kSEMAWc software

Functions for the complex refractive index modeling

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Basic relations among $\tilde{n}$, $\tilde{\chi}$, $\tilde{\epsilon}$

The theories for the light-matter interaction give the simplest expression for the complex dielectric susceptibility $\tilde{\chi} = \chi_1 - \mathrm{i}\,\chi_2$.

Refractive index, dielectric susceptibility and permittivity $\tilde{\epsilon} = \epsilon_1 - \mathrm{i}\,\epsilon_2$ are connected by the following simple equations:

$$\tilde{\epsilon} = (n - ik)^2 = 1 + \tilde{\chi}.$$

Therefore:

$$\epsilon_1 = 1 + \chi_1, \qquad \epsilon_2 = \chi_2.$$

and:

$$n = \frac{1}{\sqrt{2}}\sqrt{\sqrt{\epsilon_1^2 + \epsilon_2^2} + \epsilon_1}, \qquad k = \frac{1}{\sqrt{2}}\sqrt{\sqrt{\epsilon_1^2 + \epsilon_2^2} - \epsilon_1}.$$

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Oscillator normalization

Inside kSEMAWc $\tilde{\epsilon}$ is calculated as a sum of "oscillators" $\tilde{\chi}_i$ corresponding to different groups of electronic transitions:

$$\tilde{\epsilon} = 1 + \sum_i \tilde{\chi}_i = 1 + \sum_i C_i \tilde{f}_i$$

Sum rule on χ_2:

$$\int_0^\infty \chi_2(E) E dE = \frac{\pi(\hbar q)^2 N}{2\epsilon_0 m_e} = \frac{N(cm^{-3})}{4.61706 \cdot 10^{20}} eV^2$$

where N is electron number per unit volume of the material (all of them, including the core electrons), q is the electron charge and m_e is the electron mass.

As far as possible, the oscillator functions $\tilde{f}_i$ in kSEMAWc are normalized according to:

$$\int_0^\infty Im(\tilde{f}_i(E)) E dE = 1$$

"ideal global fit $(0 < E < \infty)$" $\Longrightarrow$ $\sum_i C_i = \frac{\pi(\hbar q)^2 N}{2\epsilon_0 m_e}$

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The Flat Oscillator

Generally the fit is limited to energies lower than a few eV.
Transitions at higher energies, not explicitly included in the oscillator sum, give anyway a substantial contribute to ϵ_1.
To simplify the fit, the 1 is replaced with a user-selectable parameter C^2_{flat}:

$$\tilde{\epsilon} = C^2_{flat} + \sum_i \tilde{\chi}_i = C^2_{flat} + \sum_i C_i \tilde{f}_i$$

C_{flat} is the only parameter of a special "flat" oscillator and, since it is squared to obtain ϵ_1, C_{flat} corresponds fairly well to the refractive index offset generated by this "Flat" oscillator: $n \simeq C_{flat} + \ldots$.

A "flat" oscillator with $C_{flat} > 1$ must be always included in the fit

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Oscillators available in ksemawc v2.6

$\tilde{\epsilon}(E)$ is calculated summing up to 20 oscillators belonging to the following 18 classes:

Flat

Lorentz
Quantum-homo
Lorentz-Dirac
Quantum-inhomo

Single peak in ε_2

Drude
Drude-ionized

Free carrier effects

Direct Gap Tauc-Exciton

Direct Gap Cody-M_1-M_2
Direct Gap Tauc-M_1-M_2

Direct Gap Cody-Lorentzian tail
Direct Gap Tauc-Lorentzian tail
Indirect Gap Cody-Lorentzian tail
Indirect Gap Tauc-Lorentzian tail

Direct Gap Cody-Urbach (exponential) tail
Direct Gap Tauc-Urbach (exponential) tail
Indirect Gap Cody-Urbach (exponential) tail
Indirect Gap Tauc-Urbach (exponential) tail

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Oscillators parameters

All the oscillators have less than four free parameters.

	C (eV^2)	E0 (eV)	D	W(eV)
Flat	C >1	-	-	-
Single peak	intensity	Peak energy	Line width	-
Lorentz-Dirac	intensity	Peak energy	Line width	Line asymmetry
Drude	intensity	-	Line width	-
Dir/Indir. Gap Lorentz	intensity	Eg	Line width	Band width
Dir/Indir. Gap Urbach	intensity	Eg	Urbach tail	Band width
Dir. Gap Exciton	intensity	Eg	Line width	Binding energy
Dir. Gap M1-M2	intensity	Eg	$(E_1-E_2)/2$	Band width

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Single peak oscillators formulas

"Lorentz"

$$\tilde{\chi} = \frac{2C}{\pi}\left[\frac{1}{E_0^2 - E^2 + 2iED}\right]$$

"Quantum-homo"

$$\tilde{\chi} = \frac{C}{\pi E_0}\left[\frac{1}{E_0 - E + iD}\right]$$

"Lorentz-Dirac"

$$\tilde{\chi} = \frac{2C}{\pi}\left[\frac{1}{E_0^2 - E^2 + 2iE(D + E^2/W)}\right]$$

"Quantum-inhomo"

$$\tilde{\chi} = \frac{C}{K}\left\{\frac{2}{\sqrt{\pi}} D_+\left(\frac{E_0 - E}{D/\sqrt{ln2}}\right) - i \cdot exp\left[-\left(\frac{E - E_0}{D/\sqrt{ln2}}\right)^2\right]\right\}$$

$C = (\pi\hbar^2 q^2 N)/(2m\epsilon_0)$ is the oscillator amplitude with dimensions $[\mathrm{eV}]^2$
E_0 is the resonance energy.
D is the line width.
W is the asymmetry parameter for the Lorentz-Dirac oscillator
D_+ is the Dawson function
K is a normalization constant for the Quantum-inhomo oscillator

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Single peak oscillators

Lorentz: standard function for the fit of peak shaped absorption spectra. Its long tails may cause problems if used for materials with a high transparency in adjacent energy range.

Quantum-homo: obtained neglecting a not-resonant term in the Lorentz oscillator. Its simpler expression allows to obtain analytical results in convolution calculations.

Lorentz-Dirac: asymmetric line shape. Useful for the fitting of noble metals optical costants.

Quantum-inhomo: obtained as the convolution between a quantum oscillator and a Gaussian distribution centered in E_0 and with HWHM equal to D ; the line width of the quantum oscillator is assumed to be much lower than the Gaussian width.
Useful to model a set of absorbing centres which cannot be considered as identical replicas due, for example, to proximity to other randomly distributed defects or to random fluctuations of strain (inhomogeneous broadening).
The fast decay of its χ_2 away from the resonance energy avoid some problems encountered using the Lorentz oscillator.

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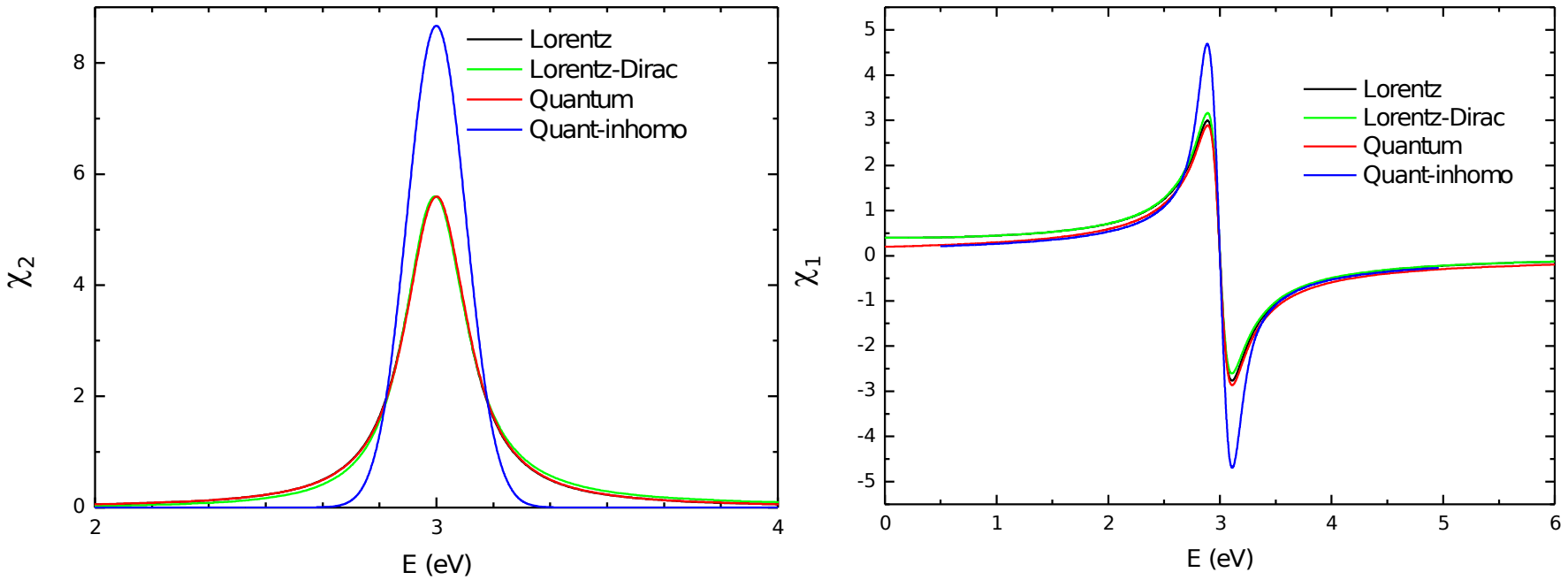
Comparison of the 4 single oscillators



The oscillator parameter used for this figure are:
C=5.6 eV^2 and $E_0 = 3$ eV.
D=0.1 eV for Lorentz, Quantum and Quantum-inhomo oscillators.
D=0.01 eV and W=50 eV for Lorentz-Dirac oscillator.

