

SCAPS Version 2.9.02, March 2010

Add-on manual

This is not a stand-alone manual of SCAPS. It only describes the novelties in SCAPS 2.9 compared to SCAPS 2.8 and earlier. A (kind of) manual of the SCAPS programme is contained in another document. Also, there is a short and recommendable document `Getting Started.pdf`, which does exactly what it promises.

Enhancements of version 2.9.02, compared to version 2.8.06 and version 2.8.02

This is the first add-on manual since the distribution of version 2.8.02 (May 2009). In between several updates of version 2.8 have been distributed (2.8.03-2.8.06, August 2009-March 2010). The main enhancements included in these updates were the introduction of batch parameters from file, the 'stop at voc'-option and the introduction of 'the blue button'. The latter two enhancements will be discussed at the end of this document, the former will be discussed together with the further extensions of the batch facilities in version 2.9.02.

The most important new feature in SCAPS 2.9.02 is the introduction of multivalent defects. Next to this other features have been added to the recombination and to the batch facilities.

1. Multivalent defects

1.1 Principles

The principles of numerical simulation of solar cells with multivalent defects are presented in:

[1] K. Decock, S. Khelifi and M. Burgelman, *to be presented at E-MRS spring meeting 2010*, Strasbourg June 7-11, 2010.

Multivalent defects are present in a lot of material systems important for solar cells. Most often such a defect will have two defect levels, but also defects with more than two levels have been reported. In this version of SCAPS you can add up to four defect levels for each defect. The charge present on a defect can be varied from -3 to +3 elementary charges. Because the most common multivalent defects are double donors, double acceptors and amphoteric defects, special facilities for them are provided in SCAPS.

1.2 How to introduce/edit a multivalent defect

A multivalent defect can be added in the same way as any other defect. On the defect properties panel however there are now more possible choices of *defect type* (see Figure 1). Next to the *neutral*, *(single) donor* and *(single) acceptor* option available in SCAPS 2.8 and earlier, the user can also introduce a *double donor*, a *double acceptor*, an *amphoteric* defect or can define a custom made multivalent defect choosing *custom defined multilevel*.

When choosing one of these four new options the user is redirected to a new panel, the *multiple level defects properties panel* (see Figure 2). Some of the properties which were already available on the defect properties panel are available here as well, together with the properties which are specific for a multivalent defect. Starting from this panel the user can edit the defect and its levels.

Only when the defect type *custom defined multilevel* has been selected the user can add up to four different levels, otherwise the number of levels is restricted to two and the charge types are predefined. The *insert* buttons are used to add a specific level. In order to remove a level the user has to click on a level with the right button of the mouse.

The charge type and the energy of a level can immediately be accessed on the *multiple level defects properties panel*. The charge types MUST be introduced in an ascending way (level 1 the most positive charge), or all levels must be neutral. In most cases the most positive level will be situated the closest to the conduction band, a warning is given if the user defines her/his defect differently, but she/he is not obliged to do so.

The other defect properties of a level can be edited by double-clicking on the text-box belonging to each level. This opens a panel similar to the *defect properties panel*, however the properties which are not level specific but general to the entire defect are dimmed and can't be edited. The only properties which can be edited are the capture cross sections (for electrons and holes), the energy level and the IPV-properties (for electrons and holes).

Several features of the energetic distribution can also be accessed on the *multiple level defects properties panel*. The *energetic distribution*, the *reference for defect energy levels* and the *characteristic energy* are the same for all levels of one defect. More info about these properties can be found in the manuals of SCAPS 2.8 and earlier. If the checkbox *Use Correlation Energy* is checked, the energy difference between level 2 and level 1 is displayed in the window next to the checkbox. When the user edits this correlation energy the energy level of level 2 will be changed accordingly with respect to level 1.

The effect of the checkbox *Put all degeneracy factors equal one* will be explained in section 1.3.

When the user has finished editing the properties of the levels the *multiple level defects properties panel* can be quitted by the *return to the defect definition panel*-button. Then the *defect properties panel* is again displayed, but the level specific properties are no longer visible. It is a kind of survey of the defect. Now the changed to the defect can be saved using the *add/accept*-button or ignored using the *cancel*-button.

