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School of Photovoltaic and Renewable Energy Engineering



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Solcore Workshop – Silicon Tandem Cell Computer Modelling

Sungkyunkwan University, 1 – 3 August 2023

N.J. Ekins-Daukes & Phoebe Pearce



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EkinsNed



www.qpvgroup.org



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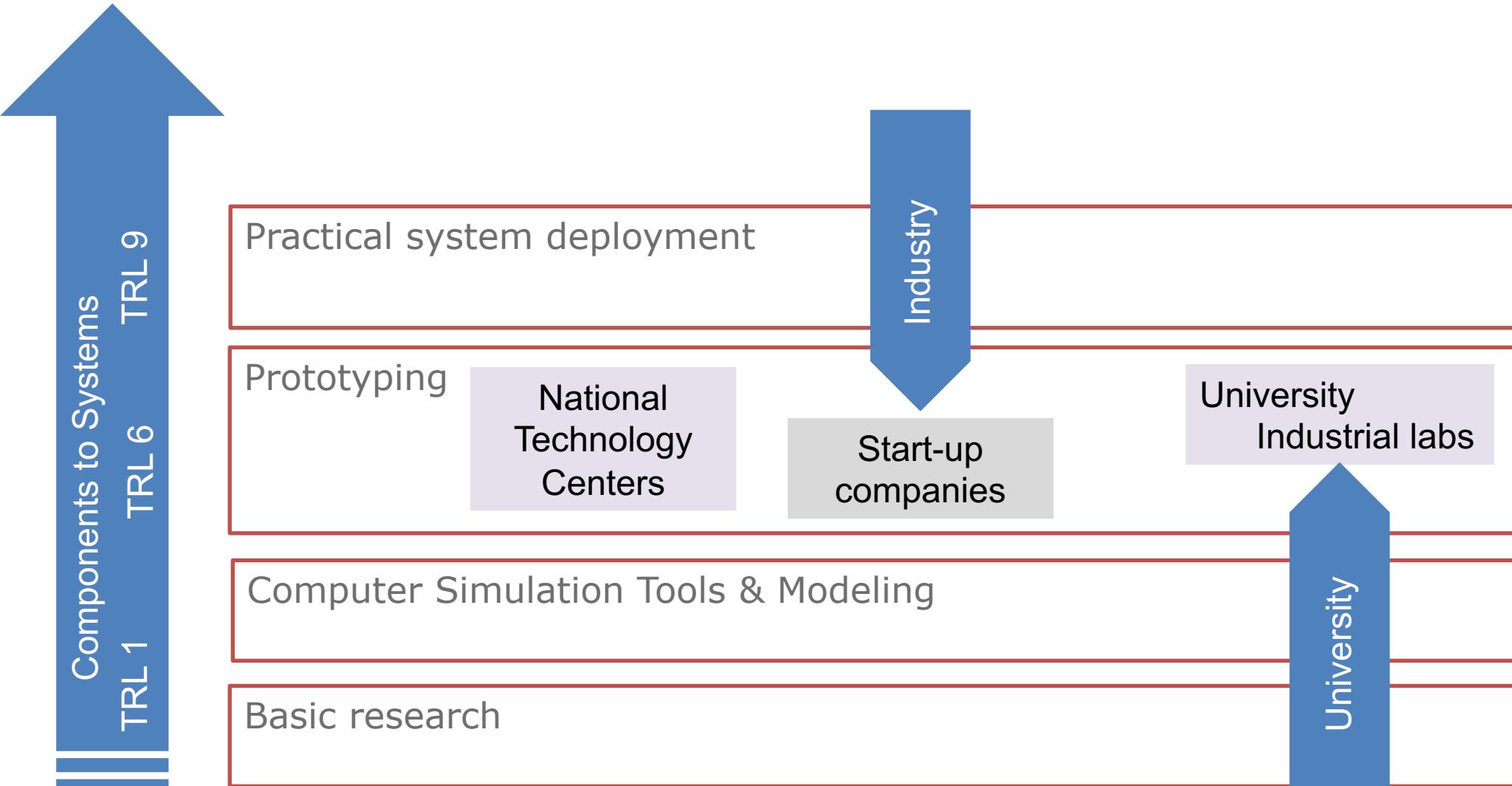
Session 1: Introduction

1 August 2023

Ned Ekins-Daukes, Phoebe Pearce



A Role for Computer Simulation in the Modern Technological Innovation Process

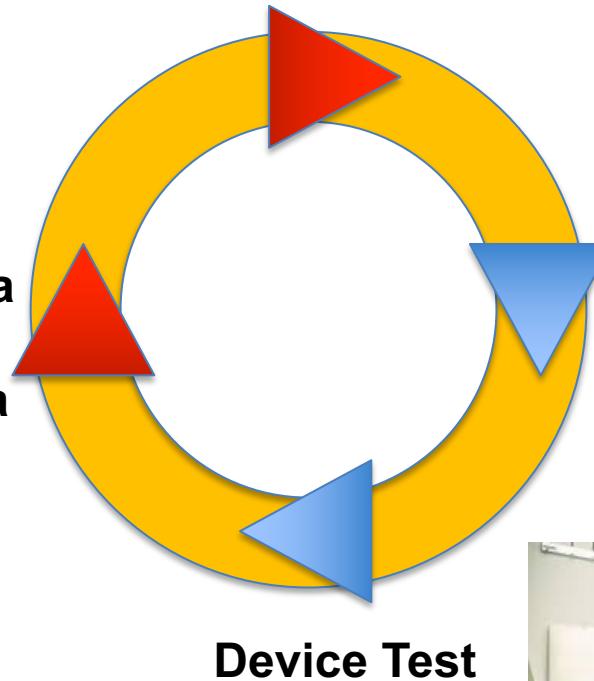


The Present Value of Computer Modelling in Research & Development

Design aided by
a computer (TCAD):



Evaluate data
through
fitting of data

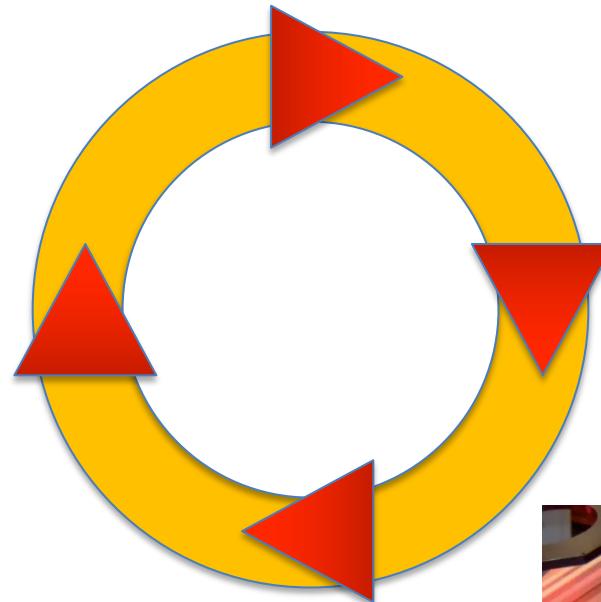


The Future Value of Computer Modelling in Research & Development

Design aided by
a computer (TCAD):



AI
assisted
fitting of
test data



Robot Device
Fabrication

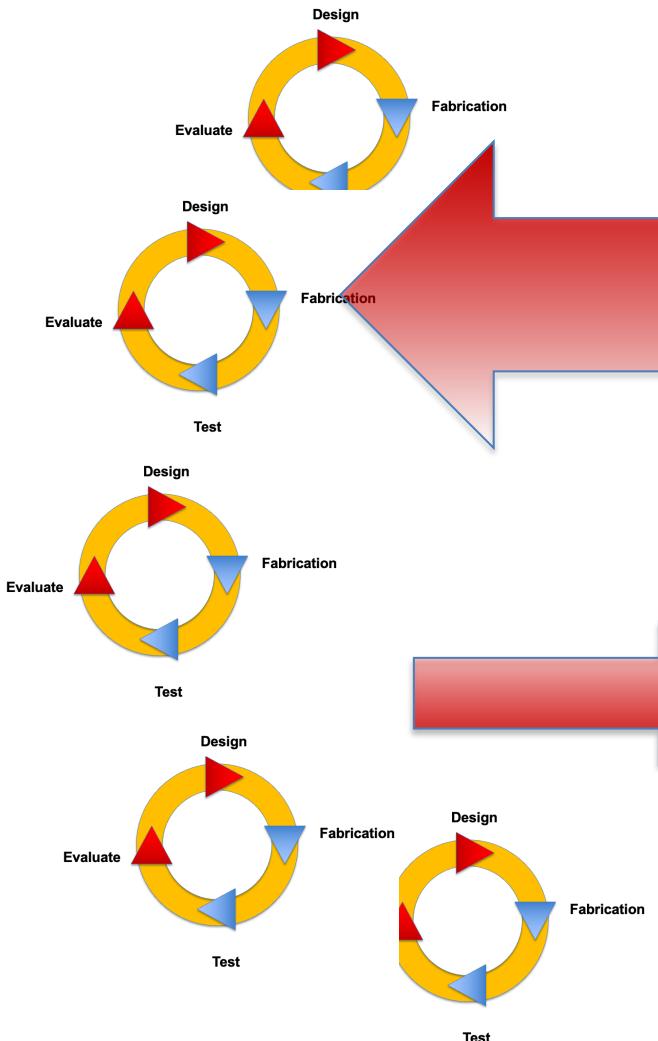


Automated
Device Test

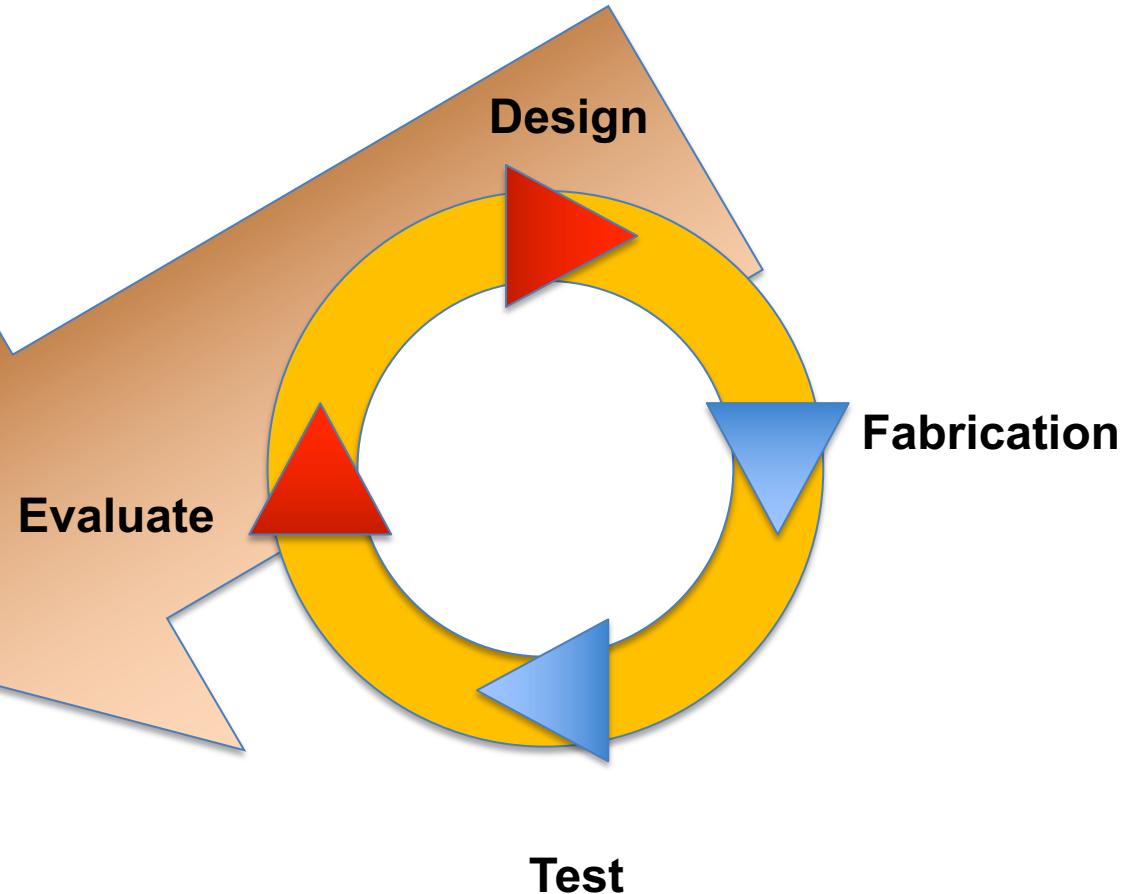


Development Process for our Computer Code:

Global PV R&D Community



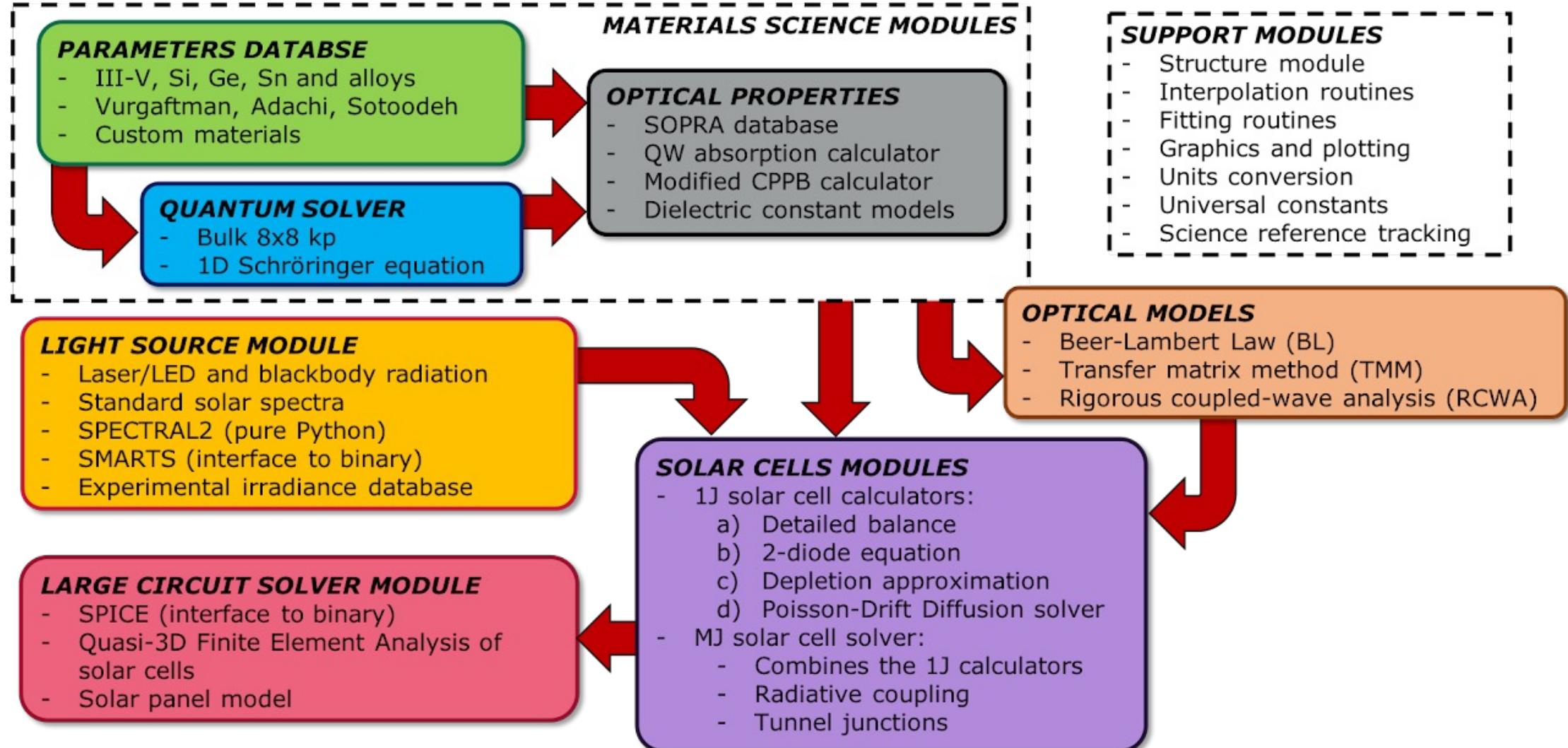
QPV Research Group



Open Source
Code Repository

SOLCORE
RayFlare

Solcore capabilities



www.solcore.solar

RayFlare capabilities

Simulations using a single method



Ray-tracing: Geometric optics for large-scale textures without diffraction effects



Transfer-matrix method: Wave optics for planar layers (coherent and incoherent)



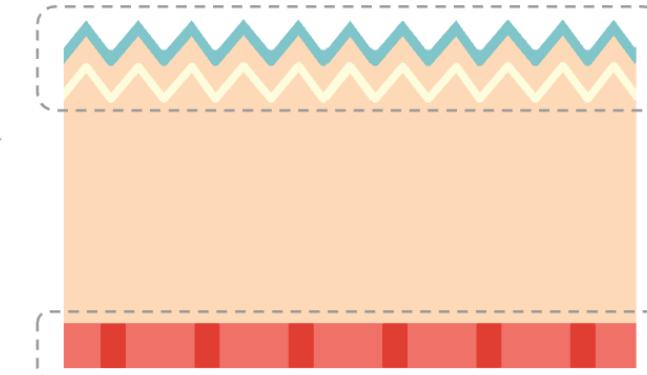
Rigorous coupled-wave analysis: Wave optics for planar or periodic structures e.g. gratings, photonic crystals

Ideal cases: E.g. perfect mirrors, Lambertian scattering

Calculate e.g. reflection, transmission, absorption per layer, depth-dependent absorption profiles

Simulations using angular redistribution matrices

Each surface is treated separately with an appropriate method



- Free, open source
- Anyone can contribute
- Modular
- Documented

<https://rayflare.readthedocs.io>

Course instructions

GitHub repository where the tutorials for this workshop are hosted:

<https://tinyurl.com/2mn6rb64>



*Look at the tutorials +
the expected outputs online*

solcore-education

Collection of teaching materials and scripts to help students learn about Solcore & RayFlare

[Click here to view the examples on GitHub Pages.](#)

View/run the examples on Binder:



