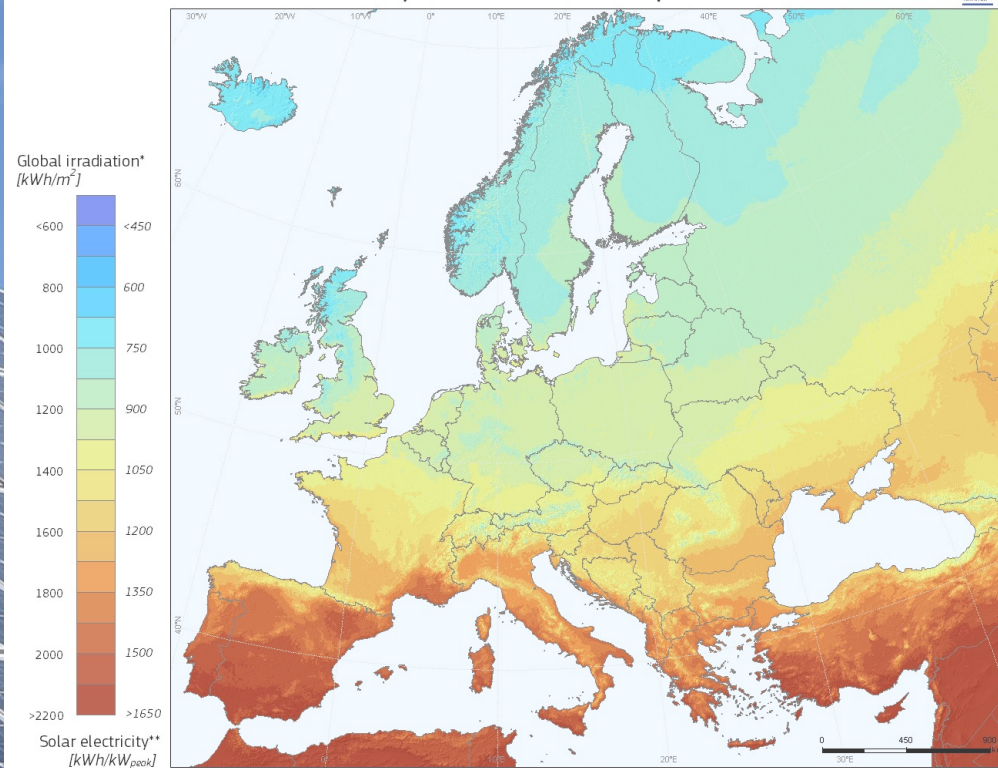


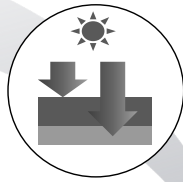


Photovoltaic Solar Electricity Potential in European Countries

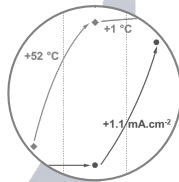


| M. Amara

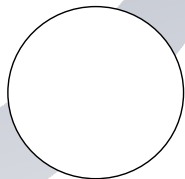
Modeling and Simulation of Photovoltaic Devices and Systems



Basic concept of solar cells

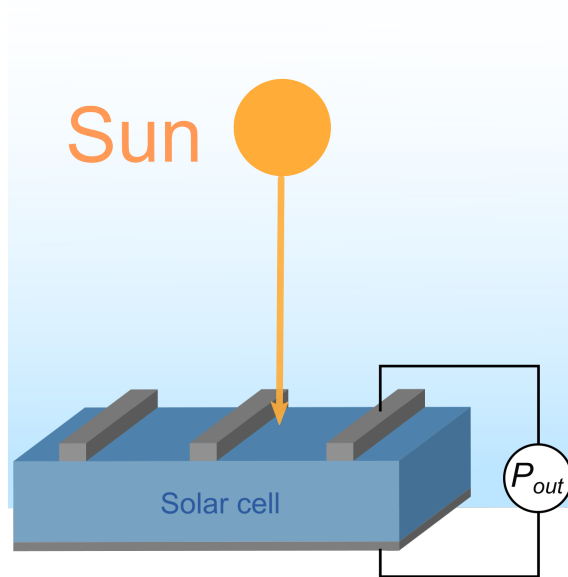


PV modeling & simulation



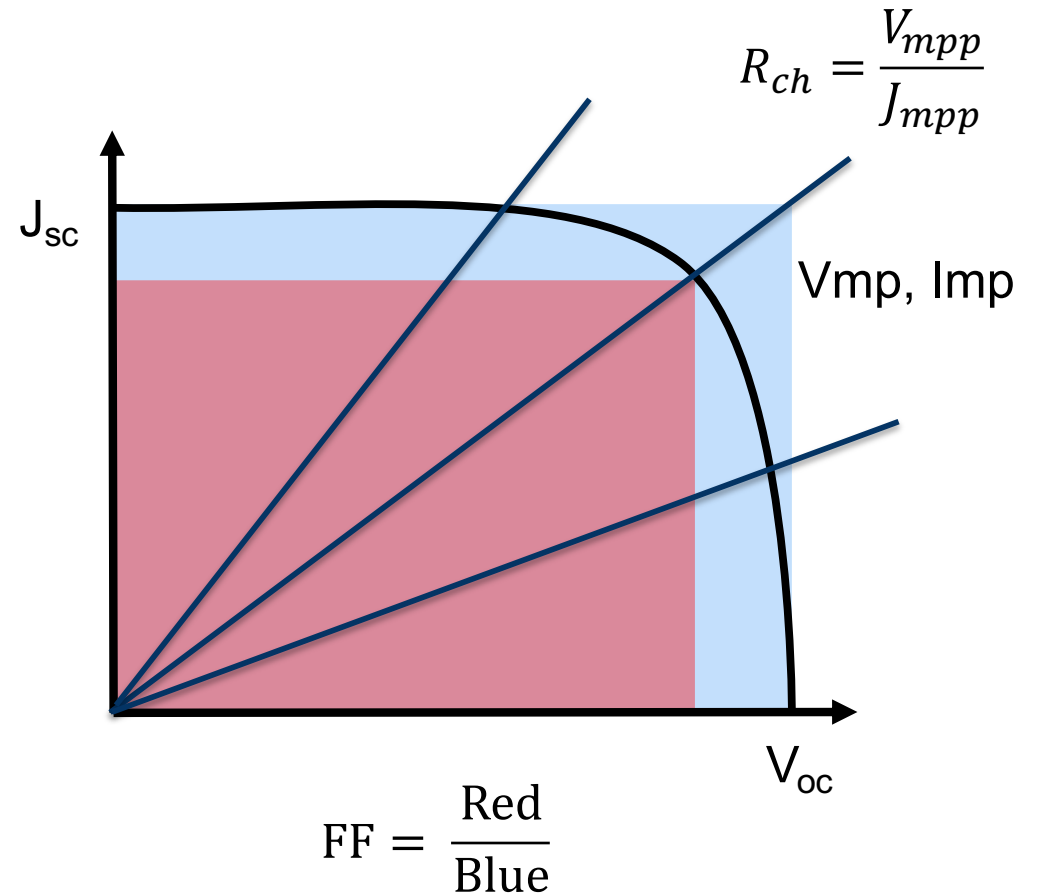
Conclusions

What is a Solar Cell ?



- Short circuit current
- Open circuit voltage
- Fill factor

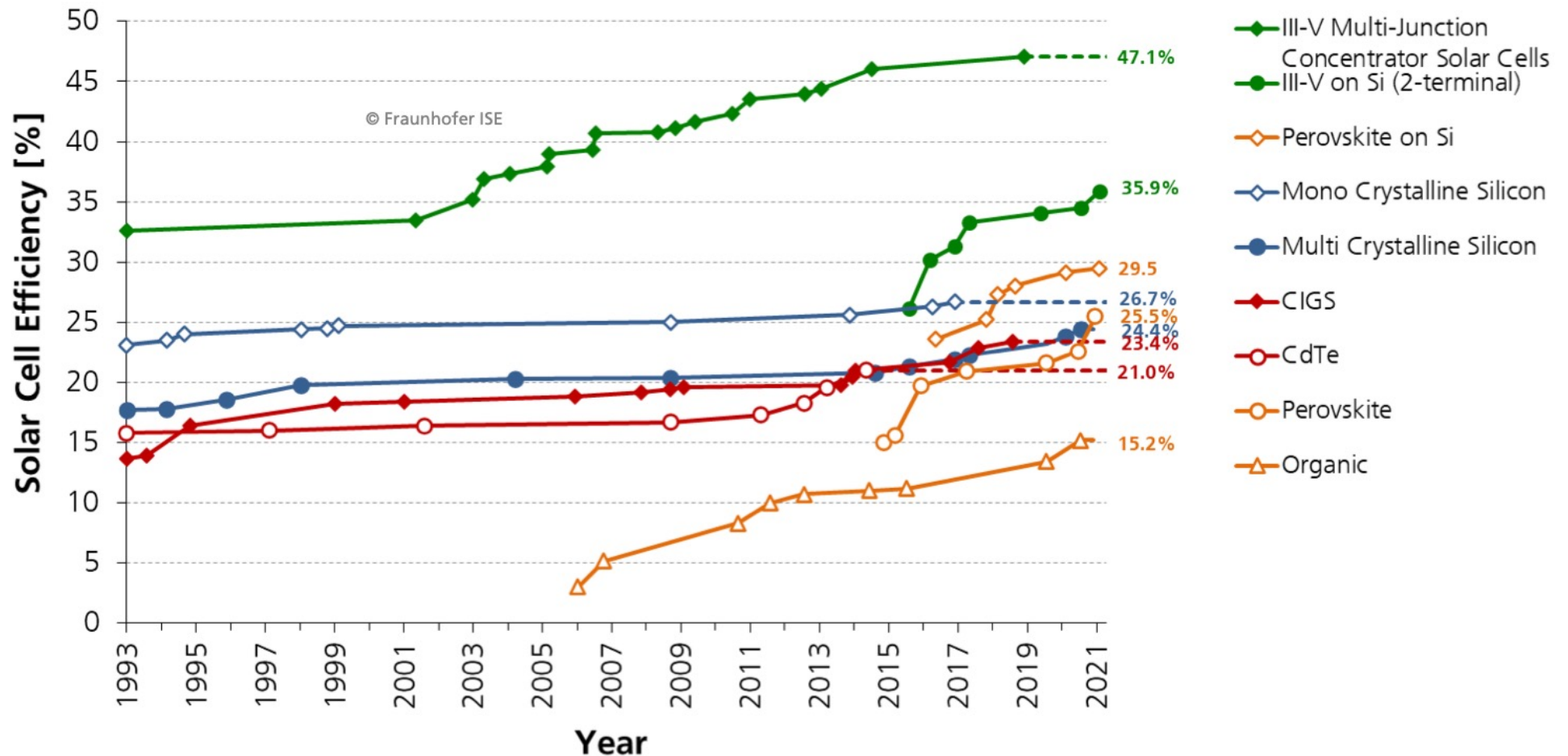
$$\eta = \frac{J_{sc} \times V_{oc} \times FF}{P_{iin}}$$



➤ What is the best solar cells performances?



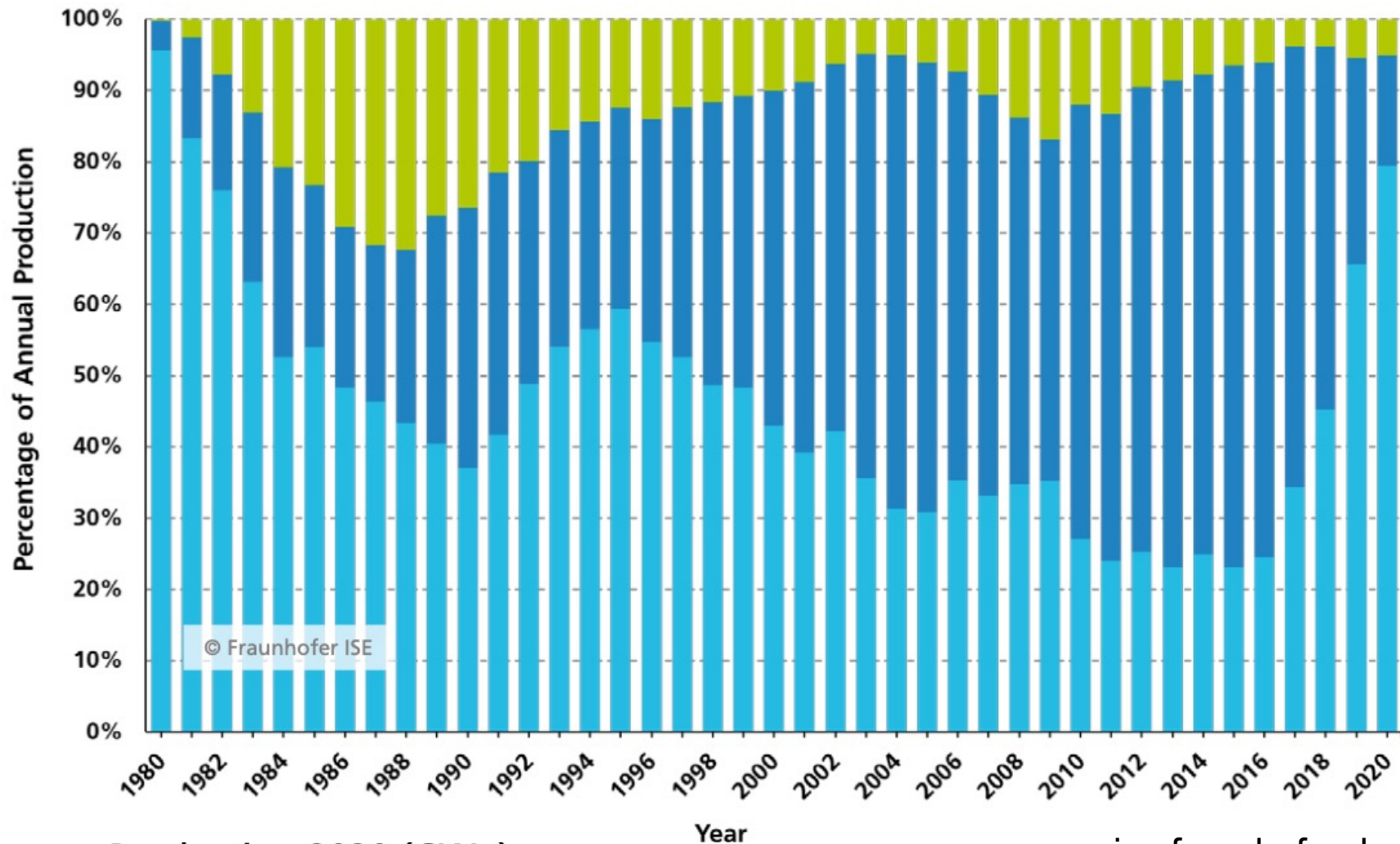
To day solar cell efficiency @ 25°C and 1000 W/m²



However !!

www.ise.fraunhofer.de

Annual PV production by technology



Production 2020 (GWp)