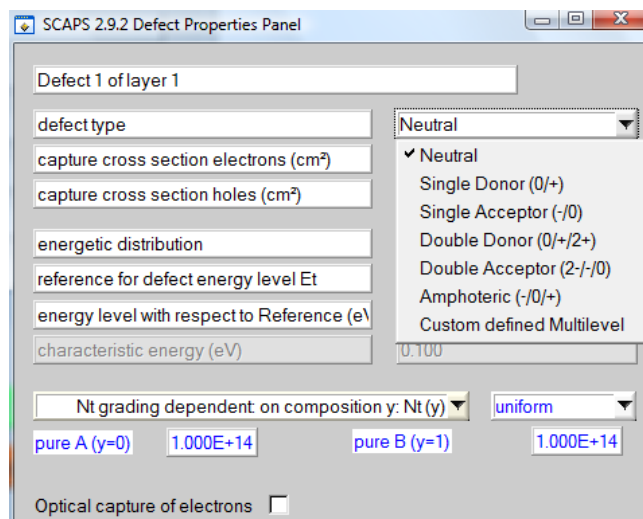


Figure 1 The definition of a multivalent defect: possible choices on the defect properties panel.

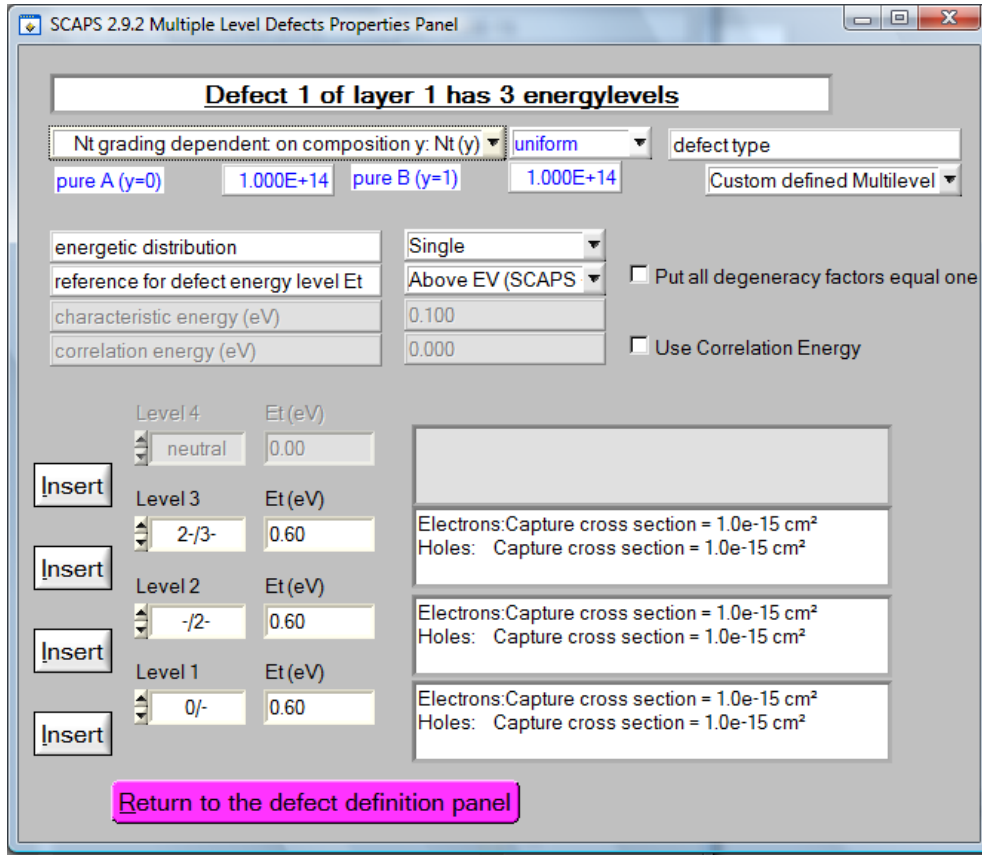


Figure 2 The multiple level defects properties panel. Only when the defect type is *Custom defined Multilevel*, the insert buttons and the properties of Level 3 and Level 4 are visible.