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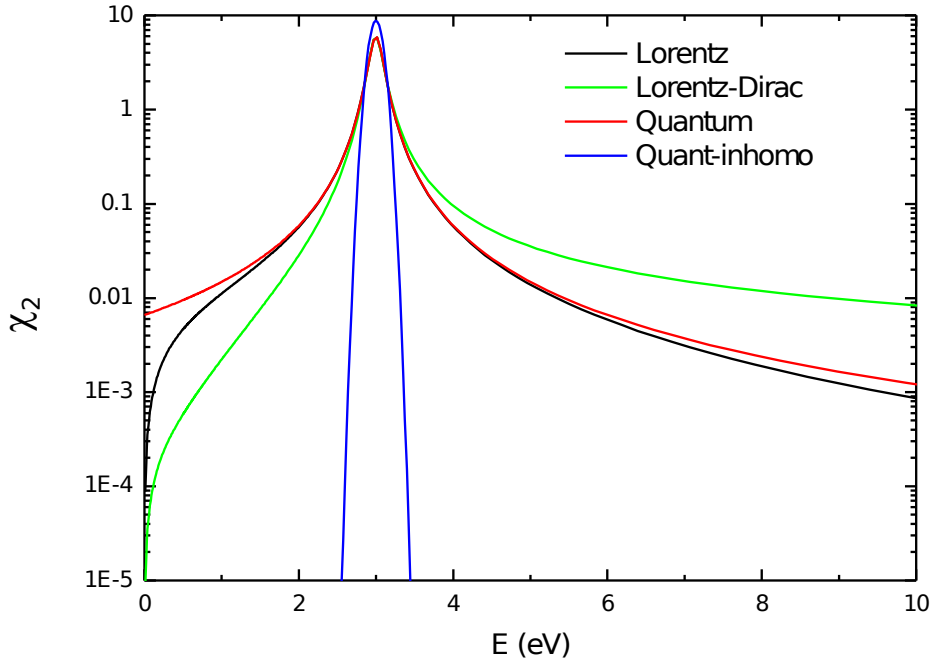
Comparison of χ_2 for the 4 single oscillators



χ_2 for the 4 single peak oscillators (Lorentz, Lorentz-Dirac, Quantum and Quantum-inhomo) with C=5.6 eV^2 and $E_0 = 3$ eV.
D=0.1 eV for Lorentz, Quantum and Quantum-inhomo oscillators.
D=0.01 eV and W=50 eV for Lorentz-Dirac oscillator.

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Drude oscillators

The "Drude" oscillator describes fairly well the response of a free electron gas.
It can be obtained simply setting $E_0 = 0$ in the Lorentz oscillator :

$$\chi_1 = -\frac{2C}{\pi}\frac{1}{D^2 + E^2}, \qquad \chi_2 = \frac{2C}{\pi}\frac{D}{E(D^2 + E^2)}.$$

D is related to the carrier scattering time τ by $D = \hbar/\tau$.

The optical mobility can be deduced from D using the equation $\mu = q\tau/m^* = (q\hbar)/(m^* D)$.

$C = (\pi\hbar^2 q^2 N)/(2m^*\epsilon_0)$ where N is the carrier density and m^* is their effective mass.

A sligthly modified version ("Drude-ionized") is available where D has an energy dependence ($D(E)$) to approximate the energy dependence of the carrier scattering time when the scattering is caused by ionized impurities.

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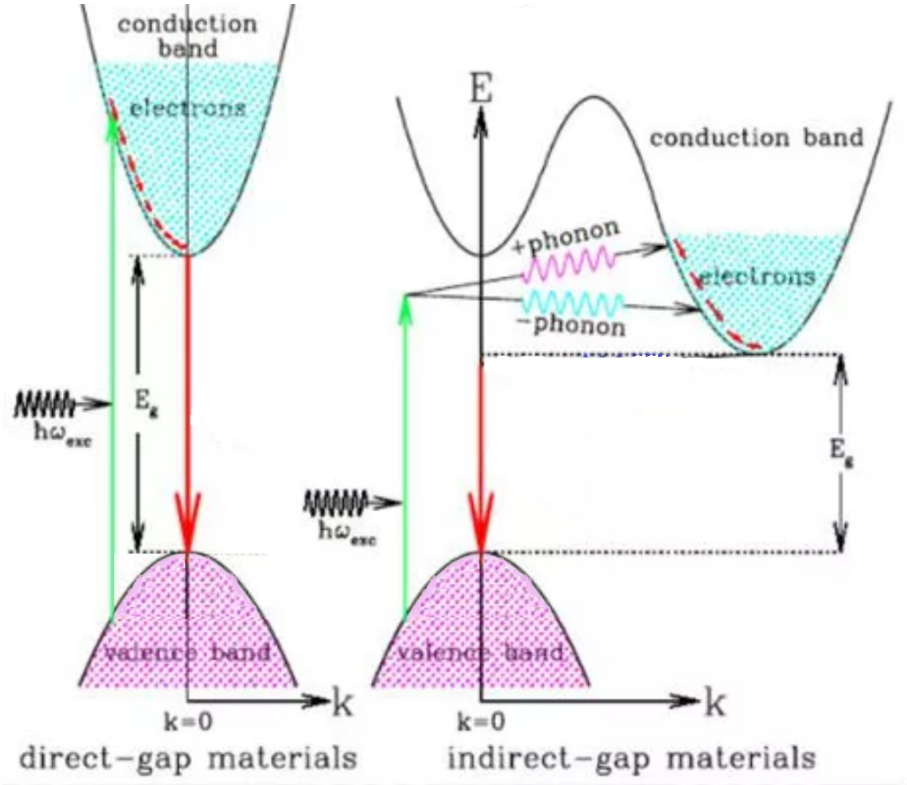
Direct and Indirect gap oscillators



The oscillators introduced up to now are unsuitable to describe the optical constants of systems with a continuous distribution of density of states such as semiconductors.

The theories reported in textbooks on semiconductors usually derive χ_2 only and exclusively at energies near the fundamental gap.

The calculation is made by hypothesizing that the excited states have infinite lifetime, i.e. that every transition between two states may take place only by absorbing/emitting photons and phonons with a total energy exactly equal to the difference of their energetic levels.

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χ_2^{inf} for excited states with infinite lifetime

Joint density of states

Calling χ_2^{inf} the χ_2 calculated for excited states with infinite lifetime, we have for **direct transitions**:

$$\chi_2^{inf}(\hbar\omega) \propto C^{abs}\frac{|M_{cv}|^2}{\omega^2}\int_{E_C(k)-E_V(k)-\hbar\omega}\frac{dS}{\left|\vec{\nabla}(E_C(k)-E_V(k))\right|}$$

For **indirect transitions** :

$$\chi_2^{inf}(\hbar\omega) \propto C^{abs}\frac{|M_{cv}|^2}{\omega^2}\int_{E_g}^{\hbar\omega+\hbar\omega_k} G_C(E_f-E_g)G_V(\hbar\omega+\hbar\omega_k-E_f)dE_f$$

Conduction and valence band convolution

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Tauc and Cody approximations

Tauc approximation $\Longleftrightarrow$ constant momentum matrix element $|M_{cv}|^2$

A constant $|\langle r \rangle|^2$ assumption can be also used as proposed by Cody for the amorphous semiconductor case.