Thin film

7.7

Multi-Si

23.3

Mono-Si

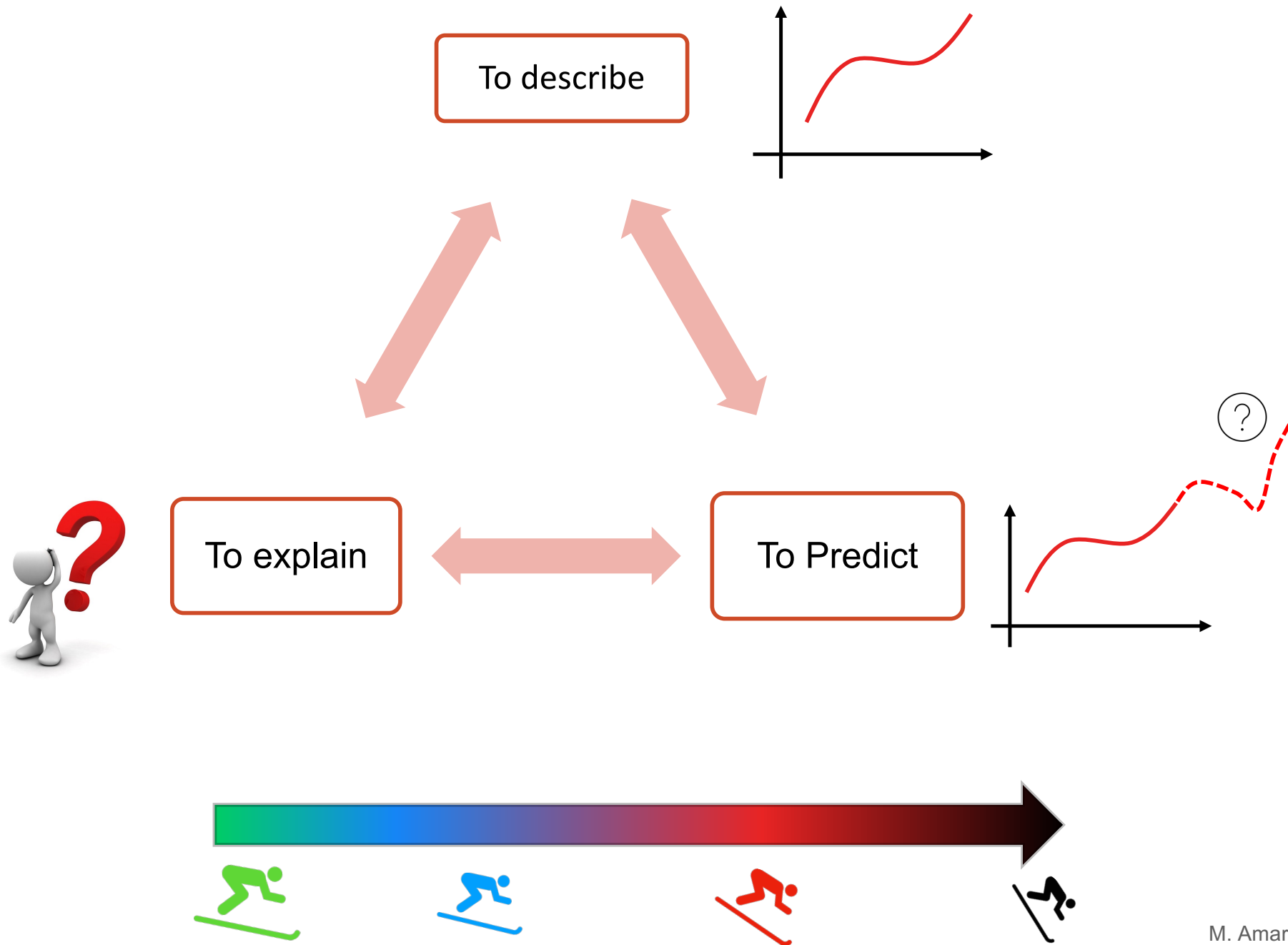
120.6

CdTe: 6.1
CIGS :1.5
a-Si : 0.2



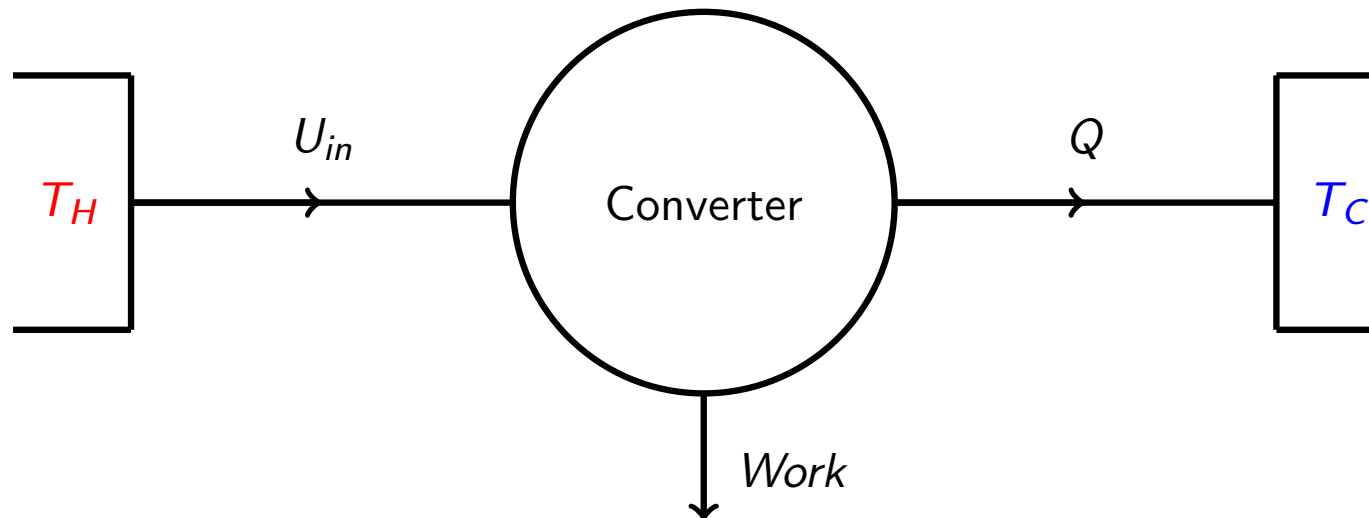
PV modeling & simulation

Why modeling & simulation





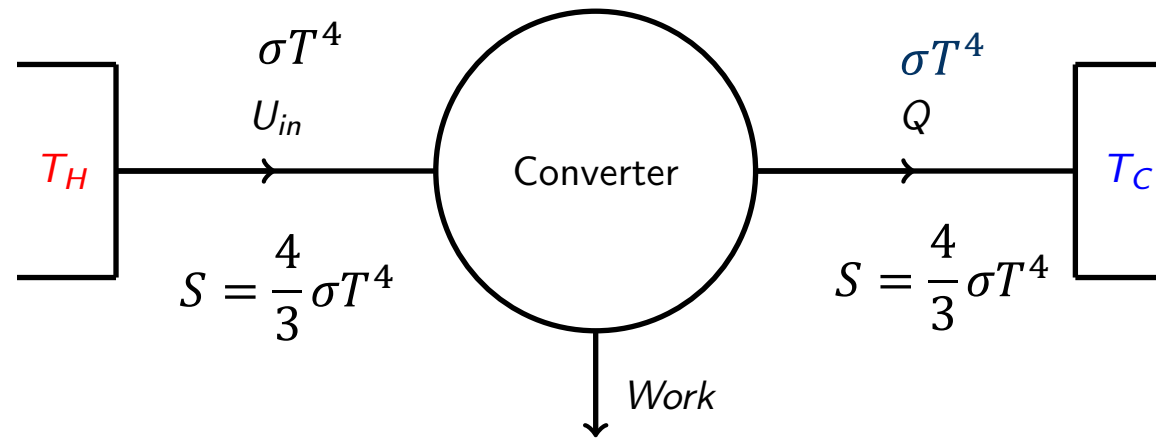
➤ What does thermodynamics tell-us: the sky is the limit



➔
$$\eta = 1 - \frac{T_C}{T_H} \approx 95\%$$

No entropy generation





Helmholtz free energy

- The useful work: $F = U_{in} - T \times S$

$$\Rightarrow \eta = 1 + \frac{1}{3} \frac{T_C^4}{T_H^4} - \frac{4}{3} \frac{T_C^4}{T_H^4} \approx 86\%$$

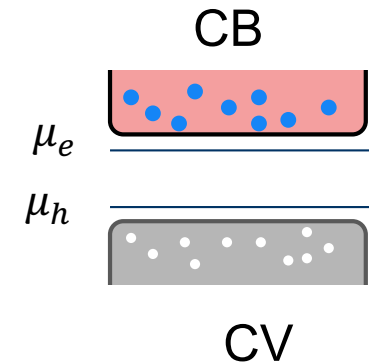
keep in mind

$$S = k_B \log \Omega$$



μ = variation of the free energy when adding/removing 1 particle

$$\mu_e = \left. \frac{\partial F}{\partial N_e} \right|_{V, T, N_h}$$



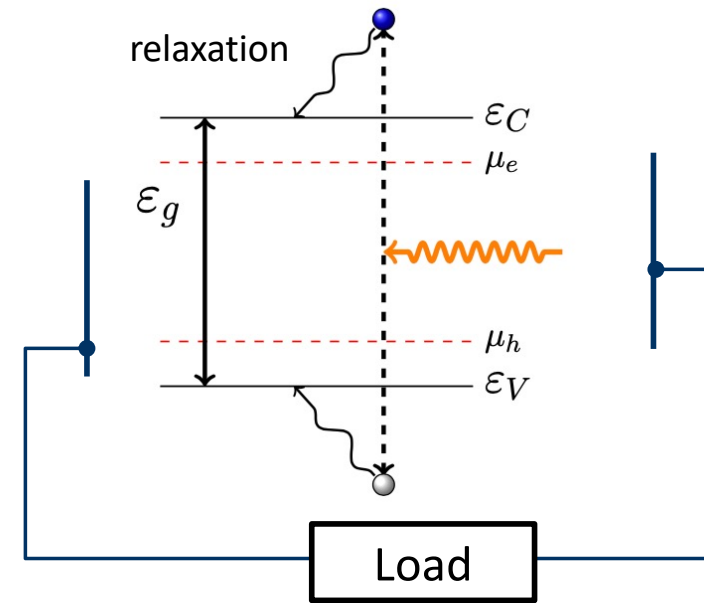
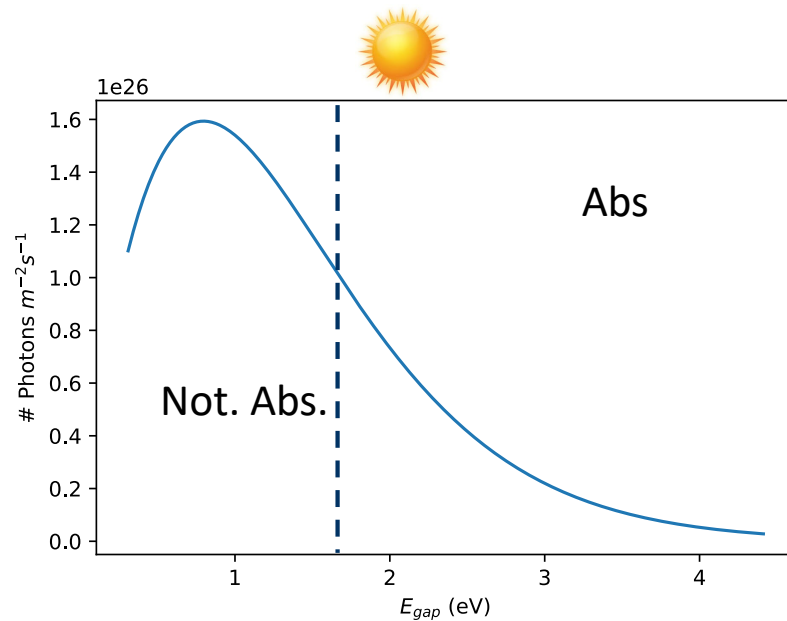
Change in free energy = maximal amount of work recoverable over the transformation

Remove 1 electron from CB, add 1 electron to VB $\longrightarrow W_{\text{out}} = \Delta F = \mu_e - \mu_h$

→ If two systems exchange energy, they will same temperature

→ If they exchange particle, they will reach same chemical potential

Basic concepts



$$J = q \dot{N} \propto q \int_{\hbar\omega > \epsilon_g}^{\infty} \phi_s(\hbar\omega) d\omega$$



→ Energy par electron $\sim \epsilon_g$

→ Useful power: $P = \dot{N} \times W = J \times q \times \Delta\mu$

$\underbrace{\hspace{1.5cm}}_V$

What is the best solar cells ?

Carriers (absorption) and collection

→ how carriers are collected ?

$$\vec{J}_{e,h} = \sigma_{e,h} \vec{\nabla} \left(\frac{\mu_{e,h}}{q} \right)$$

Selectivity:

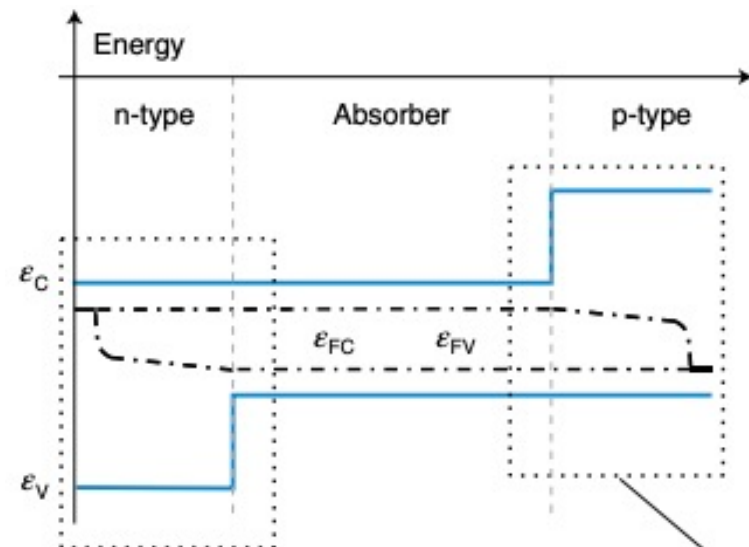
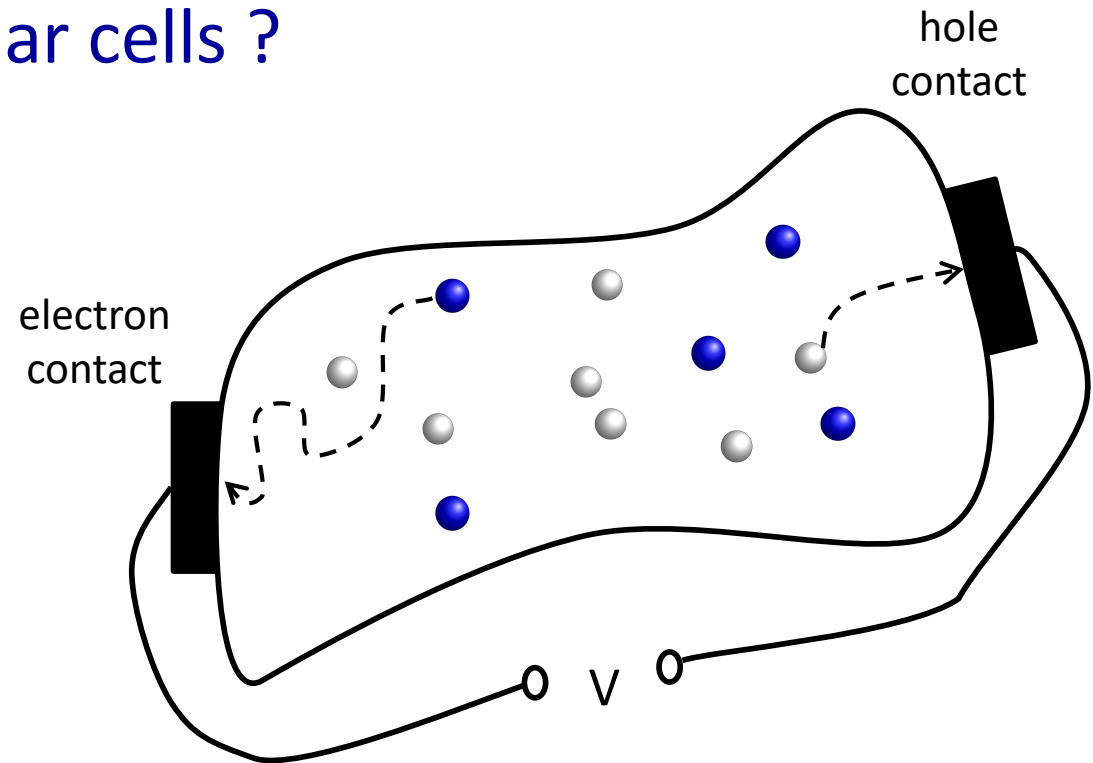
e/h have to move toward different contacts (assymetry)

