PHY661A
Thin Film Photovoltaics PVII (Master REST and STEEM)

Modeling solar cells
Tutorials for getting started with SCAPS

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1. Introduction

As shown in the title, this document is a short getting started of SCAPS software. **More detailed information can be found in SCAPS official user guide**. SCAPS user guide is located on your computer at SCAPS installation directory.

This document is focused on SCAPS software. We have added some reference (page number) which can help to go deeper by using the **SCAPS official user guide.**

In this document, we introduce SCAPS via tutorials: (i) the first tutorial shows how to build a model of a generic solar cell device; (ii) the second tutorial shows how to use SCAPS functionalities to test or evaluate the roles and impacts of some key parameters on a given solar cell device performances; (iii) the last tutorial shows some practical and useful functionalities of SCAPS.

Each of these tutorials is a starting point and useful for performing the projects.

2. About SCAPS

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. Several researchers have contributed to it's development: Alex Niemegeers, Marc Burgelman, Koen Decock, Johan Verschraegen, Stefaan Degrave. A description of the program, and the algorithms it uses, can be found in the literature.

3. SCAPS installation

The program is **freely available to the PV research community** (universities and research institutes). **It runs on PC under Windows 95, 98, NT, 2000, XP, Vista, Windows 7, and occupies about 50 MB of disk space**.

To run SCAPS on others OS (Linux and Mac) you have to install a Virtual Machine with Windows as OS. For example VMWare player: https://my.vmware.com/en/web/vmware/free#desktop_end_user_computing/vmware_workstation_player/14_0

The program can be freely downloaded (**but...: don't sell, don't distribute further, refer when you publish results obtained with SCAPS**).

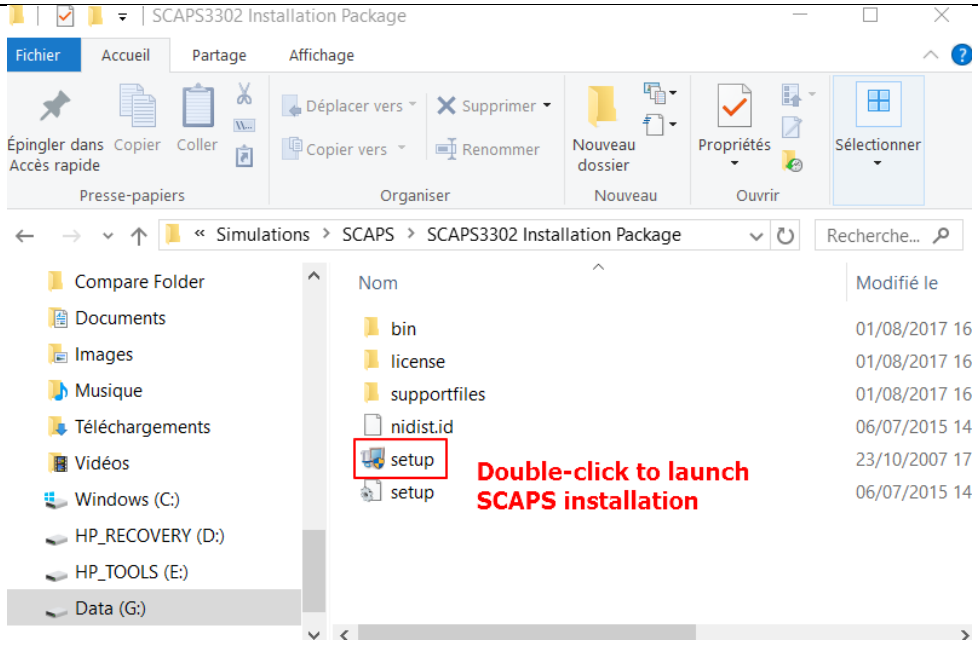
Please report to Professor **Marc Burgelman (Marc.Burgelman@elis.ugent.be)** when you have downloaded a SCAPS version: your name, your institution name and address, and the promotor's name for doctorate's students.

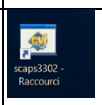
SCAPS can be found here:
http://users.elis.ugent.be/ELISgroups/solar/projects/scaps/SCAPSinstallatie.html

SCAPS installation files are compressed (zipped). To install SCAPS you have to:

1. Uncompress the files at your favorite location in your Windows Machine

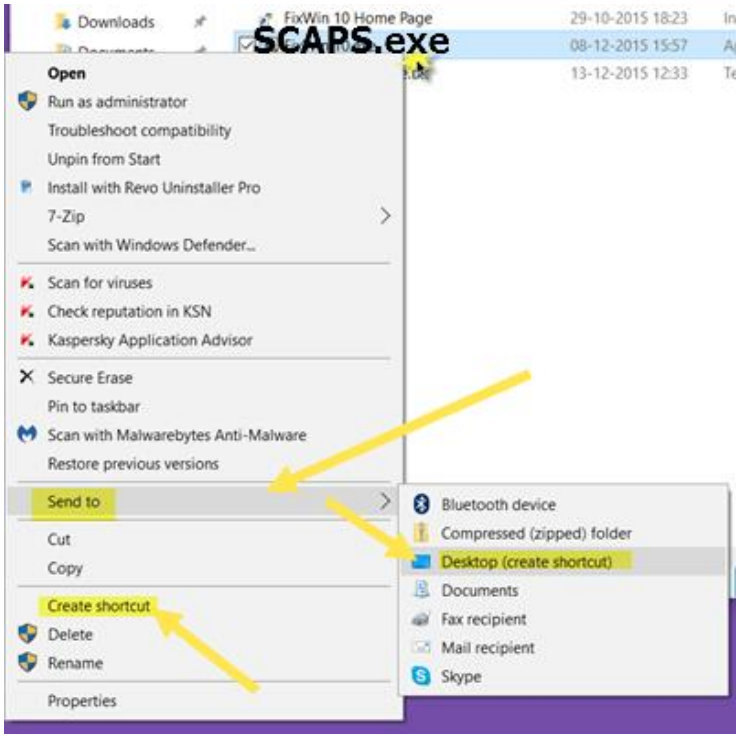
2. Double-click on the setup file to launch the installation process



3. 

Create a desktop shortcut

After a fresh installation of SCAPS you have to create the desktop shortcut**:** *go to the installation directory*, and right-click on **SCAPS.exe** file and *select Send To > Desktop (Create shortcut)*. You will see that a shortcut has been created on your Windows desktop.



4. Tutorial 1: a simplified one-dimensional generic solar cell device

In this tutorial, we will build a one-dimensional generic solar cell device.

4.1. What mean simplified one-dimensional?

The figures below illustrate the concept of "simplified one-dimensional" model for geometrical side. The left figure is the 3D architecture of the twenty-five per cent efficient PERL cell. The right figure shows how we can simplified the 3D architecture to 1D architecture.

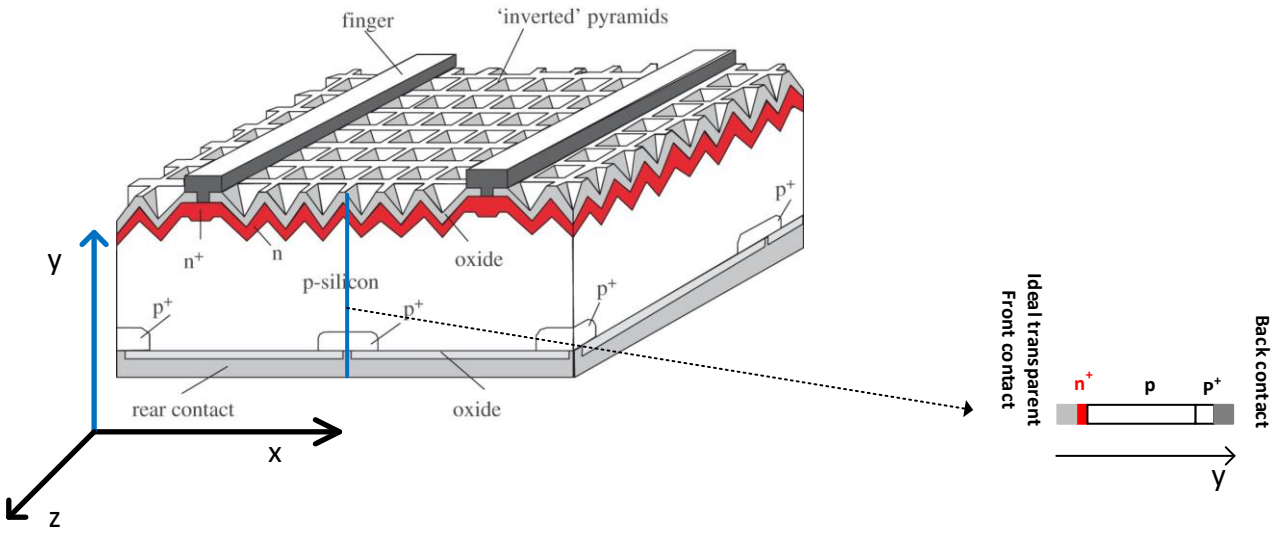


Figure 1 illustration of "simplified one-dimensional" concept: geometrical simplification

In the 1D architecture, only the flow of charge carriers in the *y* axis is studied.

SCAPS will solve the basic semiconductor equations in the *y* axis. The basic equations are:

- the Poisson equation, relating the charge to the electrostatic potential,
- the continuity equations for electrons and holes,
- the conditions to solve the equations : steady state (DC), dynamic state (AC), under dark or illumination.

In **one dimension (1D)**, the total cell length *L* is divided in N intervals, and the value of the electrostatic potential and of the electron and hole concentrations at each of the intervals will be calculated at various conditions to simulate experiments like: I-V characteristics (steady state), spectral response (steady state), capacitance measurements (dynamic)…

4.2. Setting up the generic solar cell model in SCAPS

Figure 2 shows the structure of the generic solar cell. It is an heterojunction of two different semiconductor materials. In the next sections, we will show step by step, how to use SCAPS to build a model for this cell.

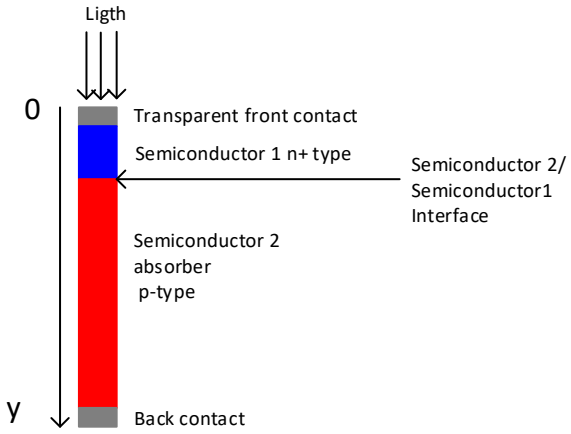


Figure 2: simple generic heterojunction solar cell structure.

4.2.1. SCAPS main window or action panel

SCAPS is a Windows-oriented program developed with **LabWindows/CVI from National Instruments (NI)**. This means that any action (click on a button) will generate a window or panel asking you to provide some values for some parameters or popping-up some graphs or results.

Figure 3 shows SCAPS main window or action panel. To start this window, double-click on the desktop shortcut (you are created in the next section). 

SCAPS main window. It is well described in SCAPS user manual (chapter 2, page 2)

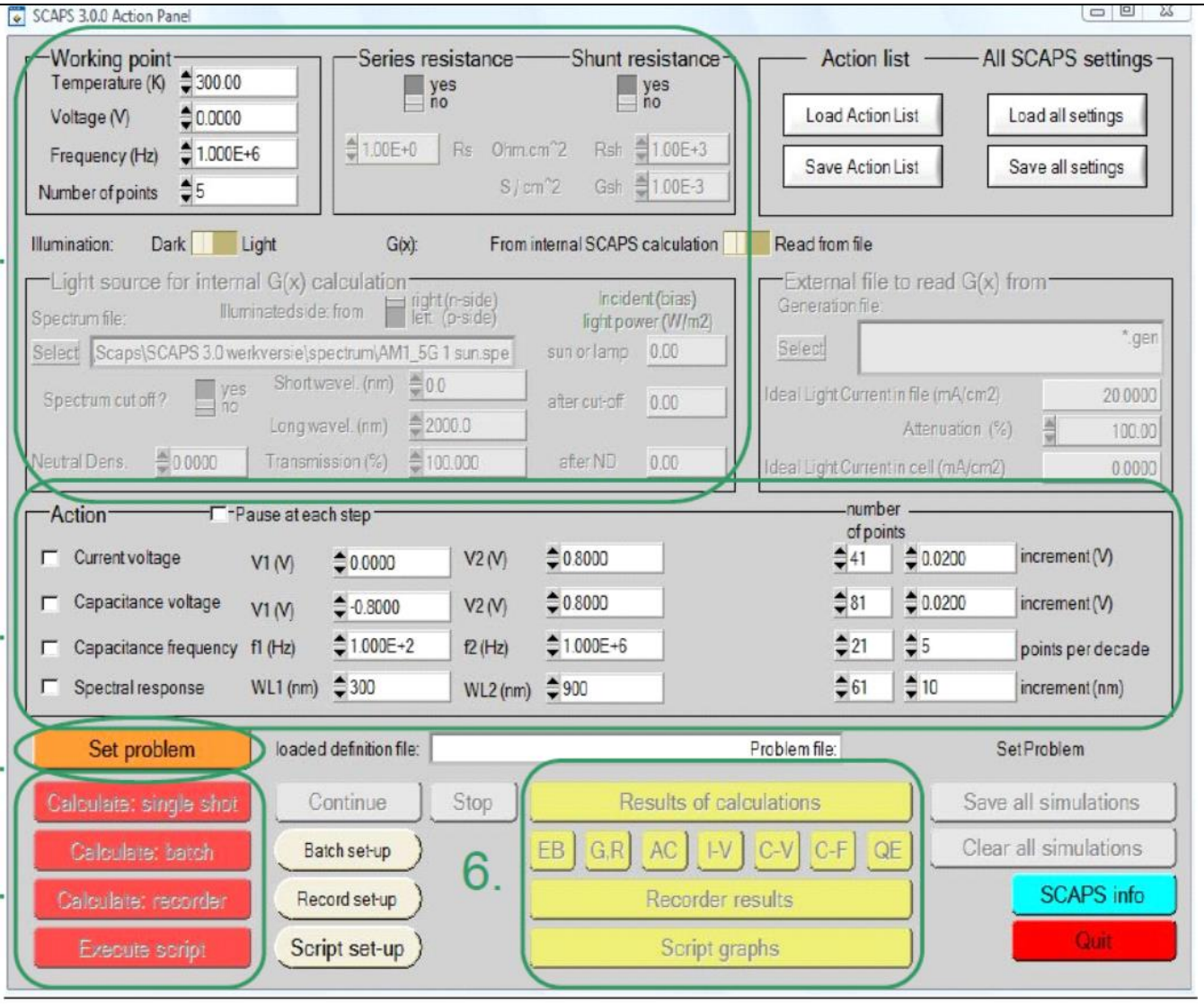


Figure 3 SCAPS main window. See in page 2 of SCAPS user manual for detailled information

number	Description
2	Define the problem, thus the geometry, the materials, all properties of your solar cell. **Remember a click will generate a panel for data input.**
3	Indicate the circumstances in which you want to do the simulation, i.e. specify the working point.
4	Indicate what you will calculate, i.e. which measurement you will simulate.
5	Start the calculation(s)
6	Display the simulated curves, ...