1.3 About degeneracy factors

In the calculation of the emission constants for a level of a multivalent defect degeneracy factors appear, see (1) where s is the number of the level. Usually they can be calculated as in (2) with H the total number of levels present, and this is the way they are calculated in SCAPS. In some cases a user might want to use other degeneracy factors, then she/he can put the values of all variables g_s equal to one. The introduction of new degeneracy factors can then be done by shifting the energy level E_s over an energy $kT \ln(g_{s-1}/g_s)$.

$$e_n^s = c_n^s \frac{g_{s-1}}{g_s} \exp\left(-\frac{E_C - E_s}{kT}\right) \quad (1)$$

$$e_p^s = c_p^s \frac{g_s}{g_{s-1}} \exp\left(-\frac{E_s - E_V}{kT}\right)$$

$$g_s = C_H^s = \frac{H!}{s!(H-s)!} \quad (2)$$

1.4 Compatibility with earlier SCAPS versions

As new features have been added, the format of the .def file has been changed, even if there isn't any multivalent defect present in the problem definition. The good news is that the new

format is both upward and downward compatible with the former format: versions 2.8 and earlier of SCAPS will correctly read the SCAPS 2.9 definition files, and SCAPS 2.9 will correctly read definition files generated by SCAPS 2.8 and earlier. Of course, the earlier SCAPS versions cannot handle all options present in the new problem definitions, but when such options are defined, they do something sensible with it.

If a multivalent defect is present in the definition file, earlier version of SCAPS will only read the parameters of “level 1” of this defect and ignore the parameters of the other levels. The nature of the defect is changed as well. Double donors and acceptors are changed in to donor and acceptors respectively. Amphoteric defects and custom defined multivalent defects are changed into neutral defects.

1.5 Energy band graph and Occupation probability graph

In SCAPS 2.8.6 and earlier only the electron occupation probability was displayed on the energy band panel and the generation panel. In SCAPS 2.9.2 it is possible to plot the hole occupation probability and the charge probability as well (See Figure 3).

In SCAPS 2.8.6 it was not necessary to make a distinction between the charge states of a defect and the defect type itself. An acceptor defect always has the charge type $-/0$. For multivalent defects this no longer holds, e.g. an amphoteric defect has two charge states: $-/0$ and $0/+$. Hence, from SCAPS 2.9.2 it is possible to choose between the defect type or the charge state to be displayed in the Energy band graph and in the occupation probability graph. In the Occupation probability graph the user can also choose to see the charge of the different levels instead (See Figure 3), right). When this option is chosen however, neutral defects can no longer be displayed. Also the electron/hole occupation option makes no sense in this case and is hidden.

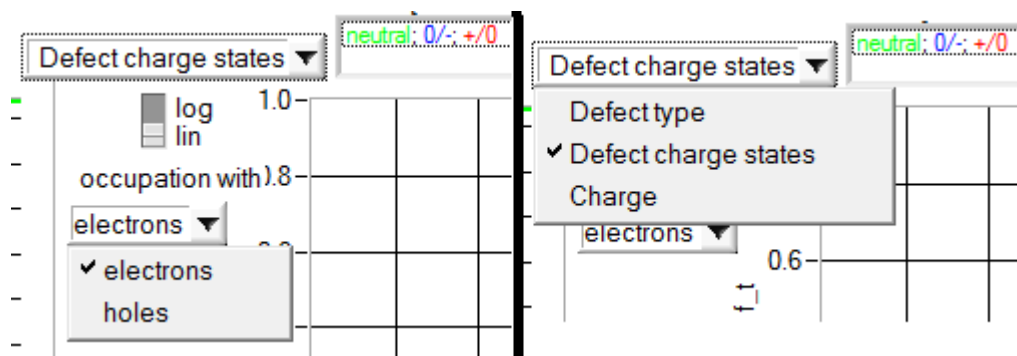


Figure 3 Left: Both electron and hole occupation can be displayed in the occupation probability graph. Right: Both defect type, charge state and charge can be displayed in the occupation probability graph.

2. Further extensions in SCAPS 2.9 concerning the recombination

On the numerical settings panel it is now possible to define the *number of discretization levels for distributed defects*. This value is not included in the problem definition file and should have a standard value of 7 when SCAPS is launched. In SCAPS 2.8.6 and earlier also 7 discretization levels are used, but they could not be user defined. As the occupation probability graph could get crowded, there exists a possibility to show only the main discretization levels in this graph when more than 7 levels are present.

From SCAPS 2.9.2 on radiative recombination and band to band auger recombination can be included. See Figure 4, which is taken from a screenshot of the layer definition panel.

Band to band recombination			
Radiative recombination coefficient (cm ³ /s)	0.000E+0	0.000E+0	uniform ▼
Auger hole capture coefficient (cm ⁶ /s)	0.000E+0	0.000E+0	uniform ▼
Auger hole capture coefficient (cm ⁶ /s)	0.000E+0	0.000E+0	uniform ▼

Figure 4 The definition of radiative and Auger recombination on the layer definition panel.