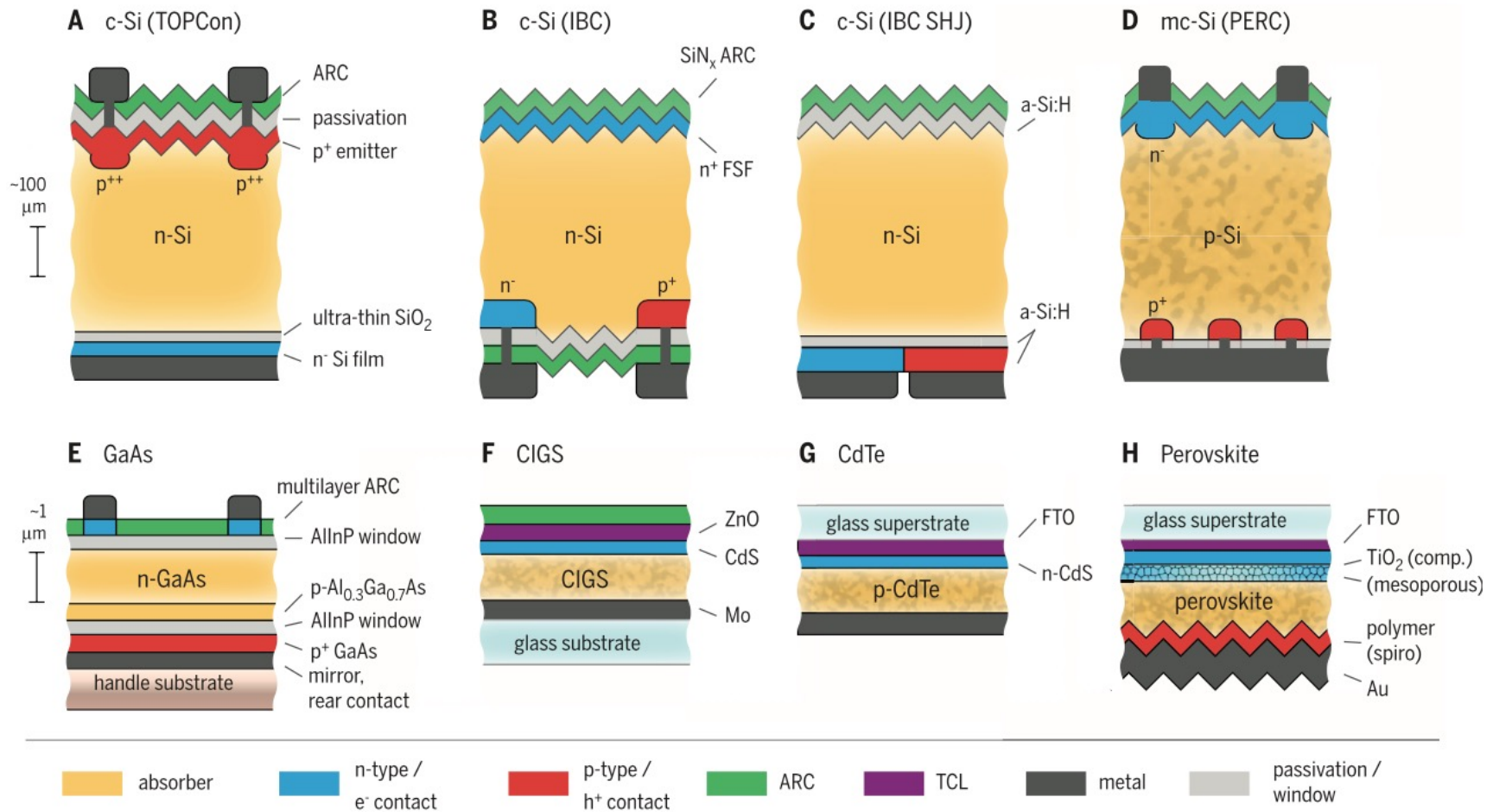
→ incomplete light absorption → α

→ Charge-carrier transport → μ

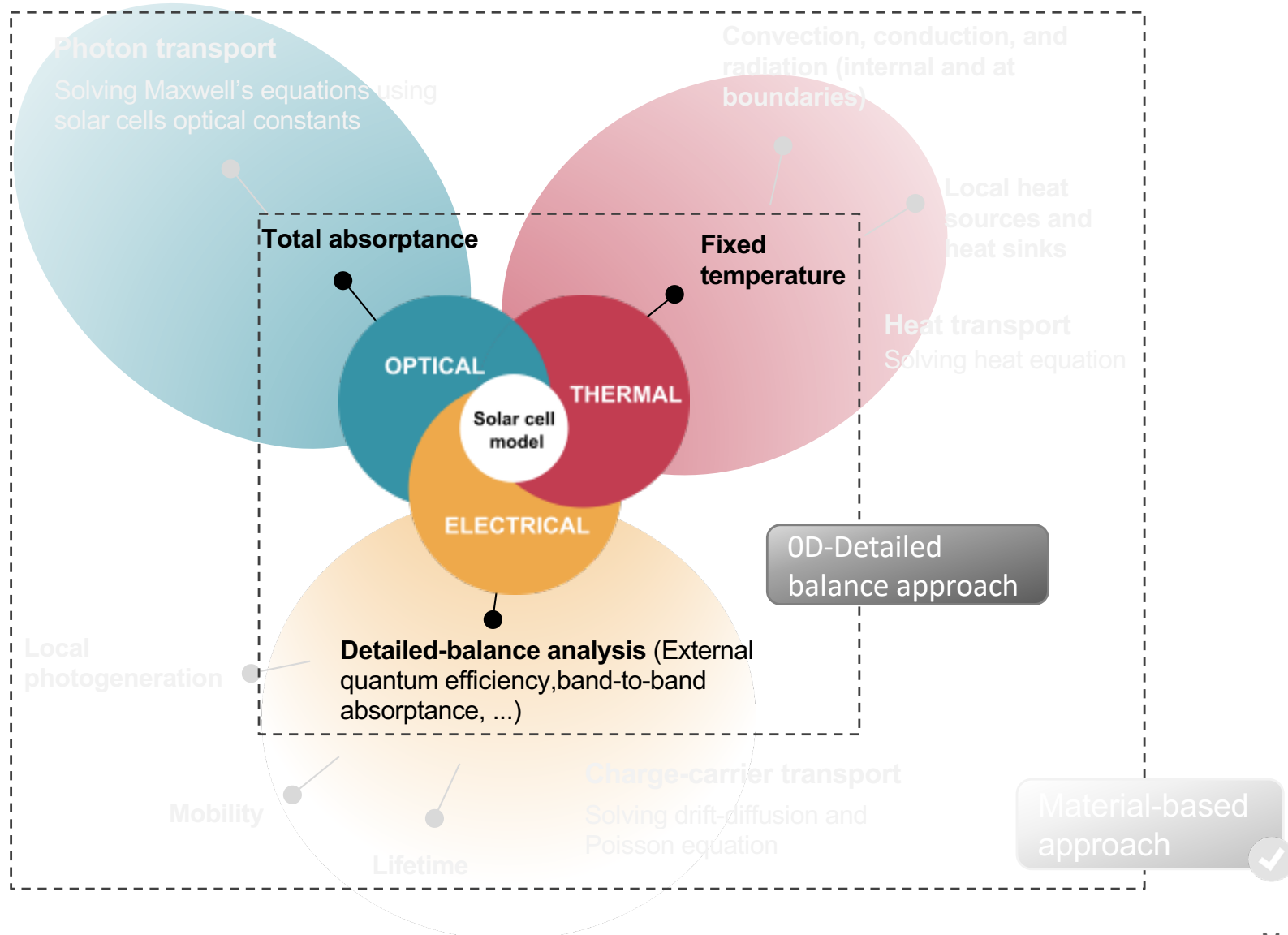
→ Charge-carrier recombination → τ

$\alpha \mu \tau$ the higher is the better



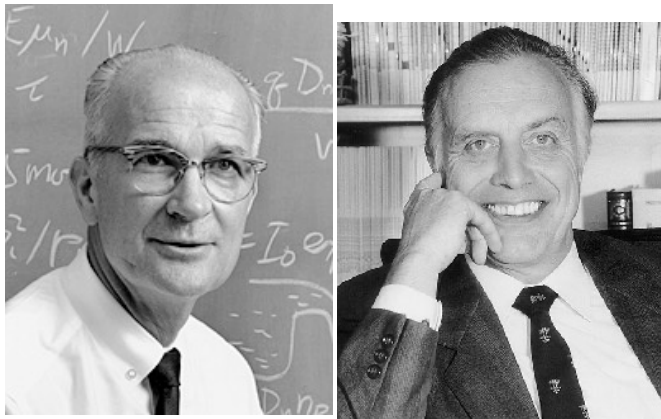


- A detailed opto-electro-thermal (OET) modelling approach



Detailed Balance Limit of Efficiency of p - n Junction Solar Cells*

WILLIAM SHOCKLEY AND HANS J. QUEISSER
Shockley Transistor, Unit of Clevite Transistor, Palo Alto, California
 (Received May 3, 1960; in final form October 31, 1960)



→ “harshly” rejected after its first submission to JAP in 1960
 → cited ~13,1700 times until its publication in 1961.

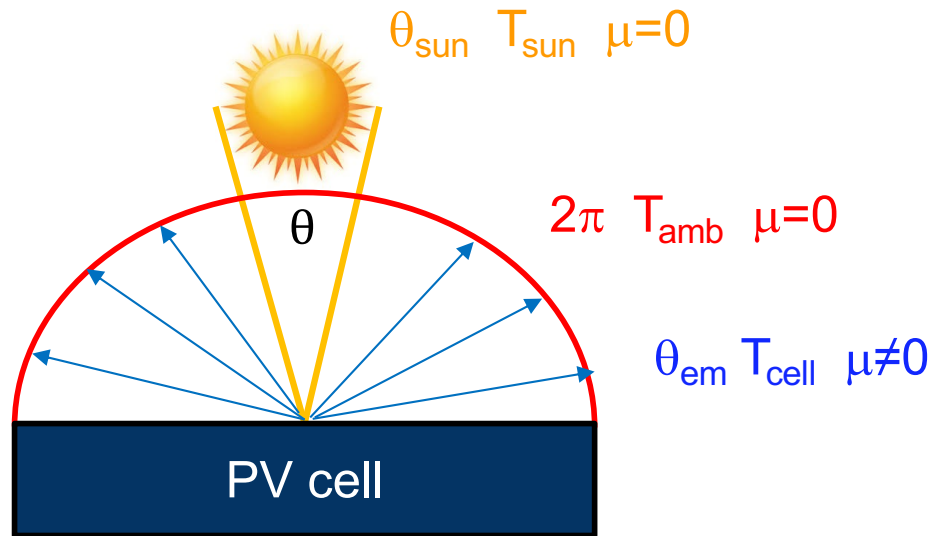
W. Shockley (1910-1989)
 Nobel Prize in Physics in 1956

H. Queisser

→ Only 3 parameters are required

- Temperature of the Sun
- Ambient temperature
- Electronic gap of the SC material

Shockley Queisser limit



$$\dot{N}(\hbar\omega) = \theta \frac{2\pi}{h^3 c^2} \int_{E_i}^{E_j} \frac{(\hbar\omega)^2}{e^{\frac{\hbar\omega - \mu}{k_B T}}} d(\hbar\omega)$$

The Würfel generalised black-body law

If the cell absorbe photon, it must emit lighth

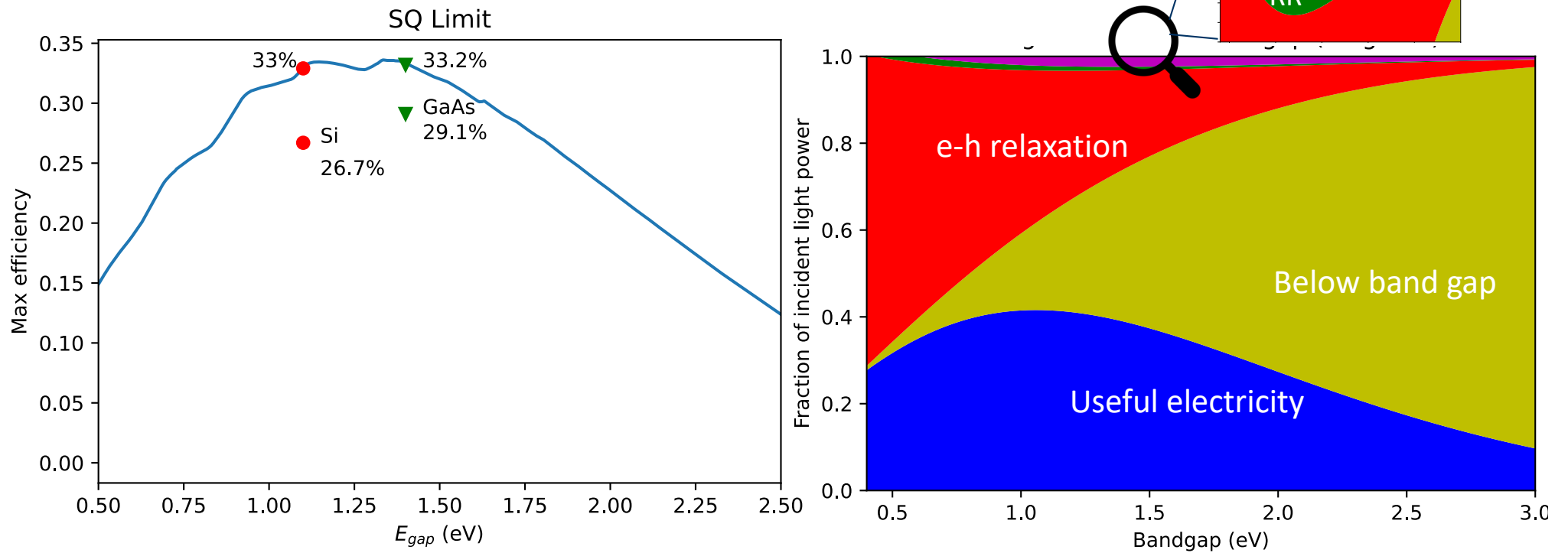
$$W_{elec} = \dot{N}_{sun}(\theta_{sun}, T_{sun}, E_i, E_j, \mu = 0) + \dot{N}_{amb}(2\pi, T_{amb}, E_i, E_j, \mu = 0) - \dot{N}_{em}(\theta_{em}, T_{amb}, E_i, E_j, \mu \neq 0)$$

→ The maximum electric work which can be extracted from a solar cell can be written as the difference between absorbed and emitted radiation.

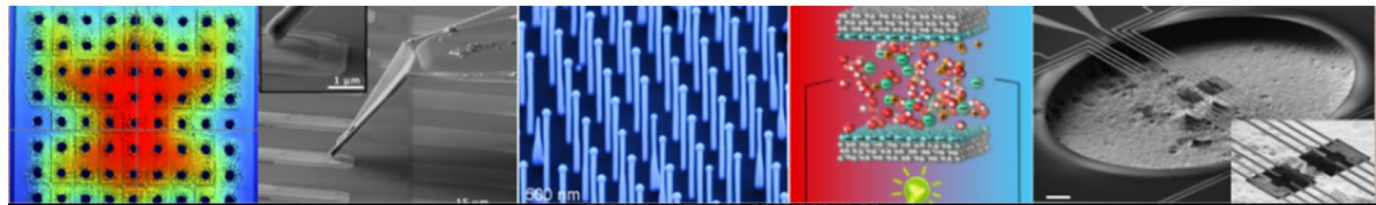
→ A loss due to radiative recombination is fundamental i.e. unavoidable



Shockley Queisser limit



→ For silicon: the more realistic limit is about 29.1 %



This tutorial was prepared by M. Amara (mohamed.amara@insa-lyon.fr) for the MONACOST School 2022

The code is adapted from the work of Steve Byrnes

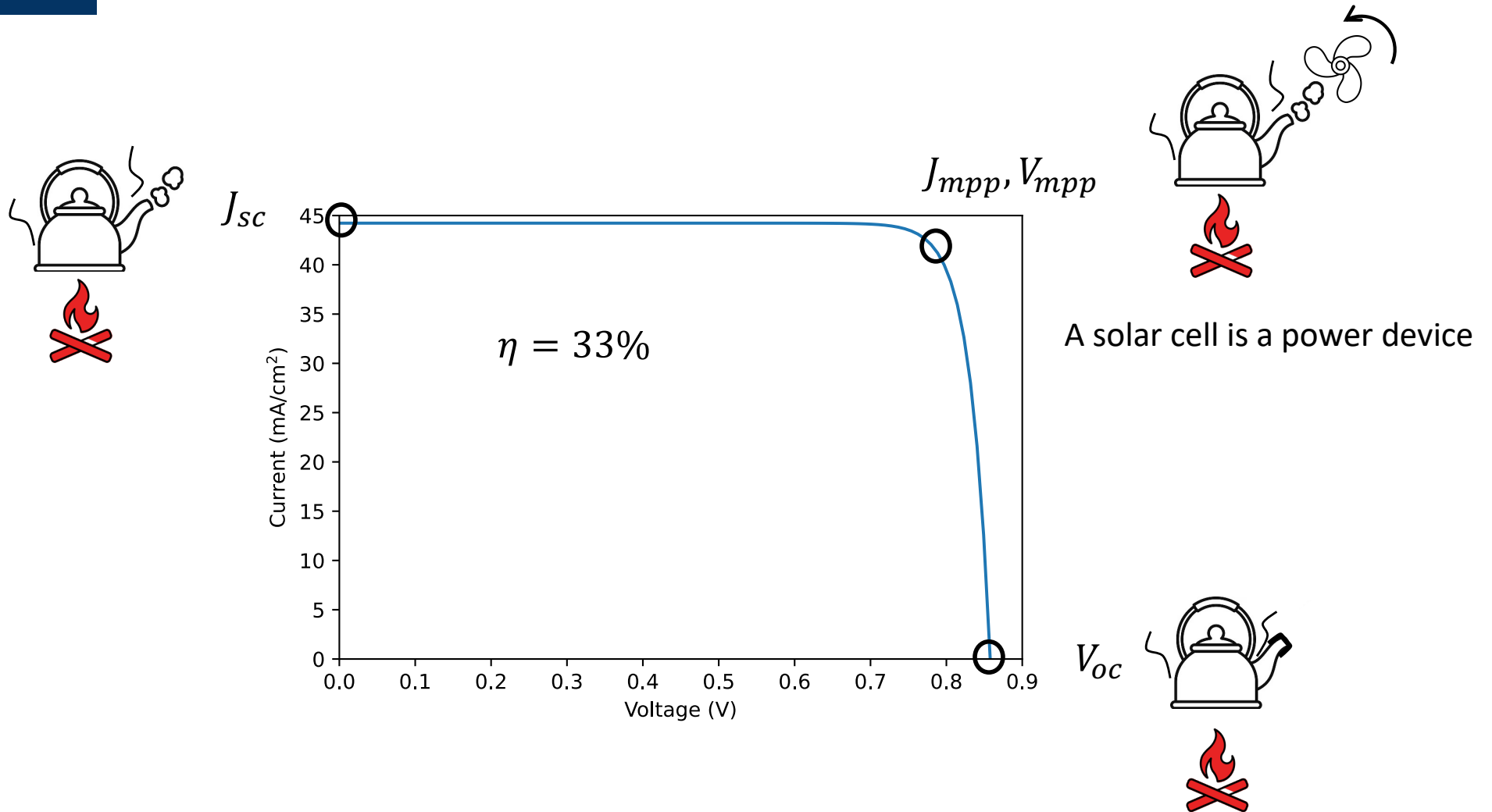
Shockley-Queisser Limit Calculator

```
Entrée [59]: import math
import numpy as np
import matplotlib.pyplot as plt
import scipy.interpolate, scipy.integrate, pandas, sys
import scipy.constants as constants

# SciPy only comes with minimization, not maximization. Let's fix that...
from scipy.optimize import fmin
def fmax(func_to_maximize, initial_guess=0):
    """return the x that maximizes func_to_maximize(x)"""
    func_to_minimize = lambda x : -func_to_maximize(x)
    return fmin(func_to_minimize, initial_guess, disp=False)[0]

#Problem constants
```

The current voltage curve

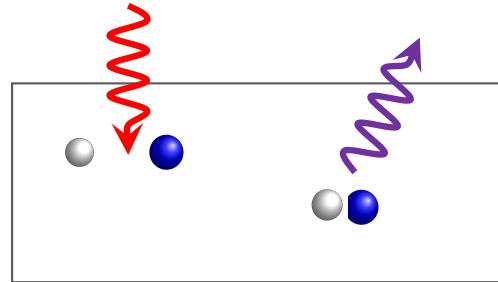


Diode equation $\longrightarrow J = J_{sc} - J_0 \left(e^{\frac{qV}{k_B T}} - 1 \right)$

How can we improve voltage ?

