# Models for the optical absorption $\alpha(\lambda)$ of materials in SCAPS

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### 1. Introduction

The SCAPS application discussed in this document uses:

• SCAPS version 3.3.07 of January 2018, or more recent.

## 2. The traditional model of optical model in $SCAPS \le 3.3.06$

Absorption model	Show / Set alpha(com	position; lambda)		
	alpha (y=0)	alpha (y=1)		
	from model from file	│ from model from file		
absorption constant A (1/cm eV^(1/2))	1.000E+5	1.000E+5 0.000E+0		
absorption constant B (eV^(1/2)/cm)	0.000E+0			
		\CIGS x=0.31 Paulson.abs		
save	absorption file for y = 0	absorption file for y = 1		

Fig. 1 The optical absorption block in the Layer Properties Panel in the 'traditional' SCAPS versions ( $\leq 3.3.06$ ). For the 'pure A material', absorption 'from model' is set, and the traditional model parameters *A* and *B* are shown. For the pure B material', absorption 'from file' is set, and the full path of the absorption file is (partially...) shown.

Fig. 1 shows the optical absorption block in the Layer Properties Panel in the 'traditional' SCAPS versions ( $\leq 3.3.06$ ). For both materials constituting a graded layer'A<sub>1-y</sub>B<sub>y</sub>, this in the 'pure A material' (y = 0) and in the 'pure B material' (y = 1), the optical absorption  $\alpha(\lambda)$  can be either read from a file, or set by a model. The traditional SCAPS model was:

$$\alpha(h\nu) = \left(A + \frac{B}{h\nu}\right)\sqrt{h\nu - E_g} \quad , A \text{ in } eV^{-1/2} \text{ cm}^{-1} \text{ and } B \text{ in } eV^{+1/2} \text{ cm}^{-1}$$
(1)

where hv is the photon energy and  $E_g$  the band gap; A and B are the model parameters. This simple square root law however is very unsatisfactory for most materials, as is illustrated in Fig. 2 for Si and in Fig. 3 for CIGS. We must conclude that the traditional SCAPS model for  $\alpha(\lambda)$  is really to coarse for real materials.



Fig. 2 The optical absorption  $\alpha$  of Si. Left: as a function of wavelength  $\alpha(\lambda)$ . Right: as a function of photon energy  $\alpha(h\nu)$ . Black symbols: the realistic  $\alpha$  values from the SCAPS absorption file Si. abs. Red solid line: the traditional SCAPS model of Eq. (1) with  $A = 5 \times 10^3 \text{ eV}^{-1/2} \text{ cm}^{-1}$ , B = 0.



Fig. 3 The optical absorption  $\alpha$  of CIGS of composition CuIn<sub>0.6</sub>Ga<sub>0.4</sub>Se<sub>2</sub>. Left: as a function of wavelength  $\alpha(\lambda)$ . Right: as a function of photon energy  $\alpha(h\nu)$ . Black symbols: the realistic  $\alpha$  values from the SCAPS absorption file CIGS Malmström.abs. Red solid line: the traditional SCAPS model of Eq. (1) with  $A = 6.7 \times 10^4 \text{ eV}^{-1/2} \text{ cm}^{-1}$ , B = 0.

We could hope to improve the model by replacing the square root in (1) with a power law with a general exponent n:

$$\alpha(h\nu) = \left(A' + \frac{B'}{h\nu}\right) \cdot \left(h\nu - E_g\right)^n \tag{2}$$

However, we would never write a physical law like this: the dimensions of the parameters A' and B' vary with the value of the exponent n, and that is really ugly. Instead we would write Eq. (2) as:

$$\alpha(h\nu) = \left(\alpha_1 + \beta_1 \frac{E_{g1}}{h\nu}\right) \cdot \left(\frac{h\nu}{E_{g1}} - 1\right)^n \quad , \alpha_1 \text{ and } \beta_1 \text{ in } \text{cm}^{-1}$$
(3)

Here the model parameters  $\alpha_1$  and  $\beta_1$  have the dimension of absorption constant (1/cm or 1/m) regardless of the value of the exponent *n*.

