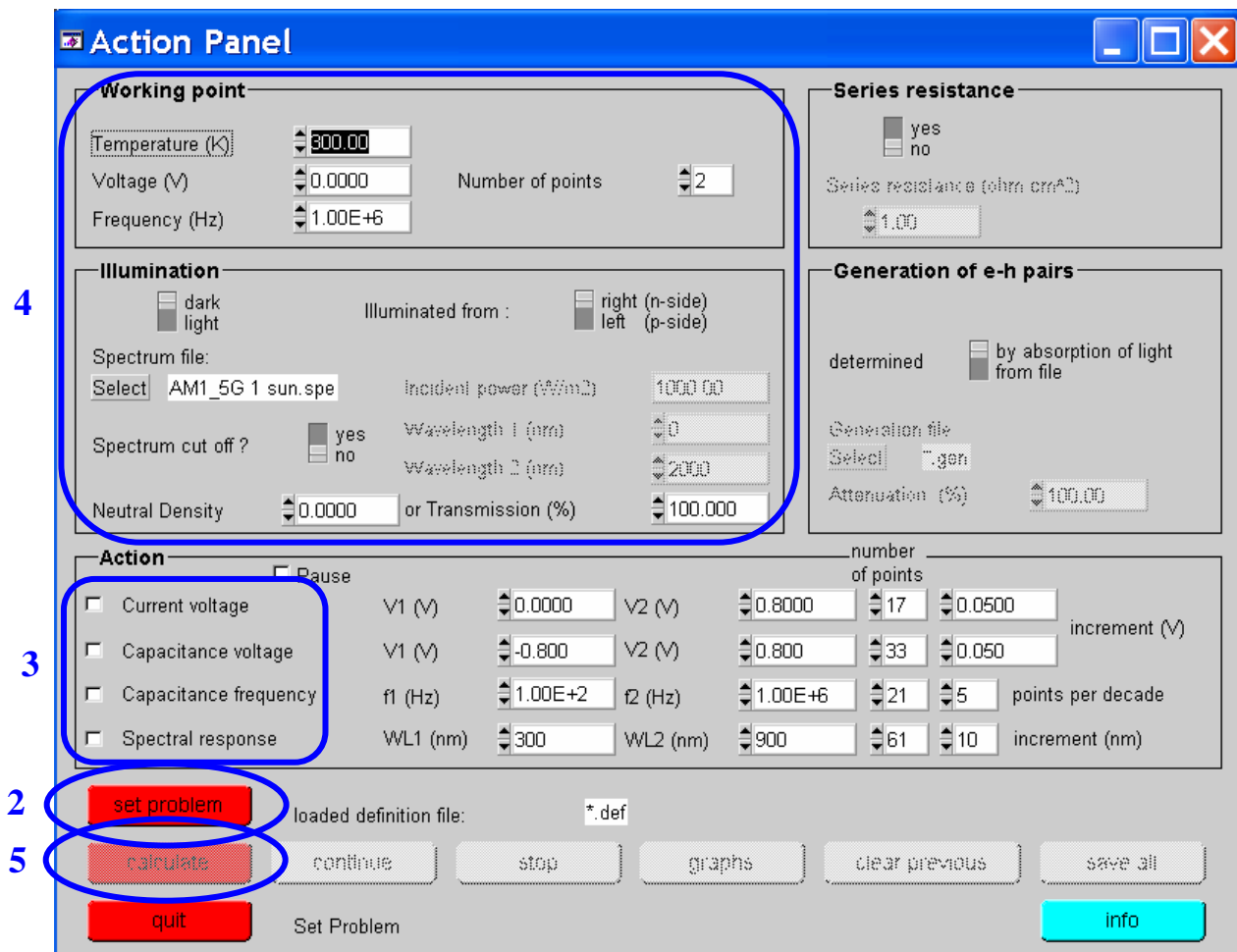# Getting started with SCAPS

SCAPS (a <u>S</u>olar <u>C</u>ell <u>Ca</u>pacitance <u>S</u>imulator) is a simulation programme developed at ELIS, University of Gent. The presentation here is based on version 2.6, march 2007.