Absorption
of sunlight

Radiative
emission

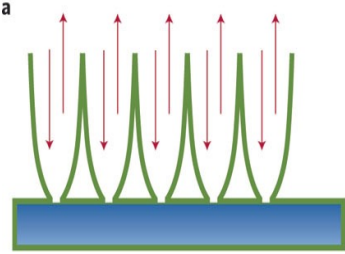


Poor light extraction

$$qV_{oc} = k_B T_c \log \left(\frac{\iint A(E, \theta) \phi_s(E) \cos \theta dE d\theta}{\iint A(E, \theta) \phi_{bb}(E, T_c) \cos \theta dE d\theta} \right) + k_B T_c \log Q_e^{LED}$$

How can we improve voltage ?

a



Directivity information
-280 meV

Photon cooling :
+77 meV

Poor quantum efficiency
- [0-300] meV

$$qV_{oc} \approx E_g \left(1 - \frac{T_c}{T_s}\right) + k_B T_c \log \frac{T_s}{T_c} + k_B T_c \log \left(\frac{\Omega_{in}}{\Omega_{out}}\right) + k_B T_c \log(Q_e^{LED})$$

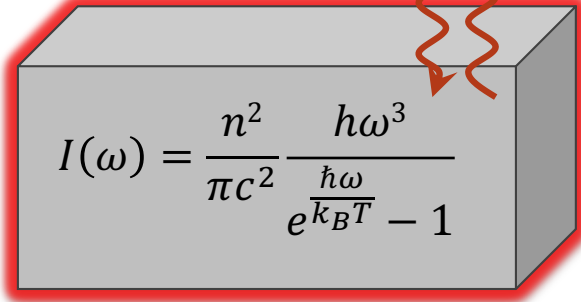
$\underbrace{\hspace{10em}}$
 $F = U_{in} \cdot$

$-$

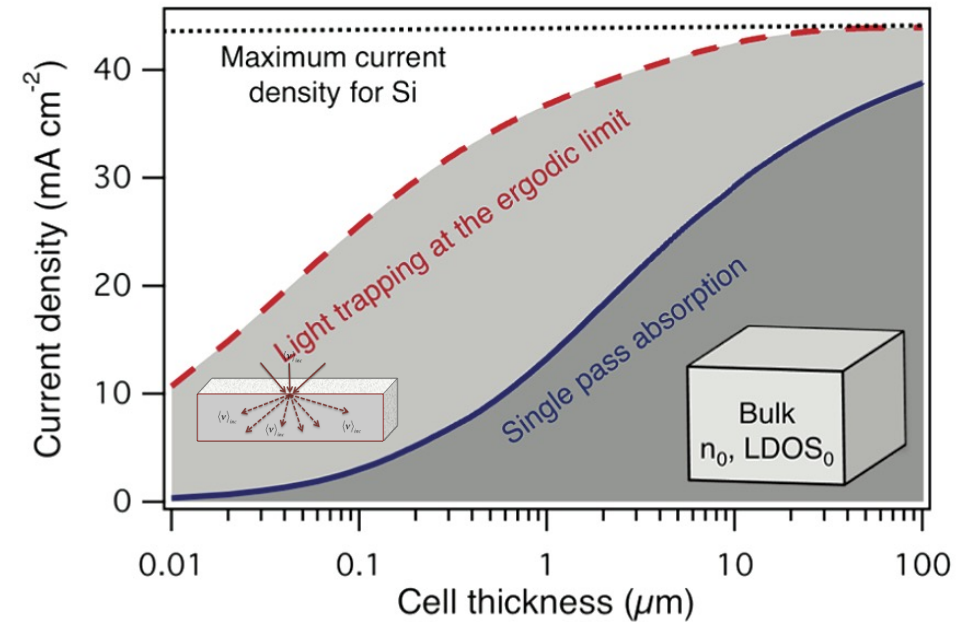
$\underbrace{\hspace{10em}}$
 $T \times S$

- A small band gaps are particularly vulnerable to entropy

How can we improve current ?

$$I(\omega) = \frac{1}{\pi c^2} \frac{\hbar \omega^3}{e^{\frac{\hbar \omega}{k_B T}} - 1}$$


$$I(\omega) = \frac{n^2}{\pi c^2} \frac{\hbar \omega^3}{e^{\frac{\hbar \omega}{k_B T}} - 1}$$

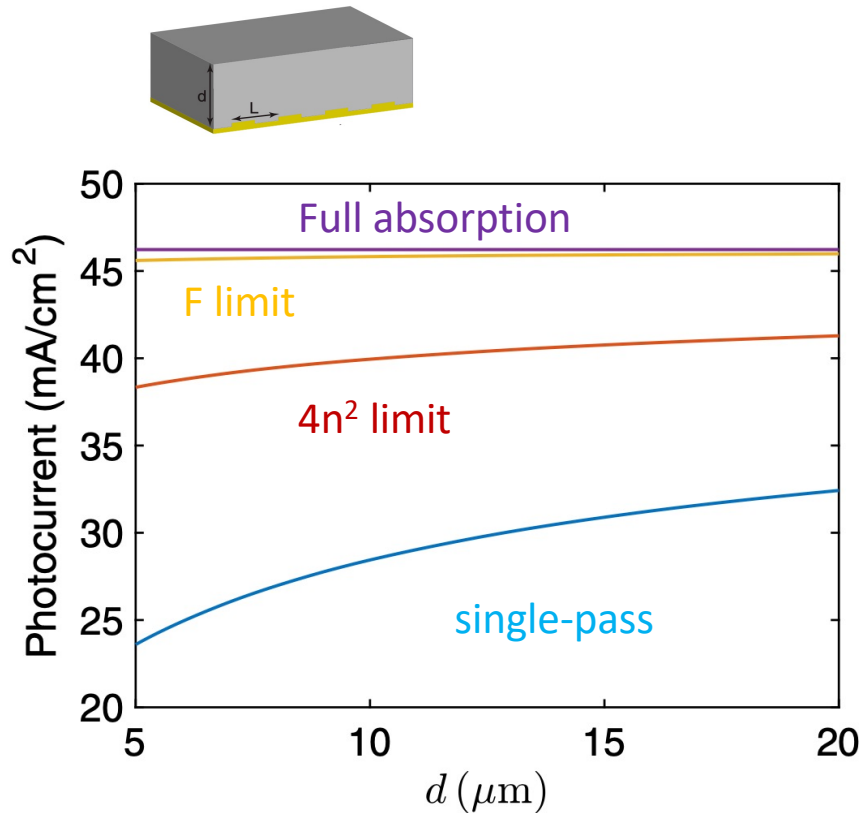


- In weakly absorbing medium, $4n^2$ absorption enhancement (for Si, ~50x)
- Reduce costs by reduced materials consumption and improved throughput (CIGS, CdTe)

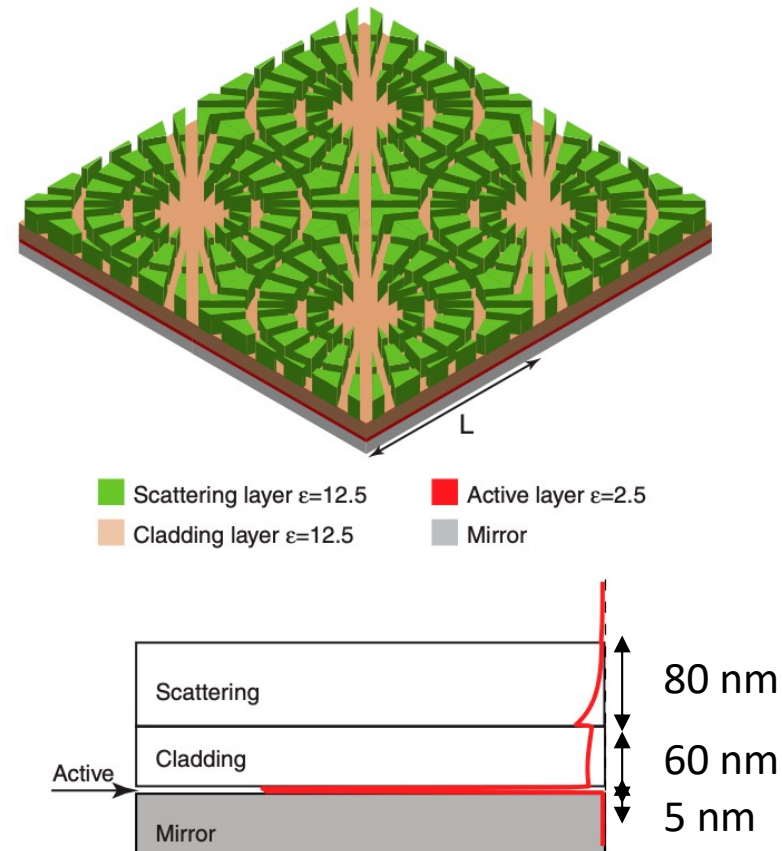
How can we improve current ?

Ultimate limit of nanophotonic light trapping : Beating the $4n^2$ ray optic limit

Numerical validation



$$F(\omega) = \left(\alpha d + \frac{\pi}{2} \left(\frac{c}{n\omega L} \right)^2 \right)^{-1}$$

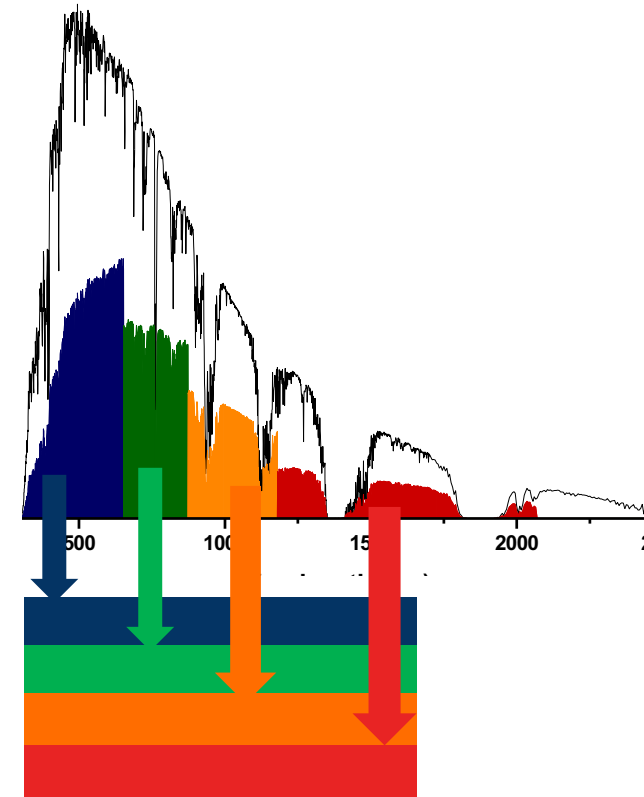


$12 \times 4n^2$ absorption enhancement

Beyond SQ: multi-junction solar cells

- MJ cells are designed assuming a given combination of: spectral content of the light ($f(\lambda)$), temperature (T_c), and illumination level (X).
- Achieving high solar → electricity efficiency requires to find the $(E_1, \dots, E_n)$ combination of band gaps for which the power of the whole stack is maximized

$$P_{ij}(X, f, T_c) = \max \left\{ \mu \left(X \int_{E_i}^{E_j} f_{\text{sun}}(E) dE \right. \right. \\ \left. \left. + \frac{2\pi}{h^3 c^2} \int_{E_i}^{E_j} \frac{E^2}{\exp\left(\frac{E}{kT_a}\right) - 1} dE \right. \right. \\ \left. \left. - \frac{2\pi}{h^3 c^2} \int_{E_i}^{E_j} \frac{E^2}{\exp\left(\frac{E - \mu}{kT_c}\right) - 1} dE \right) \right\}$$



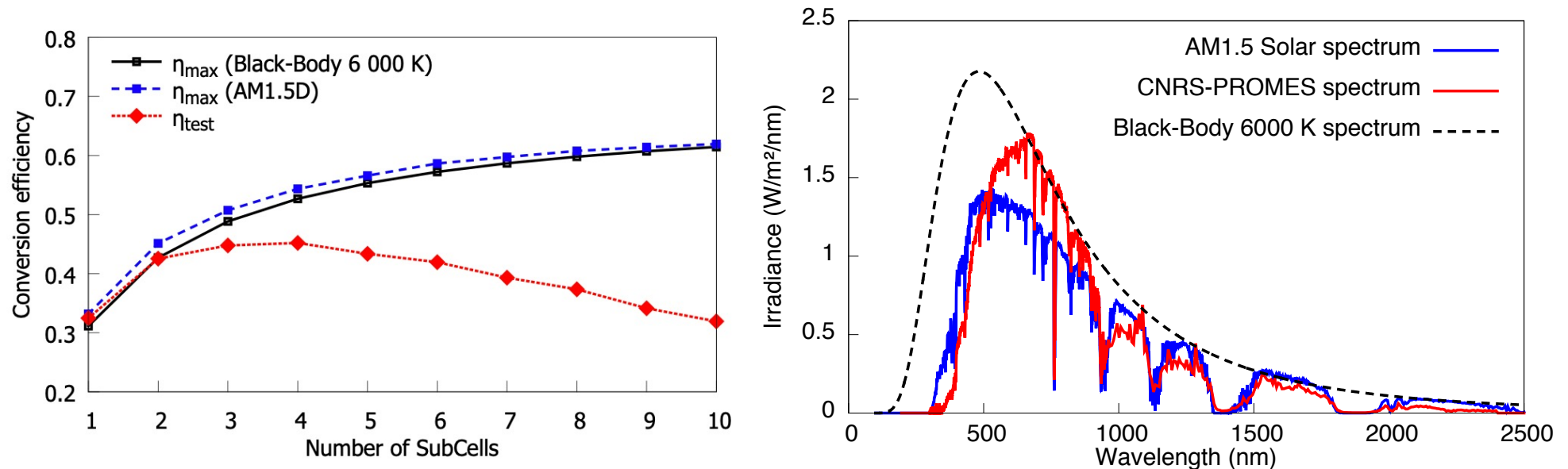
Current matching condition between subcells

TABLE I. OPTIMUM EFFICIENCIES AND BANDGAPS FOR MJ SOLAR CELLS COMPRISING UP TO 10 SUBCELLS, UNDER AM1.5D AND 6 000 K BLACK-BODY SPECTRUM, AND FOR ONE-SUN ILLUMINATION

Spectrum	N. cell	Band gap [eV]										Efficiency [%]
		Eg 1	Eg 2	Eg 3	Eg 4	Eg 5	Eg 6	Eg 7	Eg 8	Eg 9	Eg 10	
AM1.5D	1	1.14	–	–	–	–	–	–	–	–	–	33.2
	2	1.57	0.94	–	–	–	–	–	–	–	–	45.1
	3	1.75	1.18	0.7	–	–	–	–	–	–	–	50.7
	4	1.94	1.44	1.05	0.7	–	–	–	–	–	–	54.4
	5	2.07	1.61	1.26	0.99	0.7	–	–	–	–	–	56.6
	6	2.18	1.74	1.44	1.17	0.95	0.68	–	–	–	–	58.7
	7	2.27	1.85	1.56	1.33	1.12	0.92	0.70	–	–	–	59.8
	8	2.29	1.88	1.59	1.37	1.16	0.96	0.74	0.5	–	–	60.8
	9	2.35	1.96	1.69	1.47	1.26	1.09	0.94	0.74	0.53	–	61.4
	10	2.41	2.03	1.77	1.56	1.39	1.21	1.05	0.92	0.74	0.55	62
Black-Body 6 000 K	1	1.30	–	–	–	–	–	–	–	–	–	31.1
	2	1.68	0.96	–	–	–	–	–	–	–	–	42.7
	3	1.95	1.30	0.82	–	–	–	–	–	–	–	48.9
	4	2.12	1.51	1.08	0.70	–	–	–	–	–	–	52.7
	5	2.28	1.69	1.30	0.97	0.66	–	–	–	–	–	55.3
	6	2.40	1.82	1.45	1.15	0.88	0.60	–	–	–	–	57.2
	7	2.51	1.95	1.59	1.30	1.05	0.82	0.58	–	–	–	58.7
	8	2.59	2.04	1.68	1.41	1.17	0.96	0.75	0.52	–	–	59.8
	9	2.68	2.13	1.79	1.52	1.30	1.10	0.91	0.72	0.52	–	60.7
	10	2.73	2.20	1.86	1.60	1.38	1.19	1.01	0.84	0.67	0.48	61.4

