption of CZTSSe solar cells. Collaborative efforts between academia, industry, and government institutions can accelerate advancements in this technology.

   The future of CZTSSe solar cells looks promising, especially if challenges related to efficiency, stability, and manufacturing are addressed. As the demand for renewable energy sources grows, CZTSSe could play a significant role in the global solar energy market.

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