*Use Binder to run Python in your
browser & work through the examples*

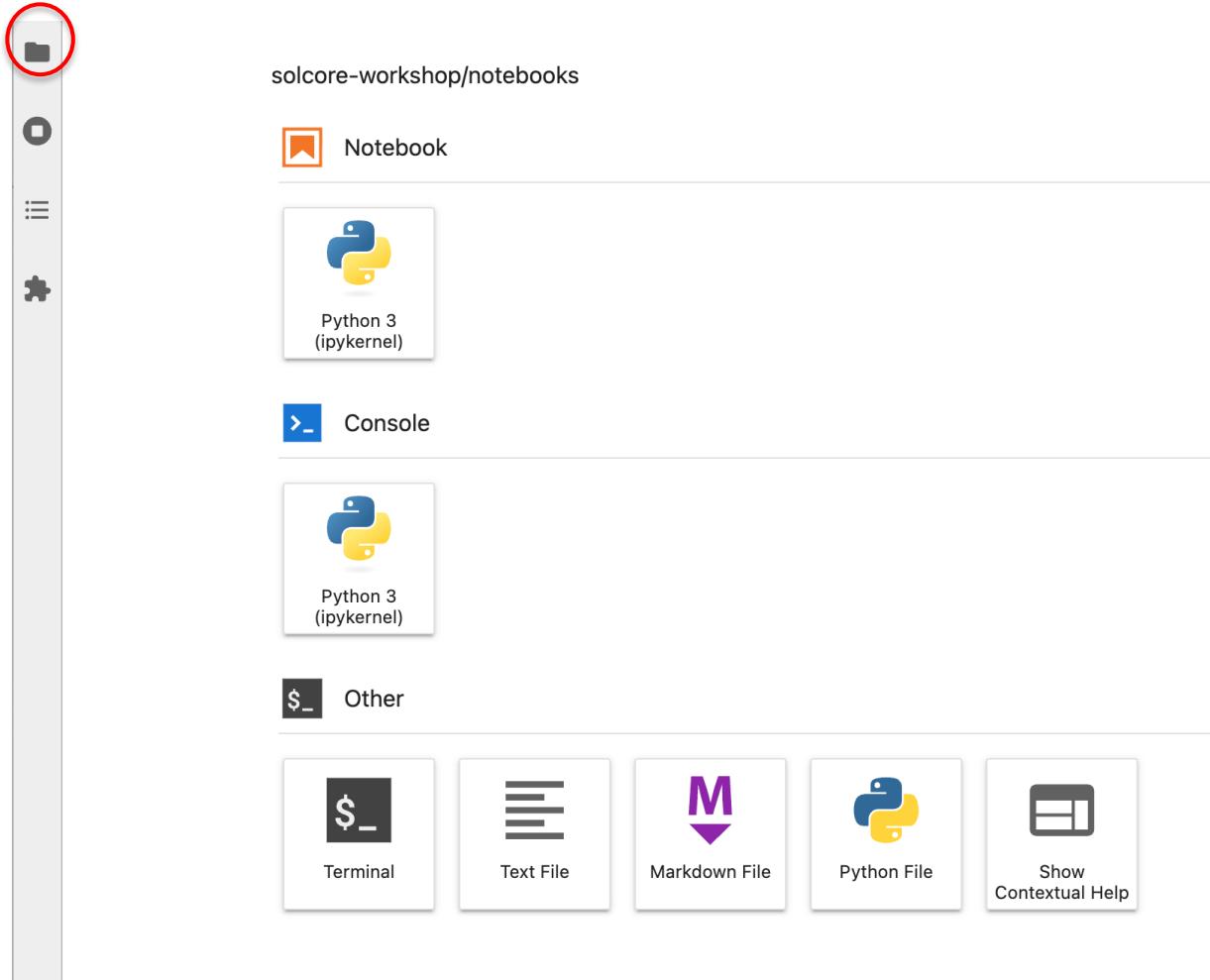
To run Solcore & RayFlare on your own computer, you will need to install Python (version 3.7 to 3.11):

Recommendations:

- On **Windows**, use **miniconda** (<https://conda.io/miniconda.html>)
- On **MacOS**, use **Homebrew + venv** (see RayFlare's installation instructions for more detail)
- On **Ubuntu/Linux**, use **system Python + venv** (see RayFlare's installation instructions for more detail)

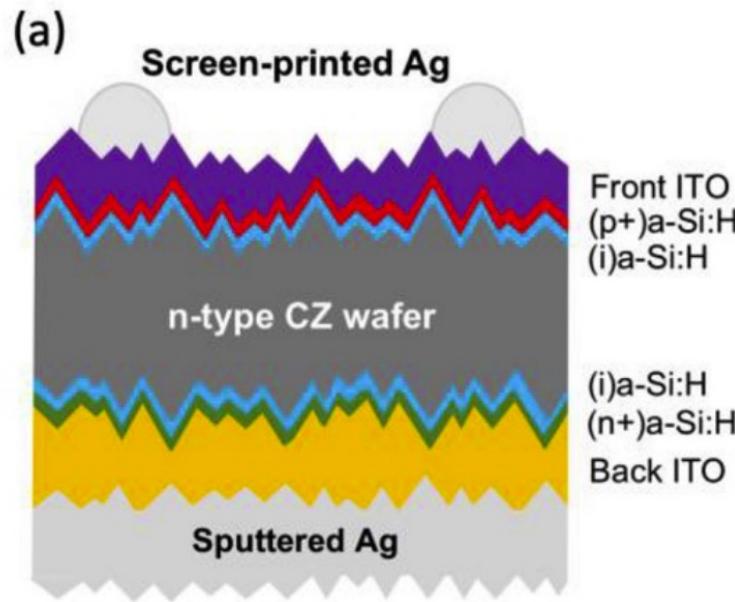
Binder

- Binder may take a long time (~ 10 minutes) to load, so please click the link to '[Launch Binder](#)' now

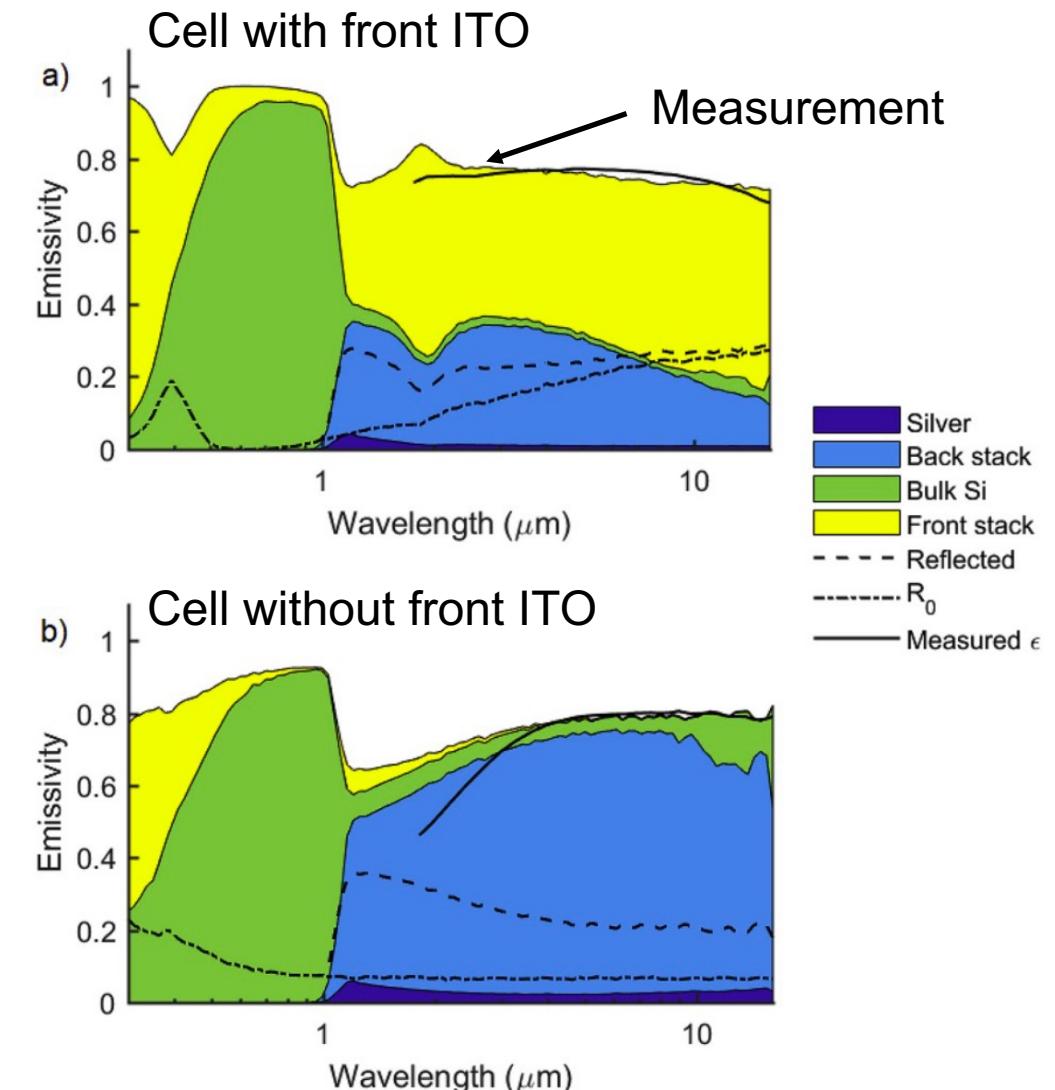


After loading, it should look like this –
click circled icon to open the examples

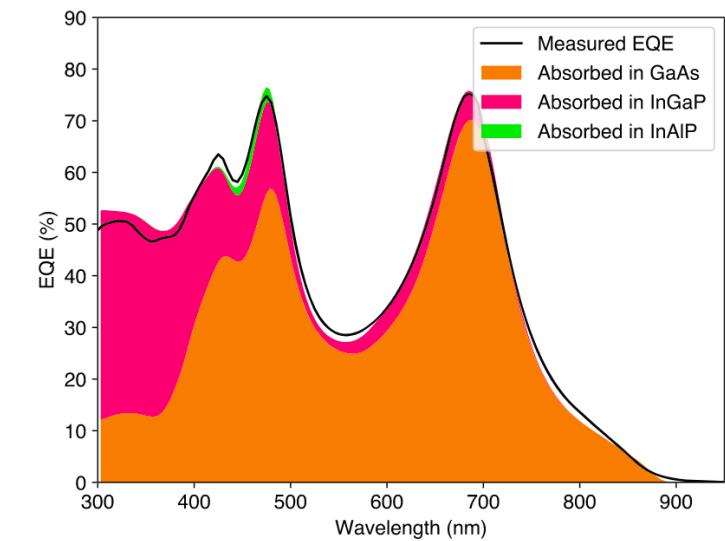
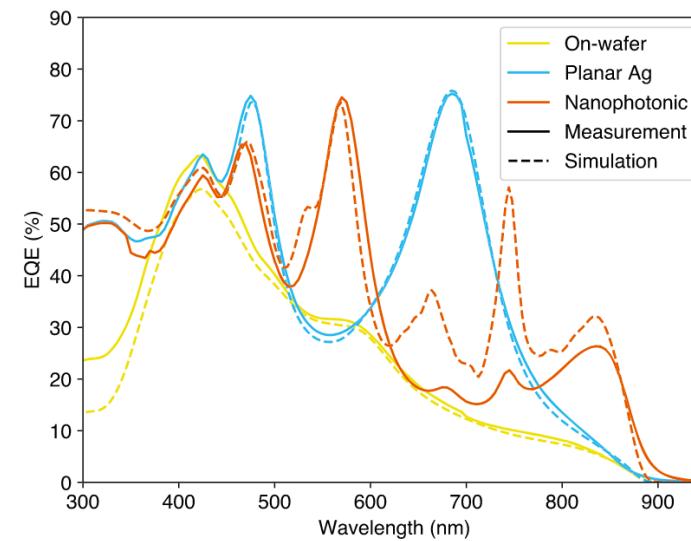
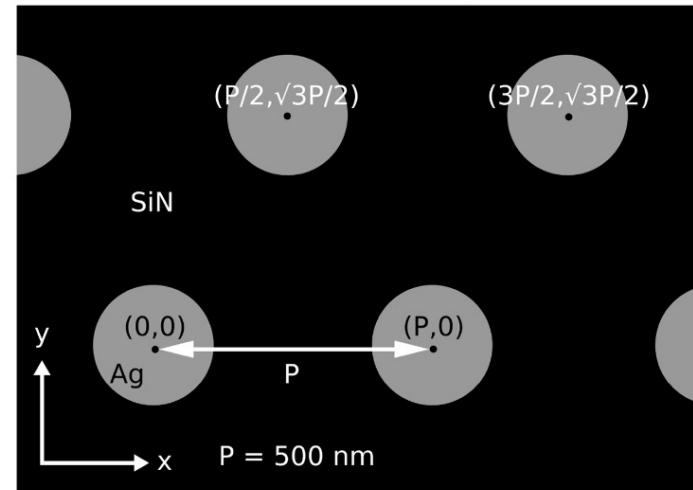
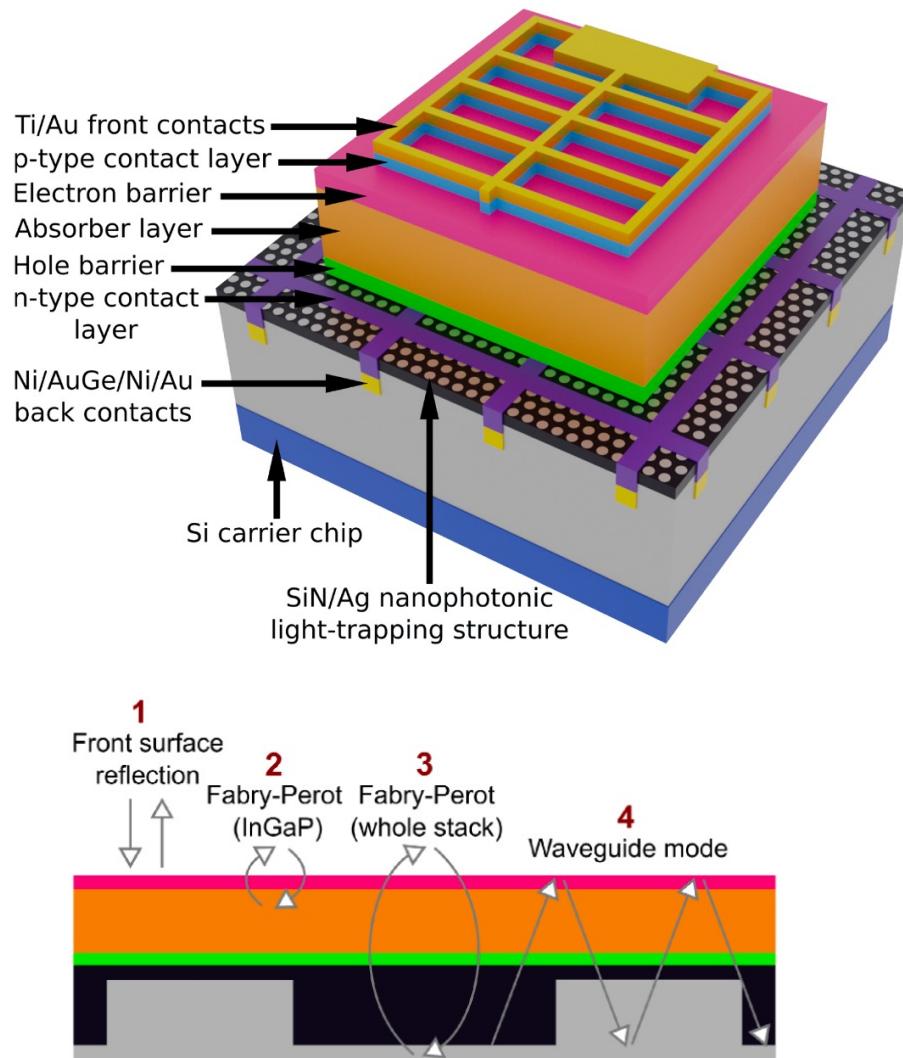
Example: Si cell emissivity



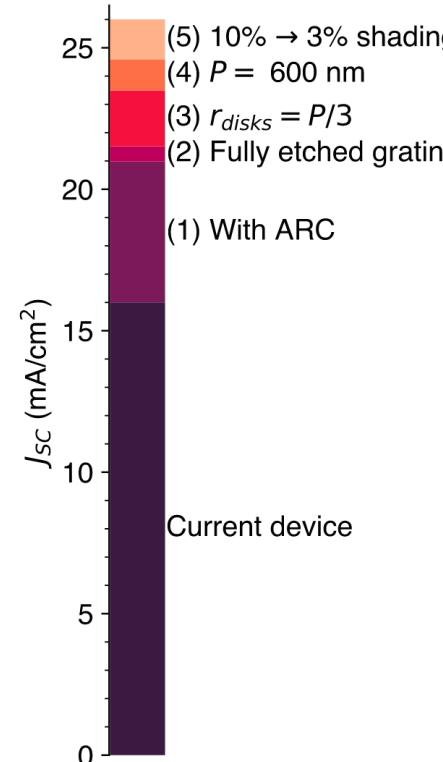
Simulations & measurement of cell absorptivity (emissivity) between 300 nm and 20 μm . This is relevant for the operating temperature of the cell. Due to free-carrier absorption in doped layers and very good light-trapping, the cell absorbs well even at wavelengths far beyond the bandgap.