Multi-junction solar cells: Influence of the spectrum

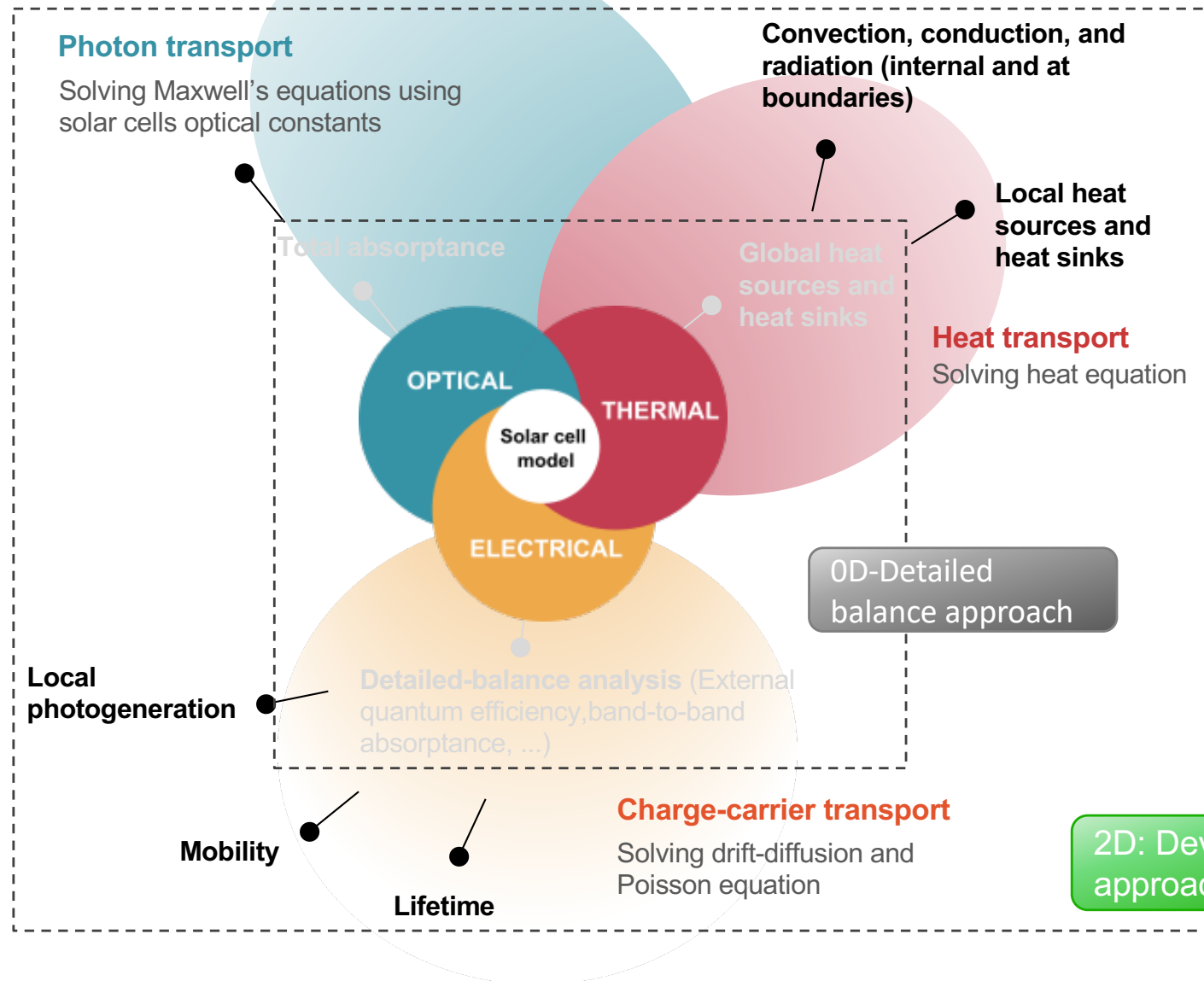
Applying AM1.5D spectrum to a 6000K BB optimized MJ solar cell



- Above 4 subcells, the penalty associated with the extra sensitivity of the device is not counterbalanced by the gain in efficiency brought by the extra subcells.

About opto-electro-thermal modelling

■ A detailed opto-electro-thermal (OET) modelling approach



Objectives

Describe ←
Explain ←
Predict ←
and optimize.. ←
the OET behavior **in real operating conditions**

Challenges

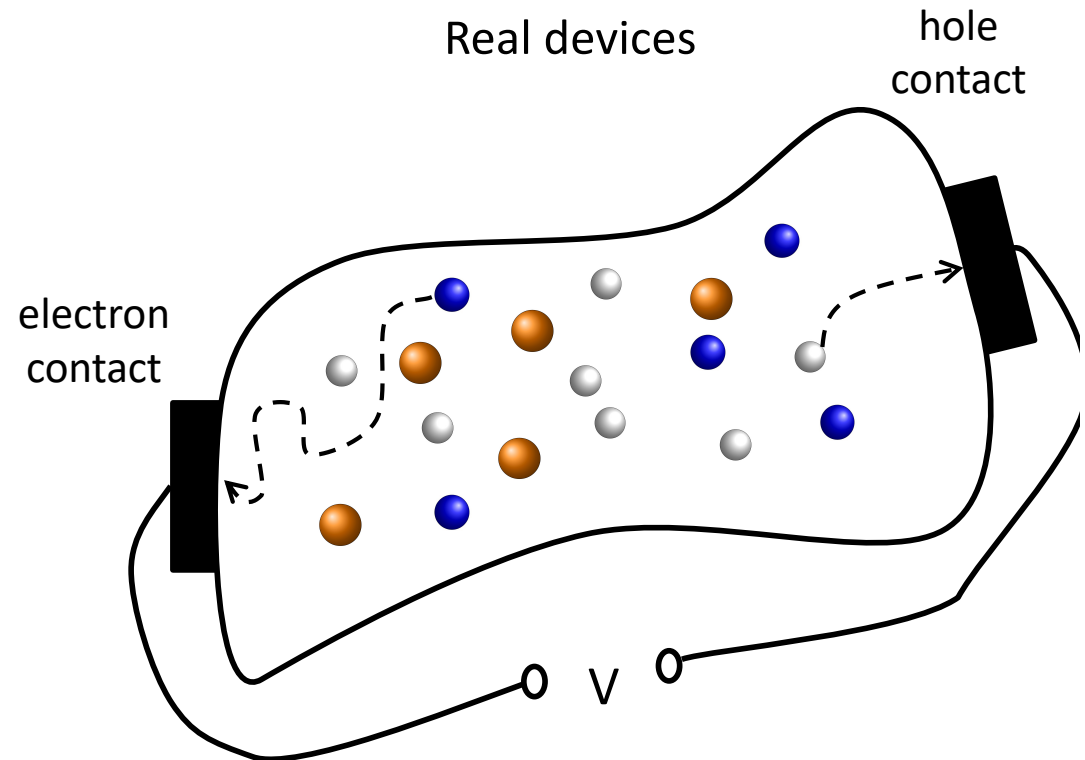
Heat transfer in active ←
layers (silicon)
Material properties ←
Multiphysics coupling ←



- Thermodynamics of irreversible processes: Onsager-Callen theory

$$-\vec{J}_N = L_{11} \frac{1}{T} \vec{\nabla} \mu + L_{12} \vec{\nabla} \frac{1}{T}$$

$$\vec{J}_Q = L_{12} \frac{1}{T} \vec{\nabla} \mu + L_{22} \vec{\nabla} \frac{1}{T}$$



$L_{i,j}$ Calculated with Boltzmann equation under the relaxation time approximation



➤ Thermodynamics of irreversible processes: Onsager-Callen theory

Current density

$$\vec{J}_n = qD_n \vec{\nabla} n + q\mu_n \Pi_n \frac{\vec{\nabla}(T)}{T} + q\mu_n n \left(\vec{E} - \frac{\vec{\nabla}\chi}{q} - \frac{k_B T}{q} \vec{\nabla}(\ln(N_c)) \right)$$

$$\vec{J}_p = -qD_p \vec{\nabla} p - q\mu_p \Pi_p \frac{\vec{\nabla}(T)}{T} + q\mu_p p \left(\vec{E} - \frac{\vec{\nabla}\chi}{q} - \frac{\vec{\nabla}(\varepsilon_G)}{q} + \frac{k_B T}{T} \vec{\nabla}(\ln(N_v)) \right)$$

Diffusion

Drift

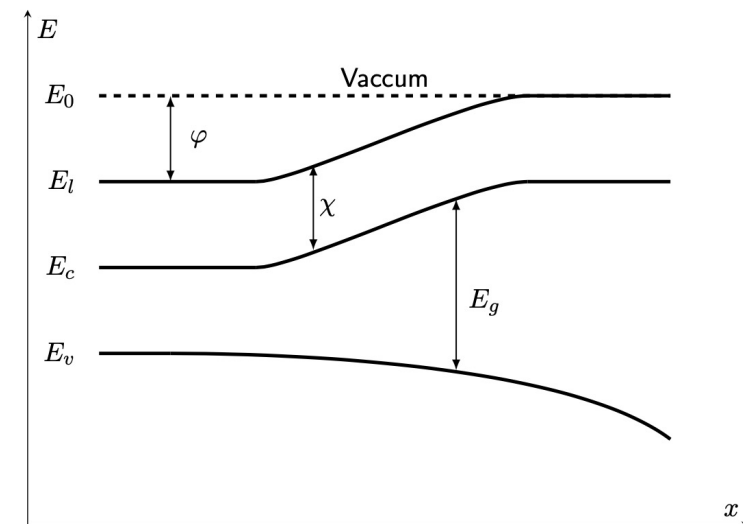
$$\vec{\nabla} \cdot \vec{J} = q(R - G)$$

$$\epsilon \Delta V = q(p - n + N)$$

Continuity

Energy current density

$$\vec{J}_u = -(\Pi_n - \varepsilon_{FC}) \vec{J}_n + (\Pi_p - \varepsilon_{FV}) \vec{J}_p - \lambda \vec{\nabla}(T)$$

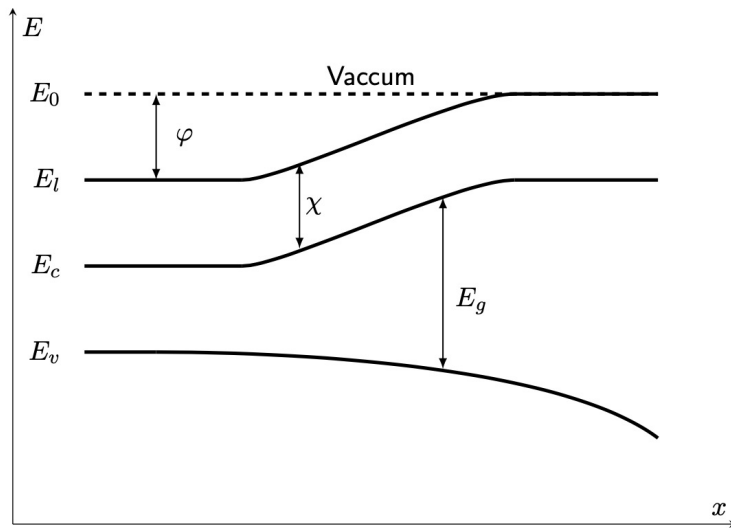




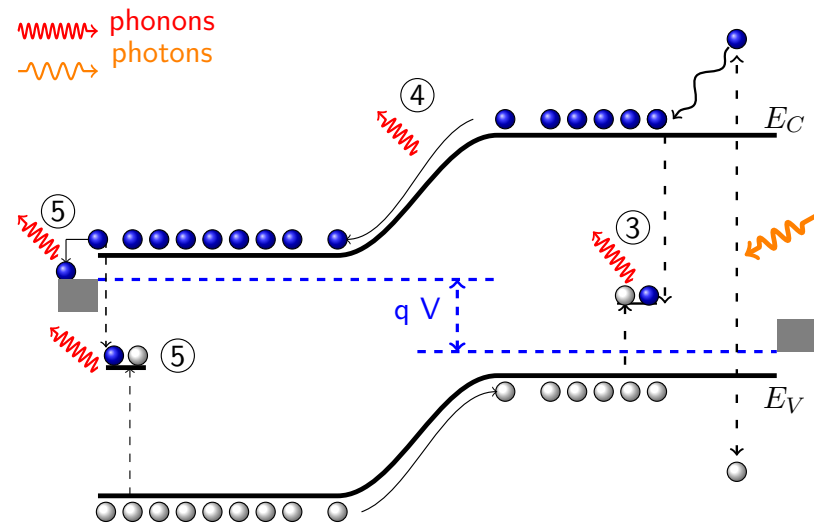
→ General formulation of heat source

$$H = \vec{E} \cdot \vec{J} + (E_g + 3k_B T) \cdot R - \vec{J}_n \cdot \vec{\nabla} \left(\chi - \frac{3k_B T}{q} \right) - \vec{J}_p \cdot \vec{\nabla} \left(\chi + \frac{1}{q} E_g + \frac{3k_B T}{q} \right) + \vec{\nabla} \cdot \{ \pi_n^0 \vec{J}_n - \pi_p^0 \vec{J}_p \} + H_T - S_r$$

ligh



A More general device

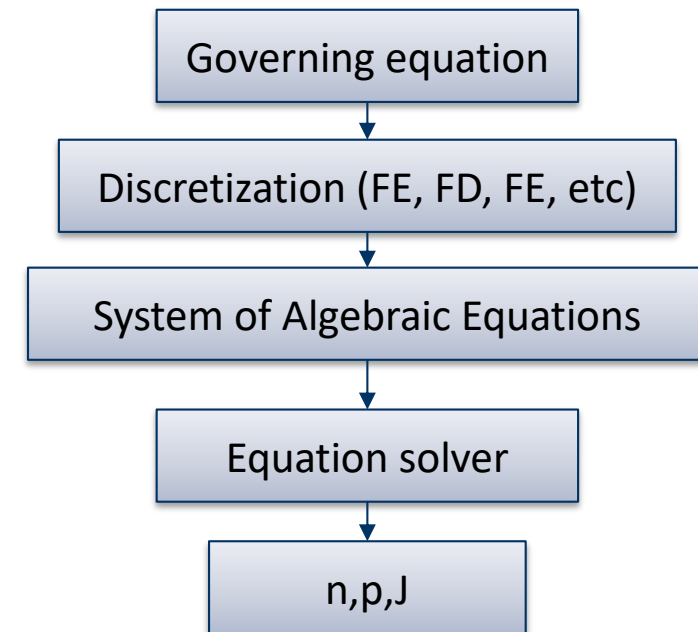


PN junction



- Scaling of variables

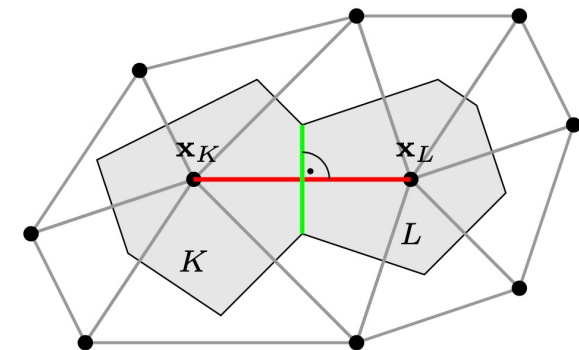
- ✓ Concentration (n, p, N_c, N_v) $\rightarrow \text{Max}(N_A, N_D) \approx 10^{20} \text{cm}^{-3}$
- ✓ Length (h_i, h_j) $\rightarrow$ cell maximum dimension $\approx 1\text{-}200 \mu\text{m}$
- ✓ Temperature $\rightarrow T_{\text{amb}}$
- ✓ Potential ($V, \frac{\varepsilon_F}{q}, E_g$) $\rightarrow \frac{k_B T_0}{q} \approx 0.0035 \text{ V}$
- ✓ mobility ($\mu_{n,h}$) $\rightarrow \mu_{\text{max}}$



- Scharfetter-Gummel discretization of the continuity equation

$$J_{K \rightarrow L} = \frac{\langle U_T \mu_n \rangle}{X_{K,L}} \left(n_K B\left(\frac{-\Delta V}{U_T}\right) - n_L B\left(\frac{-\Delta V}{U_T}\right) \right)$$