We will show how to use each part of the action panel through this tutorial.

4.2.2. Set the problem

The « **Set the problem** » button is the first button you have to click in order to tell SCAPS what is the problem you want to solve.

Figure 4 shows the “definition panel”

Solar cell definition Panel: You will get it after clicking on the “Set the Problem” on the “main Panel”.

We devised the “**Solar cell definition Panel”** into 6 regions

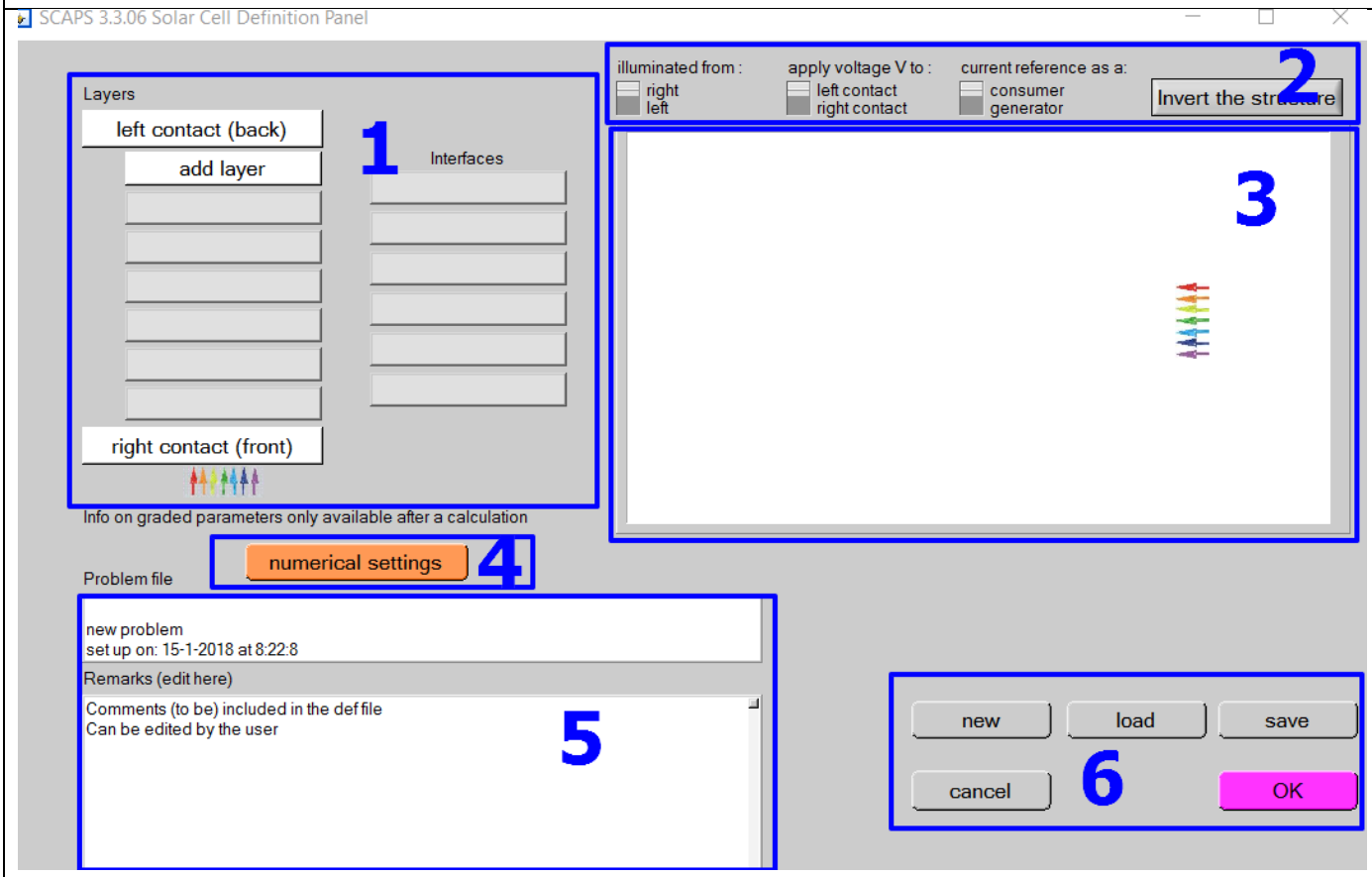
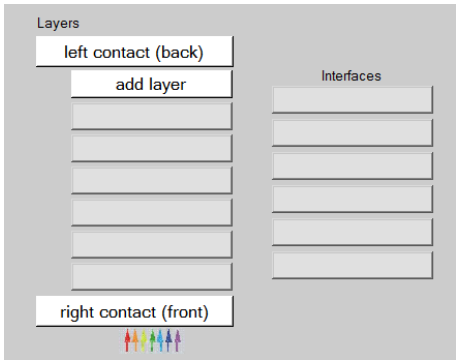
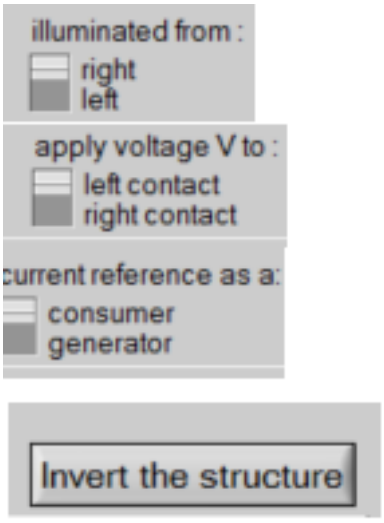


Figure 4 SCAPS “**Solar cell definition Panel**” for setting up the structure or problem to solve.

Description and illustration of the "**Solar cell definition Panel"** regions		
Number	**Illustration**	**Description or tips**
1		This region is used to build the solar cell model layer by layer. - By default, the back contact (or left contact) is at the top, and le front contact (or right contact, where light is coming in) is at back. This can be changed by clicking on the "Illuminated from" button of the region **2**  - To add a layer, click on "Add layer" button in region 1 to launch the "Layer definition Panel". This panel will be discussed more detailed later. **You can add up to 7 seven different layers** - To define contact properties, click on the "right contact" or the "left contact" buttons.
2		The region 2 is used to manage the solar cell layers stack. There are 3 buttons - Button "**Illuminated from**: ": to change the illuminated face (side). - Button "**Apply voltage V to**:" to choose the side or face to apply the voltage (during voltage sweep) - Button "**current reference as a**": choose the direction of the current. Consumer (current is positive when solar cell absorb power, negative when it generates the power); Generator is the opposite.

3		The area where SCAPS sketch the solar cell structure. Here it is blank because we are not yet start the design
4		The numerical setting button is used to change how SCAPS will do the job. After clicking on this button, you will get the "**Numerical Settings Panel**" shown on the figure 5. **There several parameters but the most important for basic simulation** are indicated on figure 5 with red rectangle - **Max. number of iterations**. **If you have convergence issues, increase this number first. By default, it is set to 250.** In general, **2500** is enough. - **Defect distribution**. You can increase the number of discrete level to be considered as Gaussian, tail-like distributions.
5		You can add some comments to document your design. For example, the date, and source of data…
6		There are five buttons: - **New**: to start a new design - **Load**: to load an existing or old design or SCAPS examples of design (there are lot of examples in SCAPS installation folder) - **Save:** to save your design. **You have to explicitly add the .def** as file extension. - **OK**: to validate your design

“Numerical Settings Panel”:

Tips: Increase the number of max. number of iterations to help SCAPS to converge

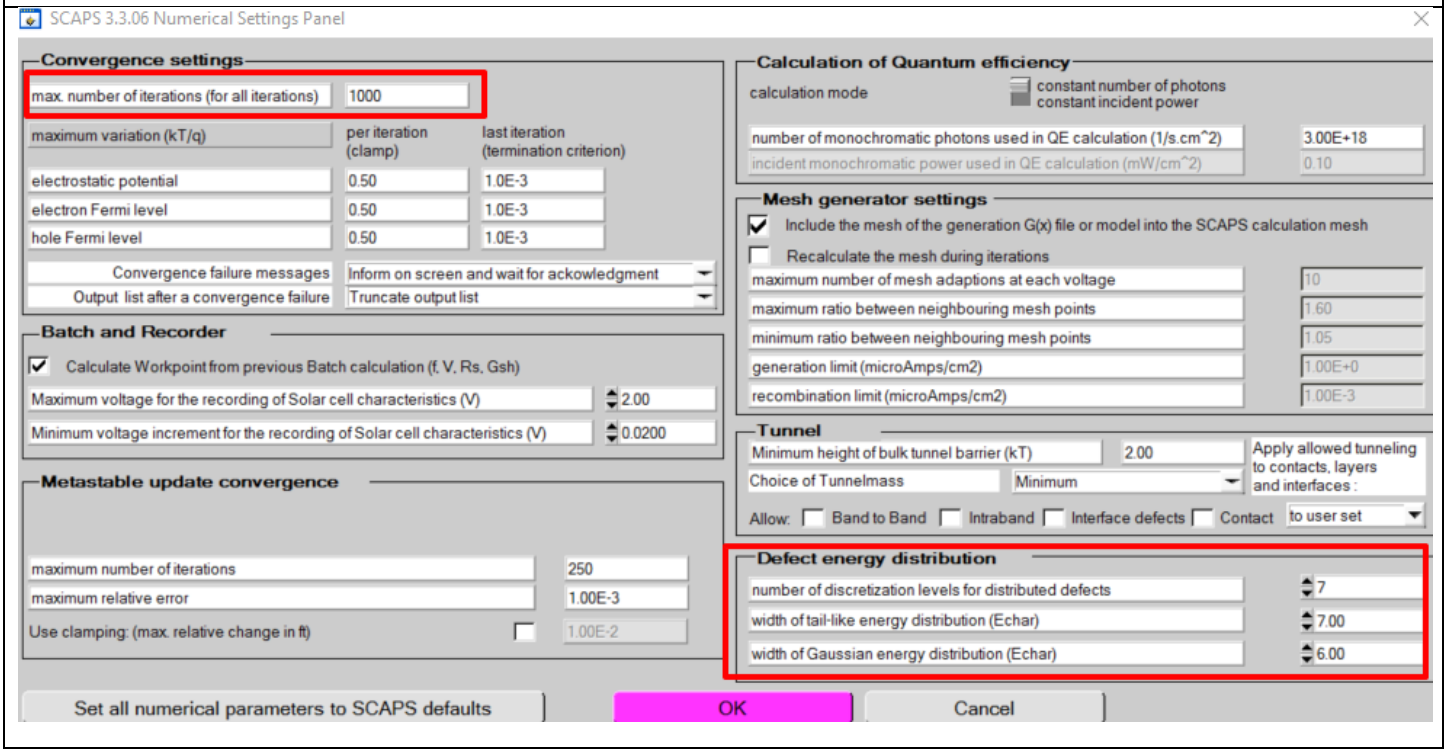


Figure 5 “Numerical Settings Panel” with main parameters indicated with red rectangles

The figure below shows the structure of the “generic “heterojunction solar cell we want to simulate.

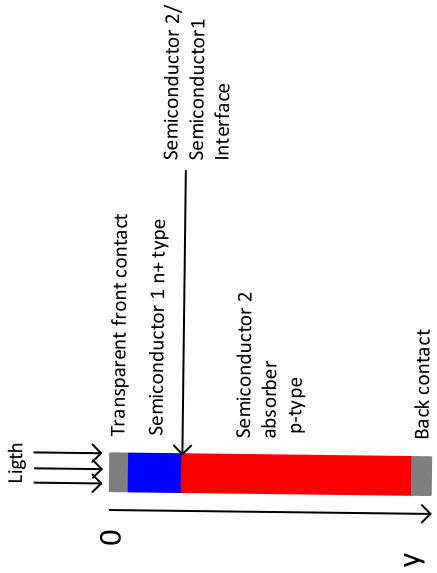


Figure 6 recall of the generic heterojunction solar cell

To build the model, we will start with the region 1 of the "**Solar cell definition Panel**" (see figure 4). The Table 1 below shows the values of the baseline values of keys parameters. To make things fun we will assume that: **semiconductor 1 is a ZnO:Al (type n ZnO doped with Aluminum) and semiconductor 2 is a crystalline Silicon**. That is a ZnO:Al/c-Si heterojunction solar cell.