The purpose of the generation-recombination panel is to investigate the recombination processes in detail. The elaborate extensions of the recombination facilities in SCAPS 2.9.2 can't but have had some repercussions on this panel, see Figure 5.

eh generation

Total recombination

SRH

Radiative

Auger

Gross IPV Generation

Net IPV Generation

electron capture

electron emission

hole capture

hole emission

gross generation of holes (IPV)

gross generation of electrons (IPV)

p-layer

defect 1 [neutral]

level 1 [neutral]

n-layer

defect 1 [neutral]

level 1 [neutral]

Show

Structure

Conditions

Generation profile G(x)

Problem definition file:

Figure 5 New features on the Generation-Recombination panel

It is possible to display the *total recombination* rate, the recombination rate at defects (*SRH*), the *radiative* recombination rate and the *Auger* recombination rate.

A tree is made visible which indicates the cell structure and allows to hide the contribution of the different defect(level)s present in the structure. This tree is situated where in SCAPS 2.8.6 and earlier a drawing of the cell structure was present. In order to see this drawing again, there is a switch button: *Structure/Conditions*.

3. Further extensions in SCAPS 2.9 concerning the batch facilities

Extra options have been added to the batch facilities of SCAPS 2.9.2 with respect to 2.8.2 and earlier: It is now possible to get *batch parameter values from file* and entire *definition files can be used as a batch parameter*.

Next to the linear and logarithmic variation of batch parameter values it is now possible to take the parameter values from a file, a *.bdf*-file (*batch definition file*), see Figure 6. The layout of this file is rather tolerant. You just add the parameter values one below the other. All lines which can not be interpreted as only one number are ignored as being comment. We strongly recommend the user to add some comments to the file, so that she/he remembers what data are present in the file, even after not using it for a while. The *bdf*-file option has been available from SCAPS 2.8.4 on.

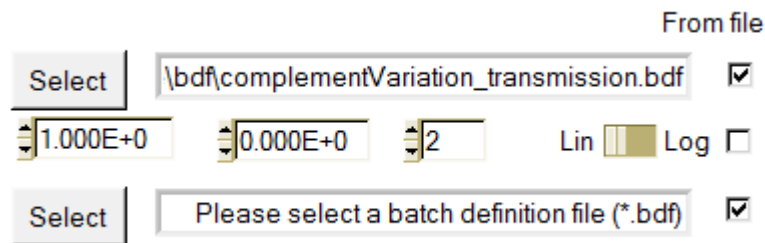


Figure 6 Selecting batch parameters from a file.

The number of batch parameters which can be varied in one batch run is limited to nine parameters. This is a practical limit imposed by the limited space on the Batch Set-up Panel. In order to allow the user to vary more than nine parameters it is possible to use entire definition files as a batch parameter, see Figure 7. The set of definition files can then be defined by clicking the *Define batch definition files*-button (which is only visible when the *Vary definition files*-checkbox is checked). Together with a variation of definition files no other parameters concerning the cell structure can be varied, only parameters concerning the ambient conditions (e.g. illumination, temperature...) can be varied together with definition files.

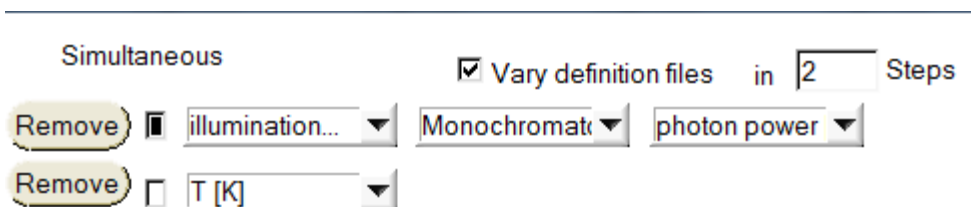


Figure 7 Using definition files as a batch parameter.

It is also possible to *print the batch panel* in order to remember your settings.

4. The recording of a batch

In SCAPS 2.8 the user can only see/save the *EB-panel*, *AC-panel* and *generation-recombination-panel* at the last calculated point. Additionally she/he had to extract the solar cell characteristics calculated in a batch from (a very large) .iv-file. This resulted in a lot of extra work to order the data when investigating the influence of a certain batch parameter. From SCAPS 2.9.2 on this can be done in a handsome way using the *record* facilities. (Almost) all properties which can be saved in one of the graph panels can be recorded as a function of the batch parameters.