Bernoulli function : $B(x) = \frac{1}{e^x - 1}$





1. Depletion approximation
2. All carriers are decoupled

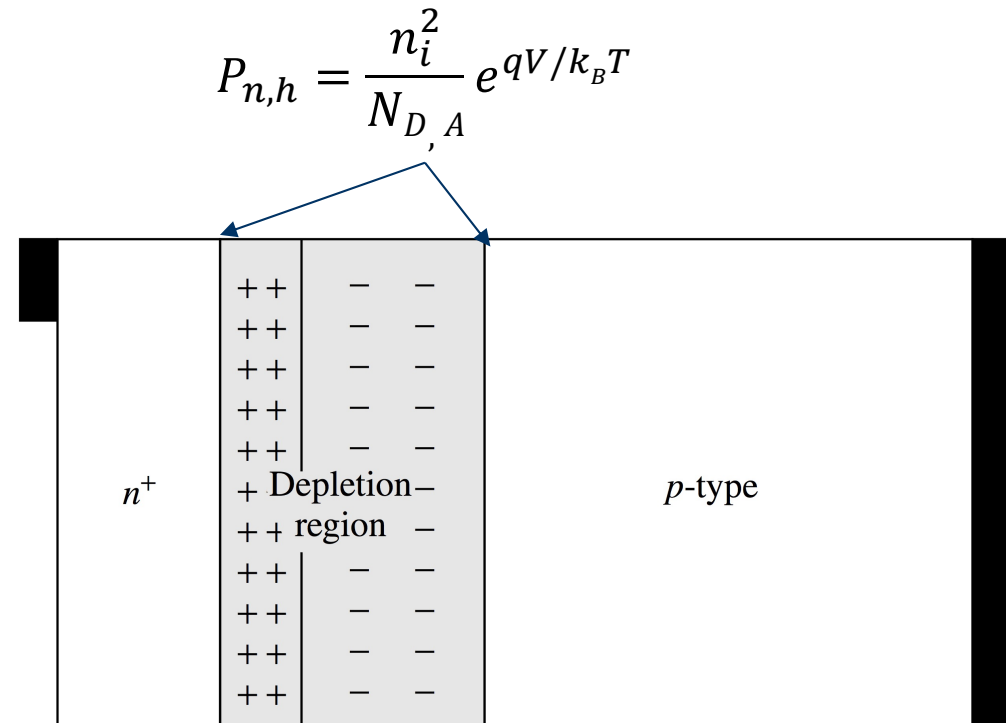
$$D_m \frac{\partial^2 m}{\partial x^2} - \frac{m - m_0}{\tau_m} = -g(x)$$

$$g_{op,\Delta\nu}(x) = \int_{\Delta\nu} \frac{\kappa_{v,interbande}(x) G_v(x)}{h\nu} d\nu$$

$$J = J_N + J_P + J_{DR}$$

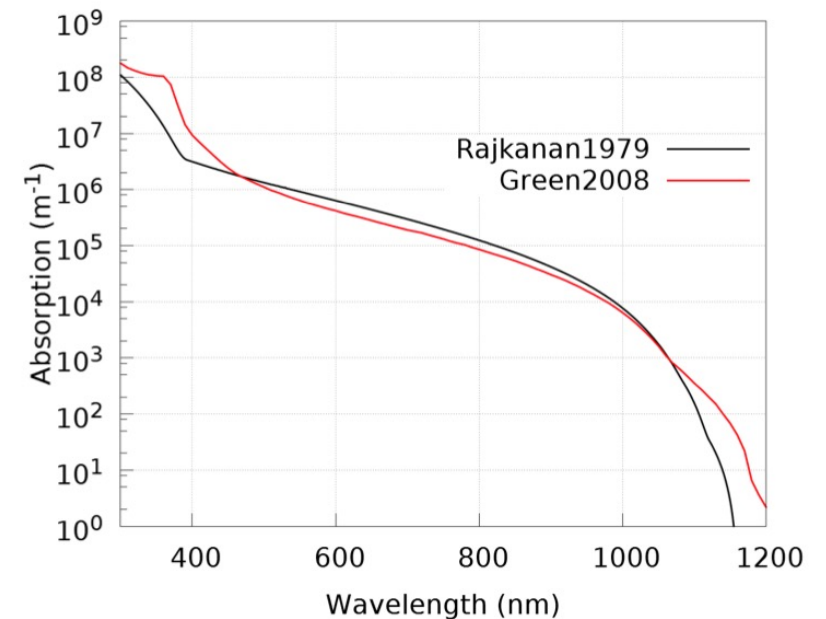
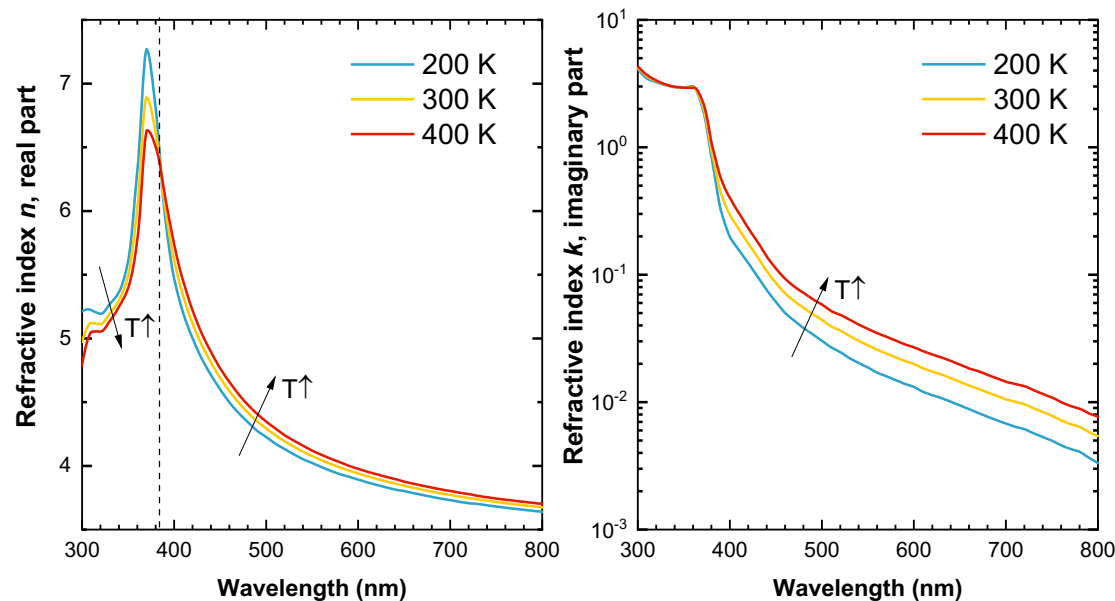
But, be aware

1. Low injection
2. Low series resistance
3. Recombination lifetime $\neq$ illumination



$$\frac{d\Delta n}{dx} = \frac{S}{D_n} \Delta n$$

- Mobility (T), lifetime (T), refractive index (T)
- Green 2008 : Parameterization to determine n and k as a function of temperature
- Rajkanan 1979: Physical model (only for k)
- How about $\lambda > \lambda_g$: very few experimental data (intrinsic silicon)
- How about other semiconductor materials: perovskite ?



$$\alpha(T) = \sum_{i,j} C_i A_j \left[\frac{(E_\lambda - E_{gi} + E_{pi})^2}{e^{E_{pi}/k_B T} - 1} + \frac{(E_\lambda - E_{gi} - E_{pi})^2}{1 - e^{-E_{pi}/k_B T}} \right] + A_d \sqrt{(E_\lambda - E_{gd})}$$

Modelling silicon VIS-NIR-MIR optical properties

→ Objective: Si complex index as a function of temperature and doping in the UV-VIS-NIR-MIR range(0.25-50 μm)

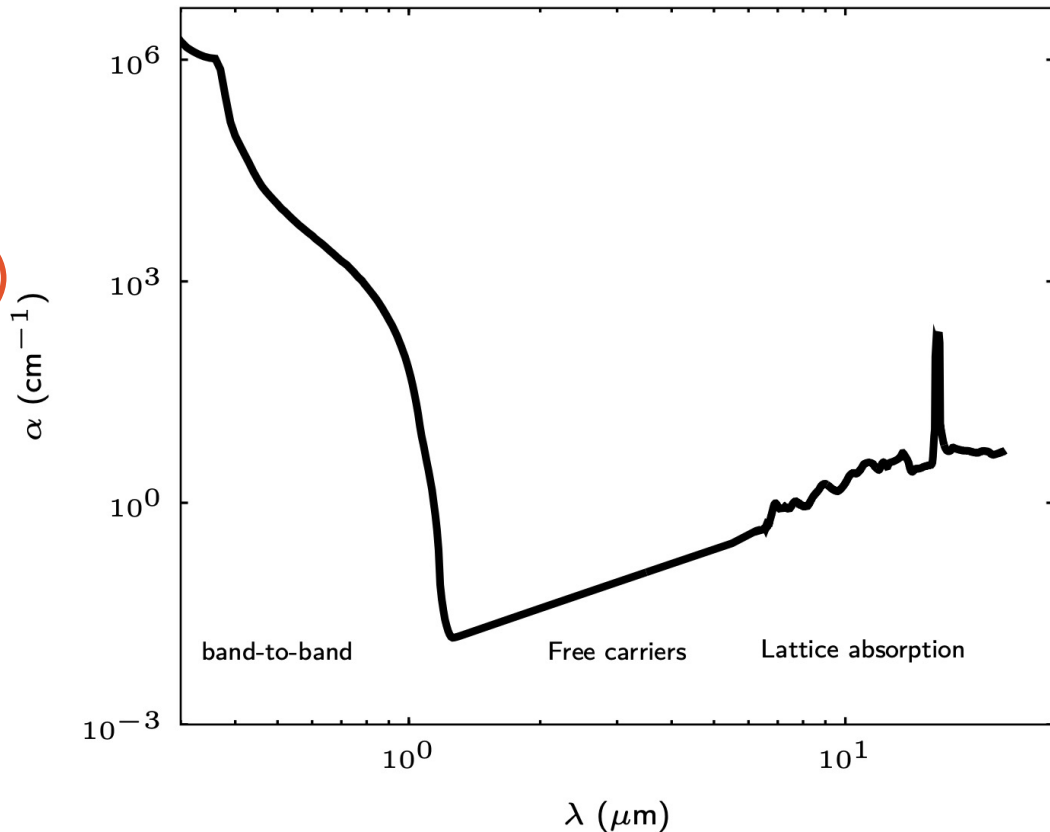
$$N(\omega, T, N_d, N_a) = n + ik = \sqrt{\epsilon}$$

$$\epsilon(\omega) = \epsilon_{bl} + \frac{N_e e^2 / \epsilon_0 m_e^*}{\omega^2 + i\omega/\tau_e} - \frac{N_h e^2 / \epsilon_0 m_h^*}{\omega^2 + i\omega/\tau_h}$$

Two contribution :

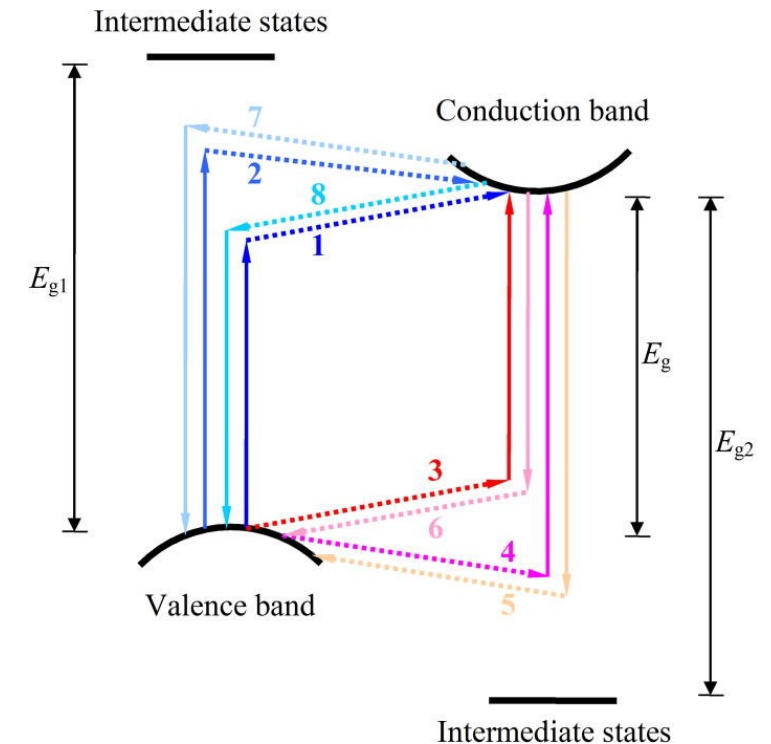
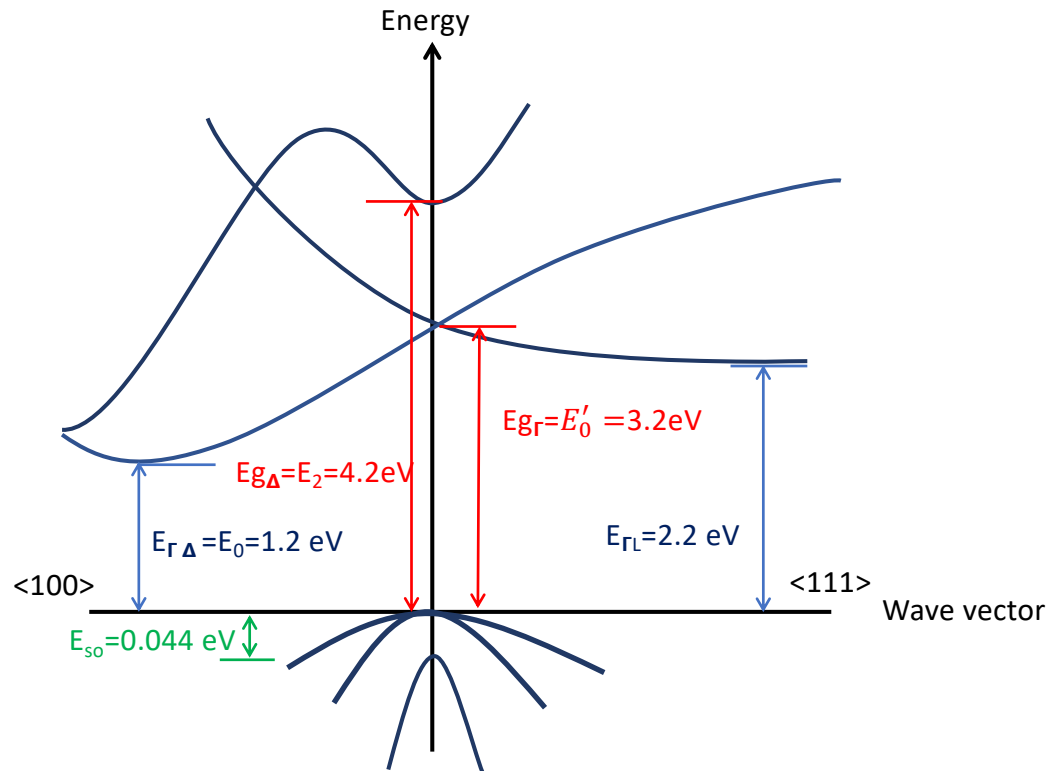
1. inter-bande = f(T)
2. Lattice

3. Free carriers: Drude model



- Effective masses
- N_e et N_h with the calculation of the Fermi level (solving the neutrality equation) = f(T, doping)
- The collision time $\tau_{e,h} = m^* \times \mu / e$

Band gap with temperature



- $E_{g\Delta} = 4.34 - \frac{3.91 \times 10^{-4} T^2}{T+125}$ 3
- $E_{g\Gamma} = 3.354 - \frac{3.5 \times 10^{-4} T^2}{T+580}$ 4
- $E_g^0(T) = E_g^0(0) - \alpha \Theta \left[\gamma + \frac{3\Delta^2}{2} \left(1 + \frac{\pi^2}{3(1+\Delta^2)} \chi^2 + \frac{3\Delta^2-1}{4} \chi^3 + \frac{8}{3} \chi^4 + \chi^6 \right)^{\frac{1}{6}} - 1 \right]$

- 16 processes : absorption/emission of photons and phonons
- $\hbar\omega_{TA} = 18.27 \text{ meV}$ and
- $\hbar\omega_{TO} = 57.73 \text{ meV}$