In tutorial 2, we will improve the model

Geometrical parameter: 1D across the junction		
Layer label or name	**ZnO:Al**	**C-Si**
Thickness [µm]	0.1	10

Table 1

Bulk electronic transport parameters		
Layer label or name	**ZnO:Al**	**C-Si**
Bandgap [eV]	3.3	1.124
Electron affinity [eV]	4.6	4.05
Dielectric permittivity (relative)	9	11.9
CB effective density of states [cm^{-3}]	2.2×10^{18}	2.84×10^{19}
VB effective density of states [cm^{-3}]	1.8×10^{19}	2.68×10^{19}
Electron thermal velocity [cm/s]	1.0×10^{7}	1.0×10^{7}
Hole thermal velocity [cm/s]	1.0×10^{7}	1.0×10^{7}
Electron mobility [cm^2/Vs]	200 [1]	1321
Hole mobility [cm^2/Vs]	93.2	461
shallow uniform donor density ND [cm^{-3}]	1.0×10^{17}	0
shallow uniform acceptor density NA [cm^{-3}]	0	$1. \times 10^{16}$

Table 2

Bulk recombination parameter		
Layer label or name	**ZnO:Al**	**C-Si**
Radiative recombination: Radiative recombination coefficient (cm^3/s) = 0		
Auger recombination : Auger electron capture coefficient (cm^6/s) = Auger hole capture coefficient (cm^6/s) =0		
Non-radiative recombination via defects:		
Defect 1		
Defect1 charge type	Neutral	Neutral
Defect1 density Nt [cm^{-3}]	1.0×10^{18}	1.0×10^{14}
Defect1 capture cross section electrons, σ_n [cm^2]	1.0×10^{-15}	1.0×10^{-15}
Defect1 capture cross section hole σ_p [cm^2]	1.0×10^{-15}	1.0×10^{-15}
Defect1 induced electrons lifetime [s], diffusion length [µm]	$\tau = \frac{1}{\sigma v_{th} N_t}$ $L = \sqrt{D\tau}$	$\tau = \frac{1}{\sigma v_{th} N_t}$ $L = \sqrt{D\tau}$
Defect1 induced holes lifetime [s], diffusion length [µm]		

Table 3

Bulk optical parameter: SCAPS accept only absorption coefficient. There are some examples files in the folder ***absorption in SCAPS installation directory***		
Layer label or name	**ZnO:Al**	**C-Si**
Absorption file name	*ZnO extrapolated.abs*	*Si Green.abs*

Table 4

C-Si / ZnO:Al Interface recombination parameter
Defect 1:
We will start without interface and add them in next tutorial

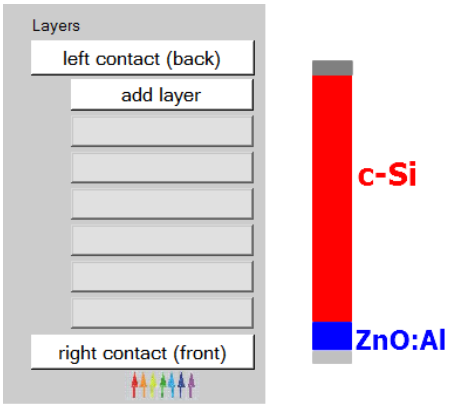
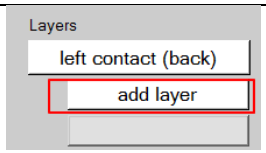
Table 5

Electronic properties of contacts		
Contact	**Front = ZnO:Al/contact**	**Back = C-Si/contact**
Thermoionic emission or surface recombination velocity electrons [cm/s]	1.0×10^7	1.0×10^7
Thermoionic emission or surface recombination velocity holes [cm/s]	1.0×10^7	1.0×10^7
Optical properties of contacts		
Reflection [%]	0	0

Table 6

4.2.3. Setting-up solar cell layers bulk parameters values

To set the solar cell layers bulk parameters values, from the “Action Panel” or “Main Panel”, follow these steps:

1	click on the “**set problem**”  button to get the “**Solar Cell Definition panel**”
Tips	As shown in the figure below, by default, SCAPS will ask you to start building your cell from the back contact. In our case, we will start from c-Si layer. 
2	Click on the “**Add layer**” button  of the “**Solar Cell Definition panel**” to get the “**Layer Properties Definition Panel**”. See on the figure 7

Layer Properties Definition Panel

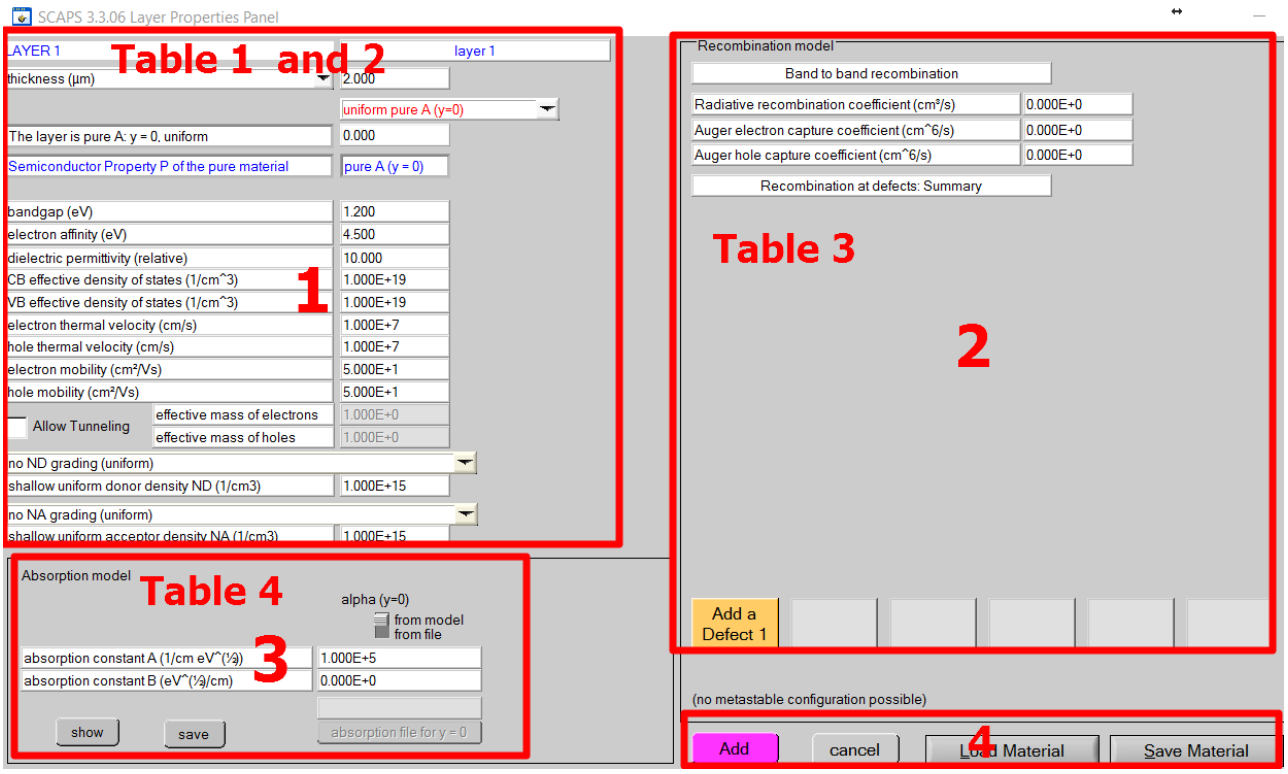
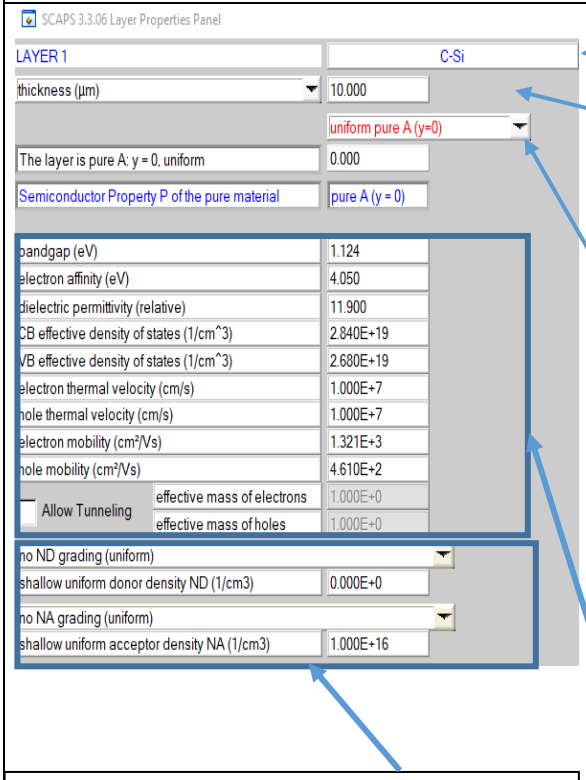


Figure 7 Layer Properties Definition Panel: regions are labeled with number for description

The “Layer Properties Definition Panel” can be divided in 4 regions.

"Layer Properties Definition Panel" Region 1: illustration for C-Si layer



Layer name: Use an explicative name: ex. p-type c-Si

Layer thickness: can change the unit (µm or nm), value **from 1 nm up to 10 cm**: for ***c-Si layer it is set to 10µm***

Composition and Parameter grading: It is possible to define a grading profile for each parameter in accordance with the chemical composition of semiconductor material. Here for c-Si layer we don't consider grading, material composition and parameter values are assumed to be uniform with position. **In the chapter 3, section 3.5 page 12, you get more information on how to use the feature.**

Doping: In SCAPS, doping charges are assumed to be ionized. This means that doping density does not change with temperature.

Temperature dependence of parameters:

Except:

(i) Effective density of states (Nc, Nv),

$$N_C(T) = N_C(T_0)\left(\frac{T}{T_0}\right)^{1.5} \quad N_V(T) = N_V(T_0)\left(\frac{T}{T_0}\right)^{1.5}$$

(ii) hole/electron thermal velocity (vth),

$$v_{th}(T) = v_{th}(T_0)\left(\frac{T}{T_0}\right)^{0.5}$$

(iii) Diffusion coefficient

$$D = \mu kT/q$$

SCAPS assume that parameters values don't change with temperature.

Tips: If needed you can calculate the temperature dependence of the parameters (with external tools), and use the values in SCAPS.

4.2.4. Bulk material Recombination parameters

"Layer Properties Definition Panel" Region 2 - recombination: illustration for C-Si layer

In SCAPS, it is not possible to set or define explicitly the value mobile charge carriers (Hole and electron) **lifetime and diffusion length**. This is true for others simulation software.

To define the lifetime and diffusion length values, we must setup the recombination mechanisms SCAPS handle **the 3 main recombination mechanism**:

1. **Radiative Recombination** via the following formula :

$$U_{\text{radiative}} = K\left(np - n_i^2\right)$$

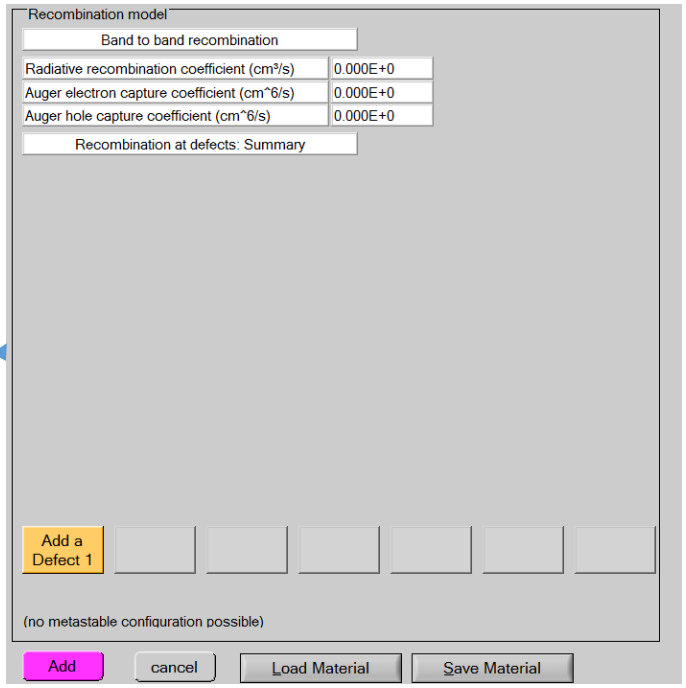
2. **Auger Recombination** via the following formula

$$U_{\text{Auger}} = \left(c_n^A n + c_p^A p\right)\left(np - n_i^2\right)$$

3. **Defect assisted or indirect Recombination**:

$$R = \frac{np - n_i^2}{\left(\frac{1}{c_p N_T}\right)(n + n_1) + \left(\frac{1}{c_n N_T}\right)(p + p_1)} \qquad \tau = \frac{1}{\sigma v_{th} N_t} \qquad L = \sqrt{D\tau}$$

(τ_n under $c_p N_T$, τ_p under $c_n N_T$)

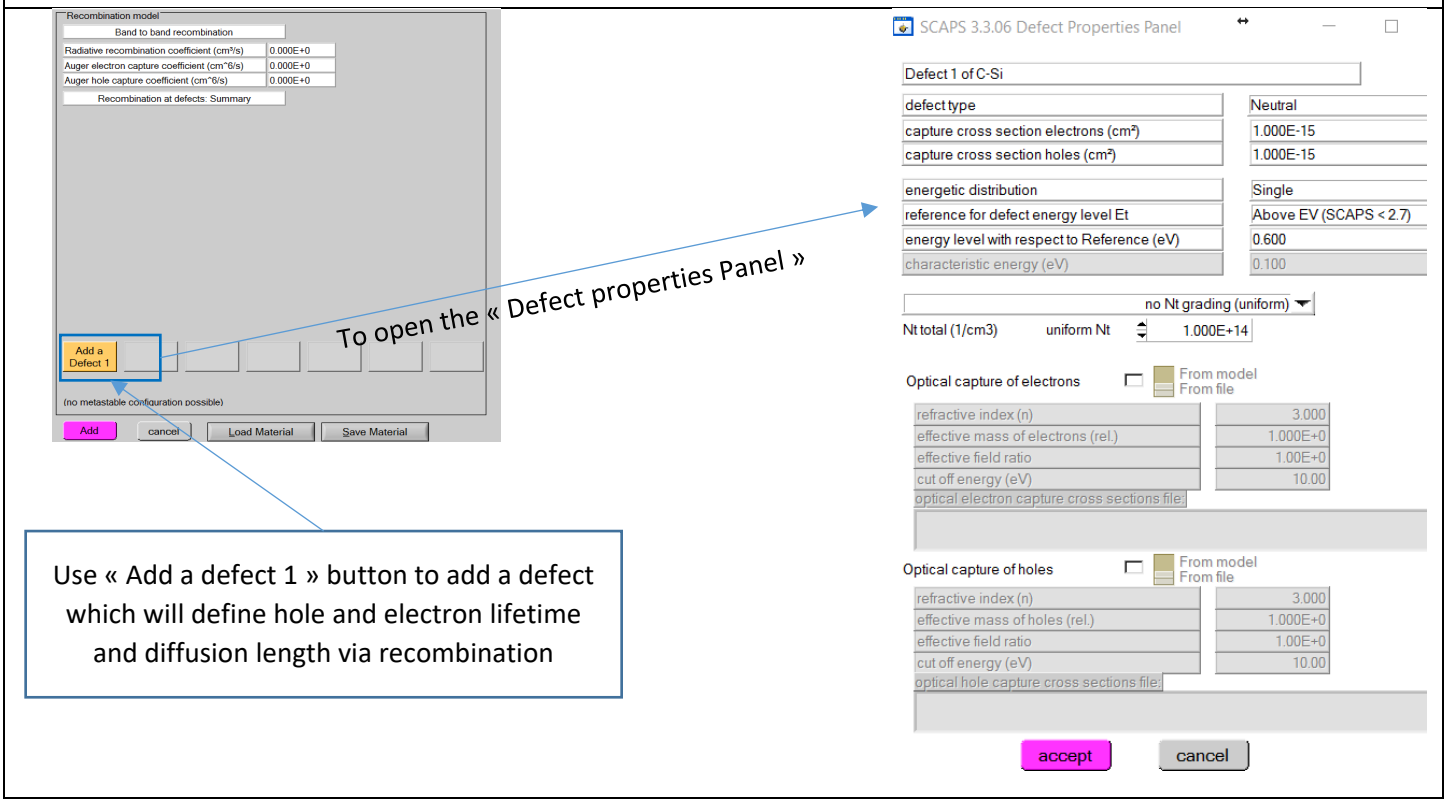


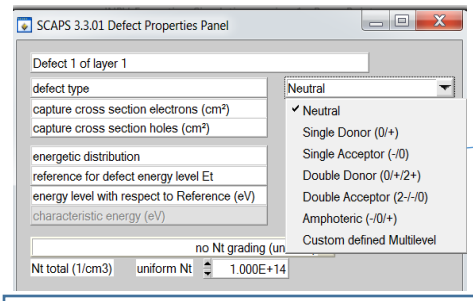
We will use only « Defect assisted or indirect Recombination ». We have to add defect by using the "Add a Defect1 "button