0. The basics

SCAPS is a Windows-oriented programme, developed with LabWindows/CVI of National Instruments. We use here the LW/CVI terminology of a 'Panel' (names used in other

softwares are: a window, a page, a pop-up…). SCAPS opens with the 'Action Panel'.

There are dedicated panels for the basic actions:

1. Run SCAPS.
2. Define the problem, thus the geometry, the materials, all properties of your solar cell
3. Indicate what you will calculate, i.e. which measurement you will simulate.
4. Indicate the circumstances in which you want to do the simulation, i.e. specify the working point
5. Start the calculation(s)
6. Display the simulated curves, ... (see section 6)

This is further explained below.

1. Run SCAPS:

Click the above pictogram on the Desktop, or double-click the file `c:\SCAPS26\scaps26.exe` in the file manager. SCAPS opens with the Actions Panel: see below.

2. Define the problem

Click the button `set problem` in the action panel, and chose `load` in the lower right corner of the panel that opens. Select and open e.g. the file `NUMOS CIGS baseline.def`: that is the example problem file of the practicum session at the NUMOS workshop, Gent, 30 march 2007. This file is supposed to be in the folder `/scaps26/def`. If necessary, browse to find this file. In a later stage, you can alter all properties of the cell by clicking `set problem` in the action panel.
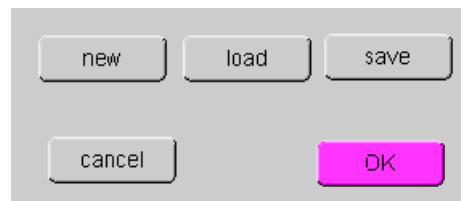
3. Select the measurement(s) to simulate

In the action-part of the Action Panel, you can select one or more of the following measurements to simulate: *I-V*, *C-V*, *C-f* and *QE*(λ). Adjust if necessary the start and end values of the argument, and the number of steps. Initially, do one simulation at a time, and use rather coarse steps: your computer and/or the SCAPS programme might be less fast than you hope, or your problem could be really tough... A hint: in a *C-V* simulation, the *I-V* curve is calculated as well, no need then to specify it separately.

4. Define the working point

The working point specifies the parameters which are not varied in a measurement simulation, and which are relevant to that measurement. Thus:

- the temperature *T*: relevant for all measurements. Note: in SCAPS, only $N_C(T)$, $N_V(T)$ and the thermal voltage *kT* are the only variables which have an explicit temperature dependence; you must input for each *T* the corresponding materials parameters yourself.
- the voltage *V*: is discarded in *I-V* and *C-V* simulation. It is the dc-bias voltage in *C-f* simulation and in *QE*(λ) simulation. SCAPS always starts at 0 V, and proceeds at the working point voltage in a number of steps that you also should specify.
- the frequency *f*: is discarded in *I-V, QE*(λ) and *C-f* simulation. It is the frequency at which the *C-V* measurement is simulated.
- the illumination: is used for all measurements. For the *QE*(λ) measurement, it determines the bias light conditions. The basis settings are: dark or light, choice of the illuminated side, choice of the spectrum. A one sun (= 1000 W/m^2) illumination with the 'air mass 1.5, global' spectrum is the default, but you have a large choice of monochromatic light and spectra for your specialised simulations.
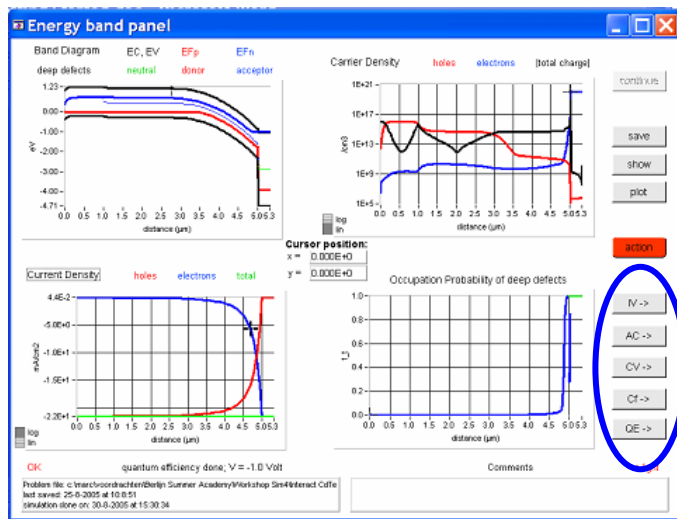
5. Start the calculation(s)

Click the button `calculate` in the action panel. The Energy Bands Panel opens, and the calculations start. At the bottom of the Panel, you see a status line, e.g. "iv from 0.000 to 0.800 Volt: V = 0.550 Volt", showing you how the simulation proceeds. Meanwhile, SCAPS stands you a free movie how the conduction and valence bands, the

While calculating I(V)...