A relation between the matrix elements of these two operators can be obtained by using commutator relations:

$$|\langle r \rangle|^2 = |M_{cv}|^2 \left(\frac{\hbar}{mE} \right)^2$$

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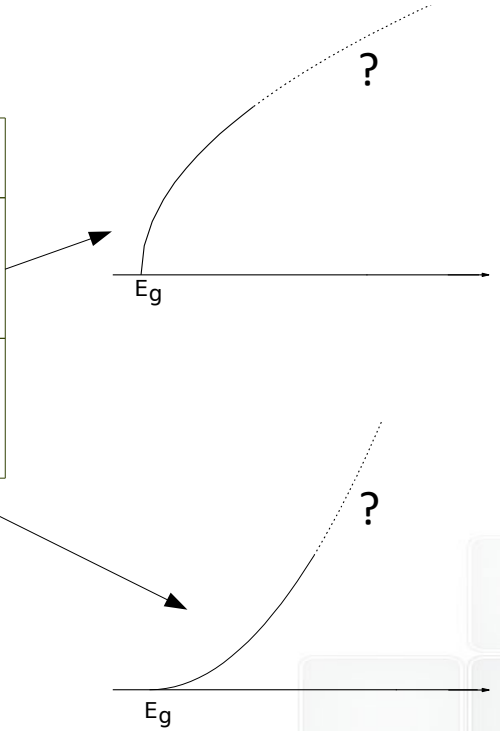
Energy dependence near Eg

If the bands are parabolic:

	Tauc	Cody
Direct gap	$\chi_2^{inf}(E) \propto \frac{\lvert M_{cv}\rvert^2}{E^2}\sqrt{E-E_g}$	$\chi_2^{inf}(E) \propto \lvert\langle r\rangle\rvert^2\sqrt{E-E_g}$
Indirect gap	$\chi_2^{inf}(E) \propto \frac{\lvert M_{cv}\rvert^2}{E^2}(E-E_g)^2$	$\chi_2^{inf}(E) \propto \lvert\langle r\rangle\rvert^2(E-E_g)^2$



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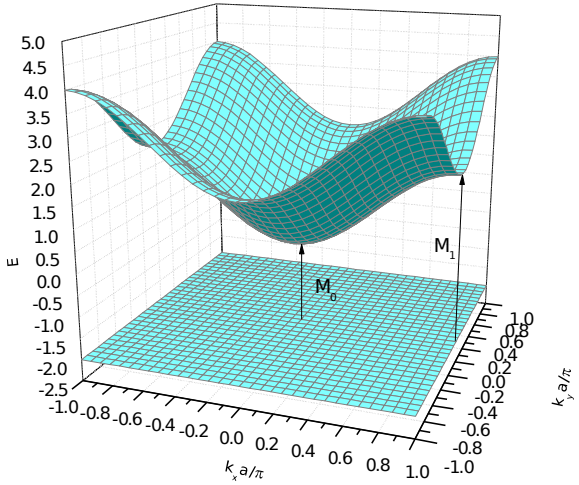
3D critical points

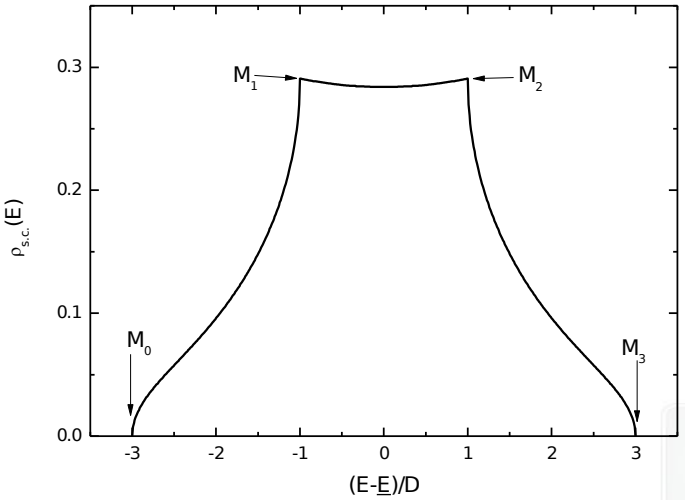
In 3 dimensions the Joint Density of States can show four types of critical points where $\vec{\nabla}(E_C(k) - E_V(k)) = 0$: M_0(minimum), M_1(saddle), M_2 (saddle), M_3 (maximum).

Band for a simple cubic lattice in the Tight-Binding s-level nearest-neighbor approximation with an overlap integral equal to D:

$$E(\vec{k}) = E_{lev} - 2D[cos(k_x a) + cos(k_y a) + cos(k_z a)]$$



Plot for the 2-D case



Density of states for the 3-D case

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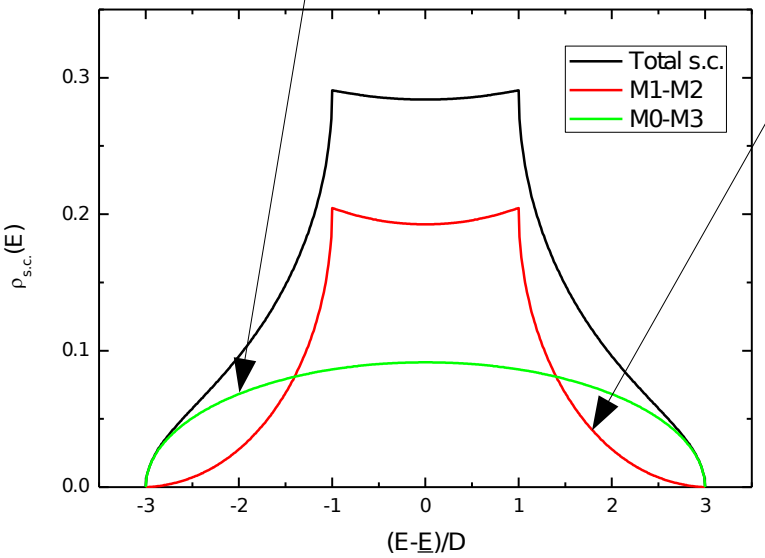
3D critical points : analytical approximation

$$\rho_{s.c.}(E) = A\sqrt{(E-E_0)(E_3-E)} + B\left[\sqrt{\frac{W}{2}-D} - \Theta(|E-\overline{E}|-D)\sqrt{|E-\overline{E}|-D}\right] + C(E-E_0)(E-E_3)$$



$$\overline{E} = (E_3+E_0)/2 \quad , \quad W = E_3 - E_0$$

$$B = C\left[2(E_3-E_0)\sqrt{\frac{E_3-E_0}{2}-D}\right]$$

To keep the oscillators simple and with 4 parameters only, M_0-M_3 and M_1-M_2 contributions to direct transitions are simulated by separate oscillators.

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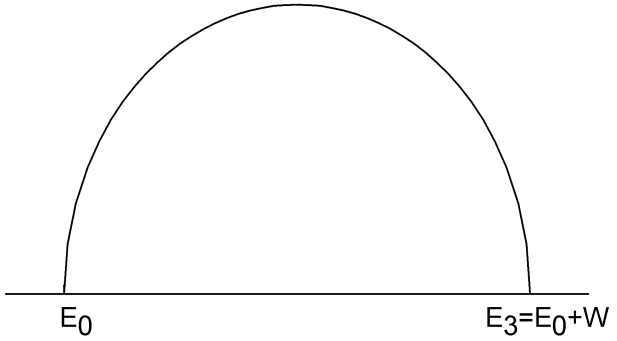
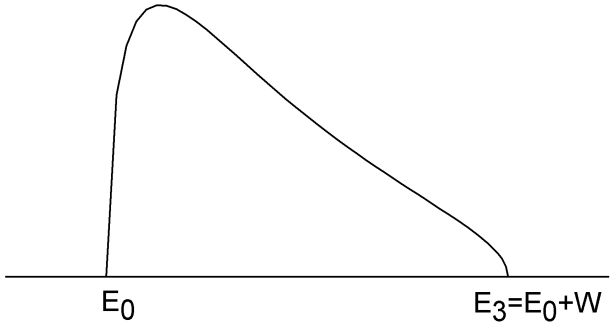
Direct gap-Cody and Direct gap-Tauc (M_0-M_3)





$$\chi^{inf}_{2-dir-Cody}(E) = \frac{C}{K_{Cd}}\sqrt{(E-E_0)(E_3-E)}$$

$$\chi^{inf}_{2-dir-Tauc}(E) = \frac{C}{K_{Td}}\frac{\sqrt{(E-E_0)(E_3-E)}}{E^2}$$

$$K_{Cd} = \frac{\pi}{16}W^2(2E_0+W)$$

$$K_{Td} = \frac{\pi}{2}(2E_0+W-2\sqrt{E_0(E_0+W)})$$

$$\int_0^\infty \epsilon_2^{osc}(E)EdE = C$$

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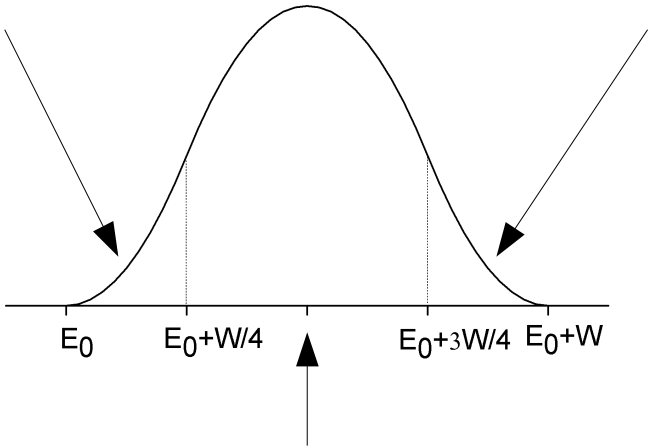
Indirect gap-Cody and Indirect gap-Tauc