Before extending the SCAPS model for optical absorption, let us shortly look up the standard theories.

#### 3. Standard theory on the optical absorption constant $\alpha$

#### **3.1** Tauc laws – power laws

Semi-empirical theory on the optical absorption  $\alpha$  proposes to make a 'Tauc plot' of  $\alpha h v$  *versus* photon energy hv in the form

$$\left[\alpha(h\nu) \times h\nu\right]_{n}^{1} \quad versus \quad h\nu \quad \text{Tauc plot} \tag{4}$$

If the plot shows a straight line for high  $h\nu$ , the intercept with the horizontal  $h\nu$ -axis is the band gap energy  $E_g$ . This implies an absorption law  $\alpha(h\nu)$ :

$$\alpha(h\nu) = \beta_0 \frac{E_g}{h\nu} \left(\frac{h\nu}{E_g} - 1\right)^n \tag{5}$$

There are examples in the literature of authors that simplify the Tauc plot a little bit, and just plot  $\alpha^{1/n}$  versus  $h\nu$  (instead of  $(\alpha h\nu)^{1/n}$ ), implying a  $\alpha(h\nu)$  law of the form:

Tauc plot 
$$\left[\alpha(h\nu)\right]^{\frac{1}{n}}$$
 vs.  $h\nu \leftrightarrow \alpha(h\nu) = \alpha_0 \left(\frac{h\nu}{E_g} - 1\right)^n$  (6)

To serve everyone, the new SCAPS absorption model will include the two laws lumped in one absorption law of the form

$$\alpha(h\nu) = \left(\alpha_i + \beta_i \frac{E_{g1}}{h\nu}\right) \left(\frac{h\nu}{E_{gi}} - 1\right)^{n_i} \text{ SCAPS models "power1" } (i=1) \text{ and "power2" } (i=2) (7)$$

The simple square root law of Eq.(1) (traditional SCAPS) corresponds to the power law Eq. (7) with exponent  $n = \frac{1}{2}$ . This law will also be included in the new SCAPS absorption model in the form of

$$\alpha(h\nu) = \left(\alpha_0 + \beta_0 \frac{E_g}{h\nu}\right) \sqrt{\frac{h\nu}{E_g} - 1} \quad \text{SCAPS model "Eg-sqrt"}$$
(8)

The model constants  $\alpha_0$  and  $\beta_0$  have the dimension of absorption constant (e.g. 1/cm) and are related to the traditional model constants *A* and *B* by

$$\alpha_0 = A\sqrt{E_g} \qquad A = \frac{\alpha_0}{\sqrt{E_g}}$$

$$\beta_0 = \frac{B}{\sqrt{E_g}} \qquad B = \beta_0 \sqrt{E_g}$$
(9)

The Tauc models Eq. (5) and generalised Tauc models Eq. (7) have a physical meaning: they are related to a property of the energy band diagram E(k) of the semiconductor (direct or indirect band gap) and to the nature of the excitation of a valence band electron to the conduction band upon absorption of a photon (allowed or forbidden transition). Text books (and also Wiki) list the values of the exponent *n* that are valid for the various excitation mechanisms, see Table 1.

Table 1 The Tauc exponent n for the various physical excitation mechanisms.

excitation mechanism	exponent n
direct bandgap, allowed transition	1/2
direct band gap, forbidden transition	3/2
indirect band gap, allowed transition	2
indirect band gap, forbidden transition	3