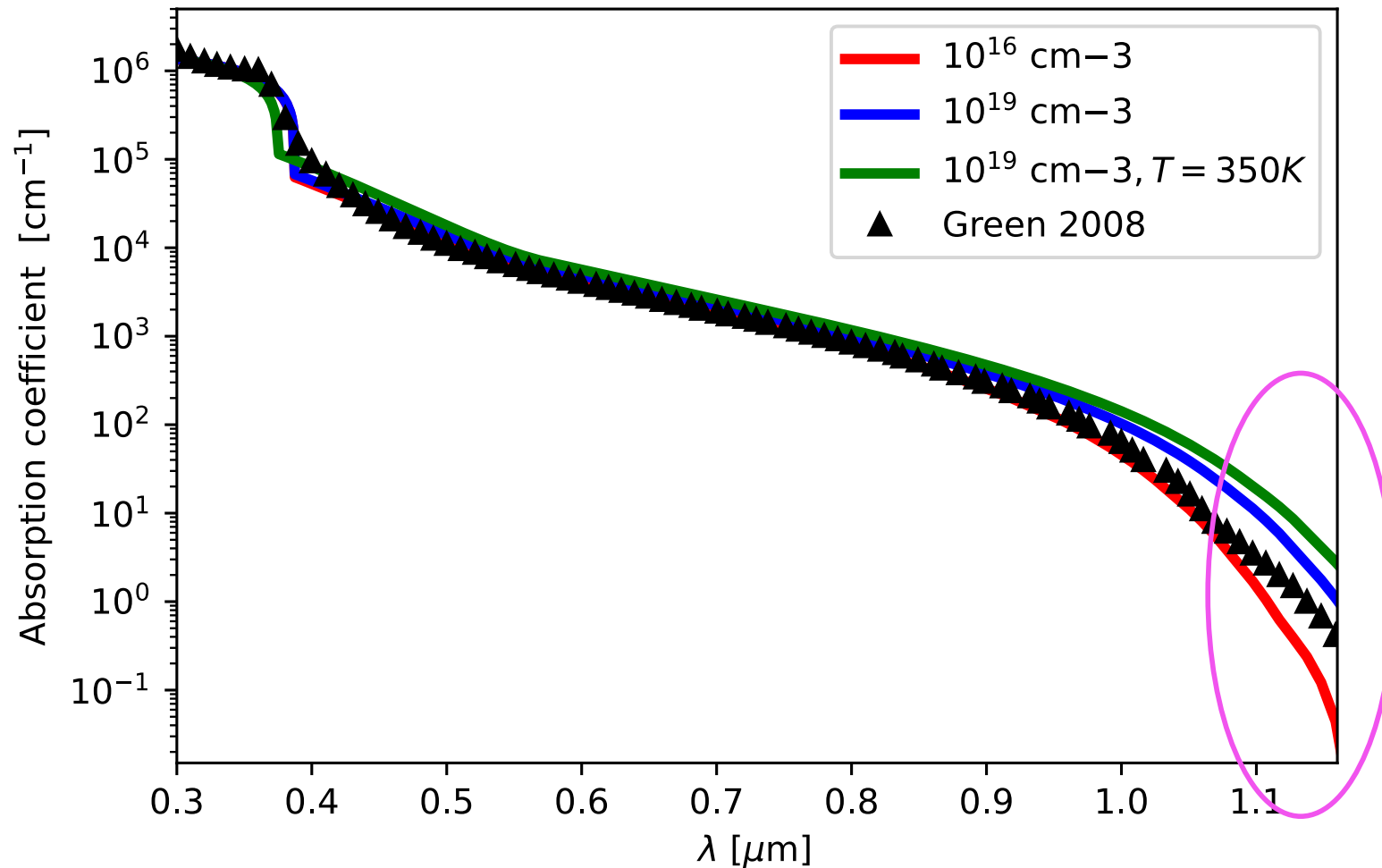


Modelling silicon VIS-NIR-MIR optical properties

Band gap with temperature

$$\begin{aligned}\alpha_{\text{ind}} = \alpha_{\text{ind}0} \frac{E_g}{E_\lambda} & \left[\frac{(E_\lambda - E_g + \hbar\omega_{ij})^2 N_q}{|E_{g1} - E_\lambda - i\Gamma|^2} \text{H}(E_\lambda - E_g + \hbar\omega_{ij}) \right. \\ & + \frac{(E_\lambda - E_g - \hbar\omega_{ij})^2 (N_q + 1)}{|E_{g1} - E_\lambda - i\Gamma|^2} \text{H}(E_\lambda - E_g - \hbar\omega_{ij}) \\ & + \frac{(E_\lambda - E_g + \hbar\omega_{ij})^2 N_q}{|E_{g2} - \hbar\omega_\lambda + i\Gamma|^2} \text{H}(E_\lambda - E_g + \hbar\omega_{ij}) \\ & \left. + \frac{(E_\lambda - E_g - \hbar\omega_{ij})^2 (N_q + 1)}{|E_{g2} - E_\lambda + i\Gamma|^2} \text{H}(E_\lambda - E_g - \hbar\omega_{ij}) \right]\end{aligned}$$

Modelling silicon VIS-NIR-MIR optical properties



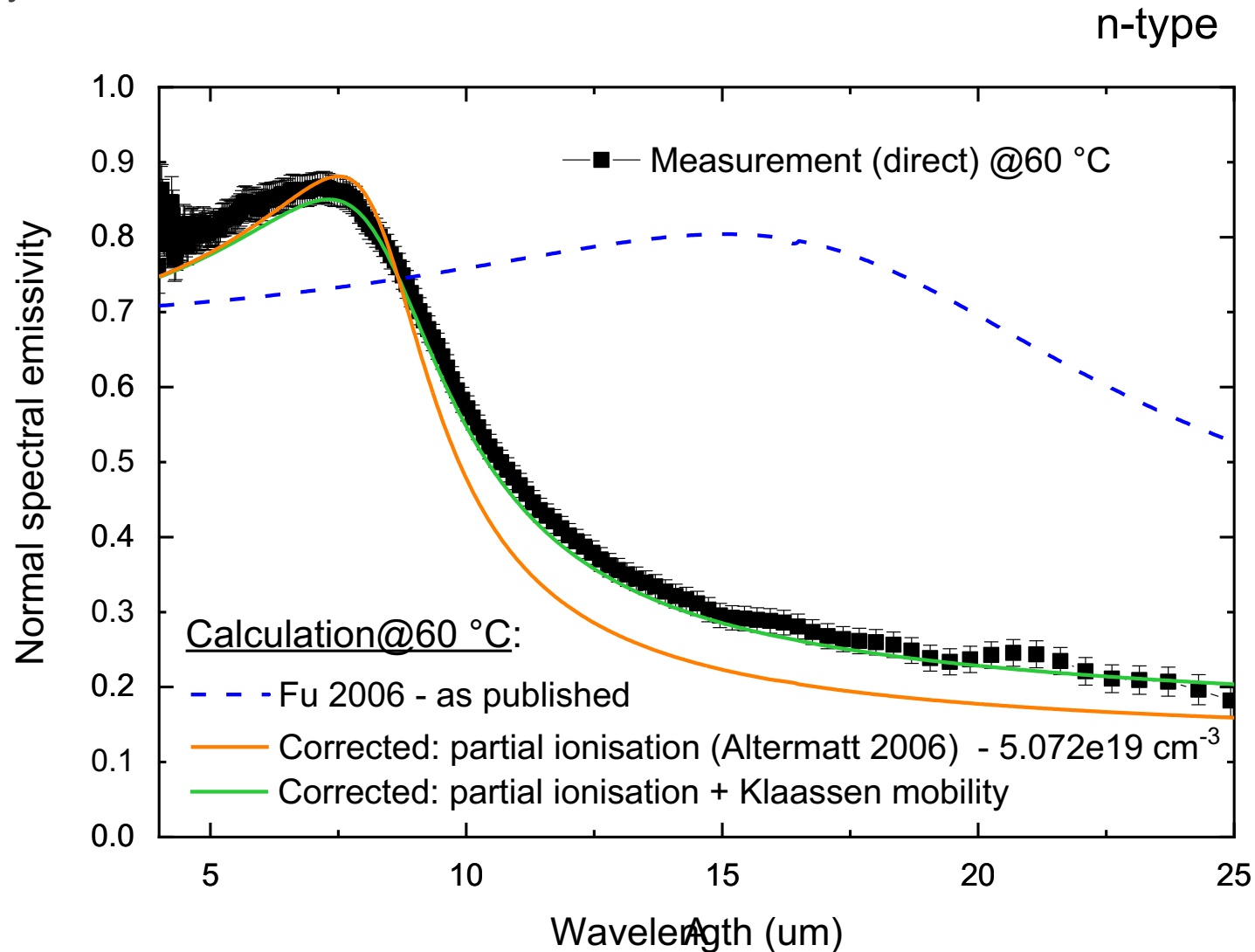
Free carriers



Modelling silicon VIS-NIR-MIR optical properties

■ n-type: OK, after correction of two ingredients

- Partial ionization of dopants
- Mobility model

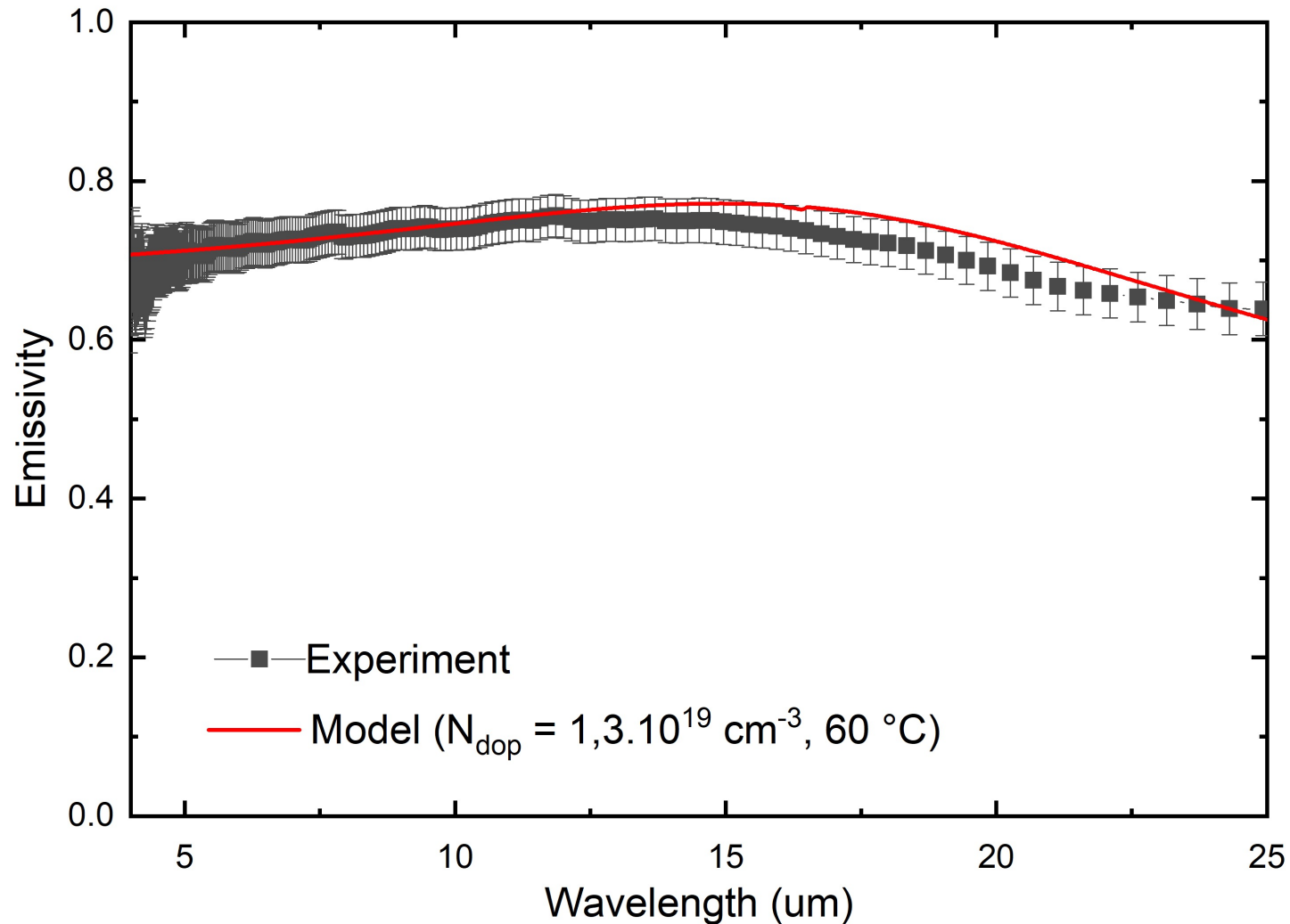




Modelling silicon VIS-NIR-MIR optical properties

■ p-type: OK, after correction of two ingredients

- Partial ionization of dopants
- Mobility model

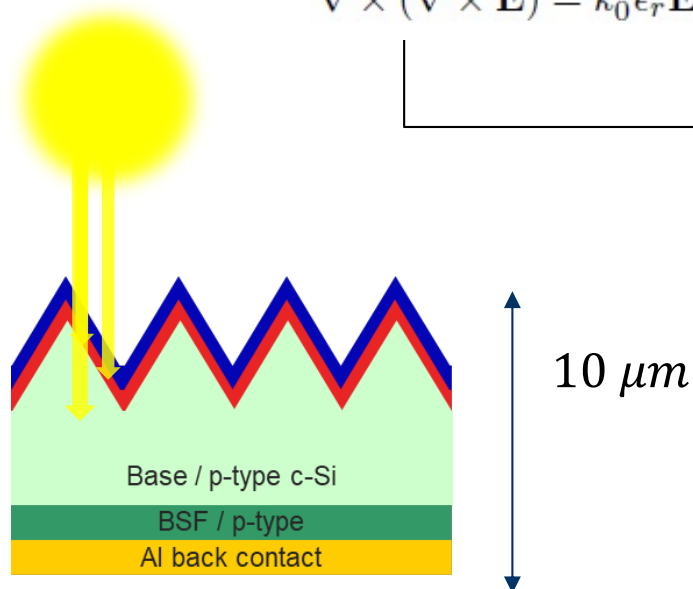
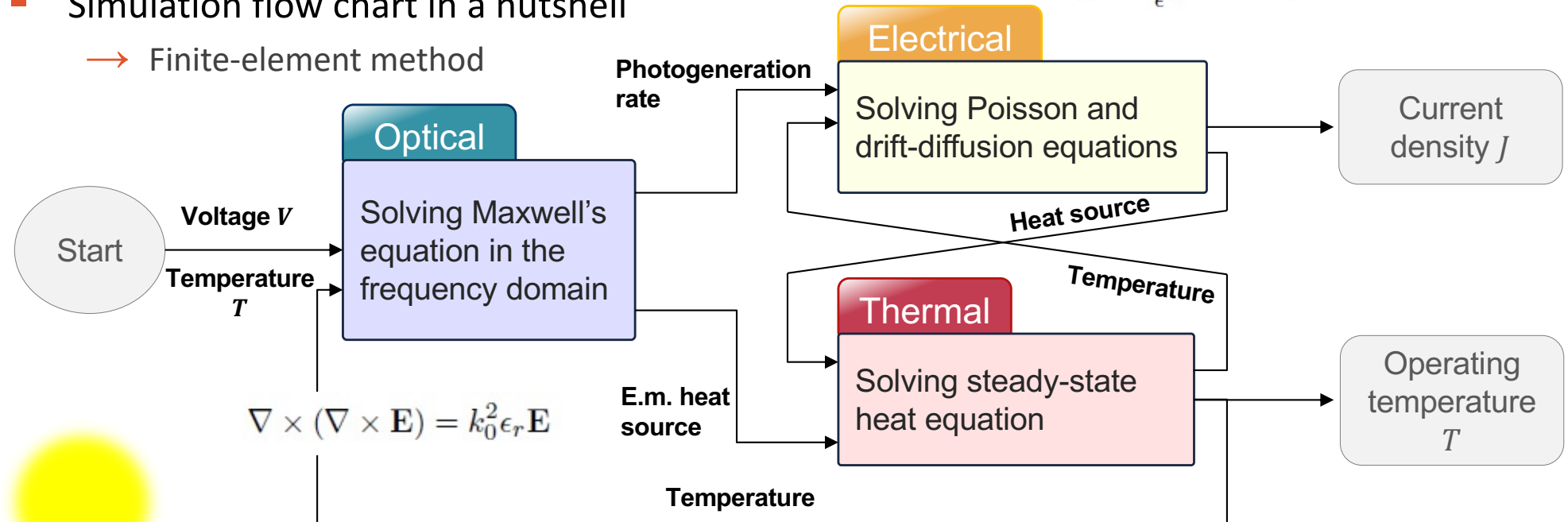


$$\frac{J_n}{q} = n\mu_n \nabla E_c + D_n \nabla n - nD_n \nabla \ln(N_c) + nD_{n,th} \nabla \ln(T)$$