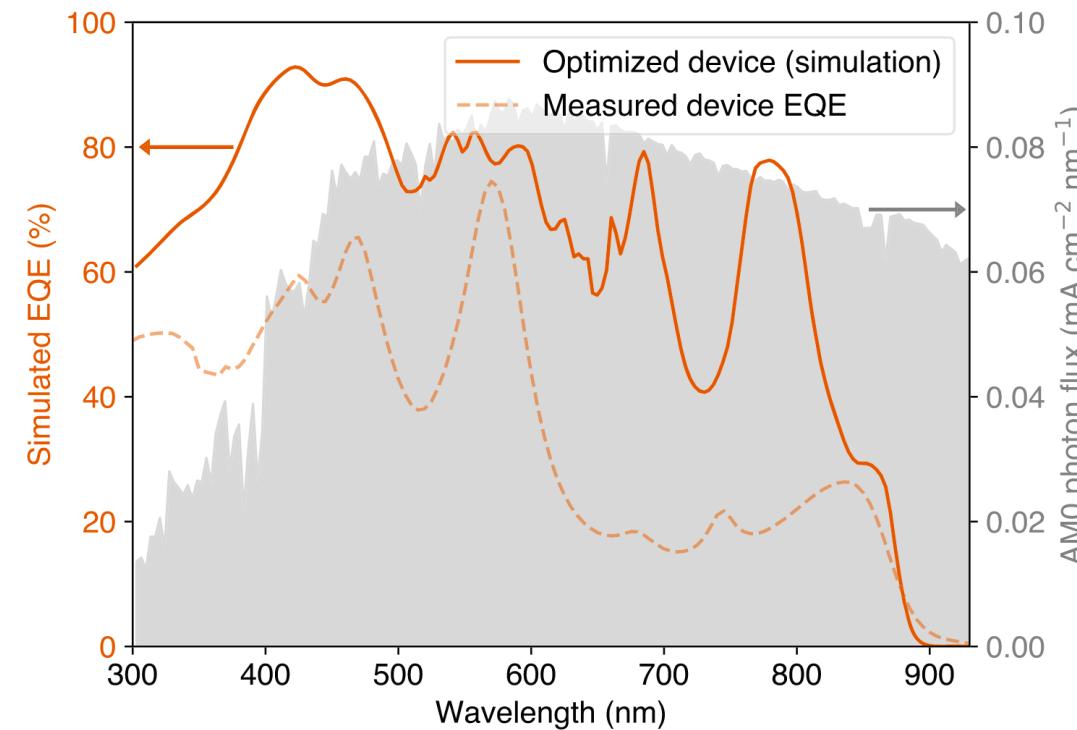
Example: ultra-thin GaAs cell



Example: ultra-thin GaAs cell (cont.)

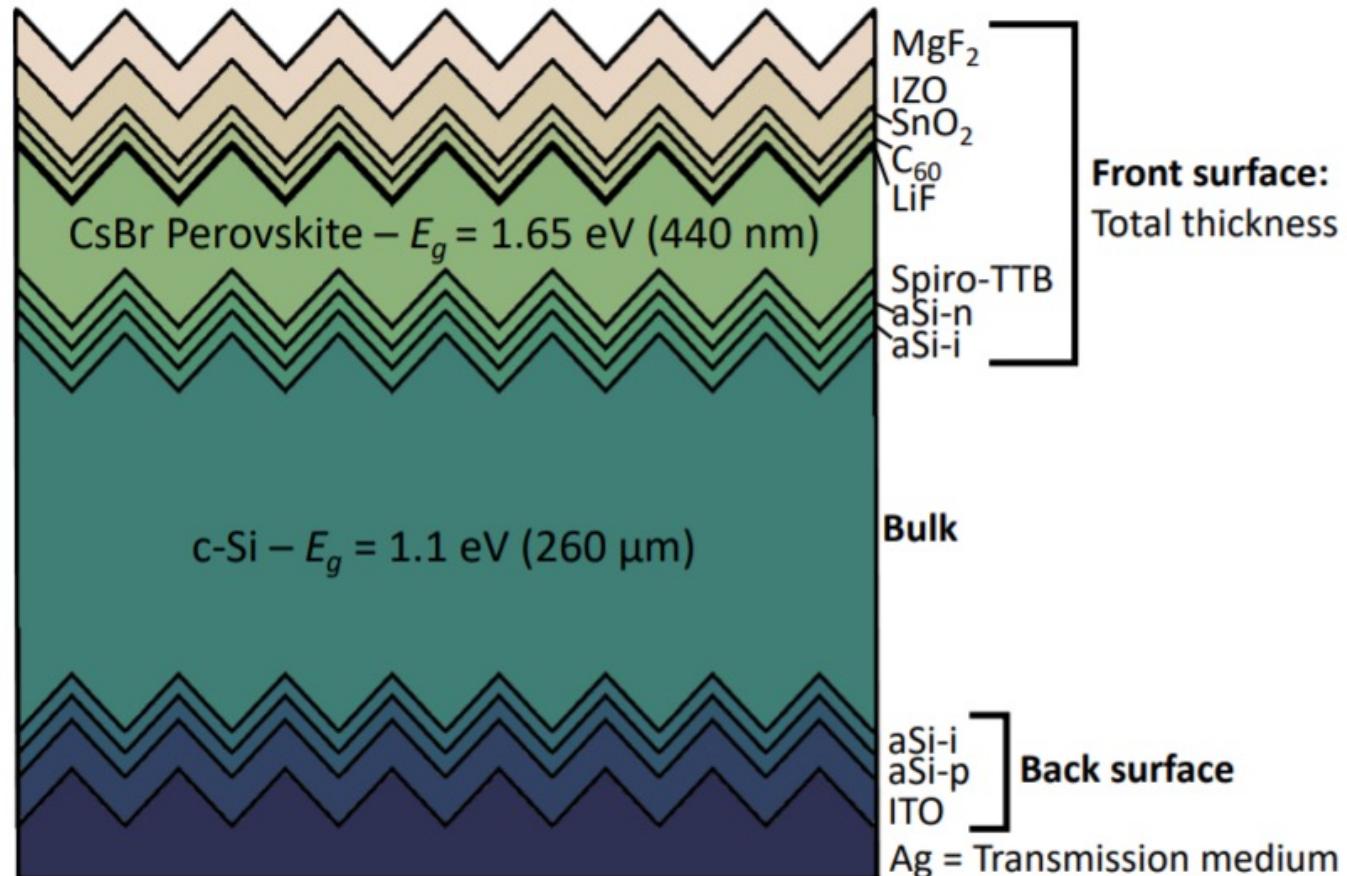


(A)



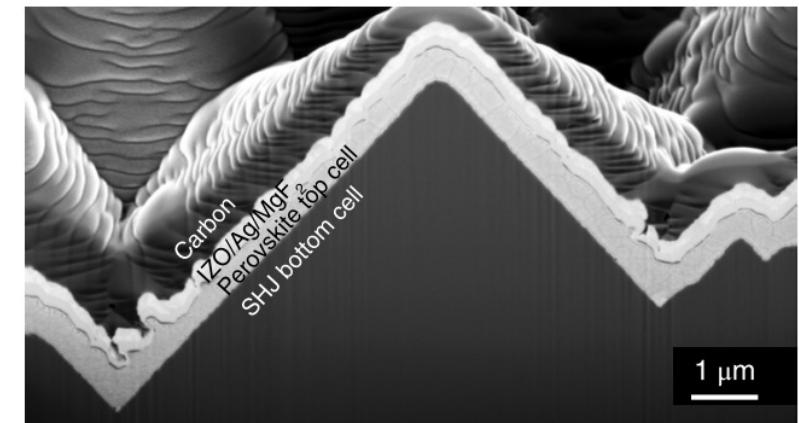
(B)

Example: Perovskite/Si tandem cell



Perovskite on silicon heterojunction (SHJ) tandem cell

Perovskite is deposited conformally on standard etched Si pyramid texture

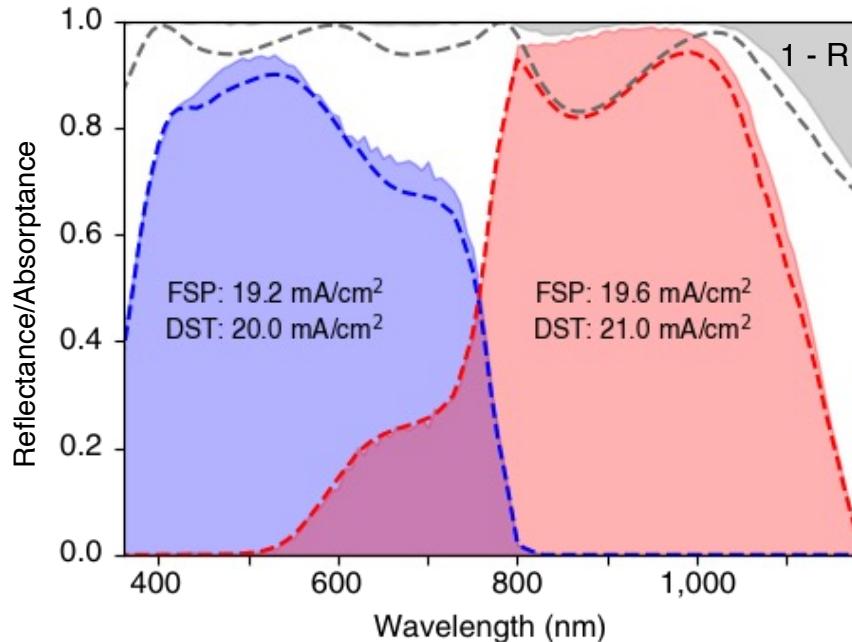


From [1]

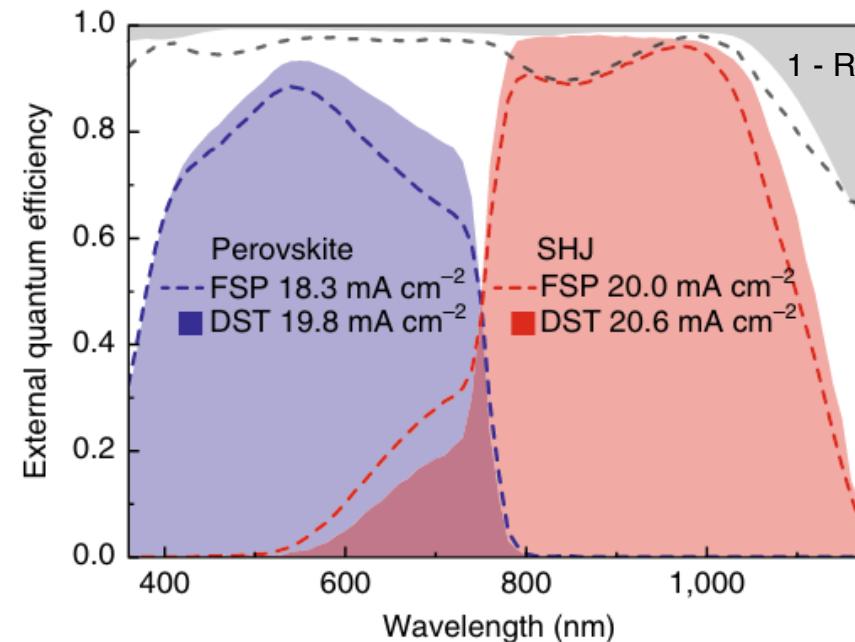
[1] Sahli, F., Werner, J., et al. (2018) 'Fully textured monolithic perovskite/silicon tandem solar cells with 25.2% power conversion efficiency', *Nature Materials*. Springer US, 17(9), pp. 820–826.

Example: Perovskite/Si tandem cell (cont.)

RayFlare simulation



EQE measurement



FSP = Front-side polished



DST = Double-side textured



From [1]

As a result of the front surface texture:

- Peak in R around 830 nm is reduced (lower front-surface reflectivity)
- Perovskite absorption slightly enhanced
- Boosts long-wavelength absorption (better light-trapping inside Si)

[1] Sahli, F., Werner, J., et al. (2018) 'Fully textured monolithic perovskite/silicon tandem solar cells with 25.2% power conversion efficiency', *Nature Materials*. Springer US, 17(9), pp. 820–826.



Session 2: Hands-on exercise Using SolCore to calculate the Shockley-Queisser Efficiency limit

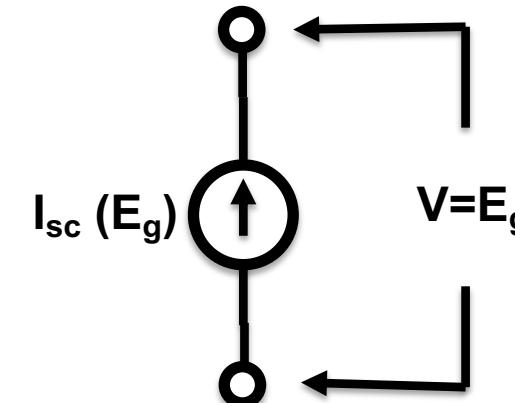
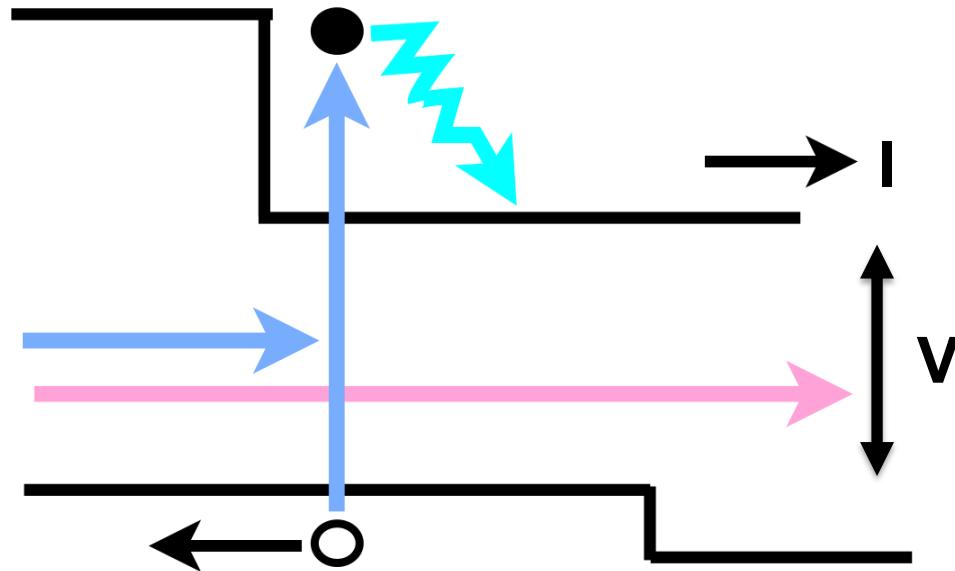
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What is the Maximum Efficiency of a Solar Cell?

Trivich-Flynn Limit (1955)

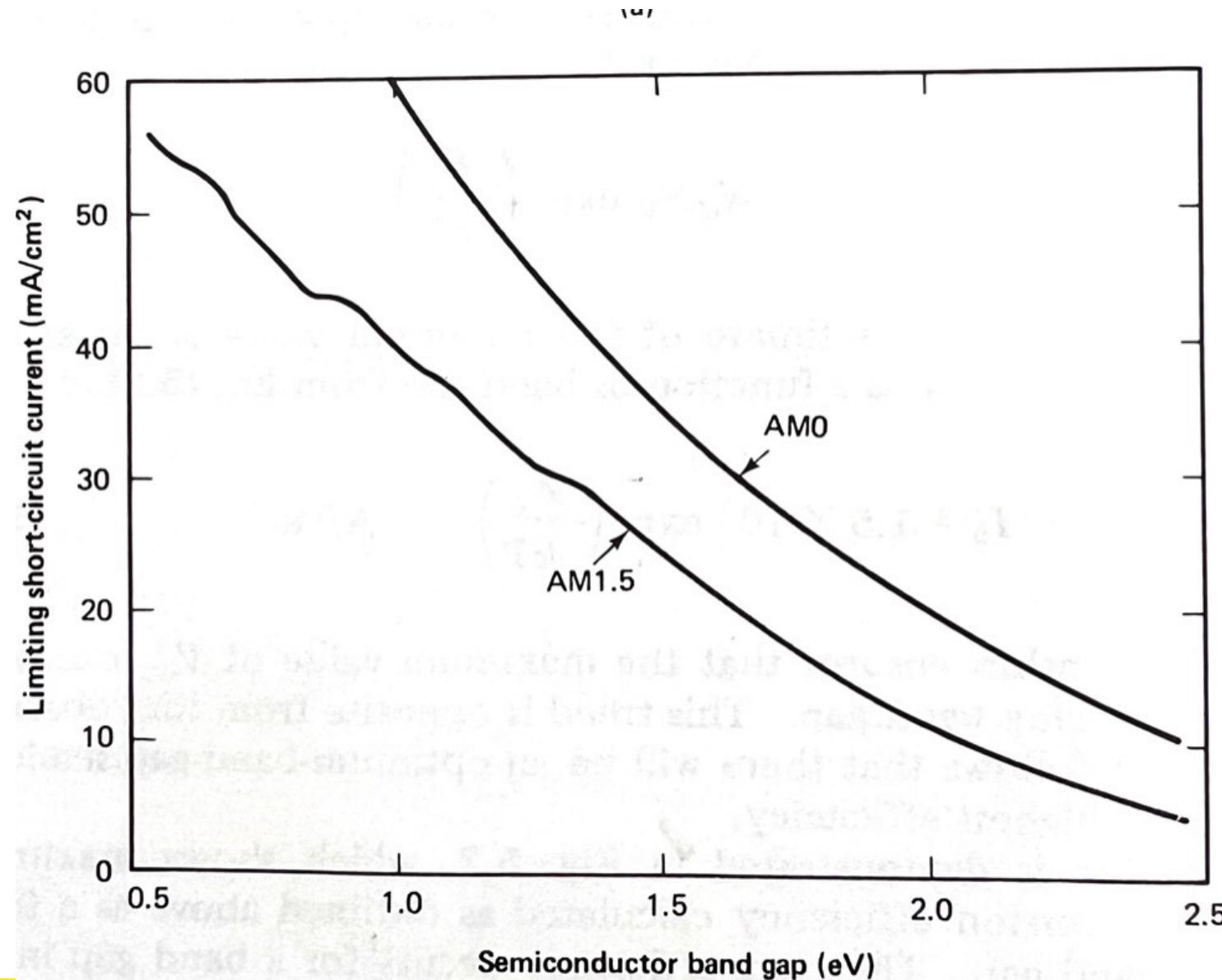
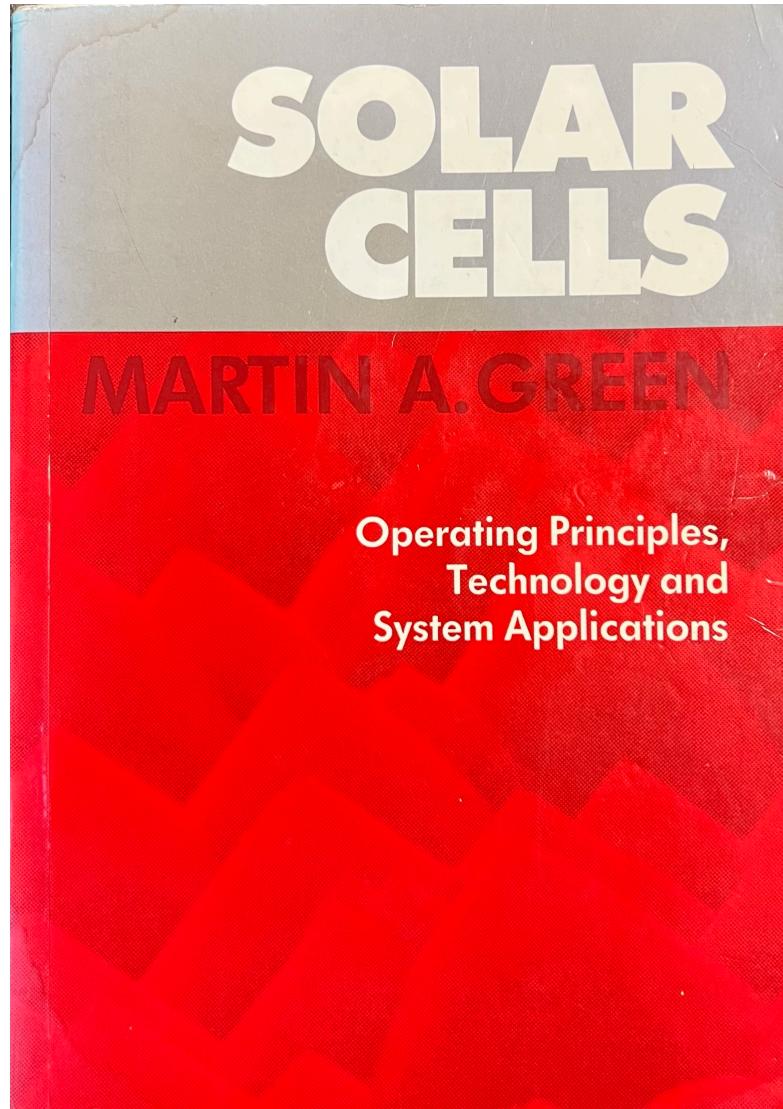


Warning : Limit is invalid for $T > 0K$!