$$\chi^{inf}_{2-ind-Cody}(E) = \frac{16\,C}{K_{Ci}W^2}(E-E_0)^2$$

$$\chi^{inf}_{2-ind-Cody}(E) = \frac{16\,C}{K_{Ci}W^2}\left[E-(E_0+W)\right]^2$$

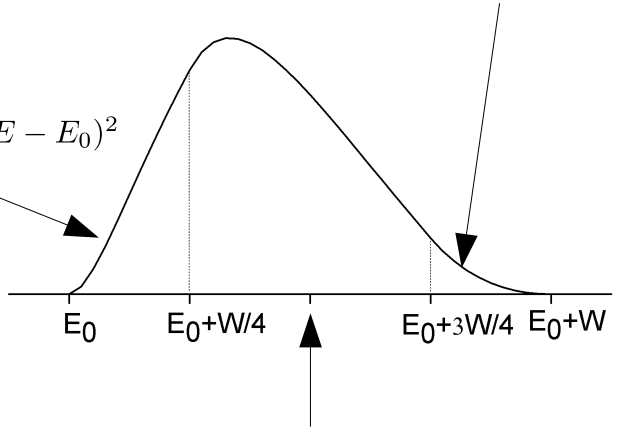


$$\chi^{inf}_{2-ind-Cody}(E) = \frac{C}{K_{Ci}}\left\{2-\frac{16}{W^2}\left[E-(E_0+W/2)\right]^2\right\}$$

$$\mathrm{K}_{Ci} = E_0W + \frac{W^2}{2}$$

$$\chi^{inf}_{2-ind-Tauc}(E) = \frac{16\,C}{K_{Ci}W^2E^2}\left[E-(E_0+W)\right]^2$$

$$\chi^{inf}_{2-ind-Tauc}(E) = \frac{16\,C}{K_{Ci}W^2E^2}(E-E_0)^2$$



$$\chi^{inf}_{2-ind-Tauc}(E) = \frac{C}{K_{Ti}E^2}\left\{2-\frac{16}{W^2}\left[E-(E_0+W/2)\right]^2\right\}$$

$$K_{Ti} = f(E_0/W)$$

$$f(r) = 2\left[8r^2ln\left(\frac{4r+1}{4r}\right)+8(r+1)^2ln\left(\frac{4r+4}{4r+3}\right)-(1+8(r^2+r))ln\left(\frac{4r+3}{4r+1}\right)\right]$$

E_0 is the gap energy , W is the absorption band width

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The convolution approach

The analytical expressions for $\tilde{\chi}(E)$ are obtained by performing the convolution between a suitable χ_2^{inf} calculated for infinite lifetime and the normalized complex $\tilde{\chi}_{qo}$ describing the response of a quantum oscillator:

$$\tilde{\chi}(E) = \int \chi_2^{inf}(E_r)\tilde{\chi}_{qo}(E_r - E)dE_r$$

The function $\tilde{\chi}_{qo}$ is given by the expression given before, normalized so that the integral of its imaginary part is equal to 1:

$$\tilde{\chi}_{qo}(E, E_r) = \frac{1}{\pi}\left[\frac{1}{E_r - E + iD}\right]$$

The result of the convolution can be expressed as analytical functions in the four previous cases.

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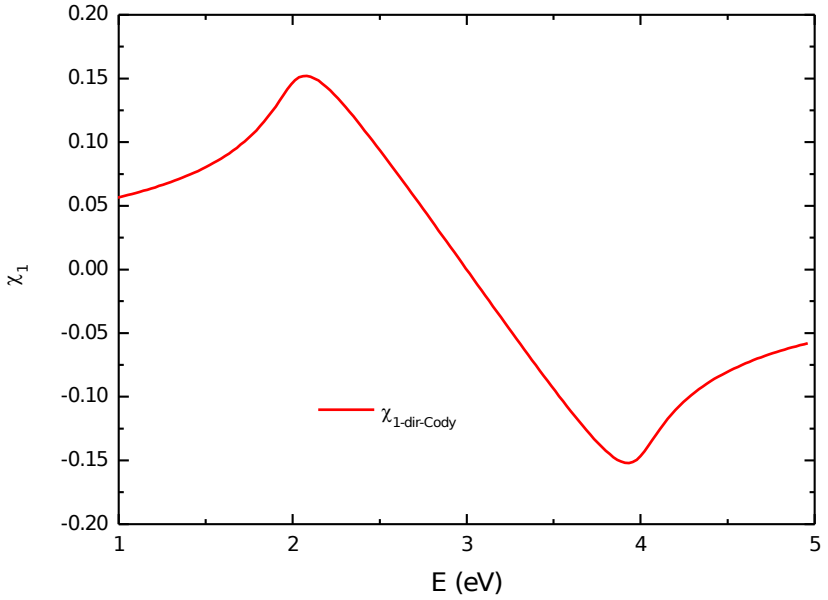
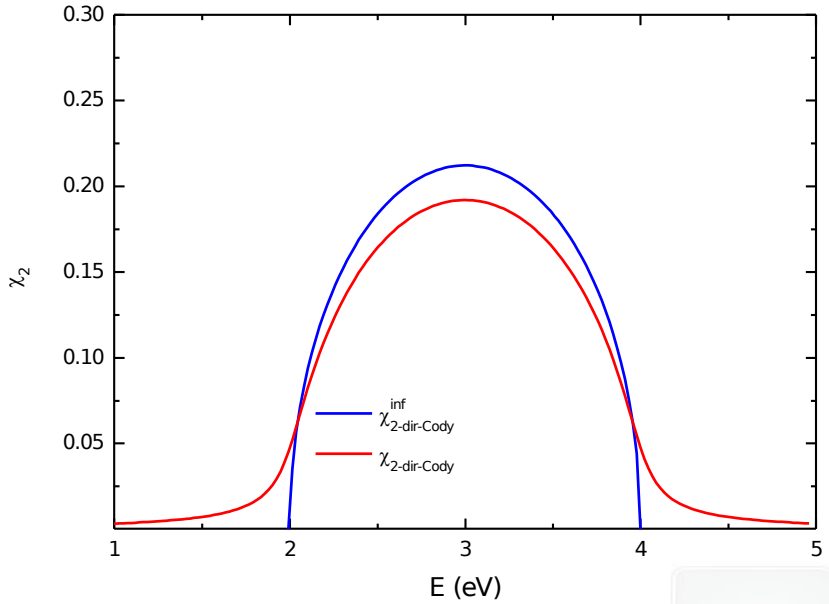
Direct gap Cody - Lorentzian tail

convolution with $\tilde{\chi}_{qo}$

$$\chi^{inf}_{2-dir-Cody}(E) = \frac{C}{K_{Cd}}\sqrt{(E-E_0)(E_3-E)} \Rightarrow \tilde{\chi}_{dir-Cody}(E) = \frac{C}{K_{Cd}}\left[\frac{E_0+E_3}{2} - E + iD - \sqrt{E_0 - E + iD}\sqrt{E_3 - E + iD}\right]$$





The example in this figure has: C=1, $E_0 = 2$ eV, $W = E_3 - E_0 = 2$ eV, $D = 0.1$ eV.

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Direct gap Tauc - Lorentzian tail

The convolution between the $\chi^{inf}_{2-dirTauc}$ and the normalized complex $\tilde{\chi}_{qo}$ gives:

$$\chi_{1-dir-Tauc}(E) = \frac{C}{2DK_{Td}} \Re\left\{ \frac{1}{2(D-iE)} \left(2iD + 2E - 2\sqrt{E_0E_3} \right.\right.$$
$$\left. -(i-1)\sqrt{2}\sqrt{D-i(E-E_0)}\sqrt{-iD-E+E_3}\right)$$
$$+ \frac{1}{2(D+iE)} \left(-2iD + 2E - 2\sqrt{E_0E_3} + (i+1)\sqrt{2}\sqrt{D+i(E-E_0)}\sqrt{iD-E+E_3}\right)$$
$$+ E(D-iE)^2\sqrt{D+i(E-E_0)}\sqrt{D+i(E-E_3)}/\left(D^2+E^2\right)^2$$
$$+ E(D+iE)^2\sqrt{D-i(E-E_0)}\sqrt{D-i(E-E_3)}/\left(D^2+E^2\right)^2$$
$$\left. - ED\left(D^2(E_0+E_3) + E(-4E_0E_3 + E(E_0+E_3))\right) / \left(\left(D^2+E^2\right)^2\sqrt{E_0E_3}\right)\right\}$$

$$\chi_{2-dir-Tauc}(E) = \frac{CD}{K_{Td}}$$
$$\times \Re\left\{ -\left[(D-iE)^2\sqrt{D+i(E-E_0)}\sqrt{D+i(E-E_3)}\right] / \left(2D\left(D^2+E^2\right)^2\right)\right.$$
$$- \left[(D+iE)^2\sqrt{D-i(E-E_3)}\sqrt{D-i(E-E_0)}\right] / \left(2D\left(D^2+E^2\right)^2\right)$$
$$\left. + D\left[D^2(E_0+E_3) + E(-4E_0E_3 + E(E_0+E_3))\right] / \left(2D\left(D^2+E^2\right)^2\sqrt{E_0E_3}\right)\right\}$$