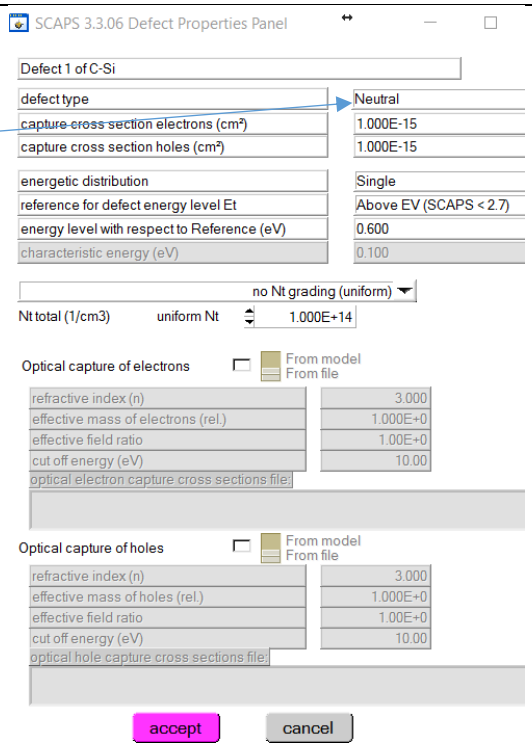
4.2.4.1. Setting up electron and hole lifetime and diffusion length via indirect recombination

See chapter 3, section 3.6 "Defects and recombination" in SCAPS manual for information on recombination and defects model.

"Layer Properties Definition Panel" Region 2 - recombination: illustration for C-Si layer lifetime and diffusion length setting up via defect

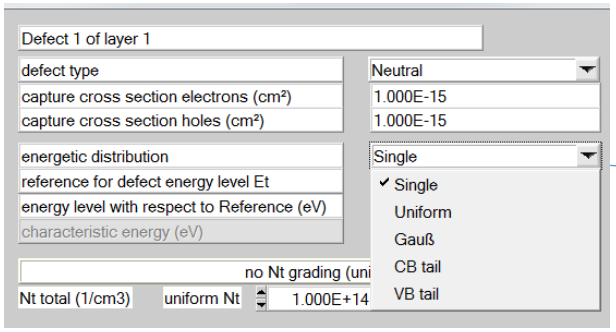


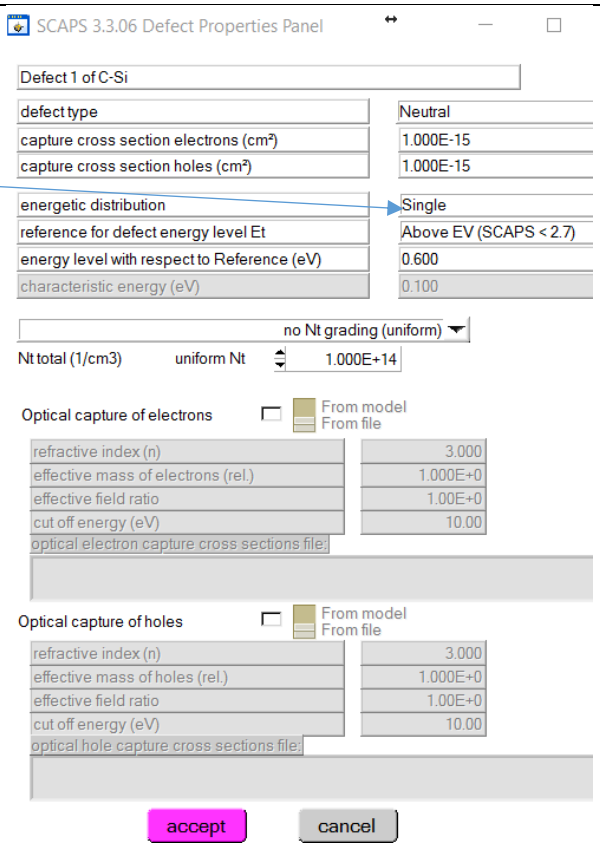




Defect can be defined to be charged or not (Neutral):

- Charged defects have two distinct effects: (i) recombination and (ii) electrostatic
- Neutral defects have only one effect: recombination. **There are called "lifetime killer"**. There are useful if you want to setup a lifetime value without affecting the charge or electrostatic in the device

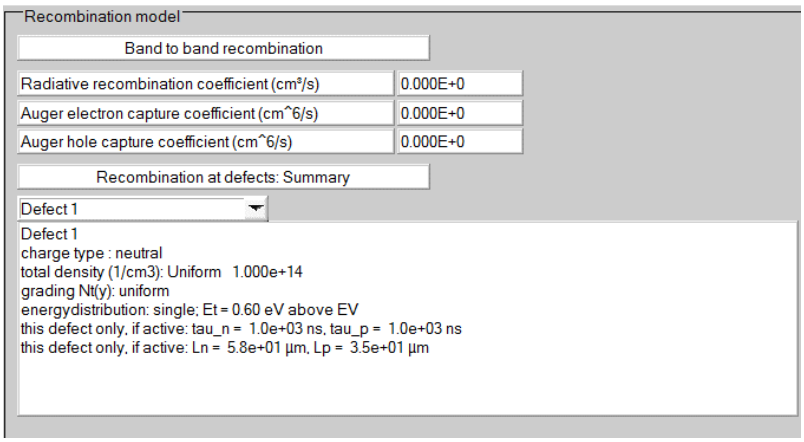




You can set the defect to be distributed in energy**. For simplicity we use a « SINGLE » non-distributed defect**

	Range	$N_t(E)=\ldots$	remarks
Single	$[E_t;E_t]$	$N_t \times \delta_{E_t}$	
Uniform	$\left[E_t-\frac{E_c}{2};E_t+\frac{E_c}{2}\right]$	N_t	
Gauss	$\left[E_t-\frac{w_G}{2}E_c;E_t+\frac{w_G}{2}E_c\right]$	$N_t \times \exp\left[-\left(\frac{E-E_t}{E_c}\right)^2\right]$	w_G can be defined on the numerical panel default value: $w_G = 6.0$ see Figure 3.23
CB tail	$[E_t - w_t E_c;E_t]$	$N_t \times \exp\left(\frac{E-E_t}{E_c}\right)$	w_t can be defined on the numerical panel default value: $w_t = 7.0$ see Figure 3.23
VB tail	$[E_t;E_t + w_t E_c]$	$N_t \times \exp\left(-\frac{E-E_t}{E_c}\right)$	w_t can be defined on the numerical panel default value: $w_t = 7.0$ see Figure 3.23

Click on the button « accept » to valid the parameters values, and you will get the "recombination summary" window



SCAPS automatically calculate the values of **lifetime and diffusion length corresponding to this specific defect "defect1", by using the below formals**

$$\tau = \frac{1}{\sigma v_{th} N_t}$$

$$L = \sqrt{D\tau}$$

It is possible to add up to 7 different defects.

See chapter 3, section 3.6 "Defects and recombination" in SCAPS manual for information on recombination and defects model.

"Layer Properties Definition Panel" Region 3 – "absorption model": illustration for C-Si layer

In its default mode, SCAPS calculates the generation of electron-hole pairs (eh-pairs) G(x) from the incident photon flux, from a very coarse optical model. This model contains only reflection/transmission at the two contacts, and absorption in the semiconductor layers. Thus: no interference, no scattering, no intermediate reflectors… **See at page 38 of SCAPS manual for more information**.

To define absorption coefficients, SCAPS offer two (2) possibilities:

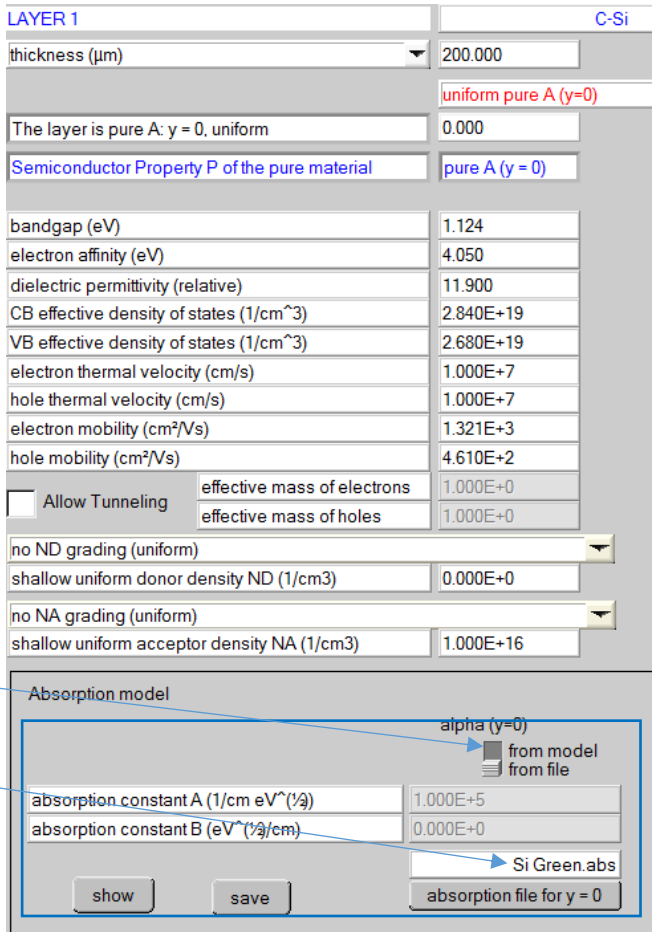
1. via a simple model where the absorption coefficients are calculated from the following formula:

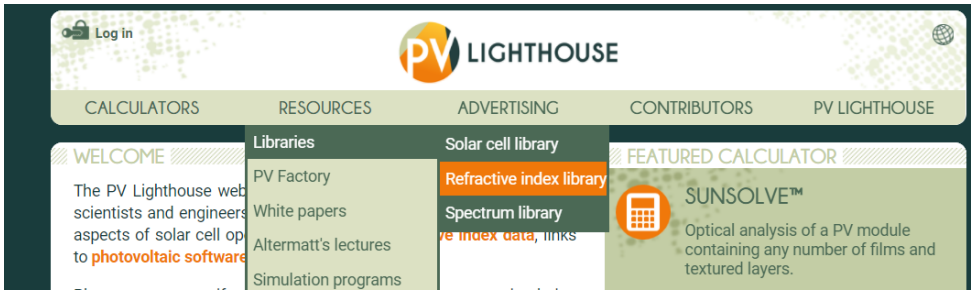
$$\alpha(\lambda) = \left(A + \frac{B}{h\nu}\right)\sqrt{h\nu - E_g}$$

2. via user input file. Some examples of absorption files can be found in the absorption folder at SCAPS installation directory. **For the c-Si layer we have use the "*Si Green.abs* " file as an input.**
For others materials: if you don't the absorption coefficient in SCAPS folders, you can use:

- the pvlighthouse refractive index library to find some optical data of https://www.pvlighthouse.com.au/