Trivich D, Flinn PA. Maximum efficiency of solar energy conversion by quantum processes. In Solar Energy Research, Daniels F, Duffie J (eds). Thames and Hudson: London, 1955.

Limit to the Short-Circuit Current

p87



What is the Maximum Efficiency of a Solar Cell?

Shockley Queisser limit (1961)

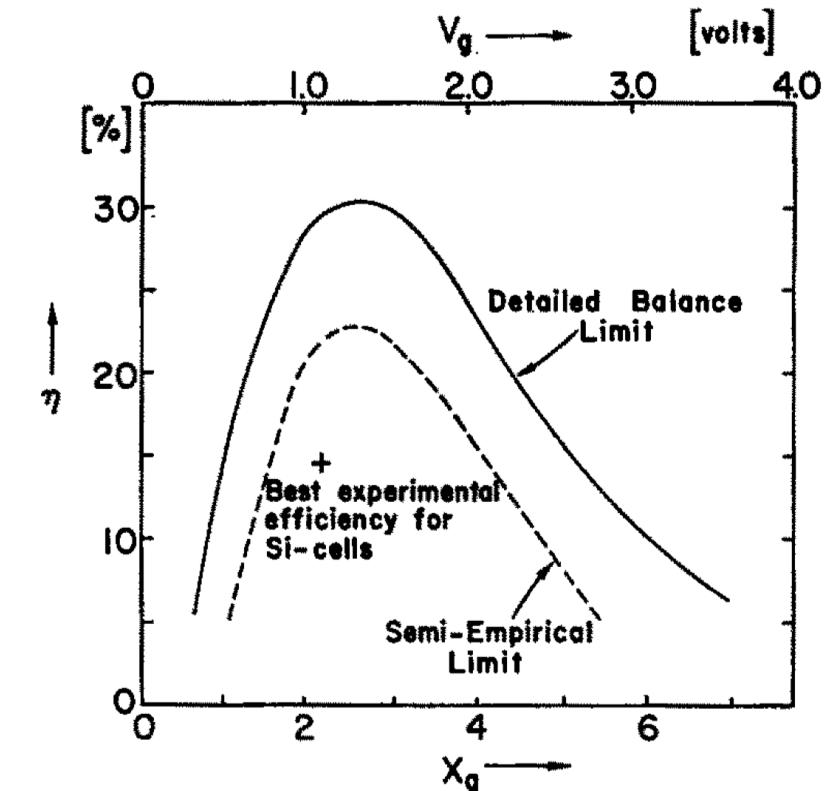
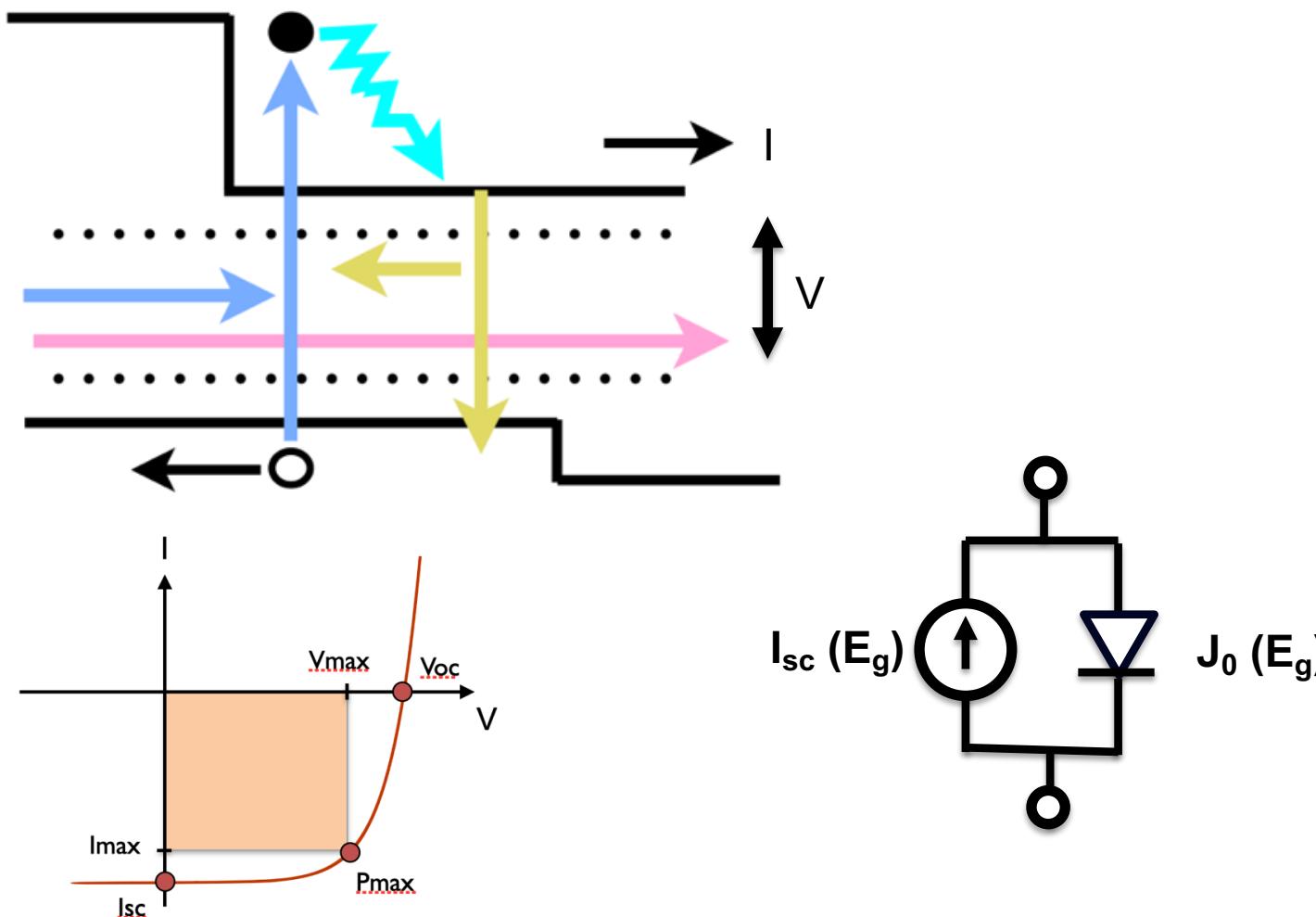


FIG. 1. Comparison of the “semiempirical limit” of efficiency of solar cells with the “detailed balance limit,” derived in this paper. + represents the “best experiment efficiency to date” for silicon cells. (See footnote 6.)

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Session 3: Shockley-Queisser efficiency limit & detailed balance junction model

1st August 2023

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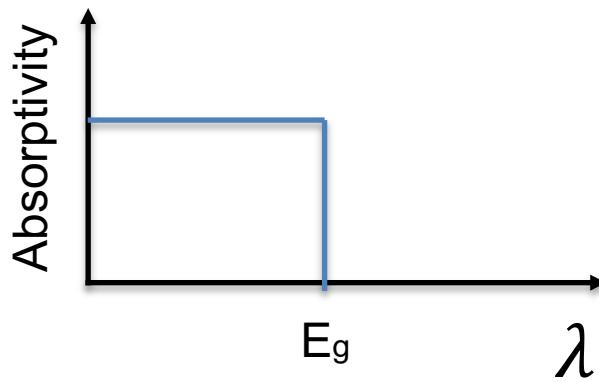


Optical Models for PV Devices

Fundamental

Shockley-Queisser (Detail Balance)

Complete absorption to band-gap energy E_g

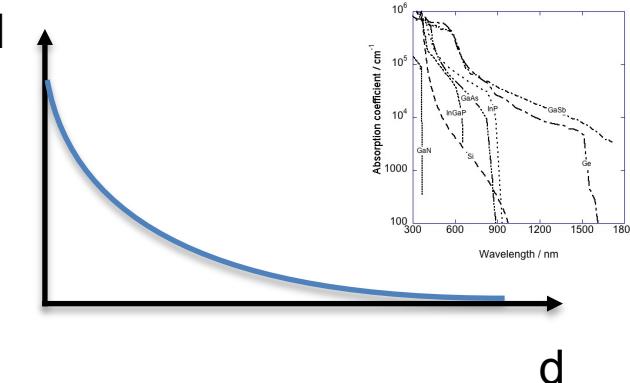


Beer Lambert Law

$$I = I_0 e^{-\alpha d}$$

Intensity of light is attenuated exponentially with increasing thickness of absorber d [m].

Absorption defined by a wavelength dependent absorption coefficient $\alpha(\lambda)[m^{-1}]$



Ray Optics

Non-uniform surfaces or PV structures $\gg \lambda$

Surface texture of a silicon solar cell

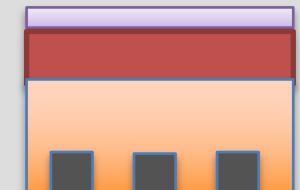


Wave Optics

Sub-wavelength structures $\ll \lambda$

Anti-reflection coating
90nm p-doped layer

800nm n-doped layer

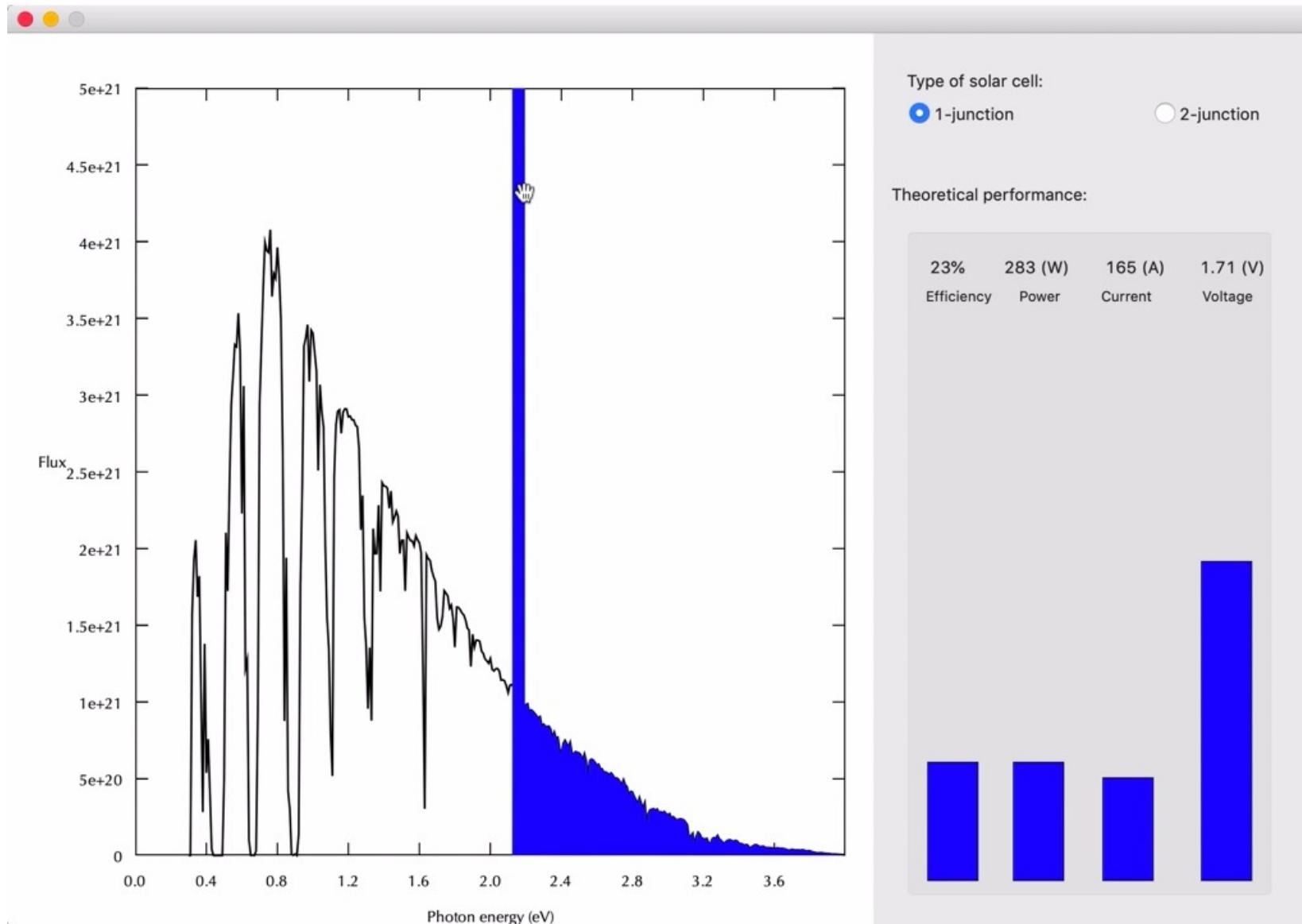


Diffractive grating
on rear side.