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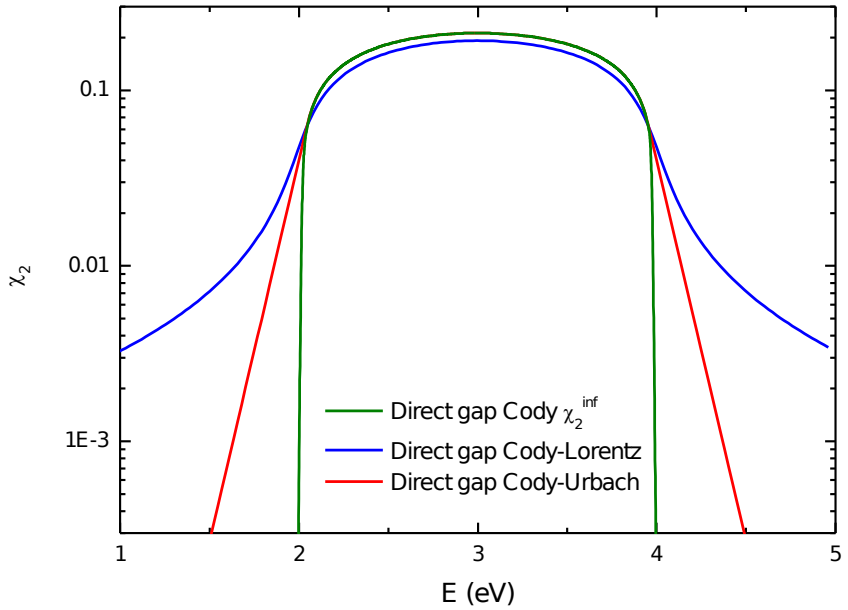
Direct and Indirect gap oscillators with Urbach tail



The parameters are: C=1, $E_0 = 2$ eV, $W = 2$ eV, $D = 0.1$ eV. D corresponds to the quantum oscillator line width in one case and to the characteristic energy D of the Urbach tail ($\chi_2(E) \propto exp(\pm E/D)$) in the other one.

χ_2^{inf} is modified adding an Urbach tail on both band edges. The real part χ_1 is then obtained by means of the numerical integration of the Kramers-Kronig relation:

$$\chi_1(E) = \frac{2}{\pi}\mathcal{P}\int_0^\infty \frac{\chi_2(x)x}{x^2 - E^2}dx$$

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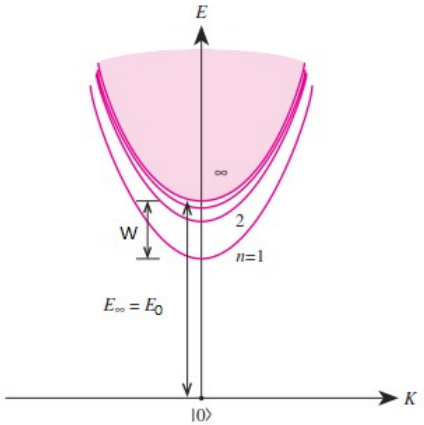
Direct gap Tauc-exciton

The oscillator included in kSEMAWc is based on an improved version of the Elliott's theory presented by Tanguy in 1995 [1] which gives a very compact expression for the susceptibility of a semiconductor with a direct gap in the Tauc approximation taking into account the excitons and a Lorentzian broadening of the states :

$$\tilde{\chi}(E) = \frac{C\sqrt{W}}{(E+iD)^2}\left[g_a(\xi(E+iD)) + g_a(\xi(-E-iD)) - 2g_a(\xi(0))\right]$$

$$g_a(\xi) = 2\ln\xi - 2\pi cot(\pi\xi) - 2\psi(\xi) - 1/\xi$$

$$\xi(z) = \sqrt{\frac{W}{E_0 - z}}$$

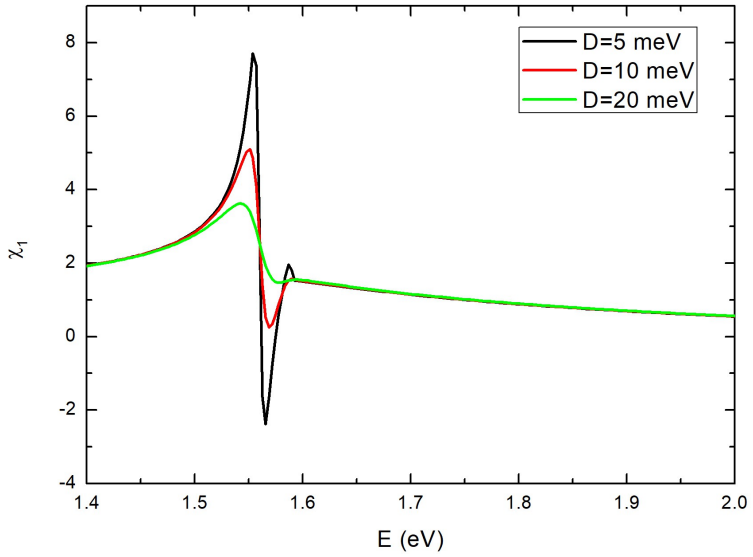


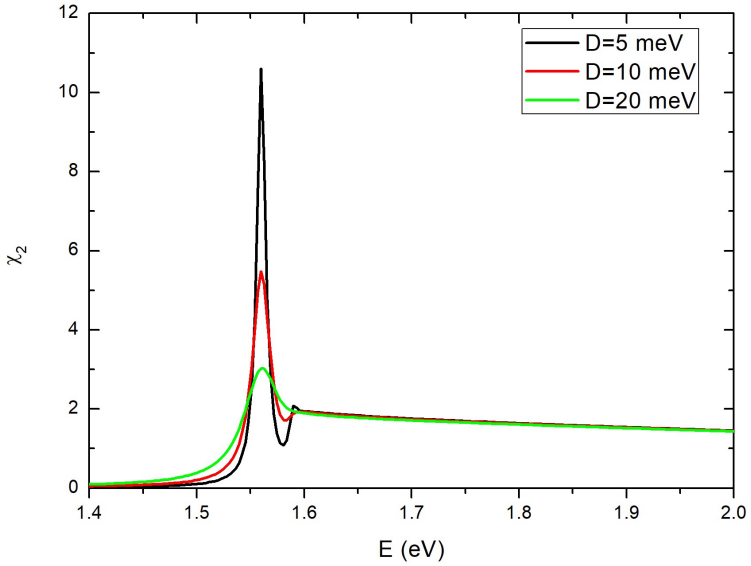
where $\psi(z) = d\ln\Gamma(z)/dz$ is the complex digamma function, D is the width of the Lorentzian broadening function, E_0 is the energy gap and W is the exciton binding energy.

[1] C. Tanguy, Optical dispersion by Wannier excitons, Phys. Rev. Lett. 75, 4090–4093 (1995).

This work was financially supported by the European Union's Horizon 2020 research and innovation programme under the grant agreement 952982 (Custom-Art)

Direct gap Tauc-exciton: broadening effect





The other parameters are: C=4, $E_0 = 1.6$ eV, $W = 40$ meV .

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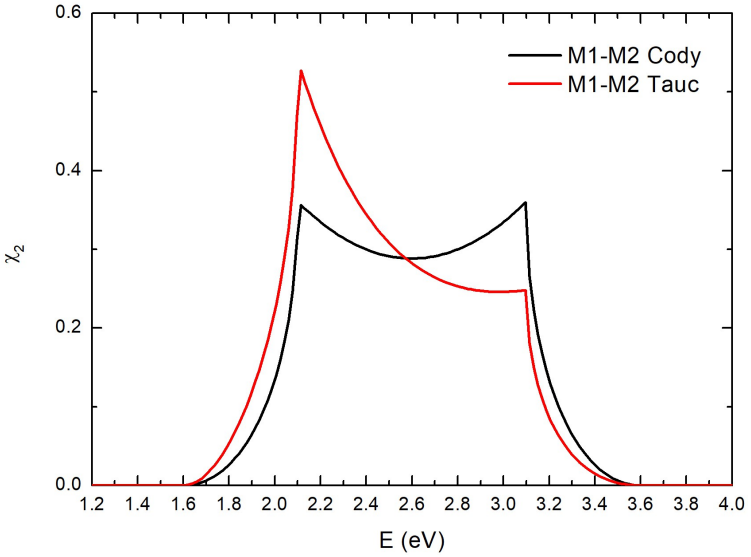
3D M_1-M_2 critical point oscillator



Plot of χ_2 for a M_1-M_2 oscillators with C=1 eV^2 , $E_0 = 1.6$ eV, $W = 2eV$ and D=0.5 eV using the Cody (black curve) and Tauc (red curve) approximations.