#### 3.2 Sub-band gap mechanism

All the power laws of the preceding sections, including the simple square root law, have in common that the absorption constant  $\alpha$  drops to rigorously zero when the photon energy is lower than the band gap energy  $E_g$ . This is illustrated in the abrupt behaviour of  $\alpha(h\nu)$  around the band gap energy  $E_g$ , or of  $\alpha(\lambda)$  around the cut-off wavelength  $\lambda_g$  in Fig. 2 and Fig. 3. Note that  $h\nu$  and  $\lambda$ , and thus also  $E_g$  and  $\lambda_g$  are related by the simple equation

$$hv = \frac{1240 \text{ nm.eV}}{\lambda} , \quad \lambda = \frac{1240 \text{ nm.eV}}{hv}$$

$$E_g = \frac{1240 \text{ nm.eV}}{\lambda_g} , \quad \lambda_g = \frac{1240 \text{ nm.eV}}{E_g}$$
(10)

(the numerical factor 1240 nm.eV equals hc, thus Planck's constant  $\times$  velocity of light, expressed in convenient units; SCAPS uses 1239.997 nm.eV O).

Instead, real materials can show considerable sub-band gap absorption, that is often taking the form of a decreasing straight line in a  $log(\alpha)$ - $h\nu$  diagram for  $h\nu < E_g$ . This behaviour can occur in materials with poor crystallinity when there are localised states in the conduction and valence bands, extending in the band gap; then the sub-band gap part of the optical absorption is described by an 'Urbach tail'. Also phonon-assisted absorption of photons can give rise to sub-band gap absorption with a similar 'tail behaviour'. Whatever the physical origin, we will describe the sub-bandgap absorption as

$$\alpha_{\text{sub-band gap}}(h\nu) \approx \exp\left(-\frac{E_g - h\nu}{E_0}\right), \quad h\nu < E_g$$
(11)

The parameter is  $E_0$  is the tail energy.

#### **3.3** Components of the new SCAPS model for optical absorption

So, we have hope to describe real materials better when we use a combination of power laws with the sub-band gap law. In the SCAPS  $\geq$  3.3.07 model for optical absorption we offer the possibility to add a few more sub-models or model components. In section 4 below, it is explained how all this is arranged in the new user interface. The full SCAPS  $\geq$  3.3.07 model is described by:

$$\alpha(hv) = (+) \quad \alpha_{bg} \qquad \text{back ground constant } \alpha$$

$$(+) \quad \alpha_c \cdot u(hv - E_g) \qquad E_g \text{-step} \qquad \alpha_c \text{ if } hv > E_g, 0 \text{ if } hv < E_g$$

$$(+) \quad \left(\alpha_0 + \beta_0 \frac{E_g}{hv}\right) \sqrt{\frac{hv}{E_g} - 1} \qquad E_g \text{-sqrt} \qquad \text{and } 0 \text{ if } hv < E_g$$

$$(+) \quad \left(\alpha_1 + \beta_1 \frac{E_{g1}}{hv}\right) \left(\frac{hv}{E_{g1}} - 1\right)^{n_1} \qquad \text{power1} \qquad \text{and } 0 \text{ if } hv < E_{g1} \qquad (12)$$

$$(+) \quad \left(\alpha_2 + \beta_2 \frac{E_{g2}}{hv}\right) \left(\frac{hv}{E_{g2}} - 1\right)^{n_2} \qquad \text{power2} \qquad \text{and } 0 \text{ if } hv < E_{g2}$$

$$(+) \quad \approx \exp\left(-\frac{E_g - hv}{E_0}\right) \qquad \text{sub-bandgap "glued to other mechanisms"}$$

Here (+) means that the sub-model can be omitted or can be added by the user to the total  $\alpha(h\nu)$  in the SCAPS user interface. The names 'back ground', 'E<sub>g</sub>-step'... are the sub-model names that are used by SCAPS. A few remarks should be made:

- There should always be at least one absorption sub-model active. When the user tries to unclick all sub-models in the SCAPS user interface (see below), the back ground model will be forced to be present.
- The model 'Eg-step' is there mainly to please theoreticians. It delivers a constant absorption constant  $\alpha_c$  'above the band gap', thus  $h\nu > E_g$  or  $\lambda < \lambda_g$ , and zero  $\alpha$  'below the band gap'. The band gap is always the band gap  $E_g$  that was input as one of the electronic properties of the material/layer. Hence it will also be varied when  $E_g$  is varied as a batch parameter, or in the script.
- The 'Eg-sqrt' model is the only model that was implemented in traditional SCAPS  $\leq$  3.3.06. In the new SCAPS  $\geq$  3.3.07, this model can be active or not, as the user decides. The user interface shows the model parameters  $\alpha_0$  and  $\beta_0$  also in their traditional form *A* and *B*. The band gap is always the band gap  $E_g$  that was input as one of the electronic properties of the material/layer. Hence it will also be varied when  $E_g$  is varied as a batch parameter, or in the script.