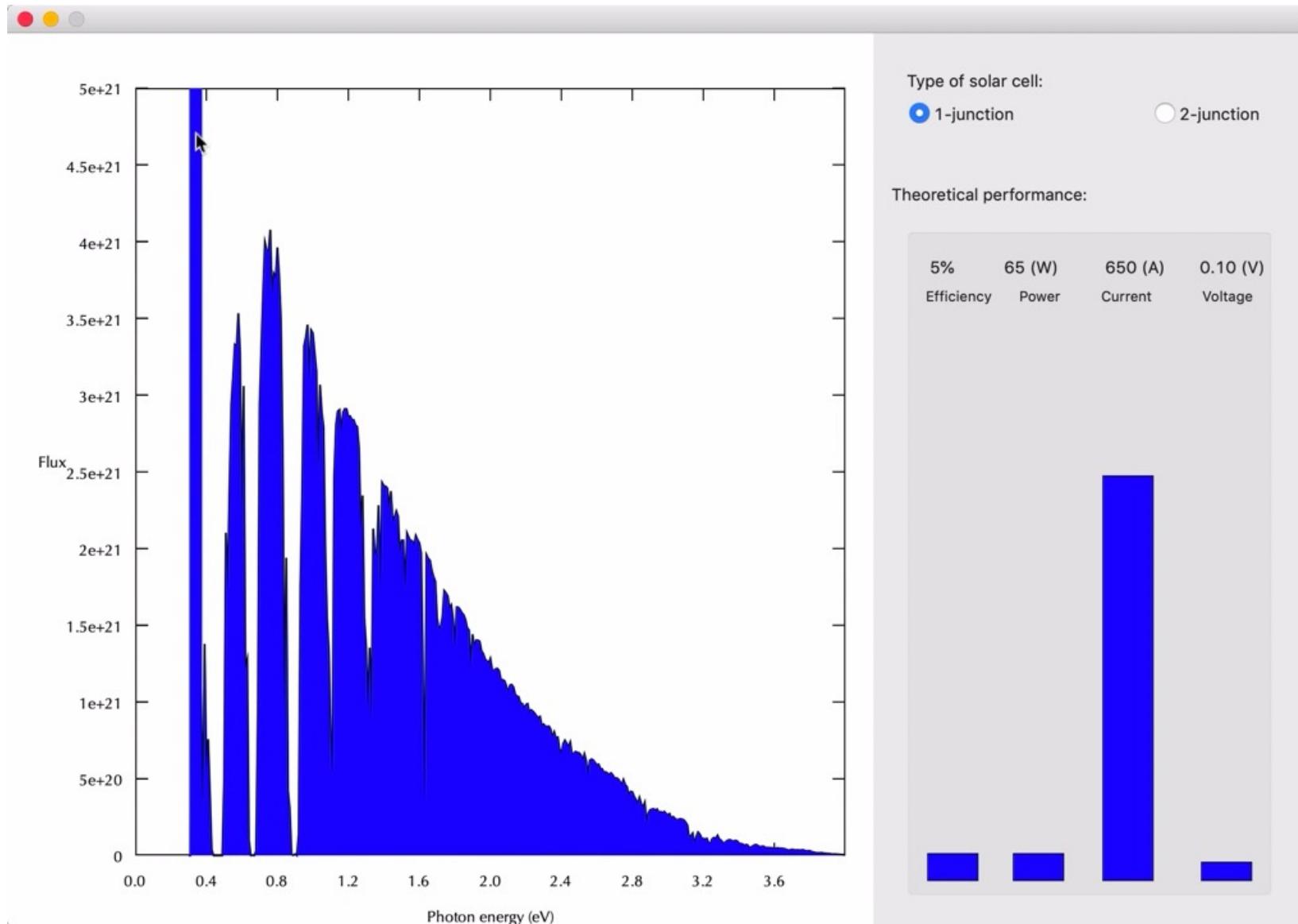


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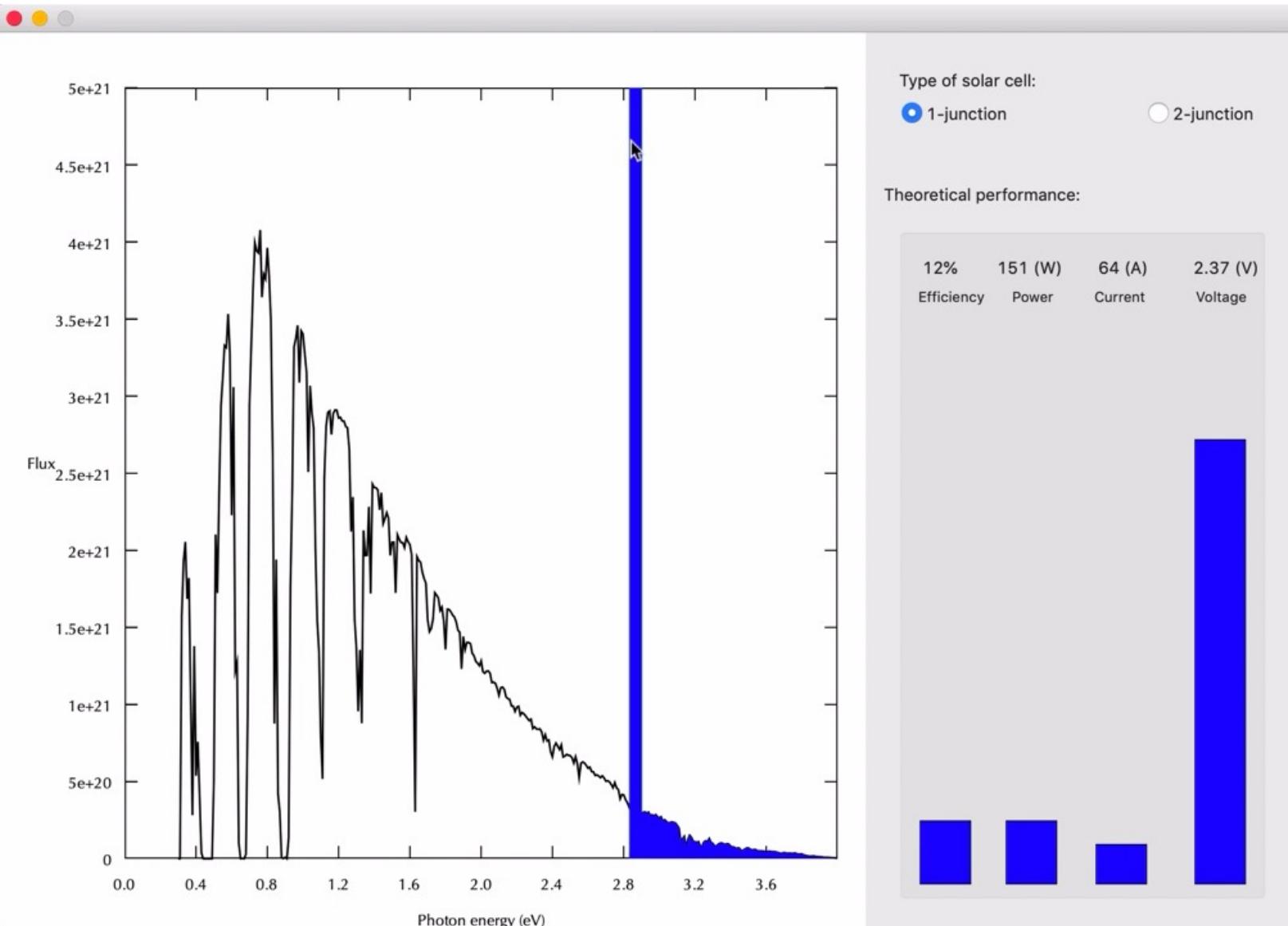
Current, Voltage, Power & Efficiency vs Eg



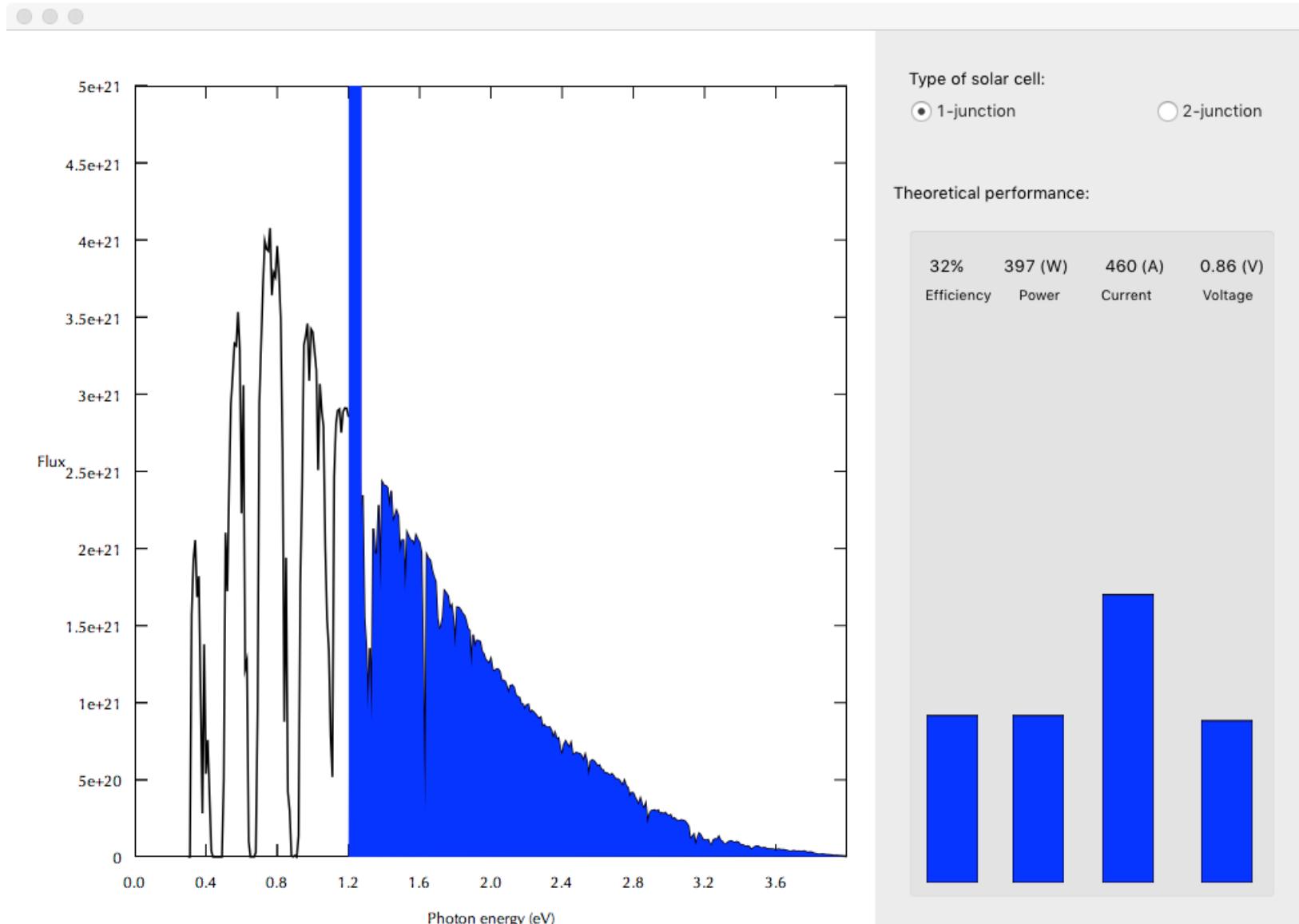
Current, Voltage, Power & Efficiency vs Eg



Current, Voltage, Power & Efficiency vs Eg



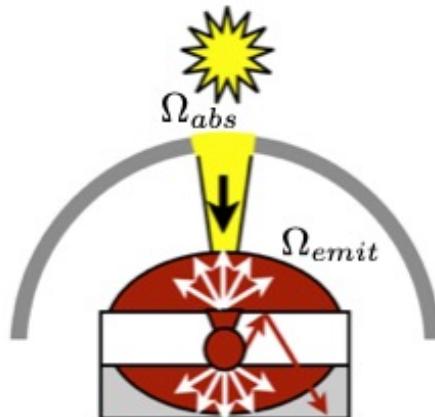
Current, Voltage, Power & Efficiency vs Eg



Electrical Models for PV Devices

Fundamental Shockley-Queisser (Detail Balance)

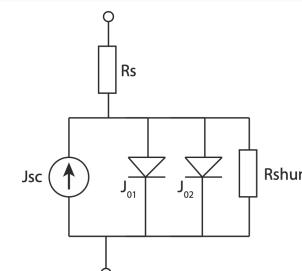
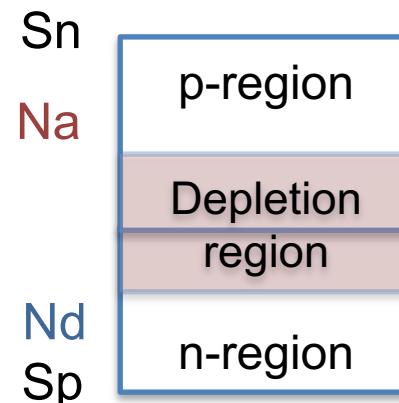
Band-gap : E_g
Temperature : T



Depletion approximation

Analytical solutions to the drift-diffusion equations for homogeneous layers.
Shockley Diode Eqn

Band-gap : E_g Mobility μ
Temperature : T Surface
Diode dimensions: x recombination S_n, S_p
Doping level: N_a, N_d Diffusion length L ,
Absorption Minority carrier
coefficient α lifetime τ

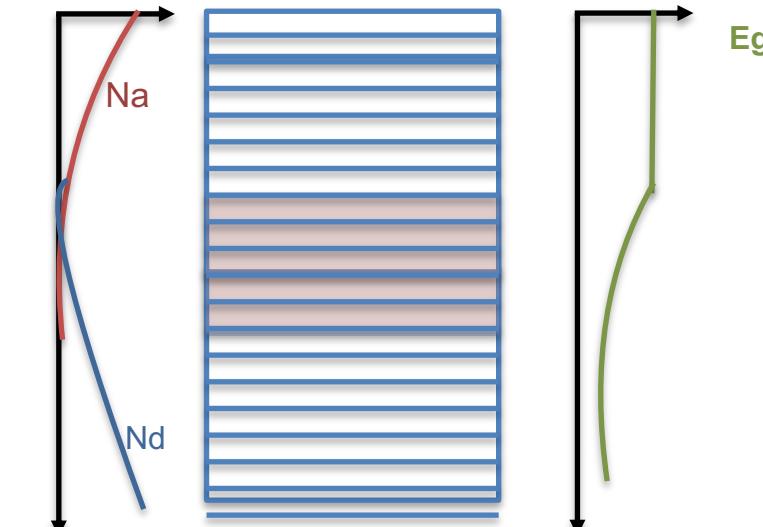


Drift-Diffusion

Numerical solution to the semiconductor drift-diffusion equations: 1D, 2D, 3D

Spatial variation of all parameters previously used in the depletion approximation.

- Variable doping profile within a region (silicon PV)
- Variable band-gap within a region (CIGS PV)
- Mobile ions under dark and illuminated conditions (Perovskite PV)



General Form of the Planck Equation



900K

Tungsten-Halogen light bulb



2800K

Sun



5800K

$$n(E) = \epsilon(E) \frac{2\pi E^2}{c^2 h^3} \frac{1}{e^{\frac{E-\mu}{kT}} - 1}$$

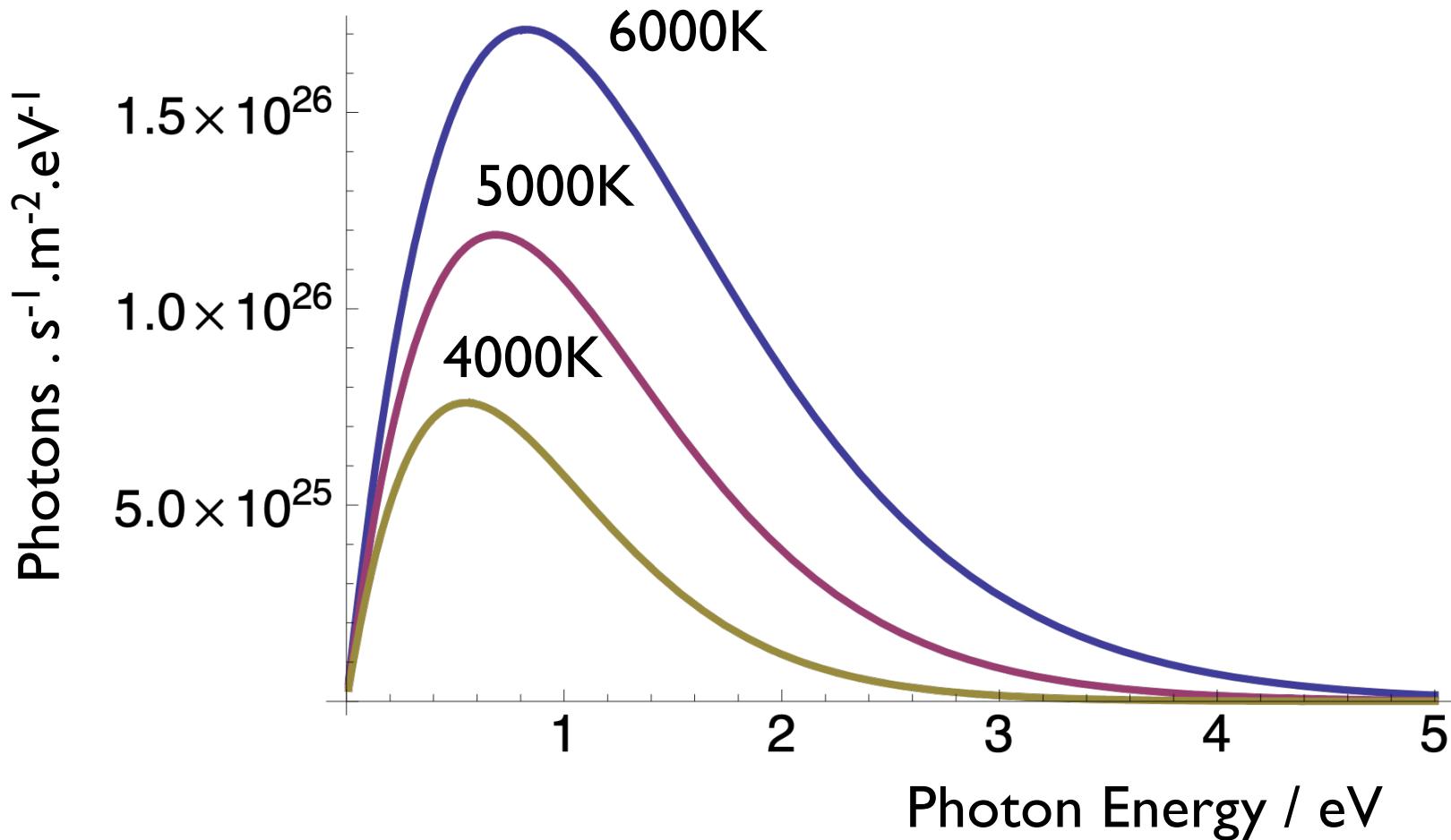
Encapsulates the electronic density of states.