The real part χ_1 is obtained by means of the numerical integration of the Kramers-Kronig relation.

$$\chi_{2-CM12}(E) = \frac{C}{K_{CM12}} \left\{ K_1 \left[\sqrt{\frac{W}{2} - D} - \Theta(|E - \overline{E}| - D) \sqrt{|E - \overline{E}| - D} \right] + (E - E_0)(E - E_3) \right\}$$

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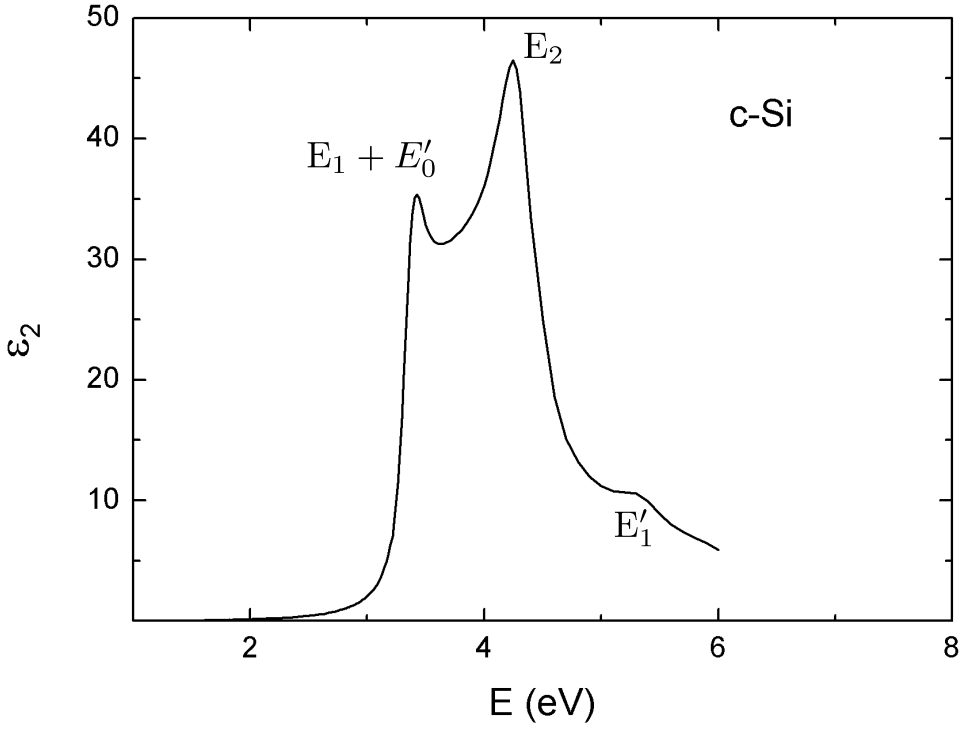
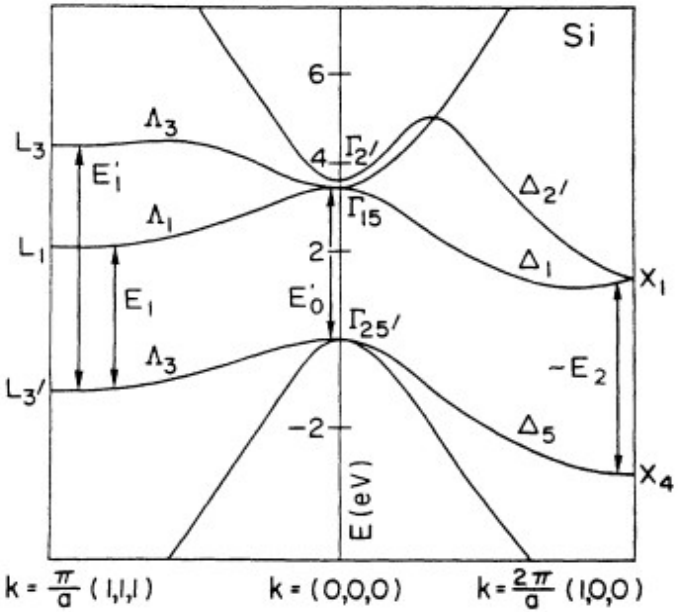
A familiar case: crystalline silicon





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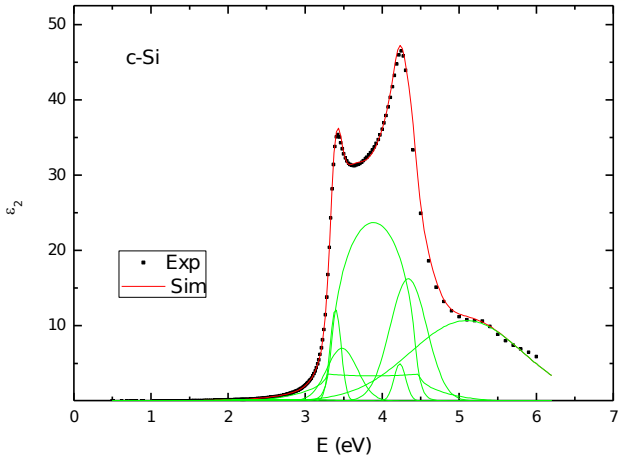
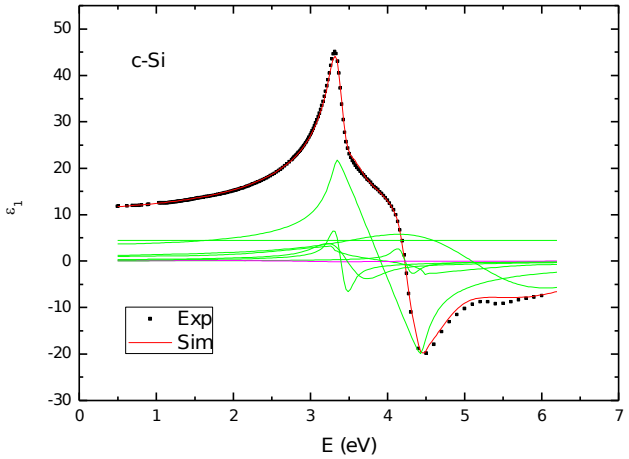
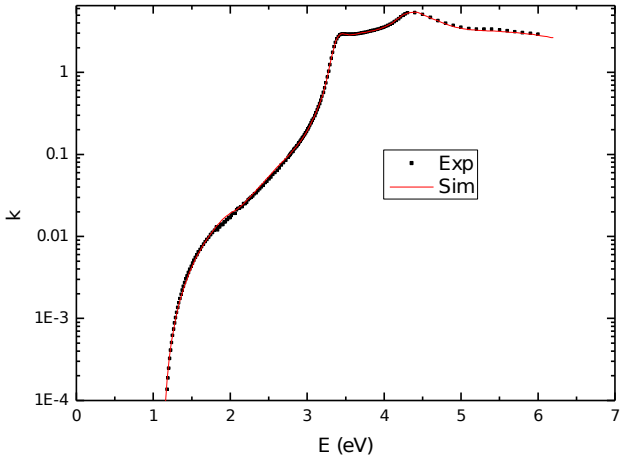
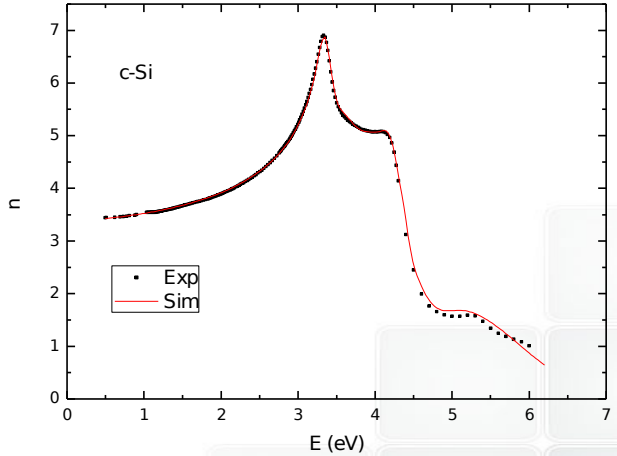
A familiar case: crystalline silicon



#Osc	type	C	E0 (eV)	D (eV)	W (eV)
1	Quant-inhomo	7.30972	3.39575	0.0831545	unused
2	Quant-inhomo	4	4.23	0.09	unused
3	Dir-Gap-Cody-M1M2	23	2.05	0.6	3.66
4	Ind-Gap-Cody-Urbach	0.85	1.1	0.03	3
5	Quant-inhomo	12.1081	3.47921	0.233499	unused
6	Quant-inhomo	42	4.34	0.28	unused
7	Flat	2.1	unused	unused	unused
8	Dir-Gap-Cody-Urbach	83.0221	3.31295	0.0600965	1.14763
9	Quant-inhomo	99.4053	5.09589	0.857884	unused