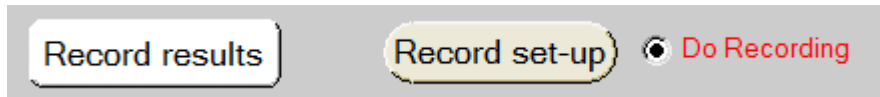


Figure 8 Detail of the action-panel: controls governing the record-facilities.

The list of properties to be recorded is made in the *Record Set-up*, see Figure 9. With the help of the five choice-menus (*type-property-layer-defect-level*) the user can chose a property and add it to the list on the left side of the panel using the *Insert* or *Replace* button. There are six types of properties to be recorded: *IV characteristics*, *General properties*, *Energy band panel*, *Generation panel*, *Occupations* and *AC panel*.

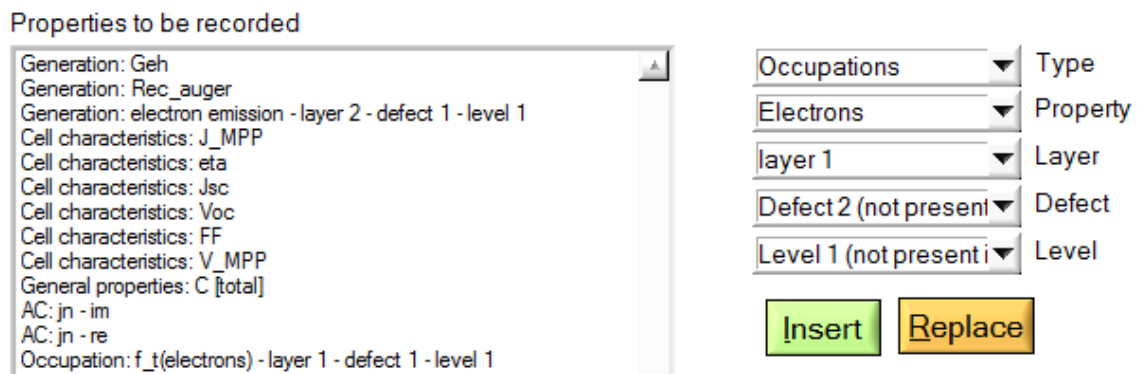


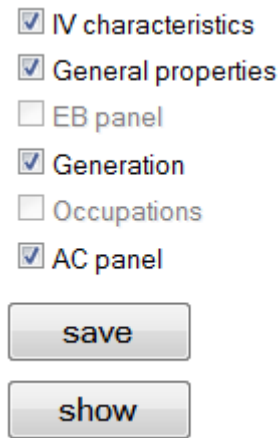
Figure 9 Setting the properties to be recorded. The list of properties to be recorded on the left. The input facility on the right.

To record a batch the *Do Recording* button should be checked when clicking the *Calculate* button. In this case the action list as it is set on the action panel will be ignored. SCAPS will determine which calculations need to be done in order to record the asked properties. For example when a property of the AC-panel is to be recorded SCAPS will perform a Cf-simulation at the frequency determined by the working point. When a cell characteristic is to be recorded an IV-simulation will be performed starting from 0V stopping at the open circuit voltage.

SCAPS doesn't a priori know the open circuit voltage. Hence it will perform an IV-simulation from 0V up to a predefined maximum voltage with the 'stop at Voc' option on. This predefined maximum voltage can be set on the numerical panel and has a standard value of 2.0V. The accuracy of the determination of the cell characteristics is determined by the increment voltage used in the IV-simulation. SCAPS uses the value which is present on the action panel unless it is larger than a predefined minimum value. This value can also be set on the numerical panel and has a standard value of 0.05V.

The results of a recording can be accessed through the *Record Results* button on the action panel. Recorded properties of the type *IV characteristics* or *General properties*, are immediately plot as a function of one of the batch parameters. Record properties of the other types are plot as a

function of the distance in the cell. The results can also be saved to a file, see Figure 10. For each type of property type a different file is saved. The user can chose which files are to be made using the checkboxes seen in Figure 10. The *show* option has the same meaning as everywhere in SCAPS. But as not all property types can be showed in one window, only the last one (= the lowest checkbox checked on Figure 10) will be showed.