- make the measurements or find it in published papers



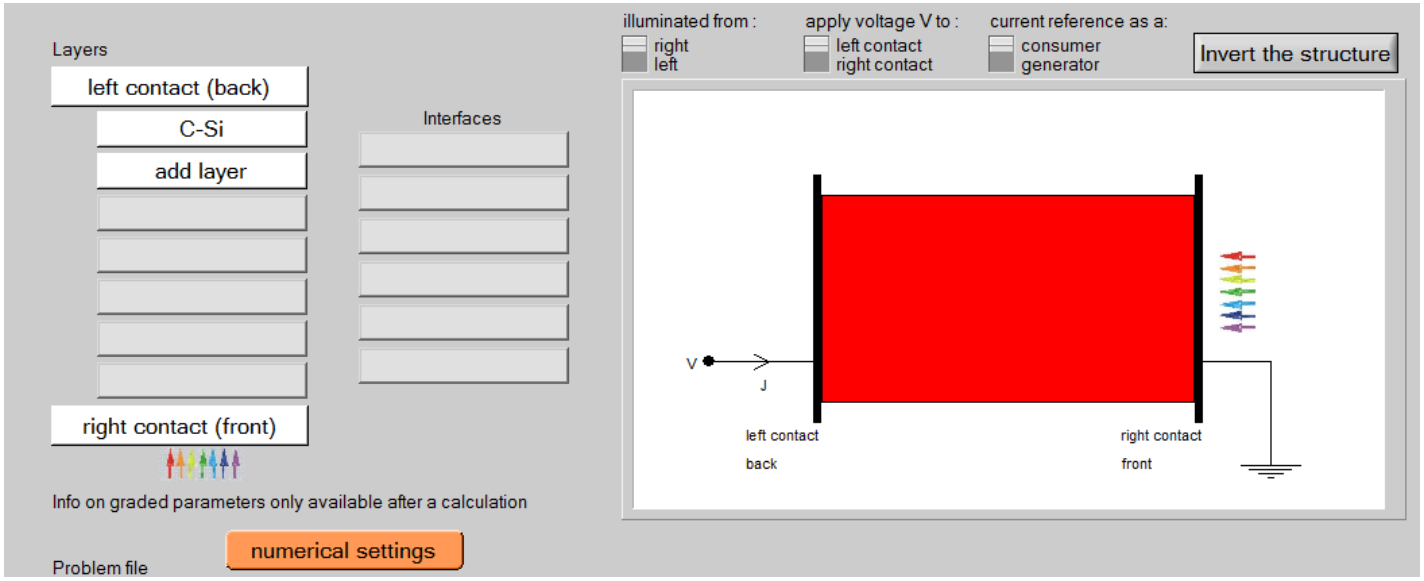


4.2.6. Adding another layer

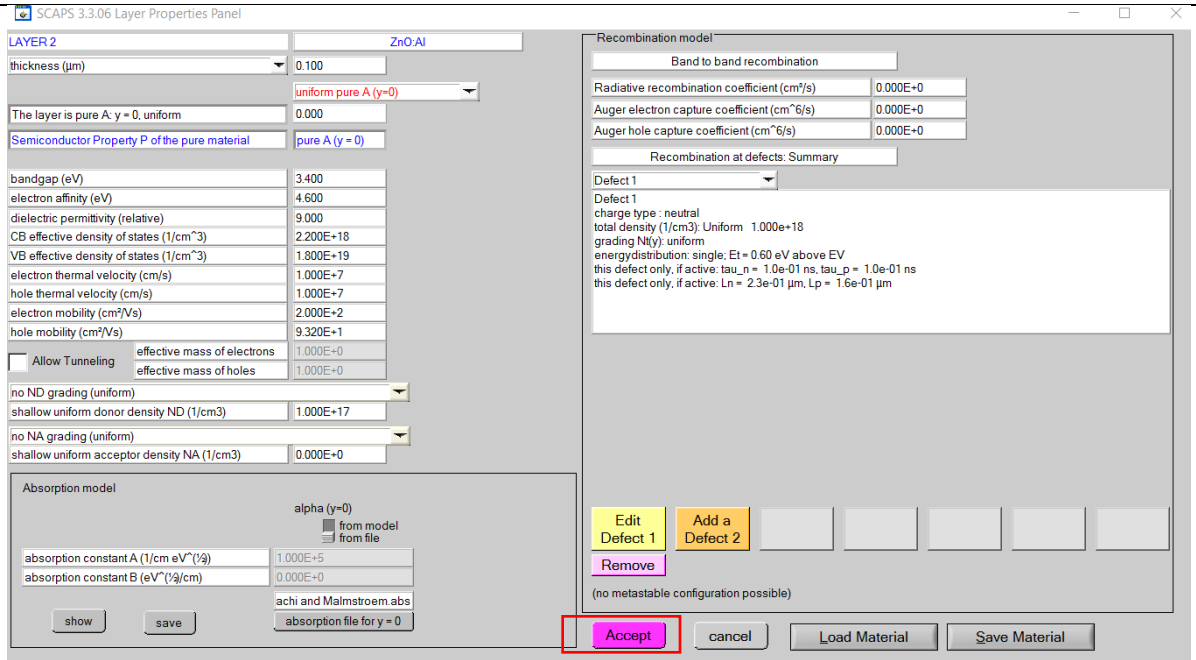
To build the ZnO: Al /c-Si junction we will add the ZnO:Al layer using the parameters values of table 1 to 4.

Add and configure ZnO :Al layer

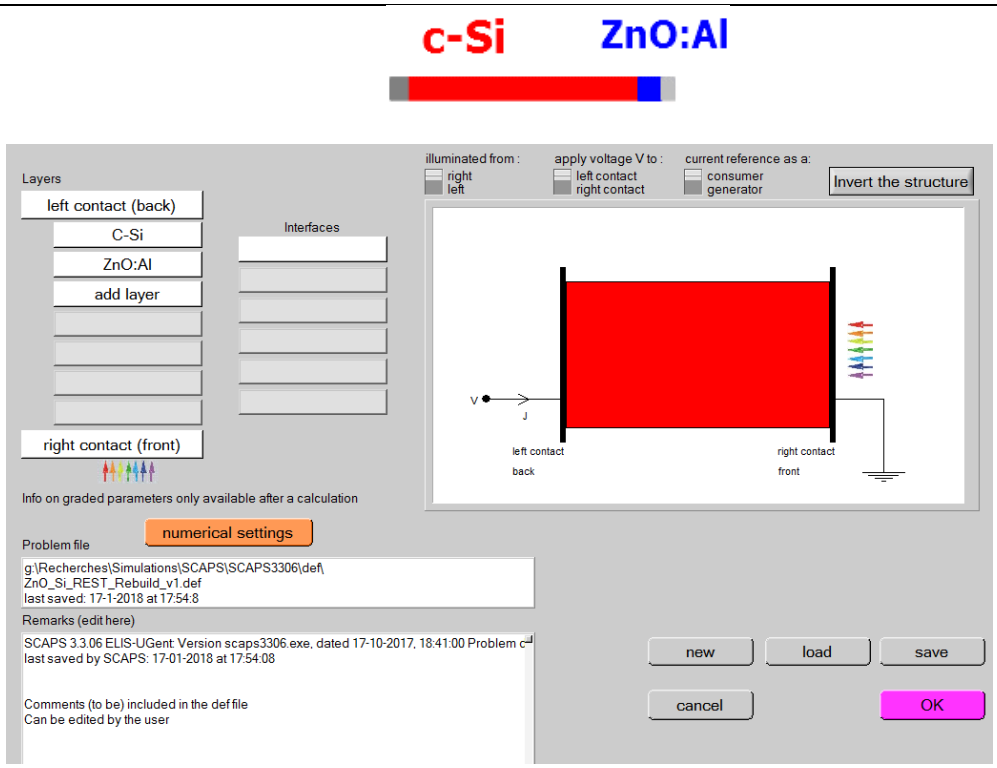
After building the c-Si layer we can now build the ZnO:Al layer in order to get the active c-Si/ZnO:Al active heterojunction. To add ZnO:Al layer click on the **ADD LAYER** button as shown below.



Parameter value of the ZnO:Al layer. **For the absorption coefficient we use "*ZnO Adachi and Malmstroem.abs*" file, located in the absorption folder at SCAPS installation directory**



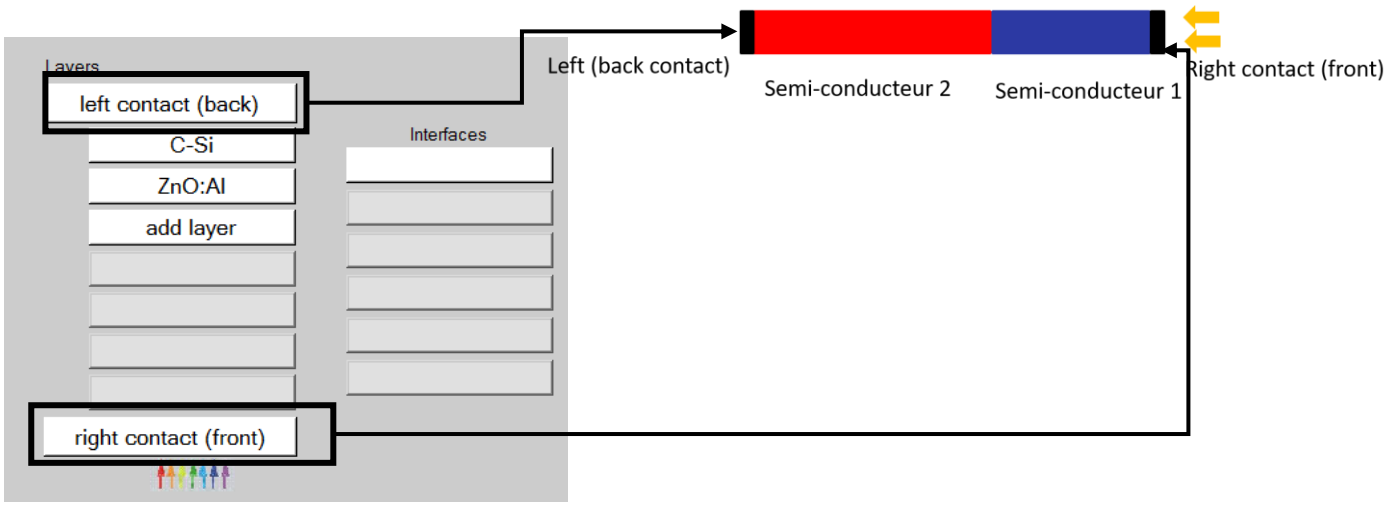
After adding the ZnO :Al layer you will get a window similar to the image below



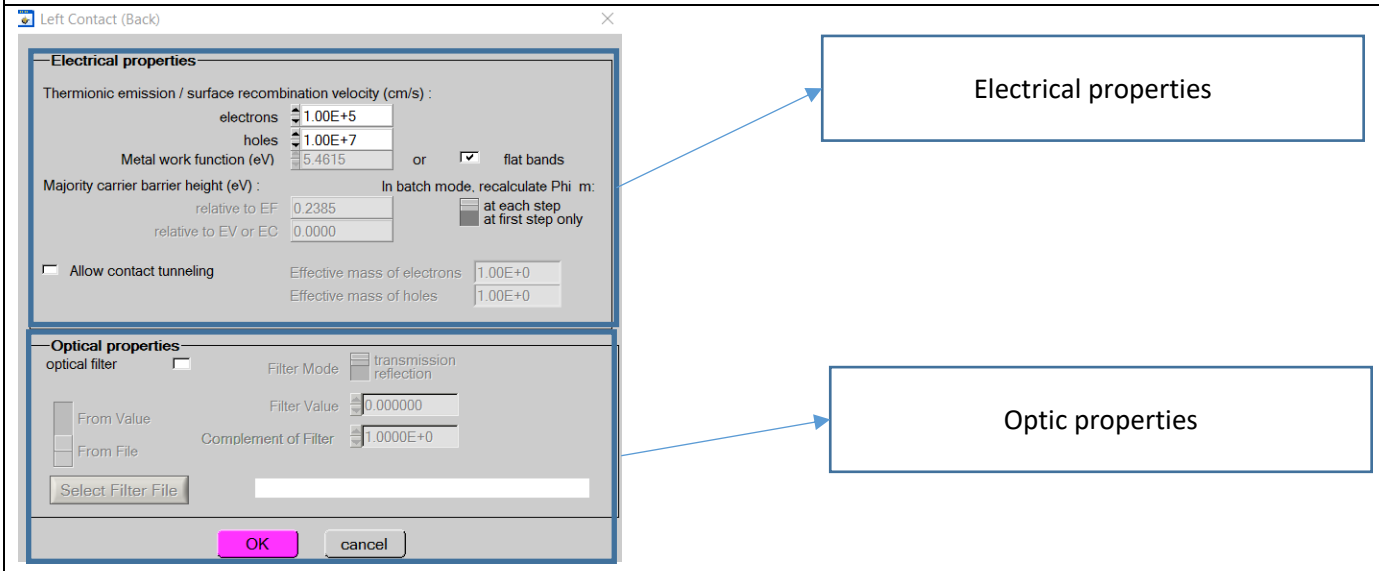
Note : **SCAPS use color code : Red=p-type, Blue=n-type and Green=Intrinsic (not doped or when donor and acceptor density are equal)**

4.2.7. Setting up contact properties

To setup the properties of the electrical contacts : launch the « contact properties panel" y clicking on **Left contact (Back) or right contact (front) button**

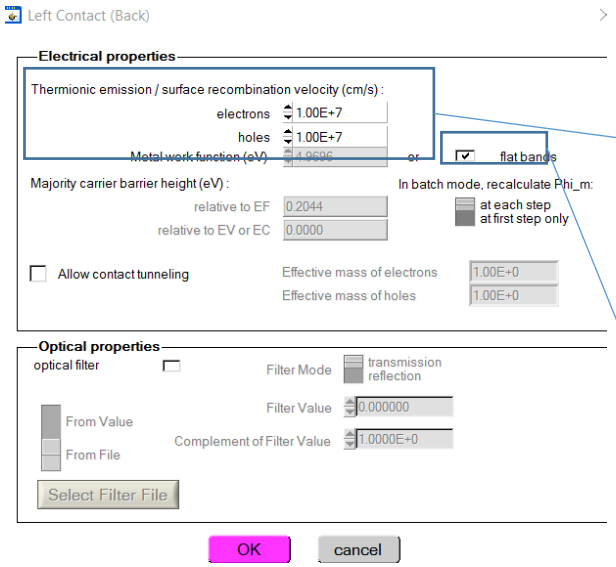


Example for the « left contact (back) properties panel ». the front contact properties panel are the same parameters.



4.2.7.1. *Contacts electrical properties*

SCAPS use the thermoionic emission model for mobile charges transport across the contacts. **The model is well described in [2, 3]. See in chapter 3 section 3.3 in SCAPS manual for more information.**



Thermoionic emission or surface recombination velocity (cm/s) :
Pay attention on the interpretation of this parameter. It can be seen as a rate of charges carriers extraction at the contact. Thus, it can be used to emulate or simulate a "**Back Surface Field (BSF)" effect or surface passivation**.

Majority carrier barrier height:
It depends on the metal work function. There are 3 possibilities here:

1. Let SCAPS calculate the metal work function in order to get: (i) flat bands conditions, but SCAPS may some difficulties to meet it if there are lot of charges or defects; (ii) give the barrier high you want and SCAPS calculate the corresponding metal work function.