Convergence failure at V = 0.900 Volt.
I(V) calculation cut at V = 0.85 Volt.

OK

Fermilevels and the whole caboodle are evolving. When you see the hated divergence message, you're entitled to get into a bad mood, but don't exaggerate on Friday night, the 30th of march… Anyway, you did not loose the *I-V* points already calculated.
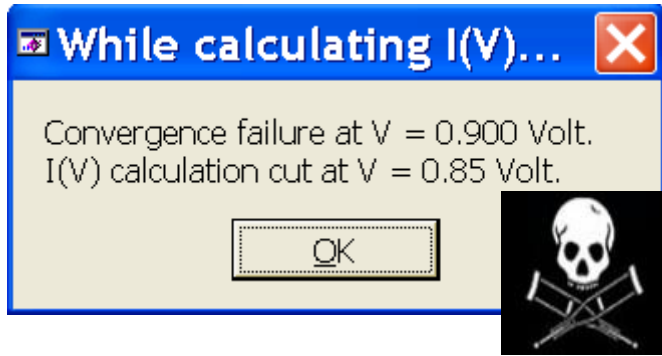
6. Display the simulated curves, ...

After the calculation(s), SCAPS switches to the Energy band panel. You can now look at your ease to the band diagrammes, carrier densities, current densities,… at the last bias point calculated (stop your calculations earlier, or use the pause button on the Action Panel if you want to look at an intermediate state at ease). You can output the results (buttons `print`, `show` (then the numbers are shown on

screen; cut&paste to e.g. Excel is possible), or `save` (then the numbers are saved to a file). You can switch to one of the specialised output Panels (if you have already simulated at least one corresponding measurement). We only show the example of the IV Panel.

7. …e.g. the *I-V* curves

The meaning of the `plot`, `show` or `save` buttons is as for the Energy Bands Panel. Again, you can switch to the other output panels (energy bands, ac, *C-V*, *C-f* and *QE*, if already calculated), and to the Action Panel to do a new calculation, or to stop (important: you can only leave SCAPS from the
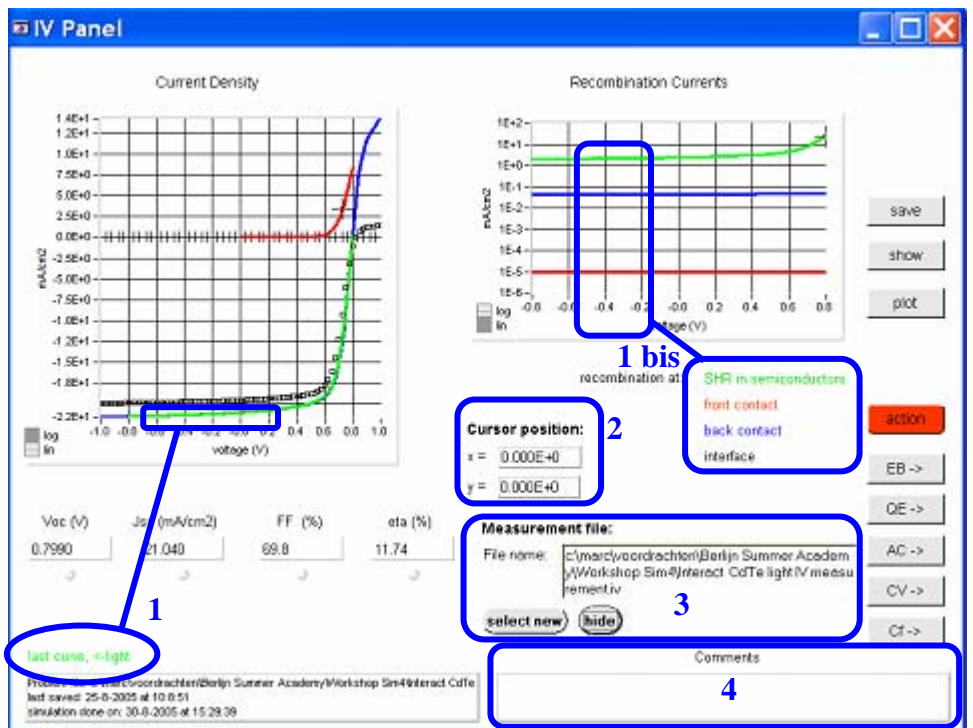
<u>Action panel!</u>). Several small remarks:

1. The color of the last calculated curve is indicated (tip: when you mess up your curves, go to the Action Panel and click `clear previous` to clear all graphs). The recombination curves are only shown for the last simulation. The color of the legend corresponds to the color of the curve (indicated as 1bis).
2. When you click the cursor on a curve in a graph, `cursor position` gives you the position in the physical units of the graph (works only for simulations, not for measurements).
3. Here you can display a measurement file (only one measurement at a time!). Select e.g. the file `Numos Ex 1 light.iv` or `Numos Ex 1 dark.iv` which you should find under /scaps26/measurements.
4. Hint: when you are doing many simulations, be friendly and helpful to yourself, and write some comments in the comment box before printing the Panel: you'll be glad to have done so when the time of writing (an article, your doctorate) comes…

8. Editing the problem

Go to the Action Panel, click `set problem` and then selecting `edit`. You are now in the Solar Cell Definition Panel. Click on a layer name, and you enter the Cell Parameters Panel (the name is not so well chosen, sorry) where you can change all parameters of that layer. Use your intuition, read the manual, or just raise your hand (the last possibility is only in Gent, Friday 30 march 2007, from 15h to 17h…).

9. New in SCAPS 2.6: batch calculations

When you want to explore the influence of one or a few parameters to the solar cell

characteristics, you can take profit now of the batch option in SCAPS 2.6. When you

click 'batch', a panel opens where you can choose which parameter to vary, over which range, and in which mode (lin or log) (see below). You can also define more than one parameter, and vary all of them (in a nested way or 'simultaneous'), but be modest to start. The calculation is only done in batch mode if 'do batch calculation' is clicked.
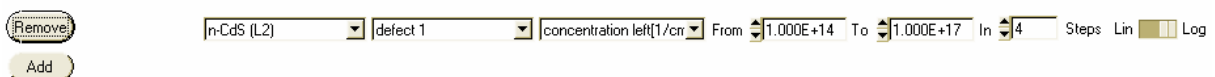
10. New in SCAPS 2.6: tunneling

Actually, two tunneling mechanisms are built in SCAPS 2.6: intra-band tunneling and tunneling to interface states. To enable intra-band tunneling, click 'intra-band tunneling' in the interface states-panel (Solar cell definition panel, click on the interface where you want to enable intra-band tunneling): see below, figure to the left. To enable tunneling to interface states, also go to the interface states panel and click on the defect where you want to enable tunneling (this type of tunneling is connected to an interface defect rather than to the interface itself, as with the previous mechanism): see below, figure to the right.

Good luck !

Interface sta

INTERFACE 1

INTERFACE STATES

Defect 1
chargetype: acceptor
concentration: N = 2.00e+01 /cm²
energydistribution: uniform; Et = 0
this defect only, if active: Sn(left)
this defect only, if active: Sp(left)

Defect 2

Defect 3

☐ Intraband Tunneling

Effective mass of elec

Interface states parame

Defect 1 of p-CIGS / n-CdS interface

defect type	▲ ac
capture cross section electrons (cm²)	1.00
capture cross section holes (cm²)	1.00
energetic distribution	▲ un
energy level (from top of left VB) (eV)	0.60
characteristic energy (eV)	1.20
concentration left (1/cm^3 eV)	2.00

☐ Allow tunneling to traps

| Relative mass of electrons | 1.00 |
| Relative mass of holes | 1.00 |

accept   cancel