The image shows a vertical list of six checkboxes with corresponding text labels to their right. From top to bottom, the items are: a checked checkbox followed by 'IV characteristics', a checked checkbox followed by 'General properties', an unchecked checkbox followed by 'EB panel', a checked checkbox followed by 'Generation', an unchecked checkbox followed by 'Occupations', and a checked checkbox followed by 'AC panel'. Below this list are two rectangular buttons with rounded corners. The top button is labeled 'save' and the bottom button is labeled 'show'. Both buttons have a light gray background and a thin border.

Figure 10 Saving record results. Only checked property types will be saved.

5. The blue button (available in SCAPS 2.8.5 and later)

In SCAPS 2.8.4 and earlier, it happened that a panel requiring input was hidden under other panels, and difficult to find; it could also happen that such panel disappeared, which caused a hang-up of the programme. These problems have been fixed now. There are some limitations to the number and kind of panels that can be opened or operated simultaneously. Above all, the F1 key acts as an emergency button that brings the cell definition panel on top; on that panel, you find a new **blue button** that displays a nicely structured list of all input panels currently open, and that allows you to navigate between them (or to quit all input at once).

6. Problem definition files distributed with SCAPS 2.9.2

The new facilities implemented in SCAPS 2.9 have made this program more powerful, but also more complicated. We therefore offer more problem definition files to illustrate the new features, and run quickly through them here. All problem definition files accompanying the distribution of SCAPS 2.8 format are redistributed, more info about them is available in the add-on manual of SCAPS 2.8. These problem definition files are:

- `Example CIGS SCAPS28.def` and `Example CdTe SCAPS28.def`: the same files as distributed with all earlier versions, but now saved in SCAPS 2.8 format.
- `CdTe-base.def`, based on the work of Gloeckler and Sites, Osaka World PV Conference 2003.
- `Numos Exercise 1.def`, `Numos Exercise 2.def` and `Numos GIGS baseline.def`: These files were distributed after the NUMOS Workshop, Gent, march 2007.
- `linear single layer N(x).def`, `linear single layer N(y).def`, `linear two layers.def`: (New) files, that illustrate three ways to implement a linearly graded diode. There is ample of information in the comment section of these .def files.

- `single_layer_N(x).def` and `single_layer_N(y).def`: (New) files, that represent two ways to implement an exponentially graded front region in a uniform base layer. There is ample of information in the comment section of these `.def` files.
- `Symmetric_graded.def` and `graded_pseudo_CIGS-ZnOS.def`: These files illustrate several grading features of SCAPS 2.8. There is ample of information in the comment section of these `.def` files.
- `IPV.def`: This problem does not simulate any real or realistic solar cell, it is just set up to illustrate the Impurity Photovoltaic Effect (IPV) in SCAPS. There is ample of information in the comment section of this `.def` file. A result obtained with this file is shown in the add-on manual of SCAPS 2.8.
- `Intraband_tunnelling.def`: This problem does not simulate any real or realistic solar cell, it is just set up to illustrate the facility of intra-band tunneling in SCAPS. There is ample of information in the comment section of this `.def` file. A result obtained with this file is shown the add-on manual of SCAPS 2.8.

Three additional `.def`-files are distributed together with SCAPS 2.9.

These files are:

- `Pin_a-Si.def`: This problem can be used as a starting point for a pin-a-Si:H diode. The structure is roughly based upon R.E.I. Schropp and M. Zeman, Amorphous and microcrystalline silicon solar cells: Modeling, Materials and Device Technology, Kluwer, Boston, 1998, pp183. *Watch out!!* The parameters used are not standard settings for a a-Si:H thin film solar cell, they only serve as a starting point.
- `DoubleDonorAcceptor.def`: This problem illustrates the set-up of double donors and acceptors, together with the use of the correlation energy.
- `MultivalentDefect.def`: This problem illustrates the set-up of a custom defined multivalent defect and the use of the 'Put all degeneracy factors equal one'-button.

And now sit back, relax and enjoy the new features of SCAPS .

As SCAPS is evolving continuously it is possible that we forgot to describe several (new) features, this should however not restrain you from using them.

Questions, remarks, identification of bugs or errors, comments... are always welcome.

Koen Decock and Marc Burgelman

University of Gent

Dept. Electronics and Information Systems (ELIS)

St-Pietersnieuwstraat 41

B-9000 Gent, Belgium.

Marc.Burgelman@elis.ugent.be

Koen.Decock@elis.ugent.be