$$\Delta\phi = -\frac{q}{\epsilon}(p - n + C)$$

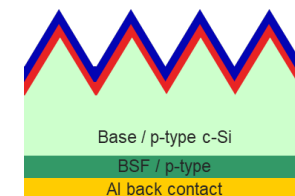
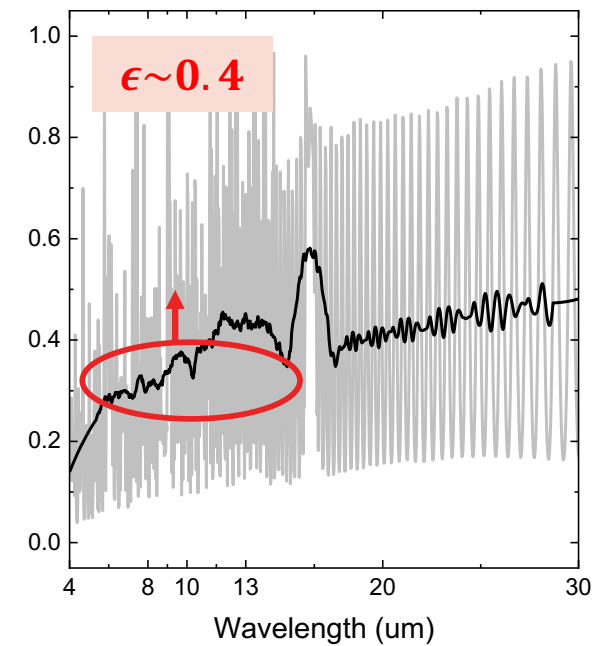
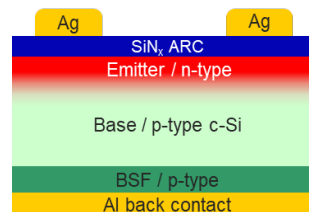
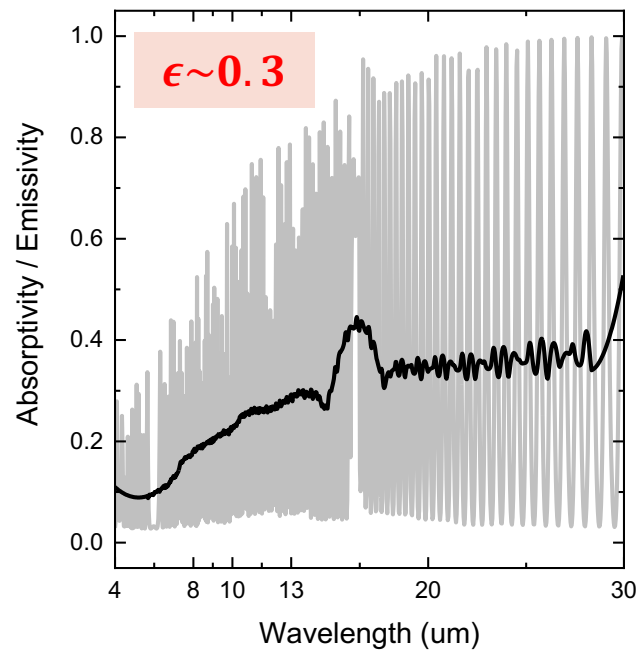
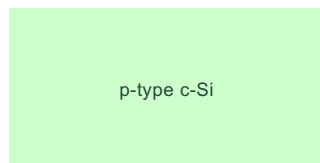
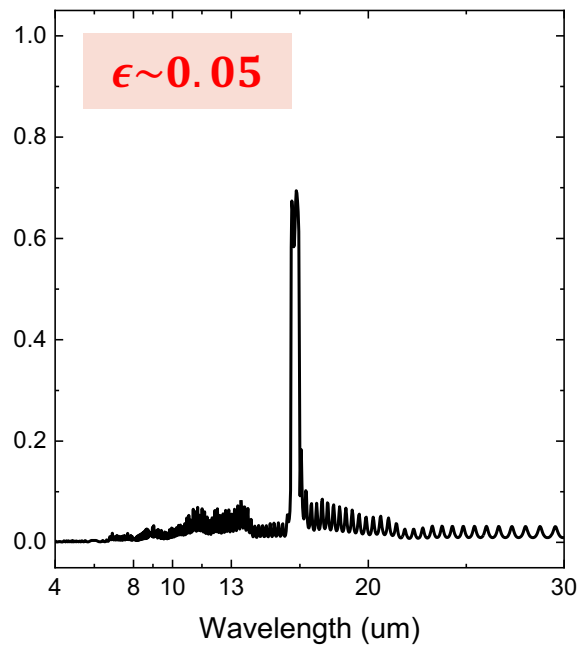
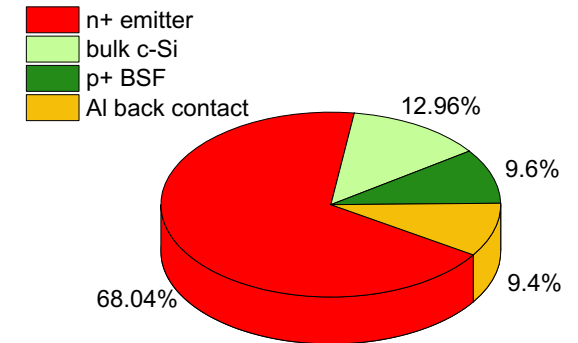
Simulation flow chart in a nutshell

→ Finite-element method



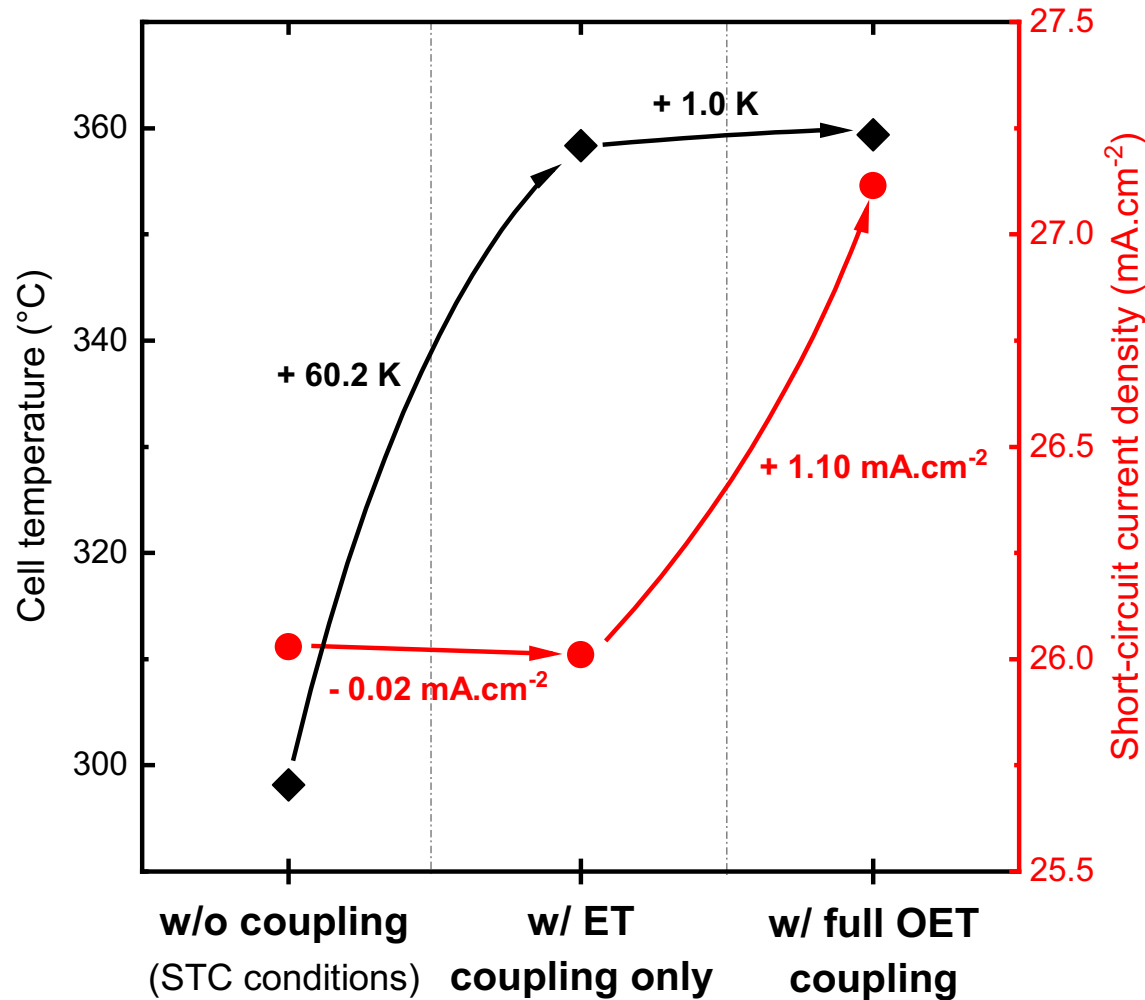
What is the impact of the different layers and surface structuration on emissivity?

→ $\epsilon(\lambda)$ should be large for $\lambda > 4 \mu m$



■ What is the importance of having a fully coupled OET model?

→ Comparing different coupling scenarios



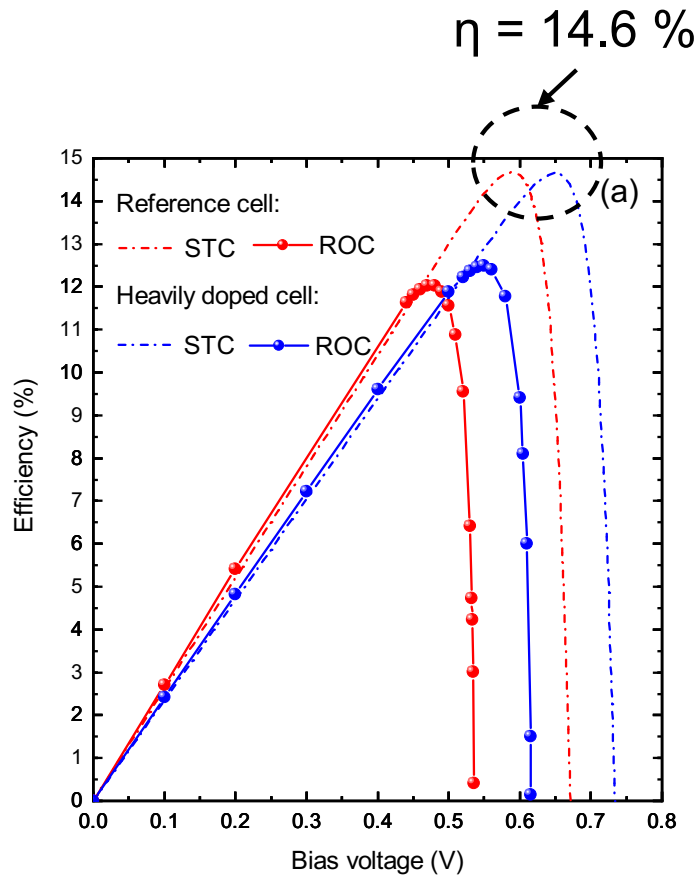
✓ ET coupling has the largest impact on the operating temperature...

✓ ... but a full coupling is required to (1) describe the increase in short-circuit current with temperature (2) accurately predict the operating temperature



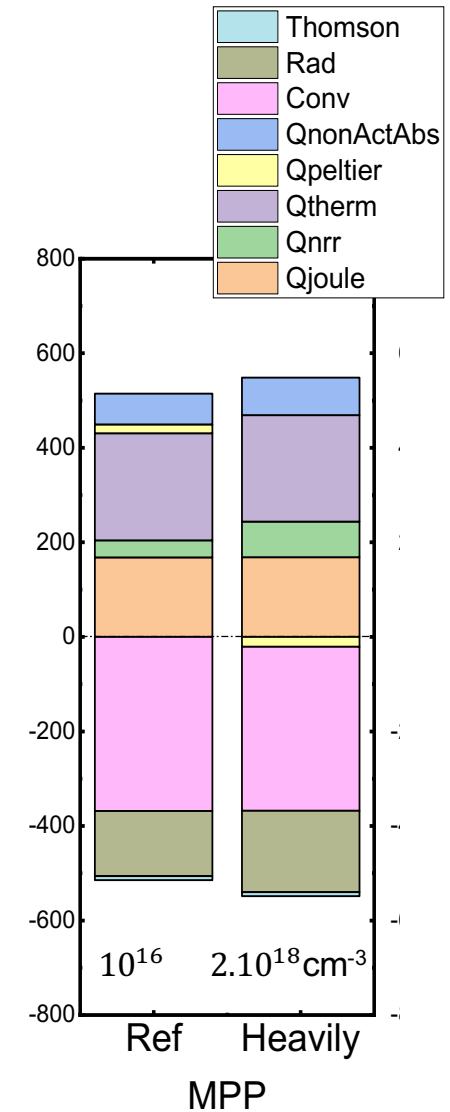
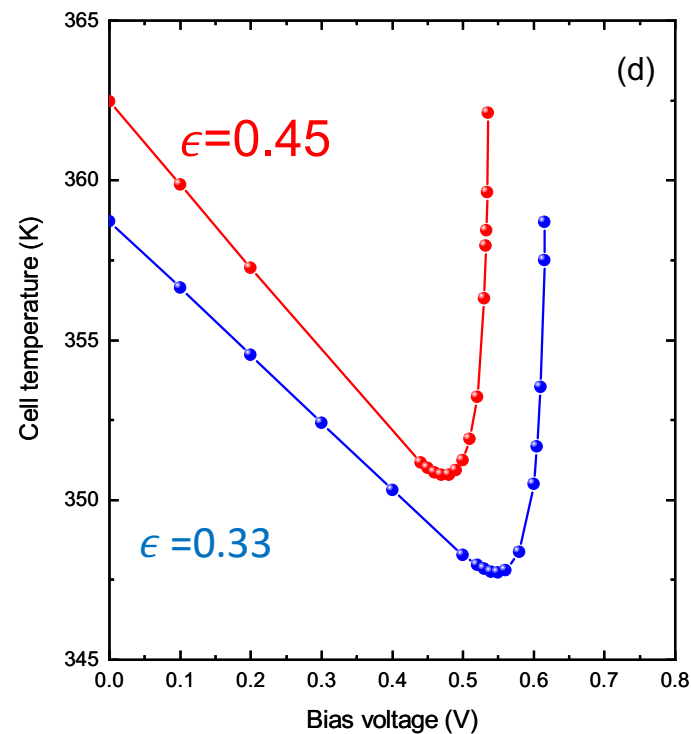
Results

→ Influence of the solar cell design



12.5 %

$\eta = 12 \%$



■ Conclusion

- ✓ Developpement of an **OET model for silicon solar cells** in real operating conditions
- ✓ Highlighting the importance of a **fully coupled simulation** for accurate output

■ Outlook

- Fine-tuning of the underlying physics and experimental validation
- Many numerical challenges: upscaling from 2D to 3D, and from a solar cell to a solar module

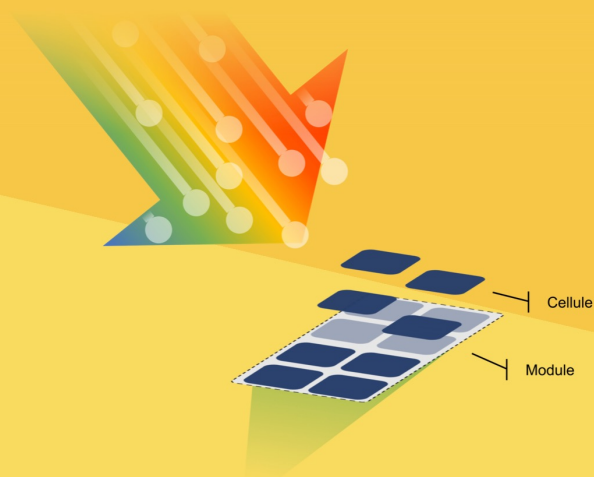
Solaire PV

Des chercheuses et des chercheurs du CNRS et de la Fédération PV répondent à toutes vos questions sur le solaire PV en France.

TÉLÉCHARGER LE GUIDE SOLAIRE PV 

AVANT-PROPOS ?

QUI SOMMES NOUS ? ?



Crédits et contact

Ce document est issu d'un atelier mené par des équipes du Centre de Nanosciences et de Nanotechnologies (C2N, CNRS, Université Paris-Saclay) et de l'Unité Mixte de Recherche de l'Institut Photovoltaïque d'Ile-de-France (IPVF, CNRS, Ecole Polytechnique), et rejointes par d'autres membres de la Fédération de recherche du Photovoltaïque (FedPV),

sous l'impulsion et la supervision de Stéphane Collin et Jean-Francois Guillemoles,

et avec la participation d'Amaury Delamarre, Thomas Vezin, Guillaume Vidon, Capucine Tong, Bérangère Frouin, Marie Legrand, Mohamed Amara, Tiphaine Mathieu, Lucas Gavotto, Daniel Suchet...

Une première étape a été menée en octobre et novembre 2021 pour préparer une soirée-débat organisée aux Journées Nationales du PhotoVoltaïque (JNPV) le mercredi 1er décembre 2021, intitulée *Le photovoltaïque solaire en France : réalité, potentiel, et défis*. Les premiers résultats de ce travail ont alors été partagés et ont reçu un accueil enthousiaste de la part de la communauté scientifique du photovoltaïque. Cette étape a permis d'étoffer l'équipe de l'atelier et d'enrichir les questions abordées.

L'équipe de l'*Atelier SolairePV* remercie Daniel Lincot pour avoir inspiré ce travail, ainsi que ses très nombreux relecteurs.

Questions



Merci pour votre attention.

Institut des Nanotechnologies de Lyon – UMR 5270

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