- The two power models 'power1' and 'power2' allow much versatility in modelling the  $\alpha(h\nu)$  or  $\alpha(\lambda)$  behaviour of a layer/material. There are 4 parameters per 'power model':  $\alpha_1$ ,  $\beta_1$ ,  $E_{g1}$  and  $n_1$  (and alike for power 2, with index 2). In the user interface panel,  $\lambda_{g1}$  is given as an alternative parameter for  $E_{g1}$ : change one of the two, and the other will be adapted in the user interface, according to Eq. (11).
- Important note on the meaning of the band gap parameters  $E_{g1}$  and  $E_{g2}$ :
  - When  $E_{g1}$  (or  $E_{g2}$ ) are positive, they should be understood as a fixed parameter: they are not related to the actual band gap  $E_g$  of the layer/material. In particular, this means that also when  $E_g$  is varied (batch or script), the parameter  $E_{g1}$  (or  $E_{g2}$ ) keeps its fixed value.
  - When  $E_{g1}$  (or  $E_{g2}$ ) are input as a negative number, they should be understood as a 'relative band gap', or a multiple of the actual  $E_g$ : their value is substituted internally with  $|E_{g1}| \times E_g$ . When  $E_g$  is varied then (batch or script), the internal parameters  $E_{g1}$  (or  $E_{g2}$ ) are varied with it.
  - Example: take a layer/material with band gap  $E_g = 1.2$  eV. When setting  $E_{g1} = 1.5$ , the internal  $E_{g1}$  parameter will always be 1.5 eV, regardless of the changes made to  $E_g$ . But when the input was  $E_{g1} = -1.5$ , the internal  $E_{g1}$  value is set to  $1.5 \times 1.2$  eV = 1.8 eV; and when one would vary  $E_g$  in a batch calculation from 1 eV to 2 eV, the internal  $E_{g1}$  would vary from 1.5 eV to 3.0 eV.
- The sub-bandgap tail mechanism is (of course) only available when the user has checked at least one of the 4 'band gap mechanisms' Eg-step, Eg-sqrt, power1 and power2.
- The proportionality constant in Eq. (11) is chosen in such a way that the sub-band gap tail is 'smoothly glued' to the  $\alpha(h\nu)$  or  $\alpha(\lambda)$  curve of all other mechanisms.
- The Eg-sqrt mechanism of the new SCAPS works with the model parameters  $\alpha_0$  and  $\beta_0$ , not with *A* and *B*. However, traditional SCAPS definition files will be read and the (*A*, *B*)  $\rightarrow$  ( $\alpha_0$ ,  $\beta_0$ ) conversion of Eq. (9) will be done automatically.
- When the Eg-sqrt model is the only 'band gap model' present, the new SCAPS  $\geq 3.3.07$  will also output the (*A*, *B*) parameters, and the new definition files will be read and treated correctly by traditional SCAPS versions.
- Also when other band gap models (than the Eg-sqrt model) are present, the new SCAPS versions will output some 'best' (*A*, *B*) values. Traditional SCAPS versions will run with these new definition files, but of course will not give exactly the same result as the new SCAPS versions, since they do not have the Eg-step, power1 or power2 models.