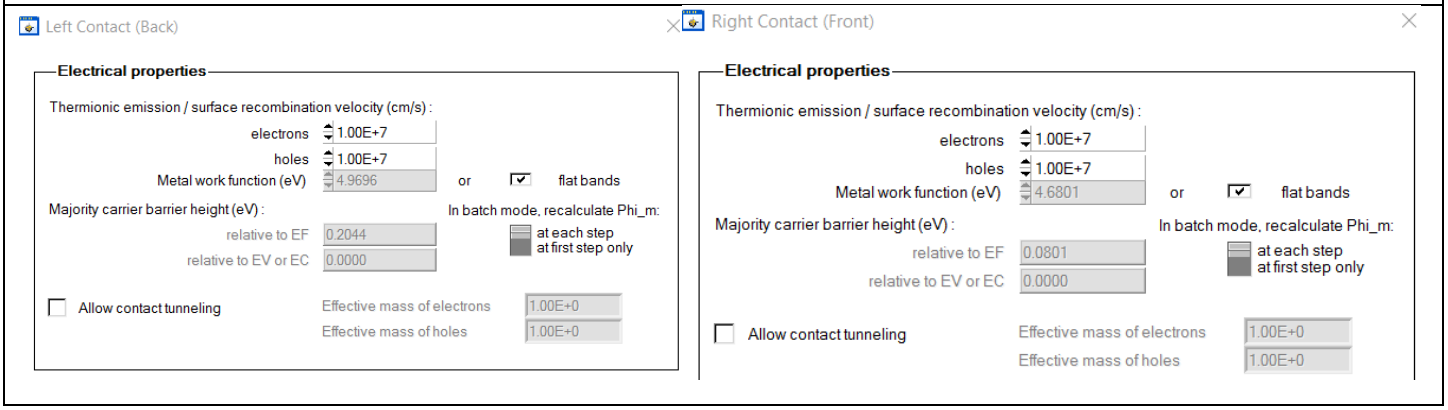
2. Set the metal work function yourself

$$\Phi_m = \chi + k_B T \ln\left(\frac{N_C}{N_D - N_A}\right)$$ Metal/type-n Contact

$$\Phi_m = \chi + E_g - k_B T \ln\left(\frac{N_C}{N_A - N_D}\right)$$ Metal/type-p Contact

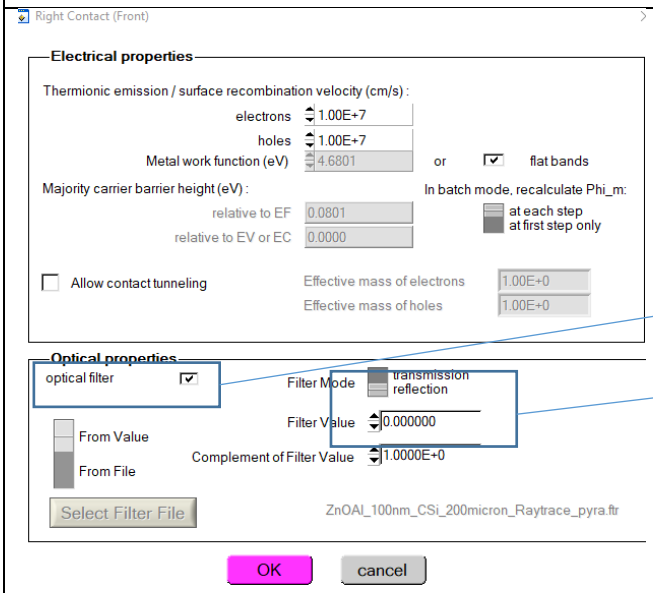
$$\Phi_m = \chi + k_B T \ln\left(\frac{N_C}{n_i}\right)$$ Metal/type-intrinsic Contact

For our cell, we have chosen "flat bands" and set Thermoionic emission or surface recombination velocity (cm/s) for hole and electron at the same value 1x10^7 cm/s (the maximum), corresponding to a maximum recombination at the contacts.



4.2.7.2. *Contacts optical properties*

At the contacts a (wavelength dependent) reflection/transmission can be set, **see chapter 4 section 4.2.1 in SCAPS manual**.
These can be set either as a constant value (wavelength independent) or as a filter file. These filter-files are standard ASCII files with the extension ***'*.ftr'***. Several files are provided with the SCAPS installation (in the folder ***filter***), however, the user can easily make his own files (from measurements or from data taken from papers or online database (for example https://www.pvlighthouse.com.au/).



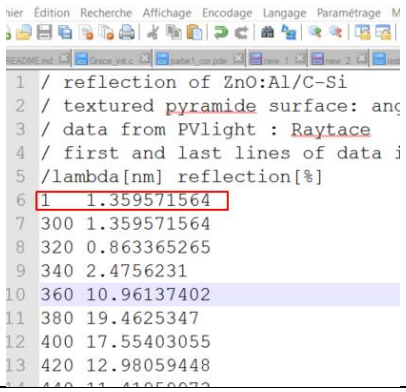
To set the optical properties of the contacts, you have to activate the option by checking "**OPTICAL FILTER**"
And choose one option :

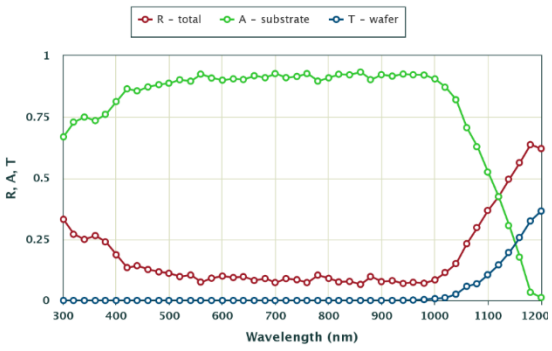
1. **FROM VALUE** for a constant value of reflection or Transmission in % (wavelength independent). **We will start with a constant value (0 refflection)**
2. **FROM FILE** for providing the filter-file

The pvlighthouse refractive index library (https://www.pvlighthouse.com.au/) is the easiest way to find some optical data. You can use the online raytrace module of pvlighthouse to calculate the optical optical properties (Reflection and Transmission) of layer or stack of layers.

You can use the online raytrace module of pvlighthouse to calculate the optical optical properties (Reflection and Transmission) of layer or a stack of layers.

The figure below show for the data ZnO:Al (100nm)/c-Si(200µm) stack obtained from pvlighthouse . R-total data are extracted to build a SCAPS filter-file. Please note that the first line of data in SCAPS filter-file has to be modified in order to help SCAPS make interpolation. **We will use these data in the next tutorial**

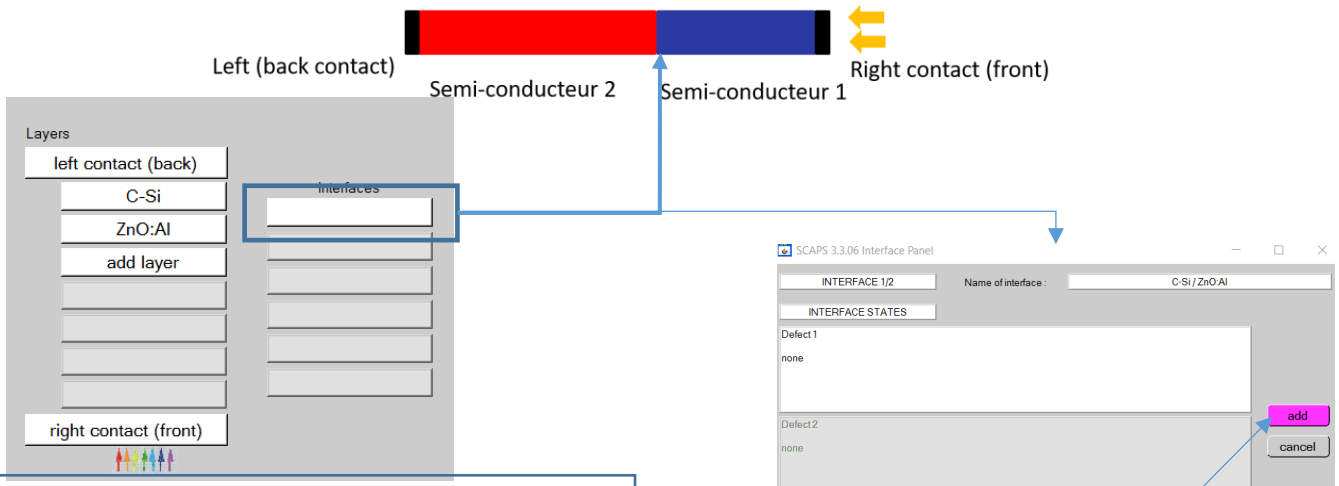




4.2.8. Setting up heterointerface electrical properties

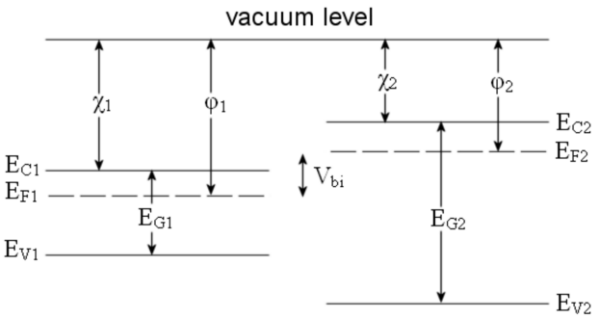
Between any two semiconductor layers an interface can be defined. The model which is implemented for interface transport in SCAPS is thermionic emission. The thermal velocity of the interface transport equals the smallest thermal velocity of the two neighboring layers. **The model is well described in [2, 3]. See in chapter 3 section 3.8 in SCAPS manual for more information.**

To setup the c-Si/ZnO :Al heterointerface, click on « Interface » button to launch the "**Interface Panel**"



Note that the bands offset values depend on the 2 semiconductors parameters: bandgap (eV) and electron affinity (eV).

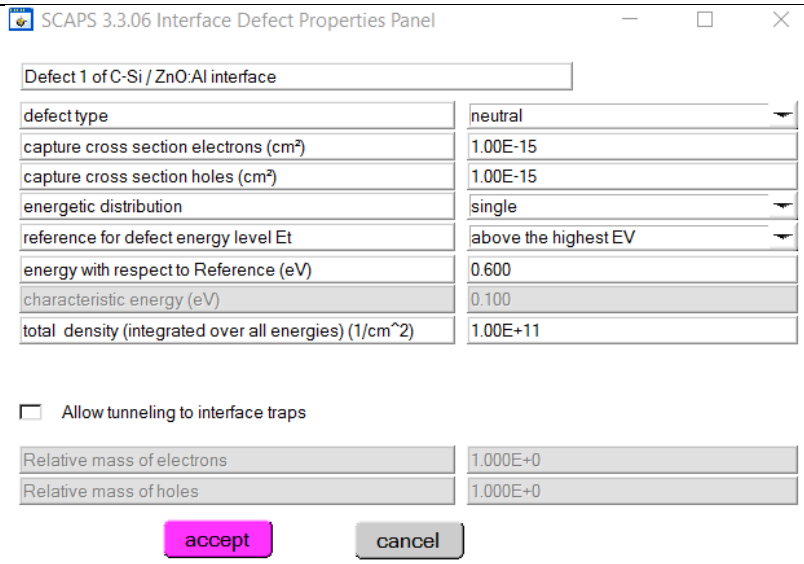
It is possible to add up to 3 different types of interface defect. The definition of interface defect is similar to that of bulk defect, except that there are quantify with surface density.
To add a defect click on "white area labelled defect 1" to launch "**Interface Defect Properties Panel**"



$$\Delta E_v = (\chi_1 + E_{g1}) - (\chi_2 + E_{g2})$$

$$\Delta E_c = \chi_2 - \chi_1$$

“Interface Defect Properties Panel”: Example of interface defect setting up. **Note that this first tutorial, we will not consider interface state**

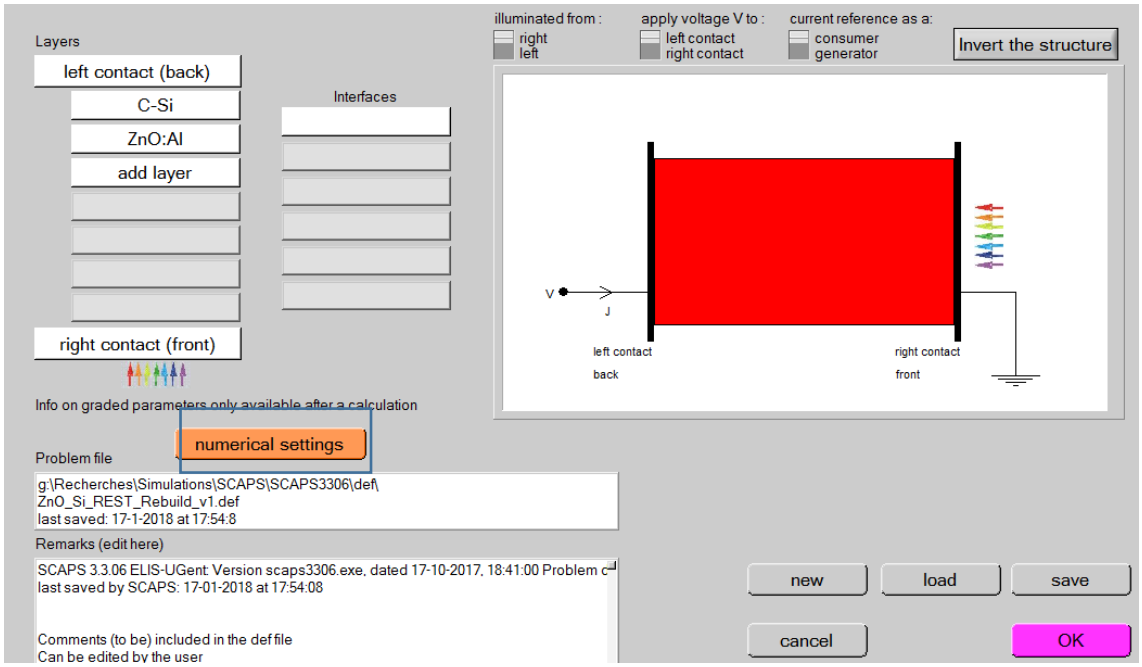


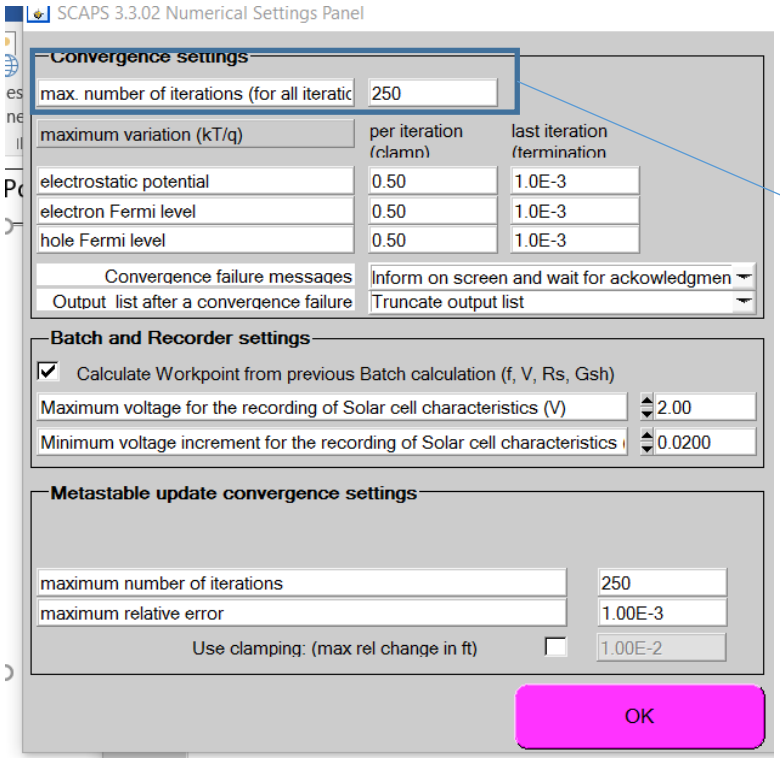
4.2.9. Save your design and configure the numerical resolution parameters

It is a best practice to save your design as soon as possible.