Photon modes

Occupation probability

Blackbody Emission

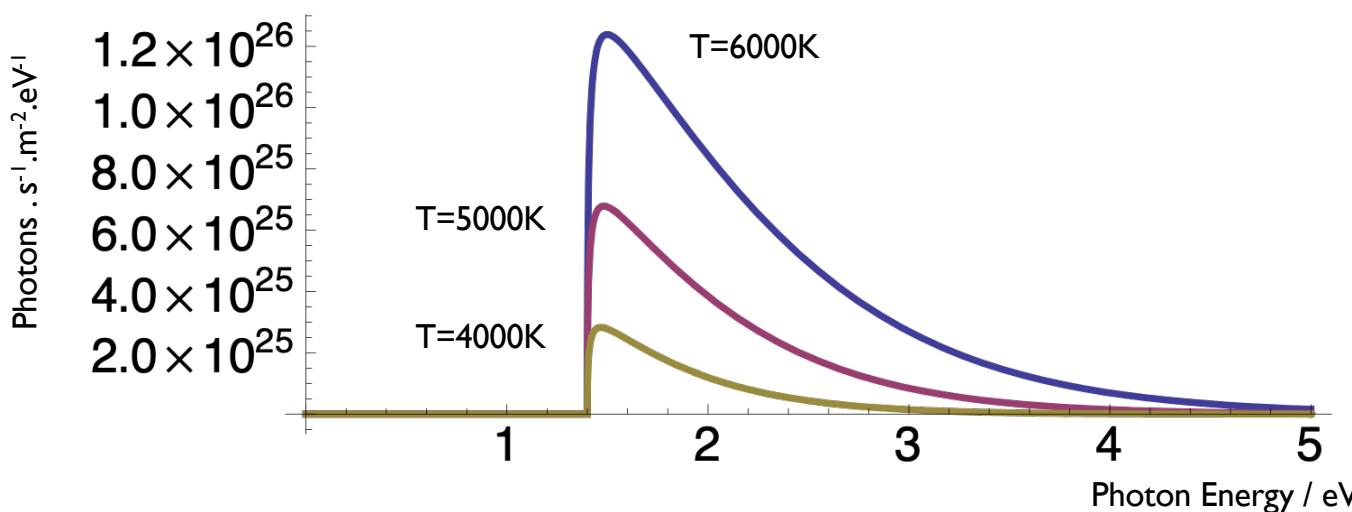
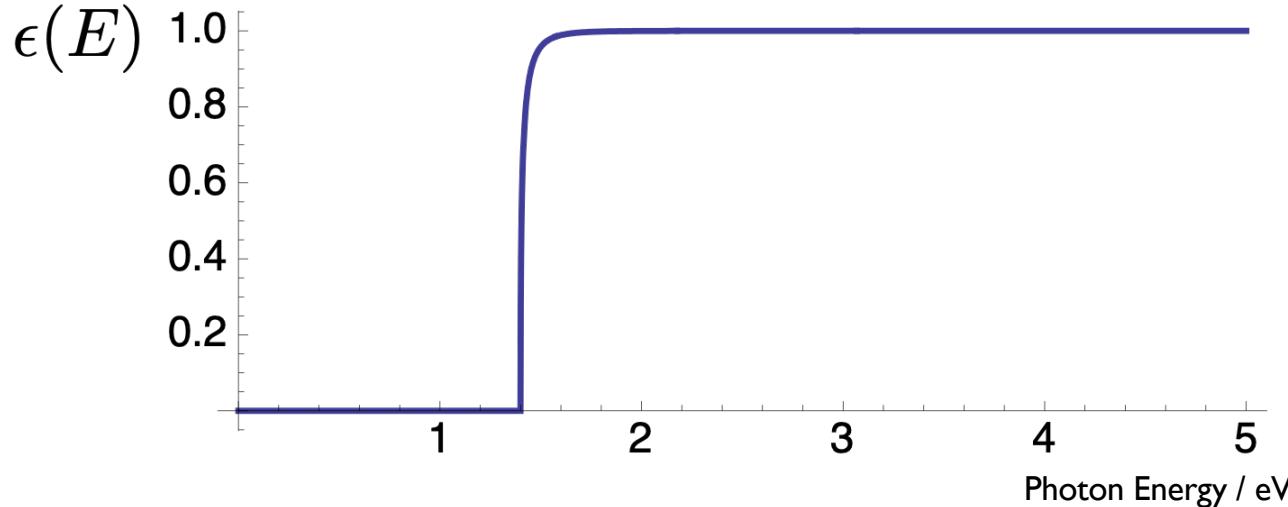
$$n(E) = \epsilon(E) \frac{2\pi}{c^2 h^3} \frac{E^2}{e^{\frac{E-\mu}{kT}} - 1} \quad \begin{aligned} \mu &= 0 \\ \epsilon(E) &= 1 \end{aligned}$$



Semiconductors are “Grey” bodies

$$n(E) = \epsilon(E) \frac{2\pi}{c^2 h^3} \frac{E^2}{e^{\frac{E-\mu}{kT}} - 1}$$

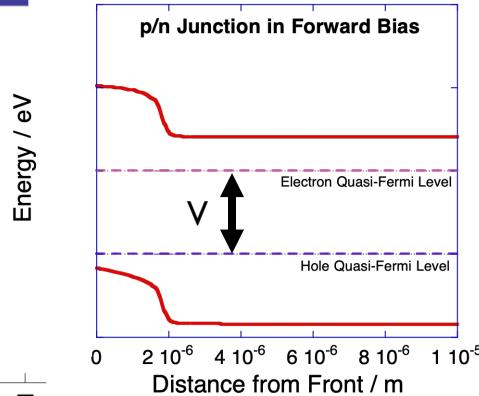
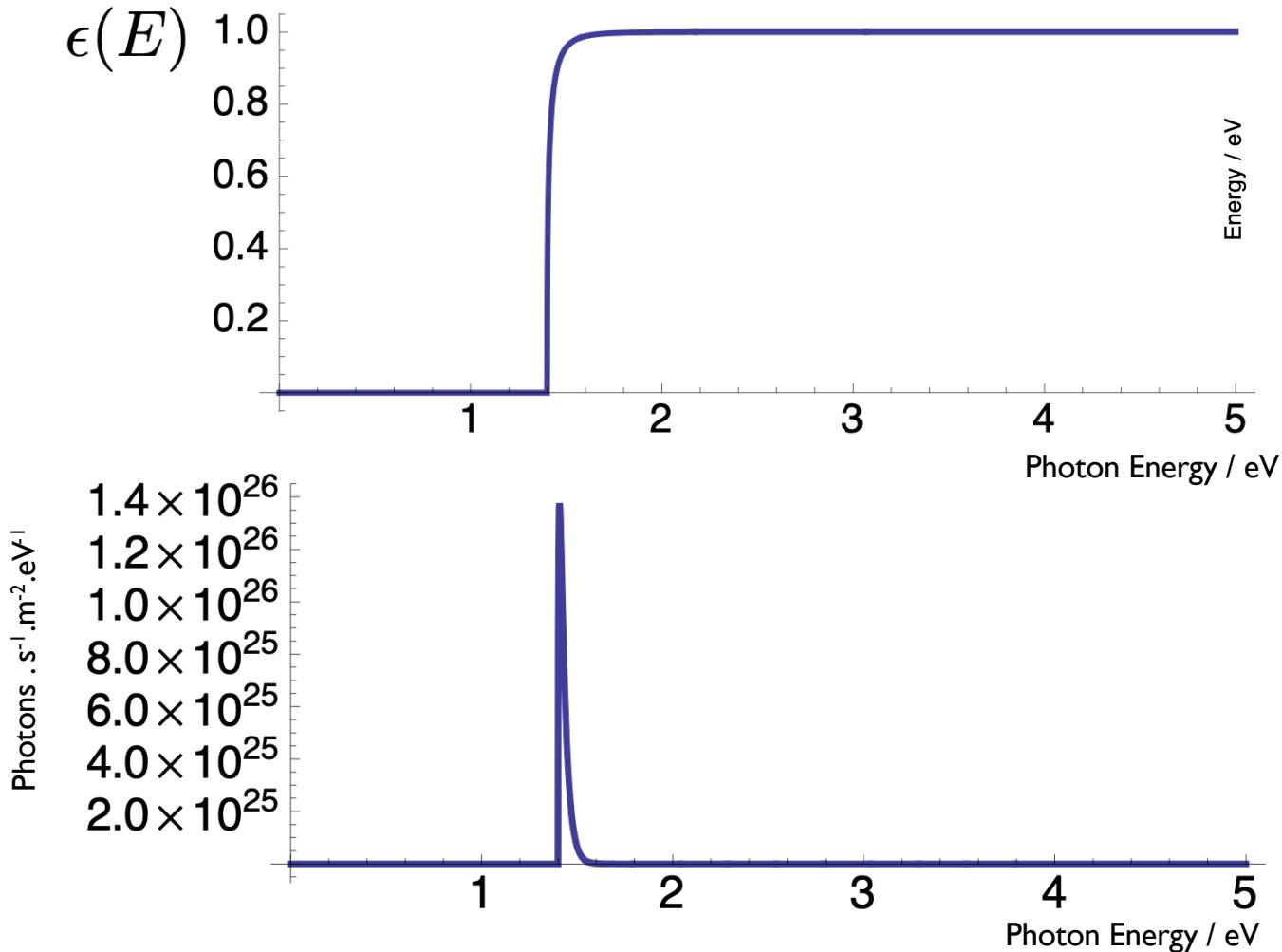
$$\begin{aligned}\mu &= 0 \\ T &> 300K\end{aligned}$$



Electroluminescence

$$n(E) = \epsilon(E) \frac{2\pi}{c^2 h^3} \frac{E^2}{e^{\frac{E-\mu}{kT}} - 1}$$

$$\mu = 1.35V$$
$$T = 300K$$

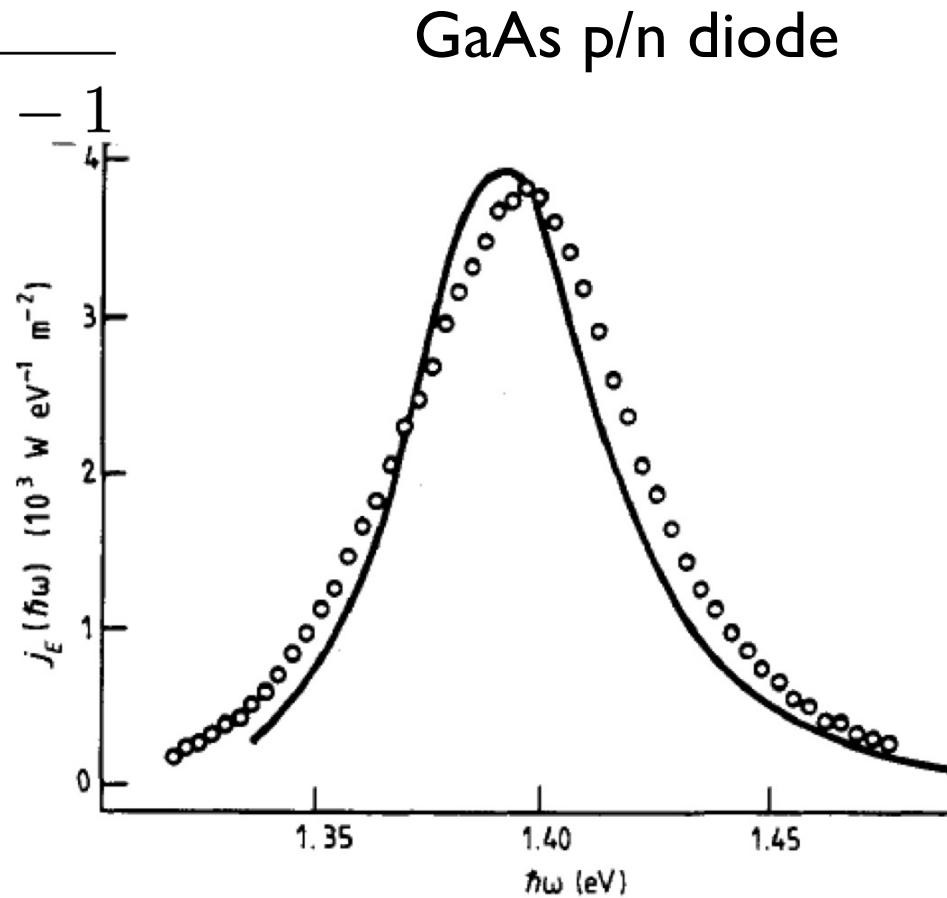


Verification of the Generalised Planck Expression

$$n(E) = \epsilon(E) \frac{2\pi}{c^2 h^3} \frac{E^2}{e^{\frac{E-\mu}{kT}} - 1}$$

$$\mu = 1.206V$$

$$T = 296K$$



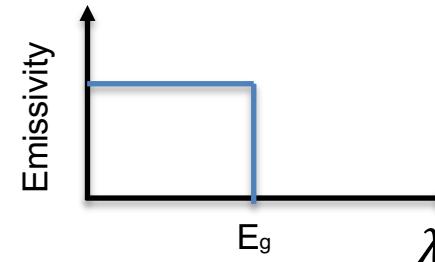
Radiative limit to J_0

$$\dot{N} = \int_{Eg}^{E_{top}} \epsilon(E) \frac{2\pi}{c^2 h^3} \frac{E^2}{e^{\frac{E-\mu}{kT}} - 1} dE$$

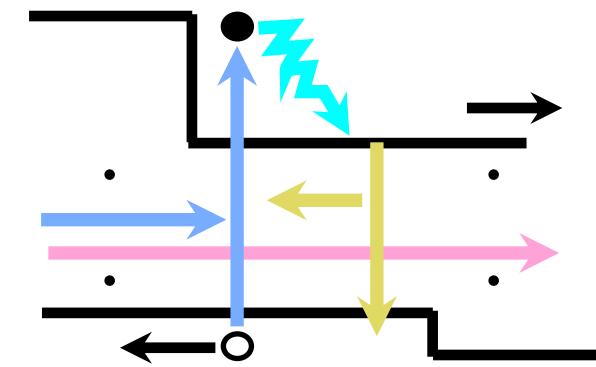
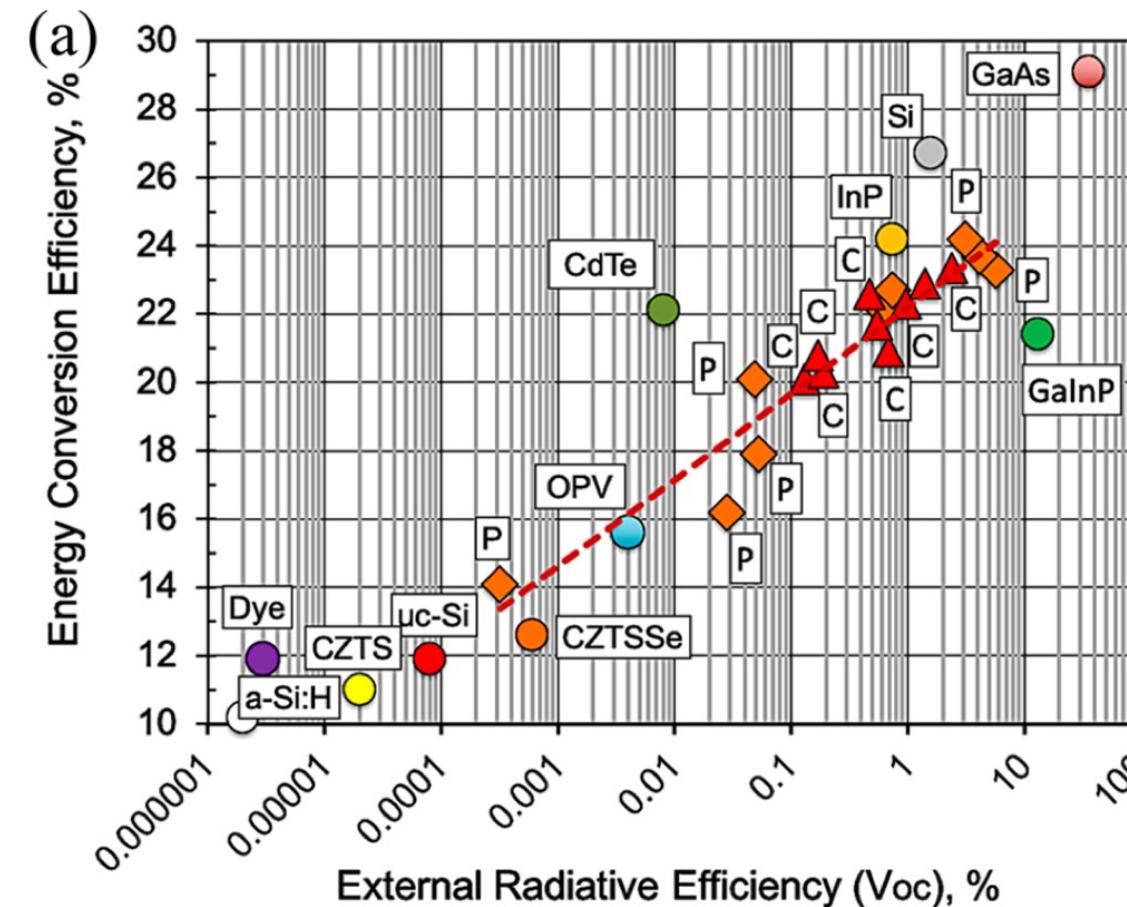
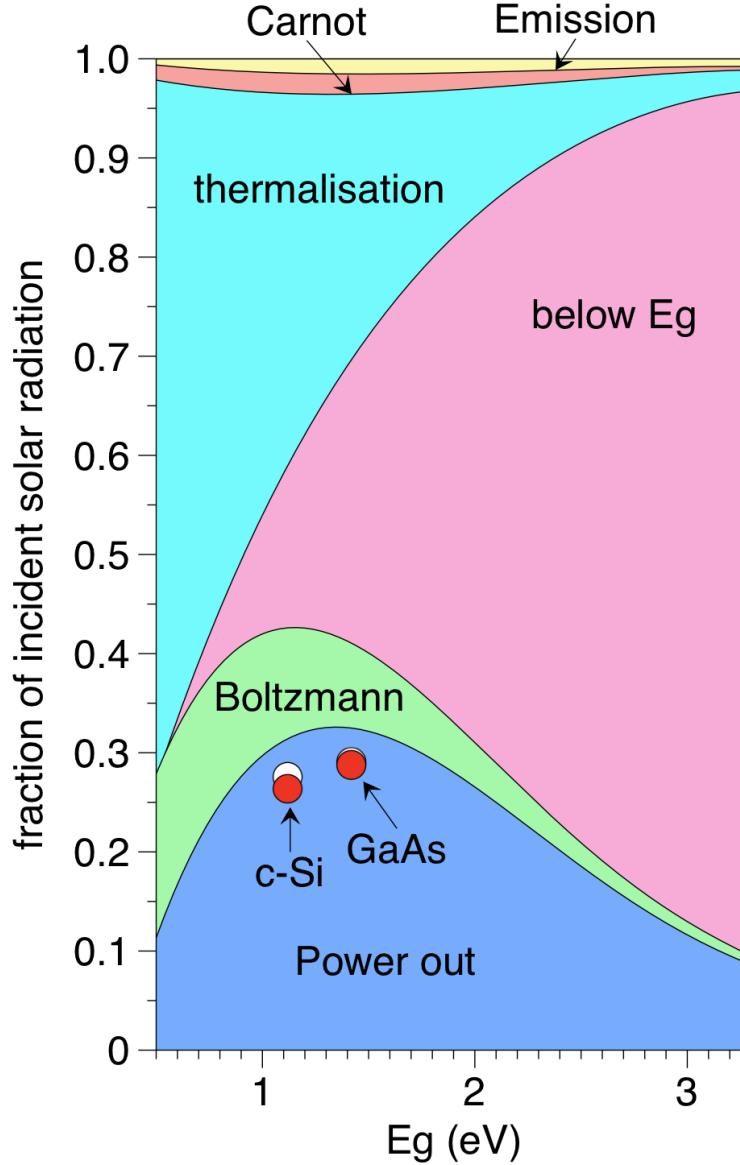
- Assume $F(E)$ Boltzmann approximation
- Bands are infinite ($E_g \rightarrow \infty$)

$$\begin{aligned}\dot{N} &= \int_{Eg}^{\infty} \epsilon(E) \frac{2\pi}{c^2 h^3} \frac{E^2}{e^{\frac{E-\mu}{kT}} - 1} dE \\ &= \underbrace{(\epsilon kT(Eg^2 + 2EgkT + 2k^2T^2)e^{\frac{-Eg}{kT}})}_{\frac{J_0}{q}} e^{\frac{\mu}{kT}} \quad \mu = qV\end{aligned}$$