# 4. The SCAPS user interface for absorption models

# 4.1 The optical absorption block

The optical absorption block in the Layer Properties Panel has been changed in the new SCAPS  $\geq 3.3.07$ , see Fig. 4. When the optical absorption of a material/layer is set to 'from model', the 'set absorption model' button is active; upon clicking, the Absorption Model Panel opens (Fig. 5). This panel is operating much like the grading panel and the (spectrum or generation) model panel, that are perhaps familiar to the SCAPS user.



Fig. 4 The optical absorption block in the Layer Properties Panel in the new SCAPS versions ( $\geq 3.3.07$ ). For the 'pure A material', absorption 'from model' is set, and a summary of the absorption models present is shown. For the pure B material', absorption 'from file' is set, and the full path of the absorption file is shown.



Fig. 5 The Absorption Model Panel of  $SCAPS \ge 3.3.07$ .

# 4.2 Description of the Absorption Model Panel:

• The title displays the layer name, here 'n-layer', and the actual value of the band gap  $E_g$ , here 1.200 eV.

- The 6 SCAPS absorption models 'back ground'... to 'sub-Eg tail' are displayed in a line below the graph. Each sub-model can be clicked on or off. The button with the sub-model name is only active when the sub-model is checked; upon clicking such button (here the 'power2' button was clicked), this button is highlighted in light blue, and the sub-model parameters (α<sub>2</sub>, β<sub>2</sub>, *E<sub>g2</sub>*, *n<sub>2</sub>*) are displayed and can be edited. Some parameters have an 'alternative form'; this can be merely another unit (α<sub>2</sub> and β<sub>2</sub>, in 1/cm or 1/m), or another informative form of the parameter (*E<sub>g2</sub>* or λ<sub>g2</sub>). (These are 'alternative facts' that are true © ).
- Upon changing a parameter value (or value of an alternative parameter), a new  $\alpha(\lambda)$  or  $\alpha(h\nu)$  curve is calculated and added to the graph. When it starts to look too messy, you can clear all graphs or all but the last calculated one.
- You can select two abscissa (horizontal axis) variables (wavelength  $\lambda$  or photon energy hv) and two ordinate (vertical axis) values (just  $\alpha$ , either in 1/cm or in 1/m). When change the abscissa or ordinate selection, all graphs but the last graph are lost.
- You can also show the  $\alpha(\lambda)$  or  $\alpha(hv)$  data contained in a SCAPS absorption file; once a file selected, you can show or hide the file data with a toggle button. <u>Remark:</u> showing file data does <u>not</u> change the absorption mode from 'from model' to 'from file'! This mode remains 'from model', but at least you can compare your model try-outs with real data.
- <u>Tip</u>: this is also a great way to look to an absorption file when setting up a SCAPS model: immediately you see what it is like!
- The number of mesh points (λ values or hν values) in the top right part of the panel of Fig. 5, is only relevant for this panel. In calculations, SCAPS decides the λ-values at which to evaluate α(λ), the generation G(x, λ),... based on the calculation settings ordered by the user: e.g. λ values in the spectrum file, λ values at which QE(λ) are ordered,...
- Of course all other familiar SCAPS facilities are there: linear/logarithmic view with only one click, saving the graph in some graphical format (great for presentations and reports usually the graphical quality is not good enough for decent publications), showing the data (and copy/paste them e.g. in Excel).

### 4.3 Examples of optical absorption models

### 4.3.1 Crystalline silicon



Fig. 6 The optical absorption of crystalline silicon, from the SCAPS absorption file Si (Green).abs (black symbols). The SCAPS model (red line) is for: power1 with  $\alpha_1=7\times10^3$ /cm,  $\beta_1=0$ ,  $E_{g1} = 1.12$  eV,  $n_1 = 2.0$  and power2 with  $\alpha_2=3\times10^5$ /cm,  $\beta_2=0$ ,  $E_{21} = 2.40$  eV,  $n_2 = 1.5$  and a sub-bandgap tail with  $E_0 = 30$  meV. The agreement is good for 400 nm <  $\lambda$  < 1150 nm or 3.1 eV > hv > 1.1 eV.