Click on the SAVE button to save your design.
Use the *extension ".def".* For *Example: "MyStructure.def"*
There is not automatic save mode in SCAPS. At each important step (major modification) save your design and name it with label. For example: v0, v1.0…

Use the « NUMERICAL SETTINGS » button to increase the “max number of iterations”: start with 1000. For thick layer it can be necessary to increase it up to 2000. **Large value will slow down the simulation**.





For a very tick material (200 µm):
MAX NUMBER OF ITERATIONS: 3500

4.3. Calculations and analysis

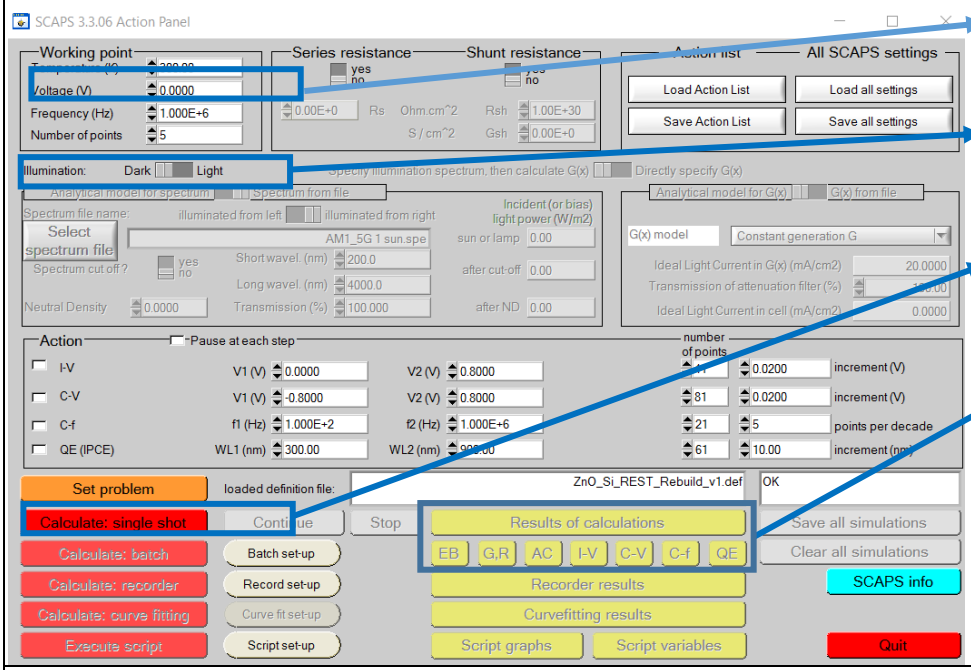
The main functionality of SCAPS is to solve the one-dimensional semiconductor equations under various conditions (dark, under bias (illumination and/or electrical bias), to simulate experiments like: I-V characteristics, Quantum Efficiency (QE)… **More information can be found in SCAPS manual, chapter 5 page 36.** Here we will show how to use some basic and useful feature of SCAPS to get deep inside solar cell operation principal or to use it as a tool to optimize your design and deeply understand solar cell internal working principle.

4.3.1. Calculate and analyze data of solar cell under illumination and at short-circuit

Analyzing solar cell internal working principle under illumination and at short-circuit is a good way to start as it is relatively easy to calculate.

At short-circuit it is possible to quantify the loss due the contacts and interface by looking and evaluating the current à the contacts.

To evaluate your device operation under illumination at short-circuit:



1. Set the applied voltage to 0

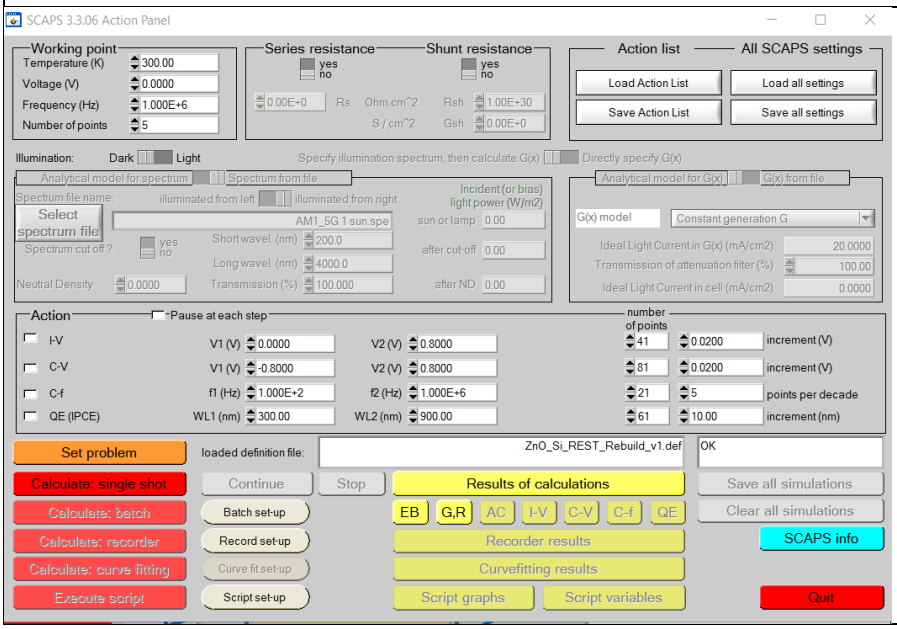
2. Turn on the light

3. Click on "Calculate: single shot "

Please note that:
(i) before any calculation, the "**Results of calculations zone**" is not active

(ii) if the design is not well saved the "**Calculate: single shot**" button is not active.

If you are correctly saved your design and click on the "**Calculate: single shot**" button, you will get the bellow window



To analyze the results :

(i) click on "**EB**" button for **E**nergy **B**and to get the energy band diagram and the charges carriers density and concentration

(ii) Click on "**G,R**" button or **G**eneration, **R**ecombination to get all the values of the internal variables of the cell.

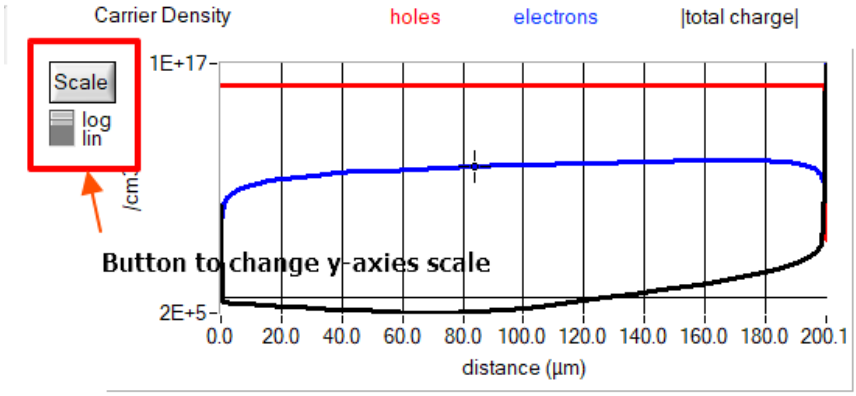
The figure below show examples of EB data, for the ZnO:Al/c-Si solar cell under illumination at short-circuit.

SCAPS "EB" output graphs : simulation done under illumination at short-circuit (V=0V):

It is possible to change the display scale:

(i) for abscises axis , click on the "**Scale distance (all graphs)"** button (in the center of the Panel), by choosing "Manual" and set up ***min*** and ***max*** values

(ii) for the energy axis for each of the for graphs you can change the scale (via the "**scale**" button)

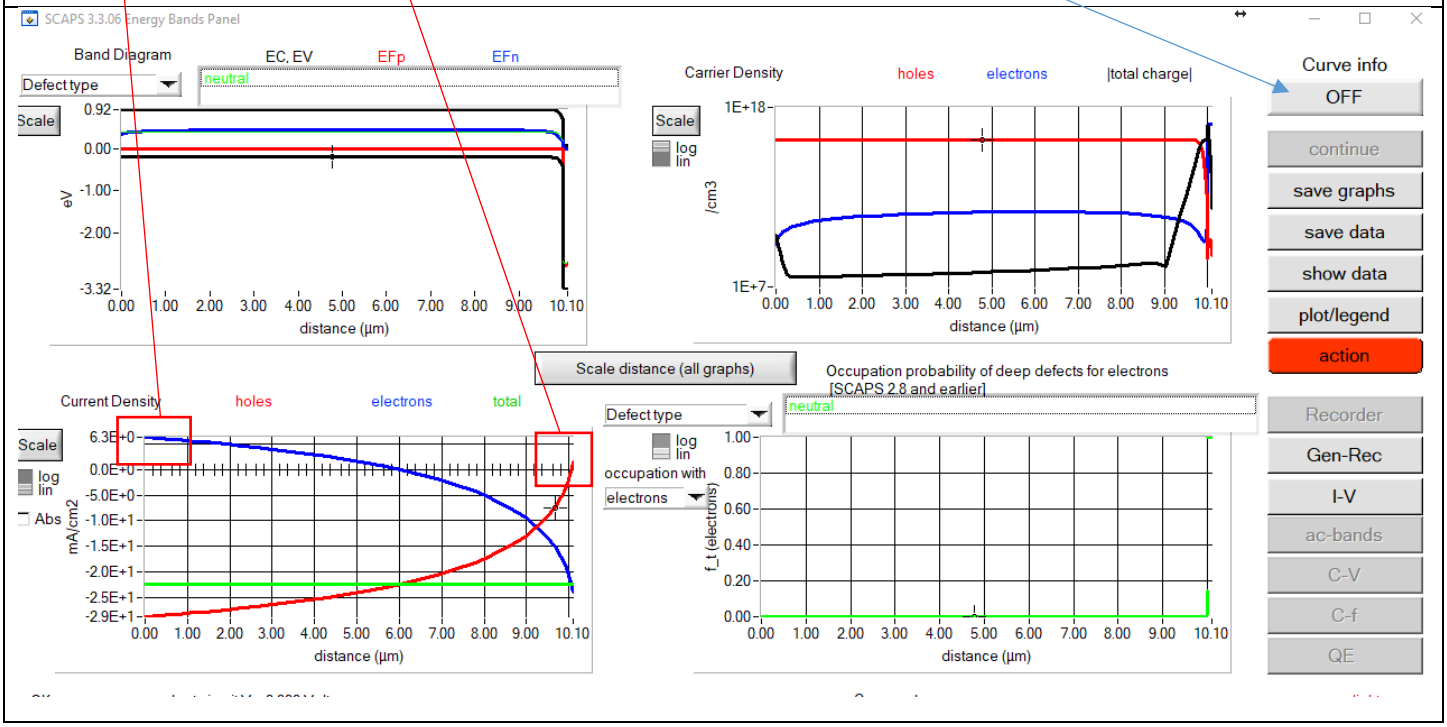


Example: To interpret these graphs, we know that at short-circuit only contacts and interface recombination are limiting factors. So, looking at the "current density" graph at the contacts we can evaluate the losses due to the contacts:

- **a hole contact, electron current is a loss (here we loss 6.3 mA/cm2);**
- **at electron contact, hole current is a loss (here we loss 1.35 mA/cm2);**

To get the value from the graph, click on **Curve info button**

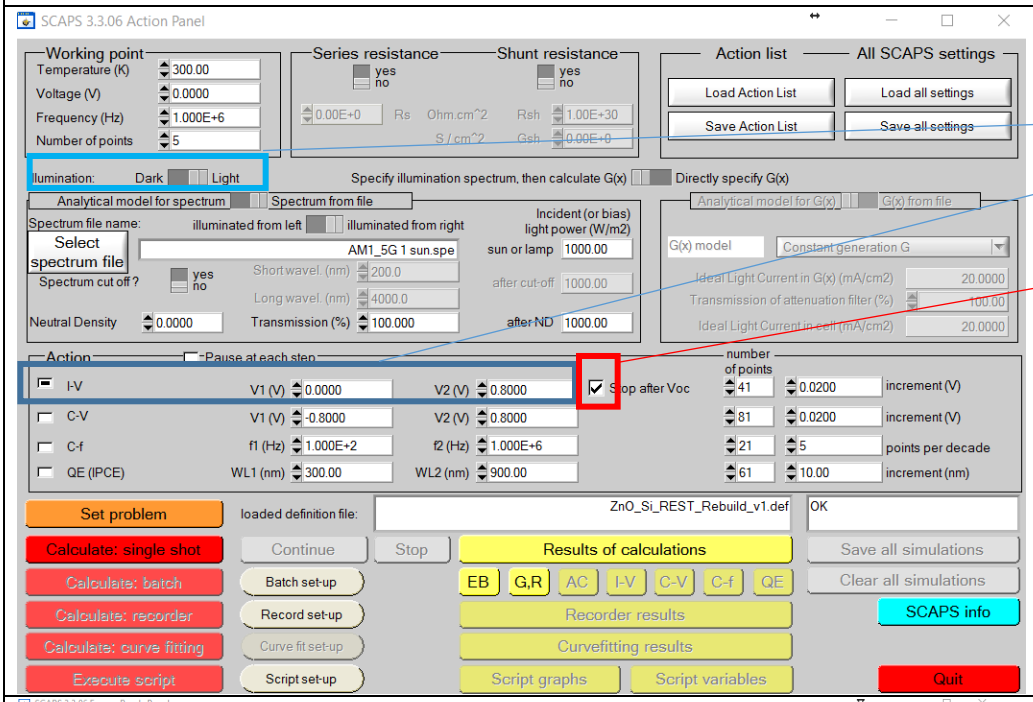
If you are in "Energy Bands Panel" and want to go back to the main panel, click on the red button "**Action**"



4.3.2. Calculate and analyze data of solar cell under illumination and at open-circuit

At open-circuit it is possible to quantify the loss due the recombination and identify where the recombination takes place in the solar cell.