$$J = J_0 e^{\frac{qV}{kT}}$$

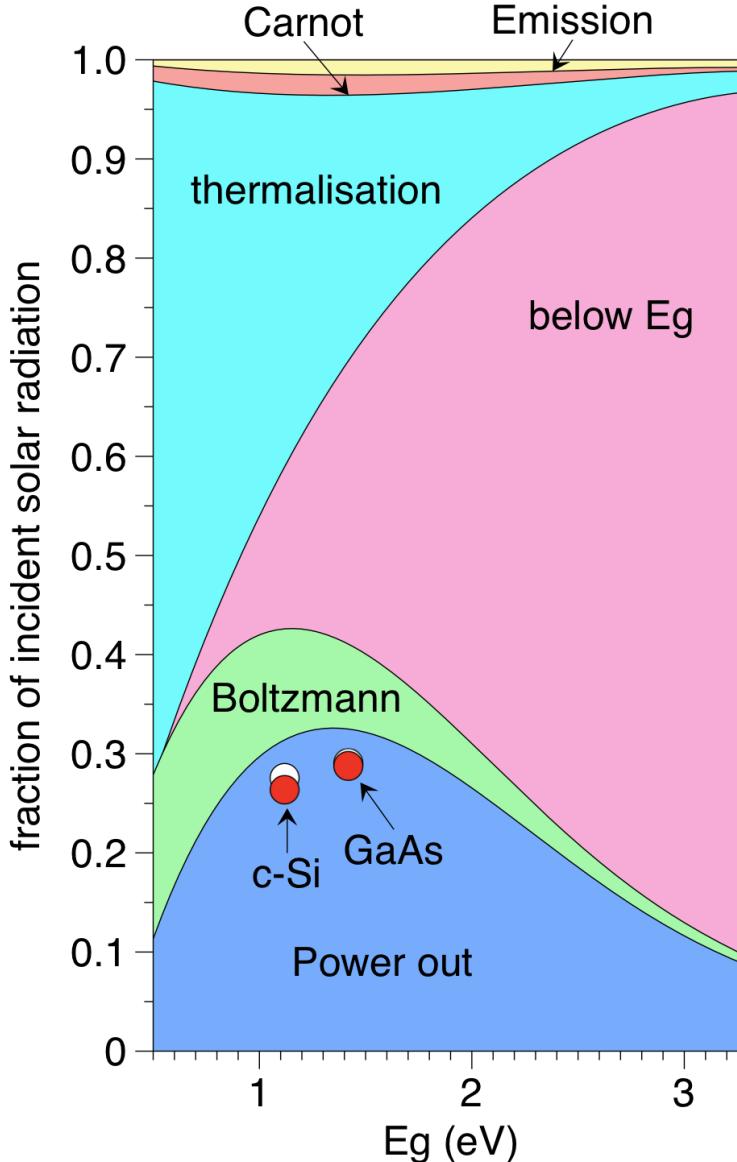


Unpacking the Shockley Queisser Efficiency limit:





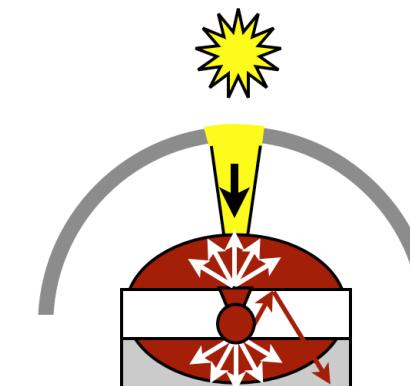
Understanding the effect of solar concentration



$$qV_{max} = E_g - E_g \frac{T_A}{T_s} - kT_A \ln \left(\frac{\Omega_{emit}}{\Omega_{abs}} \right)$$

Boltzmann loss

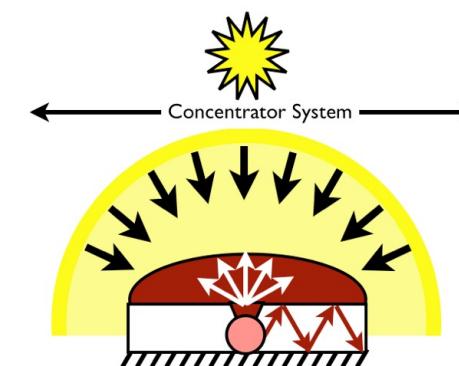
Conventional solar cell



$$\Omega_{emit} \gg \Omega_{abs}$$

Significant Boltzmann loss!

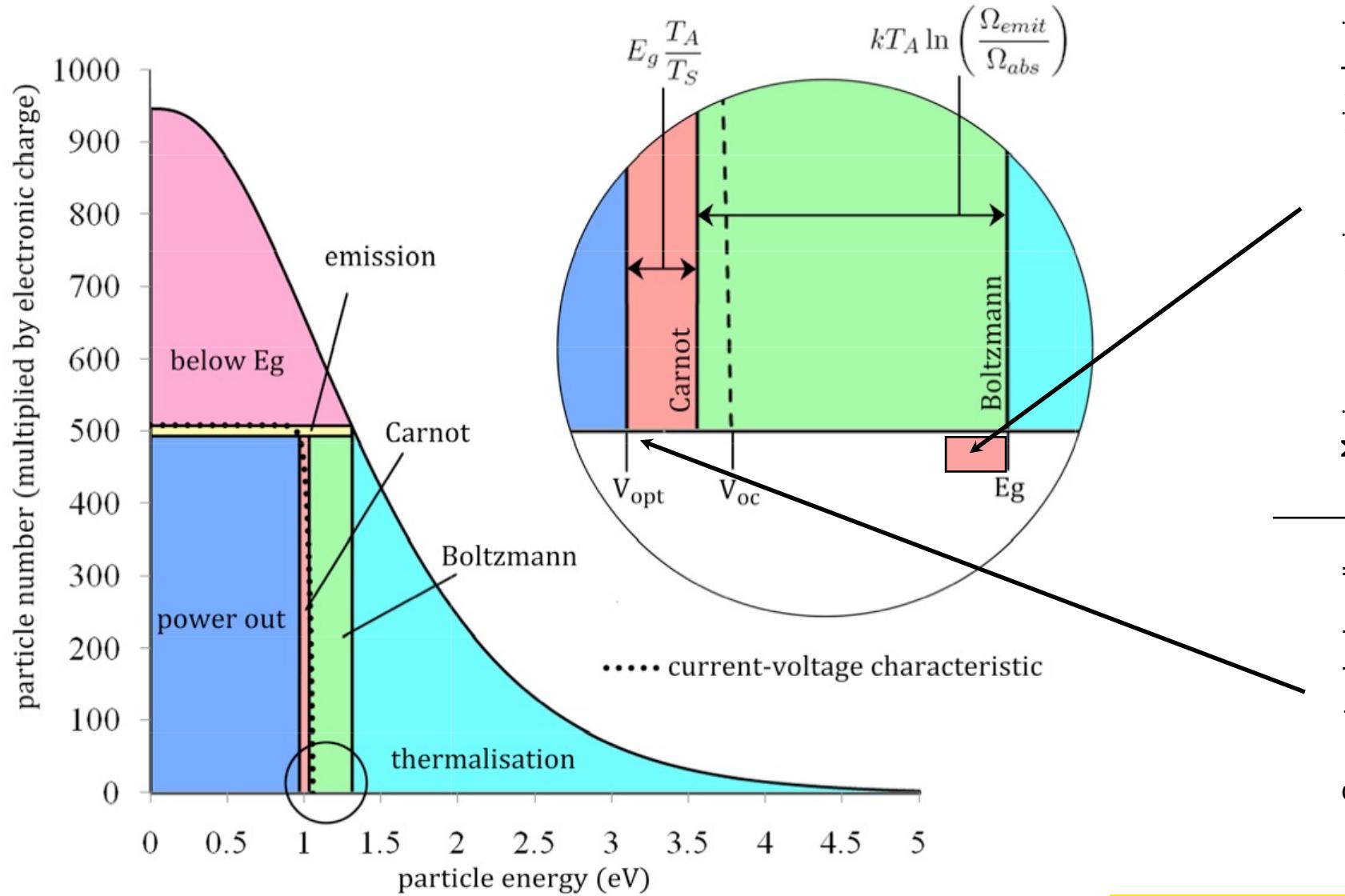
Maximum concentration



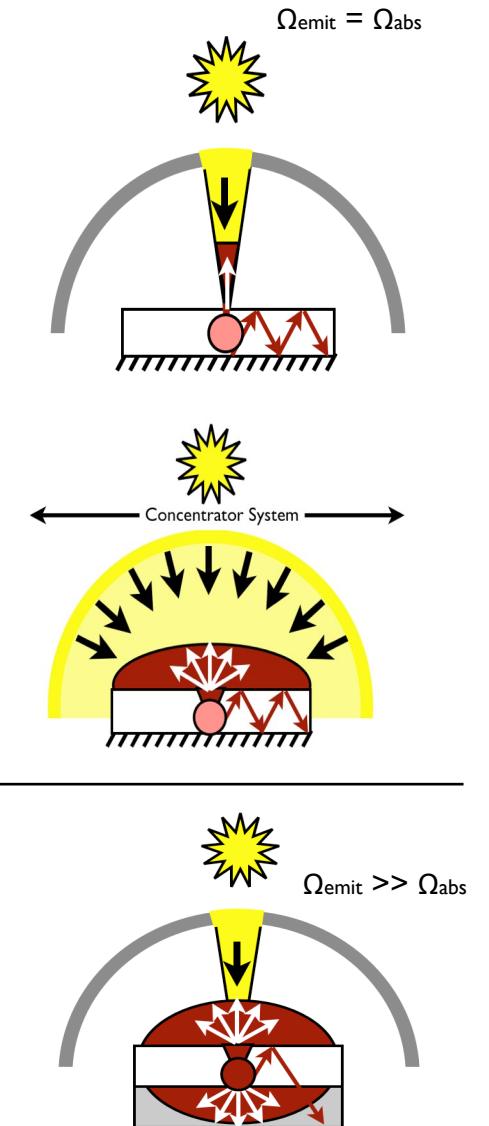
$$\Omega_{emit} = \Omega_{abs}$$

Zero Boltzmann loss.

Understanding the effect of solar concentration :



Maximum concentration or restricted emission



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Session 5: Simple Si and GaAs cells using the depletion approximation

2nd August 2023

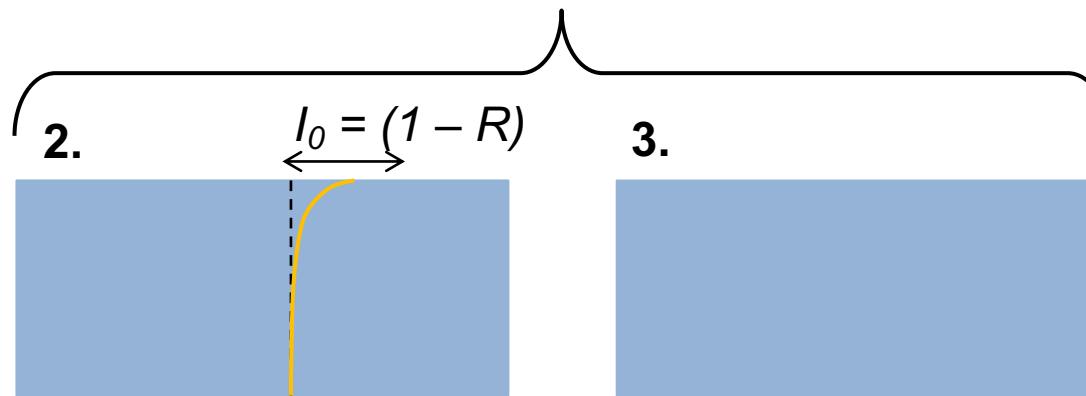
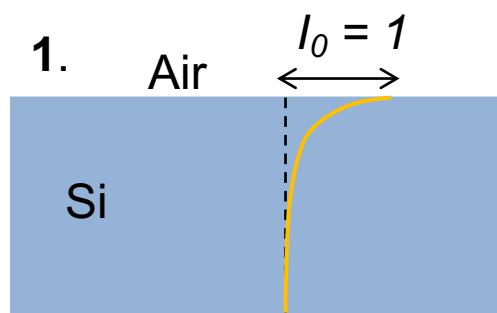
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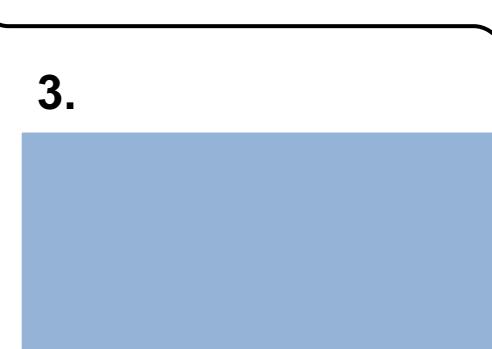
Example 5a: Simple Si cell

Si is considered infinitely thick, with 200 μm of absorbing thickness (ignore back-surface reflection)

Calculate same result in this case!



3.



4.



Beer-Lambert absorption:

$$I(z) = I_0 e^{-a(\lambda) z}$$

$$I_0 = 1$$

Fresnel eqn + Beer-Lambert absorption:

$$I(z) = I_0(\lambda) e^{-a(\lambda) z}$$

$$I_0(\lambda) = 1 - R(\lambda)$$

Transfer matrix method

(Si treated *incoherently*)

Add ARC, Transfer-matrix method

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Sessions 6 & 7: Transfer-matrix method

2nd August 2023

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Transfer-matrix method (TMM) in Solcore

Defining structures

Materials $\text{Ga}_{0.51}\text{In}_{0.49}\text{P}$ = GaInP In = 0.49

with optical properties ($n(\lambda)$, $k(\lambda)$)
retrieved from database

Layers 500 nm of InGaP

Stacks / Structures

Stack = [500 nm of InGaP
+ 1500 nm of GaAs
+ 70 nm of AlAs
+ ...]

calculate RAT of Stack with AM0 spectrum

Modelling optics

Transfer-matrix method (TMM)

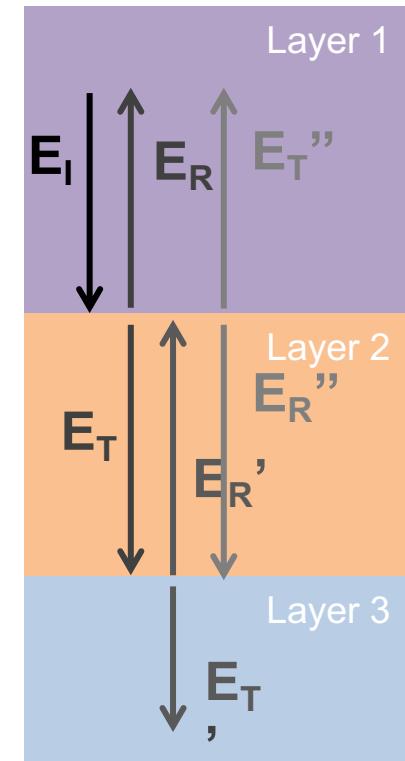
Efficiently handles **planar multilayer** stacks (including thin film interference effects)

$$\mathbf{M}_{\text{Layer 1}}$$

$$\mathbf{M}_{\text{Layer 2}}$$

$$\mathbf{M}_{\text{Layer 3}}$$

Relates waves entering and exiting layer 2 (both directions)



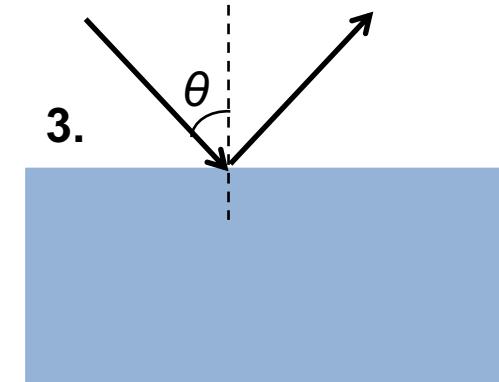
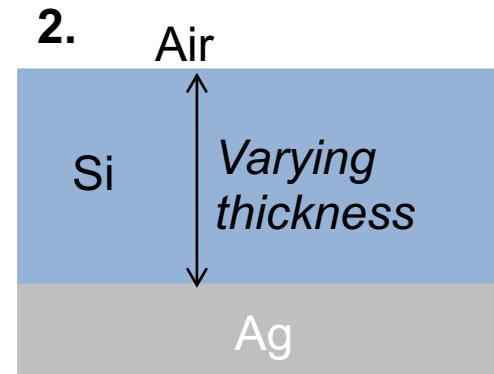
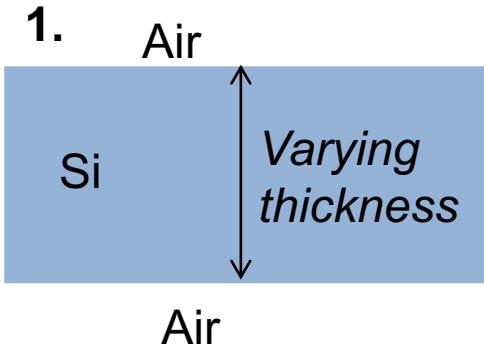
R, A, T of stack

$$\mathbf{M}_{\text{stack}} = \mathbf{M}_{01} \times \mathbf{M}_{\text{Layer 1}} \times \mathbf{M}_{\text{Layer 2}} \times \mathbf{M}_{\text{Layer 3}} \times \dots$$

Solcore integrates & streamlines the **tmm** Python package

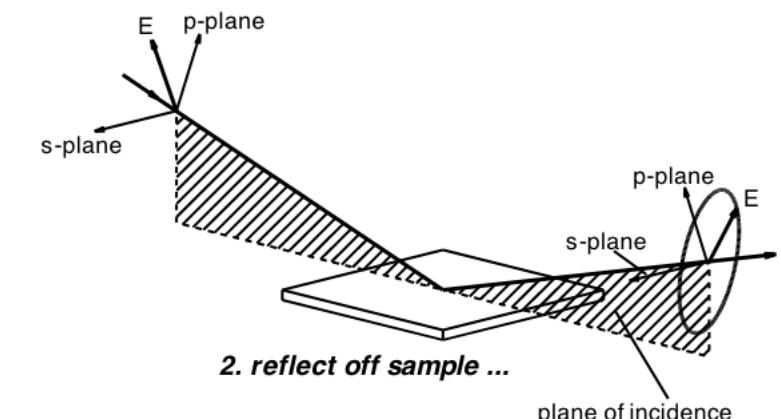
Example 6a: More exploration of TMM

No longer ignore back-surface reflection. Explore effect of different assumptions about coherency, the incidence angle, and the polarization of the incident light



Varying angle of incidence
and polarization

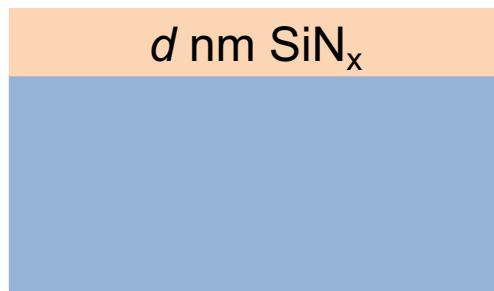
Treating a layer **incoherently** means **discarding the phase information** inside that layer; no **Fabry-Perot/thin-film interference**. The absorption profile is assumed to follow the Beer-Lambert law.