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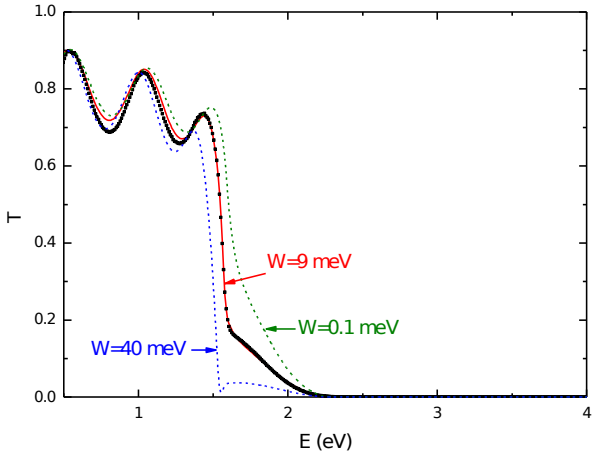
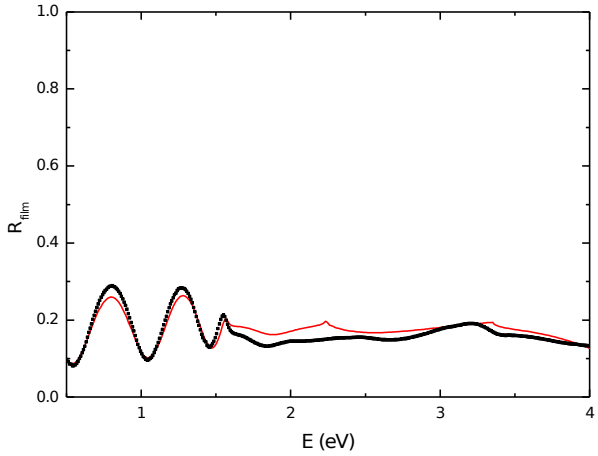
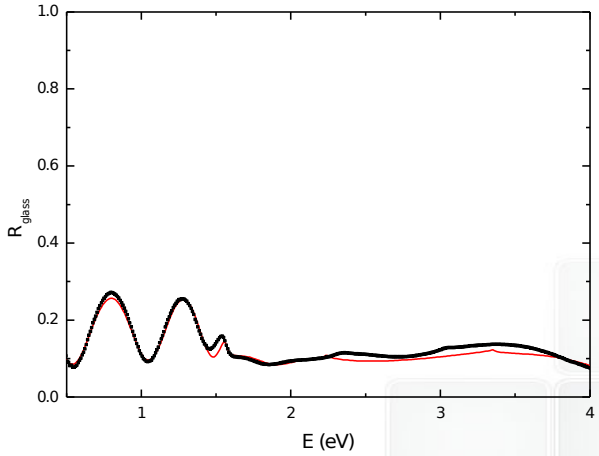
Perovskite film on glass

#Osc	type	C	E0 (eV)	D (eV)	W (eV)
1 ☑	Flat	1	unused	unused	unused
2 ☑	Lorentz	1000	17.4	1.85	unused
3 ☑	Dir-Gap-Tauc-Exciton	3.42	1.59	0.022	0.009
4 ☑	Dir-Gap-Tauc-M1M2	3.6	1.68	0.56	2.23
5 ☑	Quant-inhomo	13.3	3.52	0.67	unused







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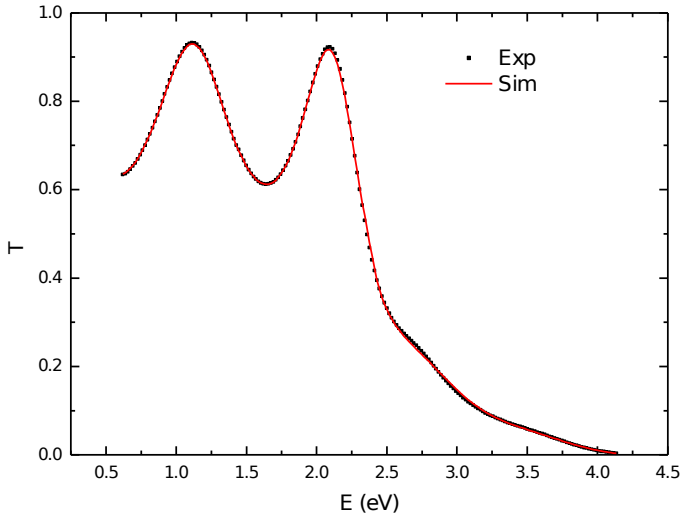
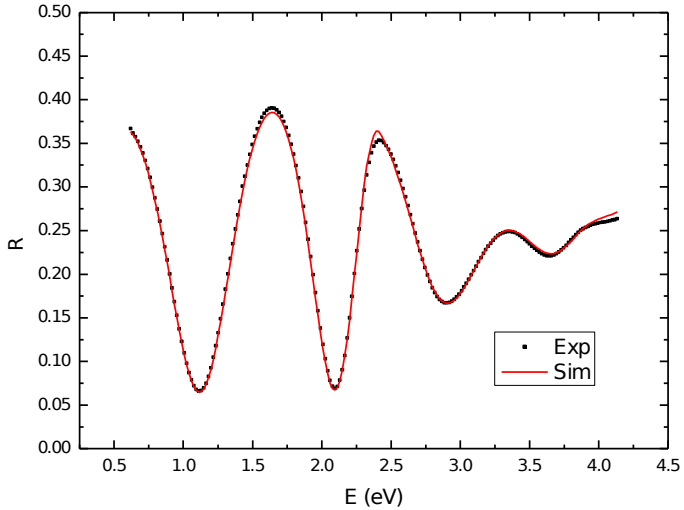
ZnSe film on glass

#Osc	type	C	E0 (eV)	D (eV)	W (eV)
1 ☑	Flat	1	unused	unused	unused
2 ☑	Dir-Gap-Cody-Urbach	122.799	2.37205	0.0948758	9.21083
3 ☑	Dir-Gap-Cody-Urbach	195.239	4.07019	0.238088	5.76904





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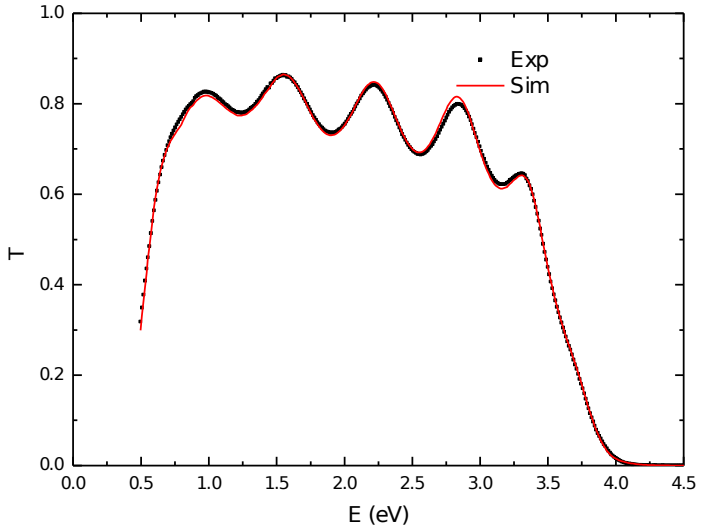
IWO film on glass

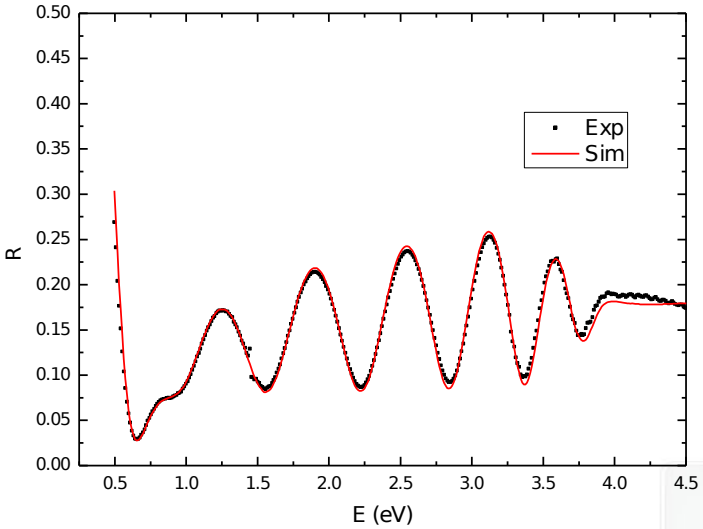
From Drude parameters, using $m^* = 0.35 m_e$, we get:

$$N(\mathrm{cm}^{-3}) = C(\mathrm{eV}^2)\frac{m^*}{m_e}4.617 \cdot 10^{20} = 2.83 \cdot 10^{20}\mathrm{cm}^{-3}$$

$$\mu\left(\frac{cm^2}{Vs}\right) = \frac{1.159}{D(eV)m^*/m_e} = 38.5\left(\frac{cm^2}{Vs}\right)$$