### 4.3.2 Copper indium selenide CIGS of composition CuIn<sub>0.6</sub>Ga<sub>0.4</sub>Se<sub>2</sub>



Fig. 7 The optical absorption of crystalline silicon, from the SCAPS absorption file CIGS Malmström.abs (black symbols). The SCAPS model (red line) is for: power1 with  $\beta_1=1.8\times10^5$ /cm,  $\alpha_1=0$ ,  $E_{g1}=1.10$  eV,  $n_1=1.5$  and power2 with  $\beta_2=1\times10^6$ cm,  $\alpha_2=0$ ,  $E_{21}=2.40$  eV,  $n_2=1.5$  and a sub-bandgap tail with  $E_0 = 10$  meV. Again the agreement is good for  $\lambda > 400$  nm or  $h\nu < 3.1$  eV; in the long wavelengths region  $\lambda > 1100$  nm or  $h\nu < 1.05$  eV the agreement is less good, but this is not so important because the low  $\alpha$  value ( $\alpha < 10^2$ /cm) in this range.

### 4.3.3 Also look to the View Grading panel!

We took the occasion to add an 'optical absorption button' to the View Grading Panel (green button in the Layer Properties Panel, available when at least one calculation was done -a work point calculation (light; V = 0) is enough).



optical absorption constant in the middle of the layers

Fig. 8 Absorption constant  $\alpha(\lambda)$  shown in the View Grading Panel, after at least one calculation.

The data in this panel are drawn from the actual parameter values used in the SCAPS calculation. In particular, you can see

- the absorption constants  $\alpha(\lambda)$  or  $\alpha(h\nu)$  of all layers together in one graph
- $\circ$  the  $\alpha$  values apply to the middle of each layer (important if the layers were graded, otherwise not)
- o the α values are shown at the actual set of  $\lambda$  values used in the calculation: this is different from the Absorption Model Panel, where some  $\lambda_{min}$  and  $\lambda_{max}$  are determined and *n* points (by default *n* = 101) are placed in between. You will notice that SCAPS uses 2 wavelengths in a calculation in dark, at 200 nm and at 5000 nm (this is a relic from vey ancient SCAPS times!), giving rise to ugly graphs (a straight line through 2 points...). In the View Grading Graph, the actual set of  $\lambda$  values in the calculation is used. Typically these are the wavelengths of the spectrum file.
- In this graph you can see how SCAPS used interpolation and extrapolation (the case for  $\alpha$  from file, or always (from file and from model) if a layer is graded).
- $\circ$  and you can see the points of the  $\lambda$ -grid, and see whether it is fine enough or too coarse for your simulation.

### 5. SCAPS simulation examples

## 5.1 Setting up a batch or a script for the absorption models

All absorption models and all parameters of them can be set as a batch parameter to be varied, see for example Fig. 9.

💽 sc	CAPS 3.3.07 Batch Set-up Panel				<b>1</b>	- • ×
Rem Ad	Vary definition files           Iayer 1 (L1)         Absorption mode          power law 1         export	onent n1 🚽	From 0.500	To €2.000	Steps	Custom list Lin 🛄 Log 🗖

Fig. 9 Example of a batch parameter setting of an absorption model, The 'power1' model is set to be present (all other models remain present or absent as was set previously by the user interface or script). The model parameter  $n_1$  will be varied over the values 0.5, 1.0, 1.5 and 2.0.

All absorption models parameters are also supported by the SCAPS script facility. The script commands should be more or less self explaining, we hope. Examples are:

```
set layer1.absorptionmodelA.egsqrt.off
set layer1.absorptionmodelA.power1.on
set layer1.absorptionmodelA.power1.exponent1 1.5
```

The SCAPS user Manual will be updated with the new script commands, I hope soon. All new script commands are already supported by the SCAPS script editor, that is already quite something. Equipped with those tools (batch, script), we are now ready to present a few simulation examples.