In SCAPS, to simulate the solar cell operation at open-circuit, we have to calculate the current versus voltage characteristics (I-V) under illumination, and stop the calculation **when the cell current is equal to 0.**



to evaluate the cell operation at open-circuit, we have to :

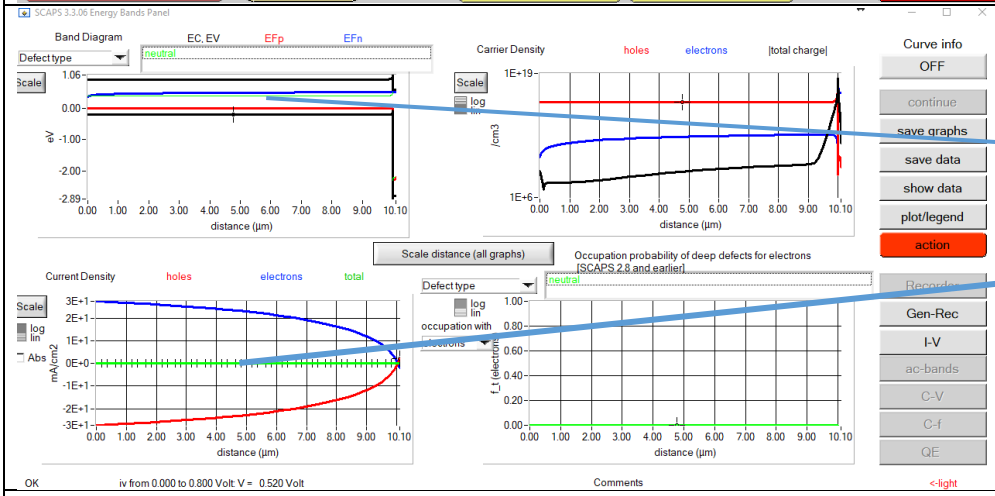
(i) turn the light ON

(ii) check the I-V box to activate the I-V calculation,

(iii) Check "Stop after Voc" to stop the I-V characteristics calculation when it reaches the open-circuit condition.

(iv) start the I-V calculation

The figure below show examples of EB data, for the ZnO:Al/c-Si solar cell under illumination at open-circuit.

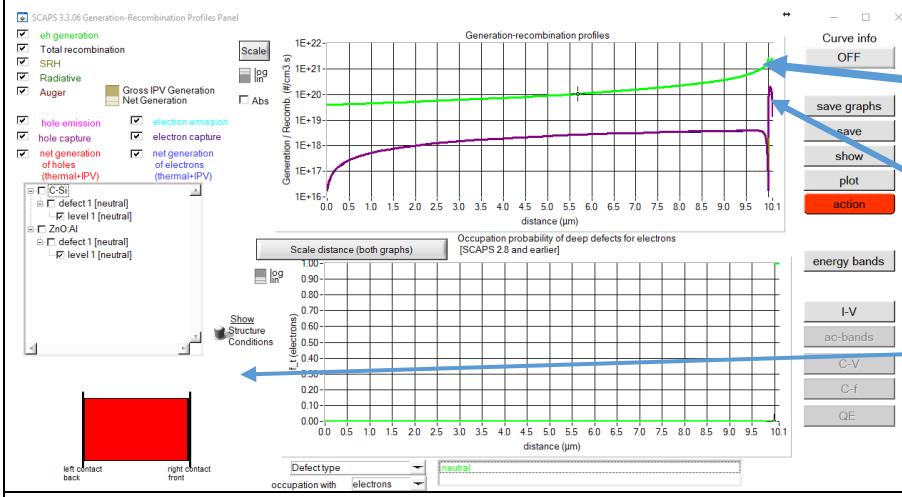


Energy band diagram at open-circuit condition:

(i) The difference between the quasi-Fermi level correspond to Voc

(ii) The total current must be 0

Click on the red button "Gen-Rec" button to analyze the generation and recombination inside the device.



Generation and recombination profiles @ Voc condition

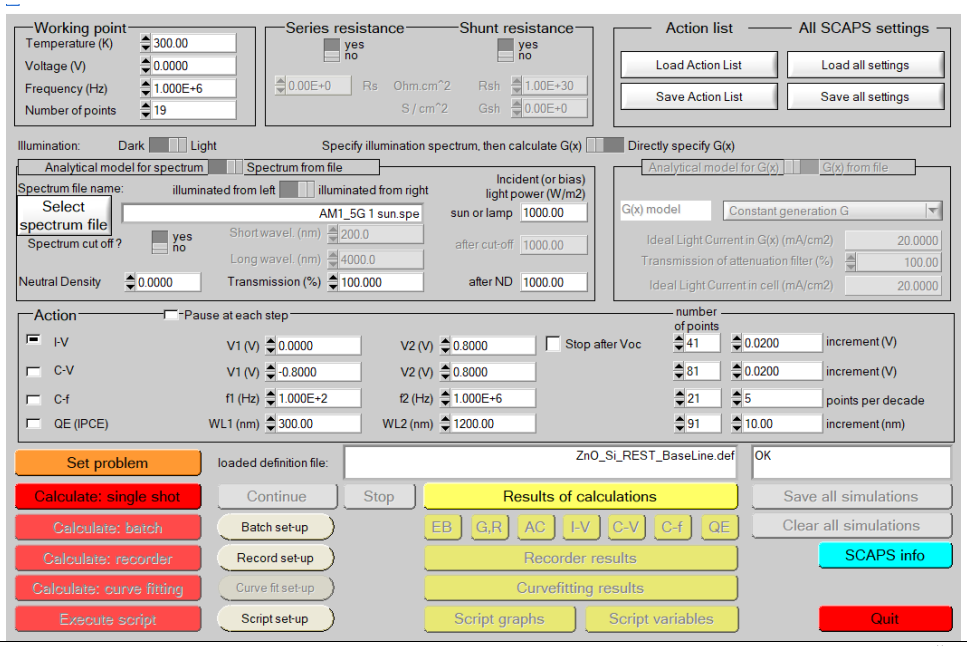
There are lot of generation at the back contact (**green curve**). That mean we can use thick layer to get current!

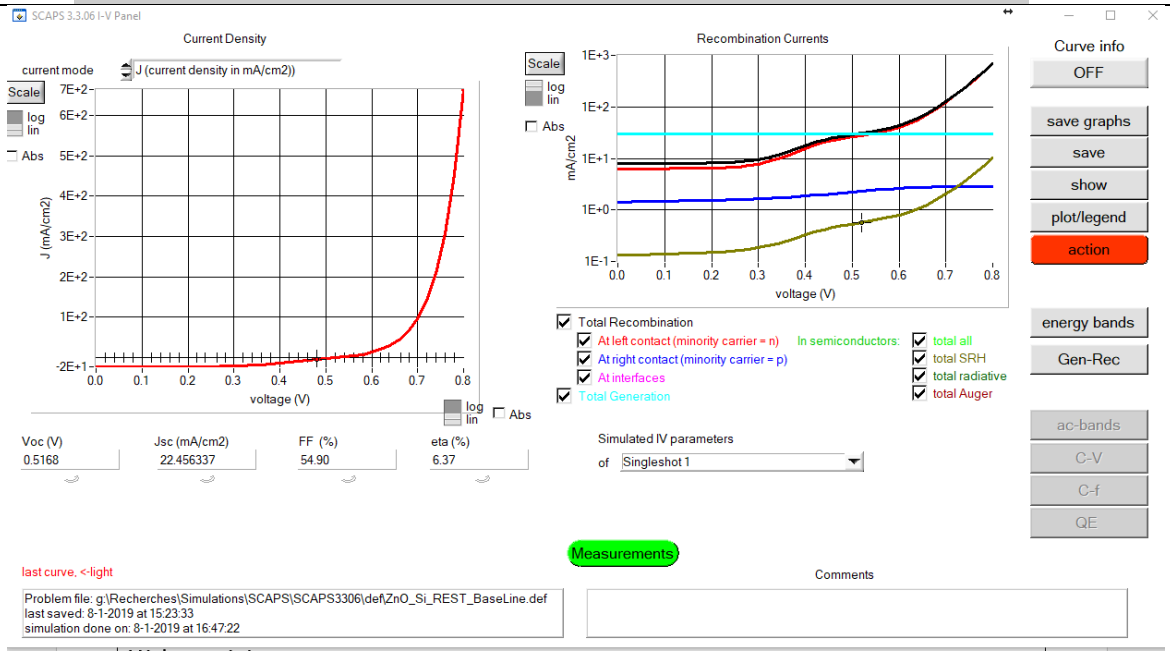
- ZnO layer have more recombination (**black curve**)

You can display or show the structure by clicking on **Show structure button** in this way can identify where the contacts are

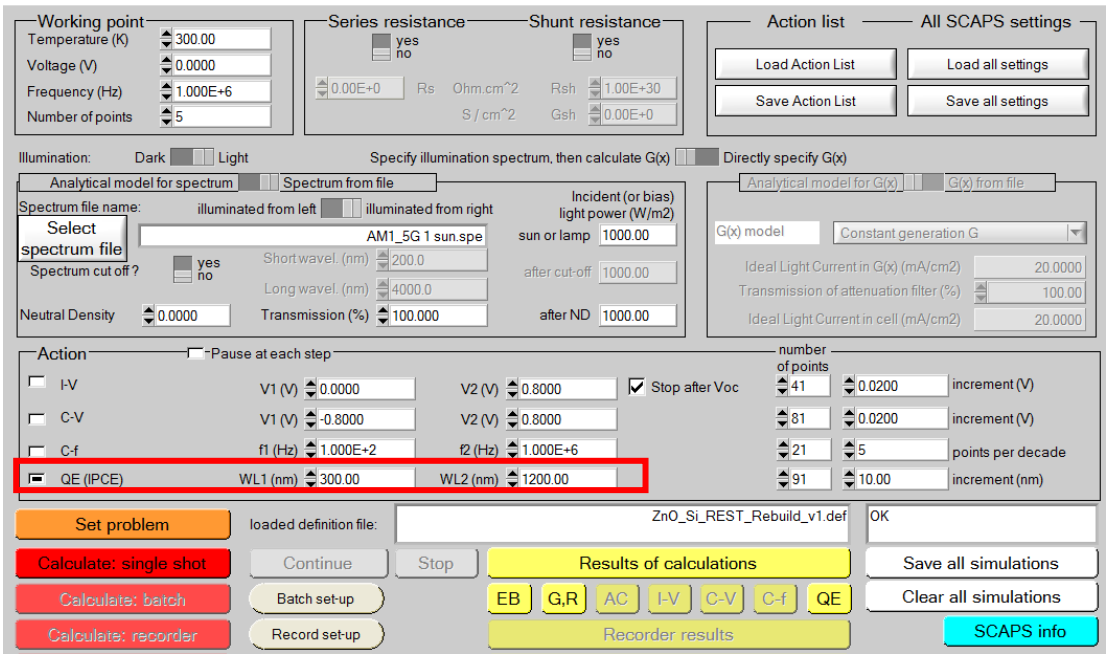
4.3.3. Calculate and analyze the I-V characteristics of solar cell under illumination and under dark

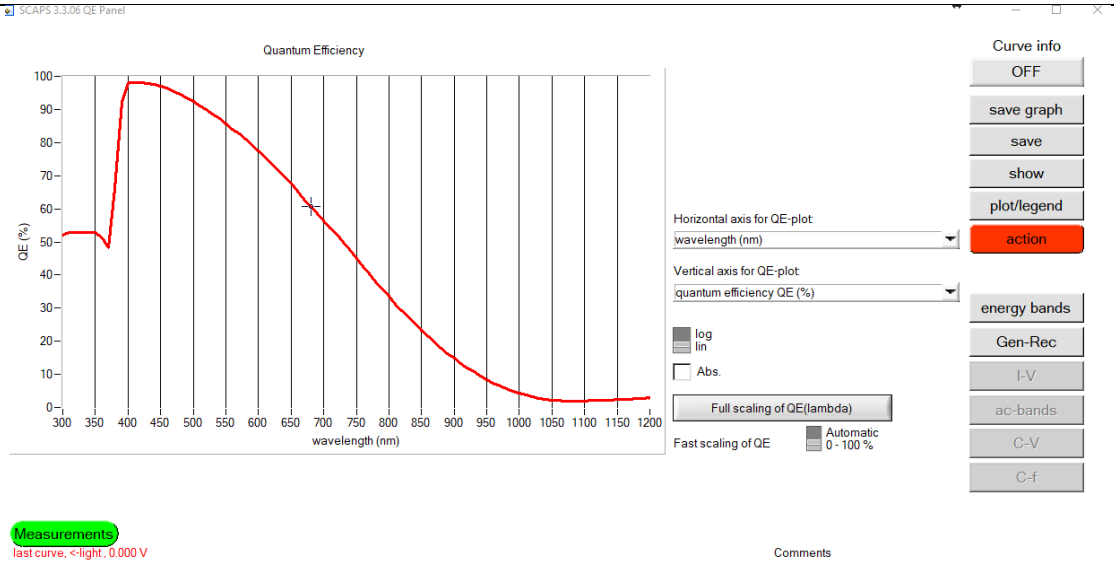
I-V characteristics under illumination





4.3.4. Calculate of Quantum Efficiency





5. Tutorial 2: improving solar cell model

In our baseline ZnO:Al/c-Si model, we are made some assumptions in order to build a getting started model. A few of these assumptions are:

- In table 6 (contacts proprieties) we consider: (i) the c-Si surface and the back contact are not reflective; (ii) the contacts (back and front) are not passivated.
- The interface ZnO:Al/c-Si is free of defects
- The non-radiative recombination centers (defects) which control the carriers lifetime don't have electrostatic effect: neutral defects and are not distributed in energy

In this tutorial, we will show how to change these assumptions in order to improve our model (let say to make it more realistic)

5.1. Contact properties

Improve the solar cell model: (i) add optical data (reflection for example) of the layers; (ii) add interface defects because there are always there in the case of heterojunction. The contact between 2 different materials generate always a defects at the hetero-interface.

5.1.1. Integration of optical data

Before jumping to interface or contacts defects setting up, we will see how we can add optical data in order to make our cell more realistic. To do this, we can get optical from 2 kinds of source:

- From experiment. In this case, we need to measure the reflection and transmission of each layer or contact and then use these data in SCAPS.
- From data base or paper. In many cases, we don't have the setup to measure the reflection and transmission of each layer or contact or we want to compare our measurement to published data. The web site of pvlighthouse (https://www.pvlighthouse.com.au/) is one of the best source of optical data base of PV material

5.1.2. Contacts recombination

5.2. Interface recombination

5.3. Defects properties

6. Tutorial 3: optimization

6.1. Comparison with experiments

6.2. Batch simulations

7. Reference

[1] S.J. Pearton, D.P. Norton ,K.Ip, Y.W. Heo,T. Steiner, Recent progress in processing and properties of ZnO, Prog. Mater. Sci. 50(2005) 293–340.

[2] A. Niemegeers, S. Gillis, M. Burgelman, A user program for realistic simulation of polycrystalline heterojunction solar cells: SCAPS-1D, Proceedings of the 2nd World Conference on Photovoltaic Energy Conversion, Wien, 1998, pp. 672-675.

[3] H.J. Pauwels, G. Vanhoutte, Influence of interface states and energy barriers on efficiency of heterojunction solar-cells, J. Phys. D-Appl. Phys., 11 (1978) 649-667.