#Osc	type	C	E0 (eV)	D (eV)	W (eV)
1 ☑	Flat	1	unused	unused	unused
2 ☑	Drude-ionized	1.75451	unused	0.0857026	unused
3 ☑	Dir-Gap-Cody-Urbach	489.375	3.80252	0.25282	13.97
4 ☑	Dir-Gap-Cody	0.139687	0.872585	2.8876e-07	2.9341





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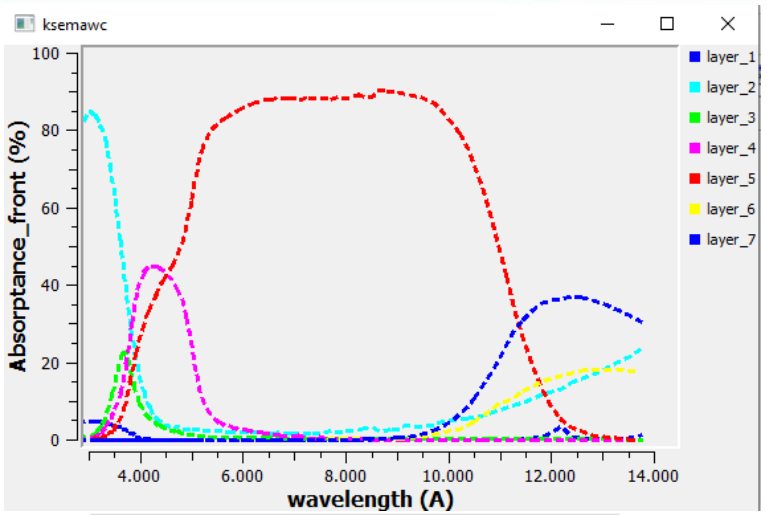
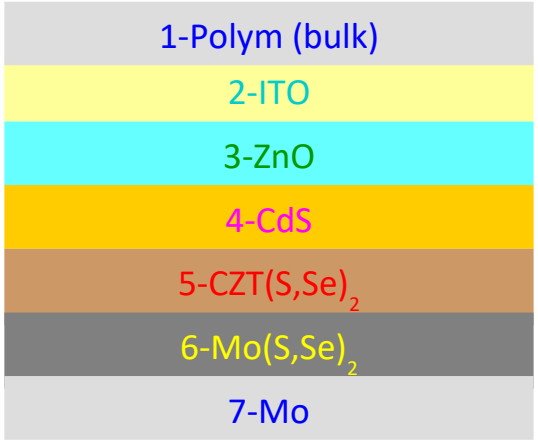
CZTSSe solar cell





Valin | Model | Simulation | Numerical Search | Data Fit | Graph Range

Model of the optical device (from Front to Back)

type	Move		d(mm-A)	rough (A)	GRAD-n	dGRAD-n/dE	CURV-n	GRAD-k	CURV-k	material
bulk	-	dw	0.10	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #6
homo. film	up	dw	2400.00	500.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #3
homo. film	up	dw	500.00	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #5
homo. film	up	dw	800.00	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #4
homo. film	up	dw	10000.00	1000.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #8
homo. film	up	dw	2500.00	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #7
homo. film	up	dw	5000.00	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #2
bulk	up	dw	0.00	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #1
bulk	up	-	0.00	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #1

N. layers 7 | Symmetric on 2nd face | inhomogeneity as 23 subfilm | computing <f(x)> with N= 5 | Plot Exp Meas ! | Simulate !

Materials

	unknown	n	k	with	EMA	f
Material #1	CZTSSe cells/Mo ENEA	1	0		air n=1 k=0	0.000
Material #2	CZTSSe cells/ITO standard	1	0		air n=1 k=0	0.000
Material #3	CZTSSe cells/CdS ENEA	1	0		air n=1 k=0	0.000
Material #4	CZTSSe cells/ZnO ENEA	1	0		air n=1 k=0	0.000
Material #5	CZTSSe cells/Polym IPC 1L 0	1	0		air n=1 k=0	0.000
Material #6	CZTSSe cells/MoSeS2 Richter	1	0		air n=1 k=0	0.000
Material #7	CZTSSe cells/CZTSSe Gokmen	1	0		air n=1 k=0	0.000
Material #8	constant nk	1	0		air n=1 k=0	0.000
output SF	constant nk	1	0		air n=1 k=0	0.000
input SF	constant nk	1	0		air n=1 k=0	0.000
input PDS	constant nk	1	0		air n=1 k=0	0.000
input ELI-1	constant nk	1	0		air n=1 k=0	0.000
input ELI-2	constant nk	1	0		air n=1 k=0	0.000
input ELI-3	constant nk	1	0		air n=1 k=0	0.000
input ELI-4	constant nk	1	0		air n=1 k=0	0.000

Load Spj! | Save Spj! | CZTSSe_cells/CZTSSe_cell_poly_IPC.Spj | info: CZTSSe cell with a 100 um front polymer encapsulant

Load nk! | Clear nk ! | CZTSSe_cells/CZTSSe_Gokmen.nk | info: CZTSSe Eg=1.13 eV k:Adachi_2015 Book+ Gokmen_2014 (DOI:10.1063/1.4890844) n: Adachi_2015 Book

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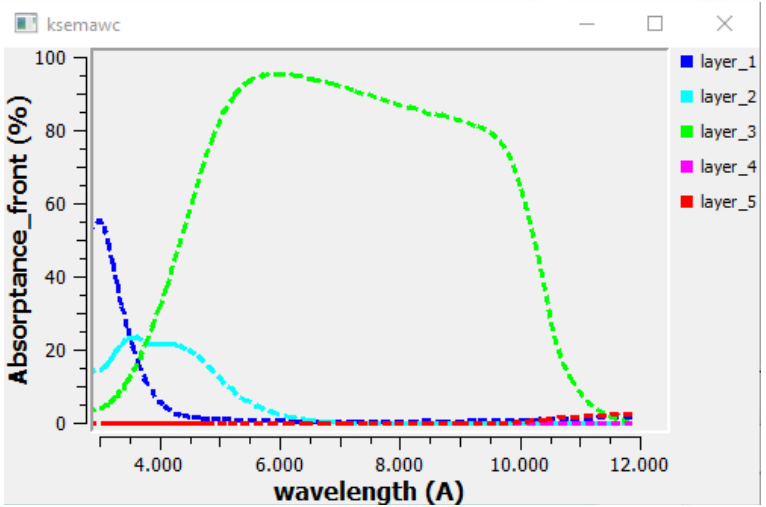
HJ c-Si solar cell



1-ITO

2-a-Si:H

3-c-Si

4-a-Si:H

5-ITO

Valin | Model | Simulation | Numerical Search | Data Fit | Graph Range

Model of the optical device (from Front to Back)

type	Move		d(mm-A)	rough (A)	GRAD-n	dGRAD-n/dE	CURV-n	GRAD-k	CURV-k	material
homo. film	-	dw	690.00	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #2
homo. film	up	dw	120.00	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #3
homo. film	up	dw	2500000.00	1000.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #4
homo. film	up	dw	150.00	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #3
homo. film	up	dw	690.00	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #2
bulk	up	dw	0.00	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #1
bulk	up	dw	0.00	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #1
bulk	up	dw	0.00	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #1
bulk	up	-	0.00	0.0	0.0000	0.000	0.0000	0.0000	0.0000	Material #1

N. layers 5 | Symmetric on 2nd face | inhomogeneity as 23 subfilm | computing <f(x)> with N= 5 | Plot Exp Meas ! | Simulate !

Materials

	unknown	n	k	with	EMA	f
Material #1	unknown					
Material #2	ITO/ITO_standard	1	0		air n=1 k=0	0.000
Material #3	HJ_stack/a-SiH_CNR	1	0		air n=1 k=0	0.000
Material #4	sili/cSixx.1	1	0		air n=1 k=0	0.000
Material #5	constant nk	1	0		air n=1 k=0	0.000
Material #6	constant nk	1	0		air n=1 k=0	0.000
Material #7	constant nk	1	0		air n=1 k=0	0.000
Material #8	constant nk	1	0		air n=1 k=0	0.000
output SF	constant nk	1	0		air n=1 k=0	0.000
input SF	constant nk	1	0		air n=1 k=0	0.000
input PDS	constant nk	1	0		air n=1 k=0	0.000
input ELI-1	constant nk	1	0		air n=1 k=0	0.000
input ELI-2	constant nk	1	0		air n=1 k=0	0.000
input ELI-3	constant nk	1	0		air n=1 k=0	0.000
input ELI-4	constant nk	1	0		air n=1 k=0	0.000

Load Spj! | Save Spj! | HJ_stack/Simulaz_HJFlat_amorfi.2.Spj | info: TCO-aSI-cSI-aSi-TCO

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- **Francesco Biccari** for his useful suggestions for simplifying the software distribution
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And...Thank You for your attention !

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