# 5.2 Influence of the exponent *n* of a 'power model' on the quantum efficiency $QE(\lambda)$

We take the definition file simple pn.def from the standard SCAPS installation, and in the *n*-layer we change  $E_g$  from 1.2 eV to 3.0 eV, and *d* from 0.5 µm to 0.1 µm: when illuminated from the *n*-side, we have then a window/absorber structure. The absorption in the *p*-layer is set to 'model', we check the power1 model and we uncheck the Eg-sqrt model (and any other sub-models). The exponent  $n_1$  of the power model is varied with the batch set-up as in Fig. 9.

The resulting  $\alpha(\lambda)$  and  $\alpha(h\nu)$  of the *p*-layer is shown in Fig. 10, and the result of a *QE* calculation is shown in Fig. 11, once as a function of wavelength, and once as a function of photon energy.



Fig. 10 Optical absorption in the *p*-layer with  $E_g = 1.2$  eV, with only the power1 absorption model present. The exponent  $n_1$  is varied from  $n_1 = 0.5$  (red curve) over  $n_1 = 1.0$  and  $n_1 = 1.5$  to  $n_1 = 2.0$  (cyan curve). Left: as a function of wavelength  $\alpha(\lambda)$ . Right: as a function of photon energy  $\alpha(hv)$ .



Fig. 11 Quantum efficiency QE of the problem of section 5.2, with absorption in then-layer as in Fig. 10, with the same color code. Left: as a function of wavelength  $QE(\lambda)$ . Right: as a function of photon energy QE(hv).

We conclude that the exponent of the power law has the effect of 'smoothing' the *QE* in the long wavelength range, but still 'above the band gap' (that is, still for  $\lambda < \lambda_g$  or  $hv > E_g$ ). The user can check that lowering the diffusion length in the *n*-material (e.g. by increasing the defect density) has a similar effect. Remember that the difference between e.g.  $n_1 = 0.5$  and  $n_1 = 1.5$  can be a consequence of a difference in physics: both values apply to a direct band gap material, but  $n_1 = 0.5$  for an allowed transition and  $n_1 = 1.5$  for a forbidden transition, see Table 1. The difference between the simulated/measured  $QE(\lambda)$  is striking (at least in this example).

### 5.3 Influence of the sub-band gap tail energy $E_0$ on the quantum efficiency QE( $\lambda$ )

We take the same modified simple pn.def file. In the *p*-layer we set only the power1 model with  $n_1 = 1.0$  (corresponding to the blue curve in Fig. 10), and we add sub-band gap absorption with tail energy  $E_0$ . In the batch set-up, we let vary  $E_0$  from 10 meV to 300 meV (series of values, in meV: 10, 20, 30, 40, 50, 70, 100, 150, 200, 300).



Fig. 12 The problem described in section 5.3. Absorption models in the *p*-layer: power1with  $n_1 = 1.0$ , and sub-band gap with varying  $E_0$ : from  $E_0 = 10$  meV (red) to  $E_0 = 300$  meV (blue-green). Left: the optical absorption  $\alpha(h\nu)$ . Right: the quantum efficiency  $QE(\lambda)$  in dark.

We conclude that the sub-band gap tail energy  $E_0$  has the effect of 'smoothing' the QE in the long wavelength range, but 'under the band gap' (that is, still for  $\lambda > \lambda_g$  or  $h\nu < E_g$ ).

### 6. SCAPS models for optical absorption: summary

- The new SCAPS models for optical absorption allow for a much more realistic modeling of  $\alpha(h\nu)$  when measured data or reliable literature data are not available.
- It can be questioned however what the advantage would be of finding and inputting up to 12 model parameters, when one just could input a file name: a reliable  $\alpha(\lambda)$  file is to be preferred in all cases!
- A real advantage is that one can very easily visualise, and thus better judge, the  $\alpha(\lambda)$  behaviour of a particular model and even of a particular  $\alpha(\lambda)$  input file.
- Another advantage of the new SCAPS version is that the  $\alpha(\lambda)$  or  $\alpha(h\nu)$  behaviour of all layers can be displayed together after calculation, exactly as they were used in the calculation.