Example 6b: Simple ARC optimization

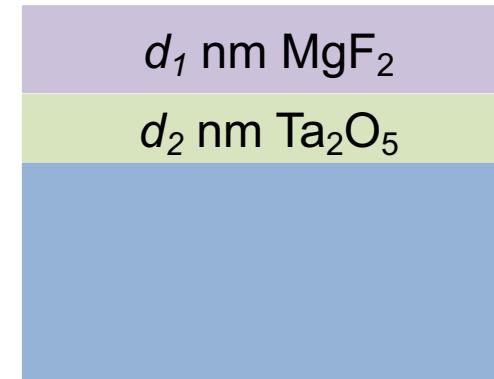
Find ARC layer thicknesses which minimize reflectance

1.



Vary d

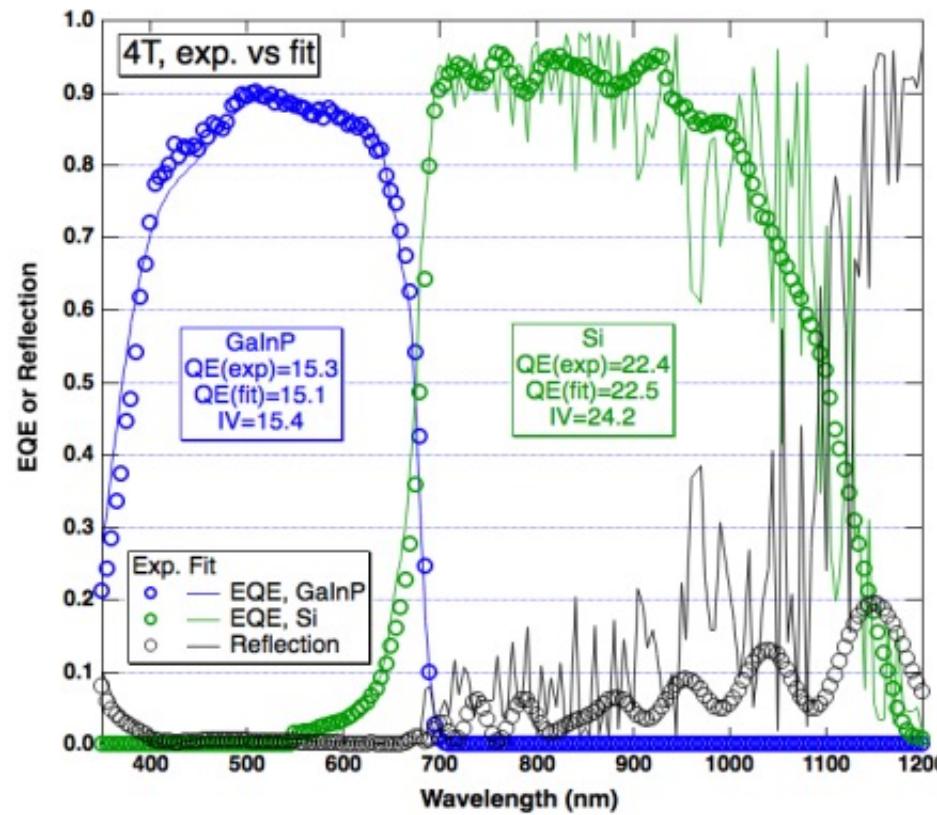
2.



Vary d_1 and d_2

Example 7: Planar GaInP/Si cell (2-terminal vs. 4-terminal)

Material	Thickness (nm)	Contrib. to j_{sc}
air	0	0
MgF ₂	97	0
ZnS	41	0
n-Al _{0.52} In _{0.48} P	17 (20)	0
n-Ga _{0.5} In _{0.5} P	950 (1000)	0.91
p-Al _{0.27} Ga _{0.26} In _{0.47} P	200	0
p-Al _{0.5} Ga _{0.5} As	500	0
ZnS	82	0
epoxy	10,000	0
glass, n=1.56	1,000,000	0
epoxy	10,000	0
PECVD SiO _x	100	0
SiN _x , n=1.91	70	0
SiN _x , n=2.4	15	0
n,p-Si	357,000 (150,000)	1
Al ₂ O ₃	15	0
SiN _x , n=1.91	120	0
Al	10,000	0



Note: the paper uses a textured Si bottom cell, while we assume all interfaces are planar. We will discuss the use of textures in III-V/Si and perovskite/Si tandem cells tomorrow.

Faculty of Engineering
School of Photovoltaic and Renewable Energy Engineering



UNSW
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Sessions 8 - 10: Advanced optical modelling

3rd August 2023

Ned Ekins-Daukes, Phoebe Pearce



RayFlare installation

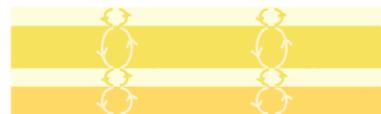
- Previously, we have used **Solcore** for all the examples.
 - Solcore has quite a lot of optics capabilities, but **it cannot do ray-tracing**
 - **RayFlare** is our dedicated optics package; it can reproduce what Solcore does, but also adds new functionality:
 - Ray-tracing
 - Angular redistribution matrix method (ARMM)
- Please go to **rayflare.readthedocs.io** and read the installation instructions
 - Basic installation: **pip install rayflare**
 - This will install everything except RCWA functionality (for diffraction gratings/2D periodic structures)
 - Installation instructions for RCWA functionality can be found in the documentation. Unfortunately, it does not work on Windows (but all other RayFlare functionality does work!)

RayFlare capabilities

Simulations using a single method



Ray-tracing: Geometric optics for large-scale textures without diffraction effects



Transfer-matrix method: Wave optics for planar layers (coherent and incoherent)



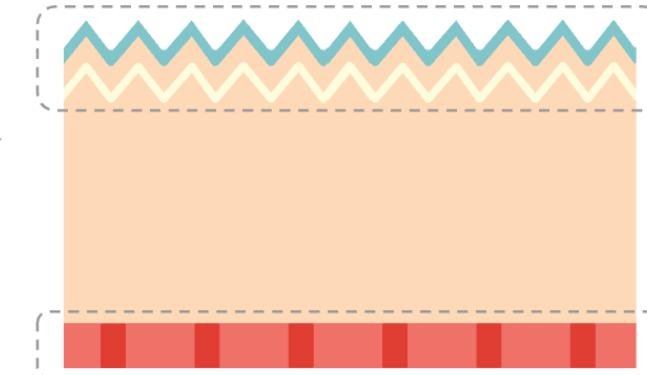
Rigorous coupled-wave analysis: Wave optics for planar or periodic structures e.g. gratings, photonic crystals

Ideal cases: E.g. perfect mirrors, Lambertian scattering

Calculate e.g. reflection, transmission, absorption per layer, depth-dependent absorption profiles

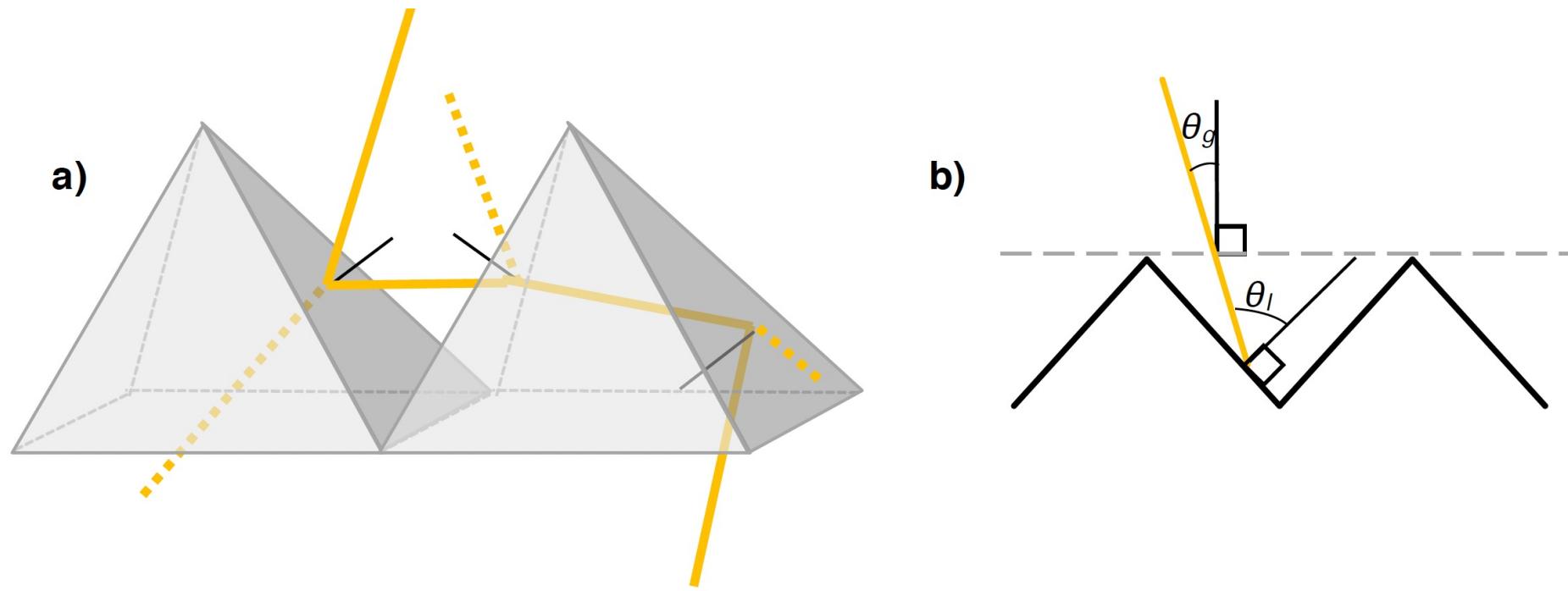
Simulations using angular redistribution matrices

Each surface is treated separately with an appropriate method



- Free, open source
- Anyone can contribute
- Modular
- Documented

Ray-tracing



Reflection and transmission probabilities can be calculated using the Fresnel equations (for simple interfaces) or TMM (for interface with thin layers). If using TMM, can also calculate absorption per layer (and absorption profiles)

Rigorous coupled-wave analysis (RCWA)

(Also called the "Fourier Modal Method")

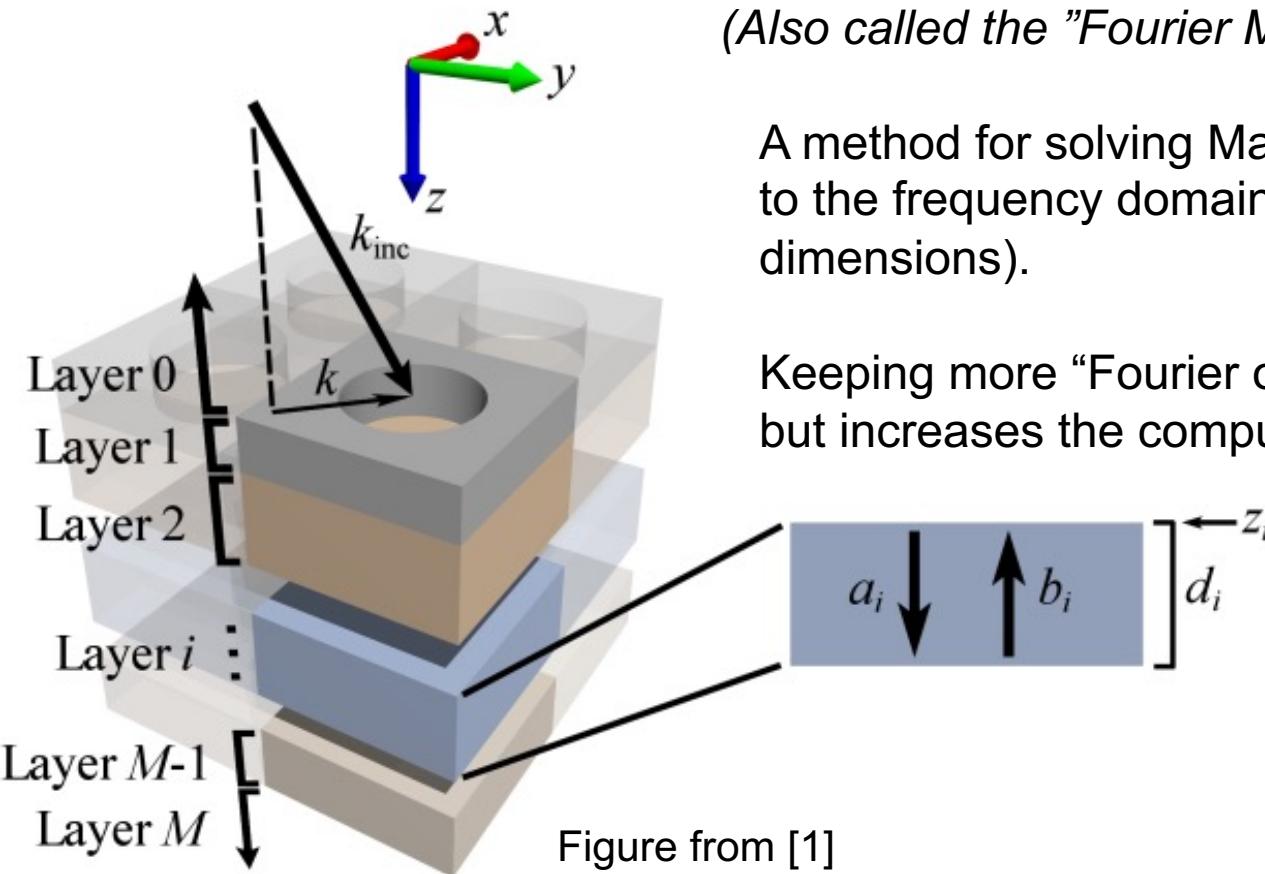


Figure from [1]

A method for solving Maxwell's equations, which transforms the problem to the frequency domain (for structures which are periodic in two dimensions).

Keeping more "Fourier orders" should make the solution more accurate, but increases the computation time

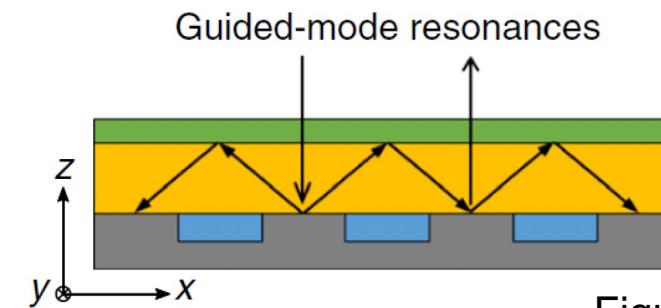
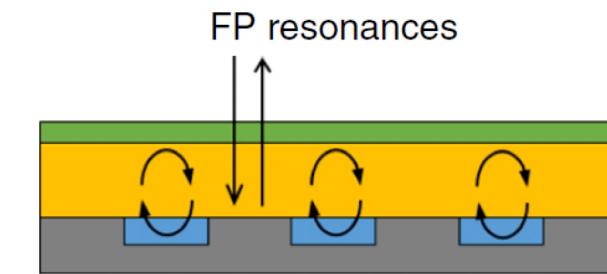


Figure from [2]

[1] H.-L. Chen et al., *Nature Energy*, vol. 4, no. September, 2019, doi: [10.1038/s41560-019-0434-y](https://doi.org/10.1038/s41560-019-0434-y).

[2] <https://web.stanford.edu/group/fan/S4>

Angular Redistribution Matrix Method

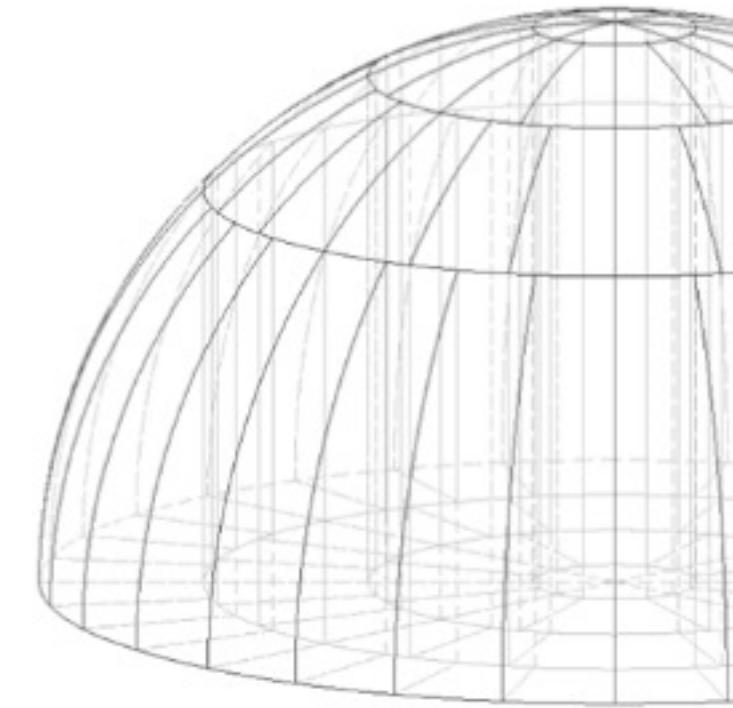
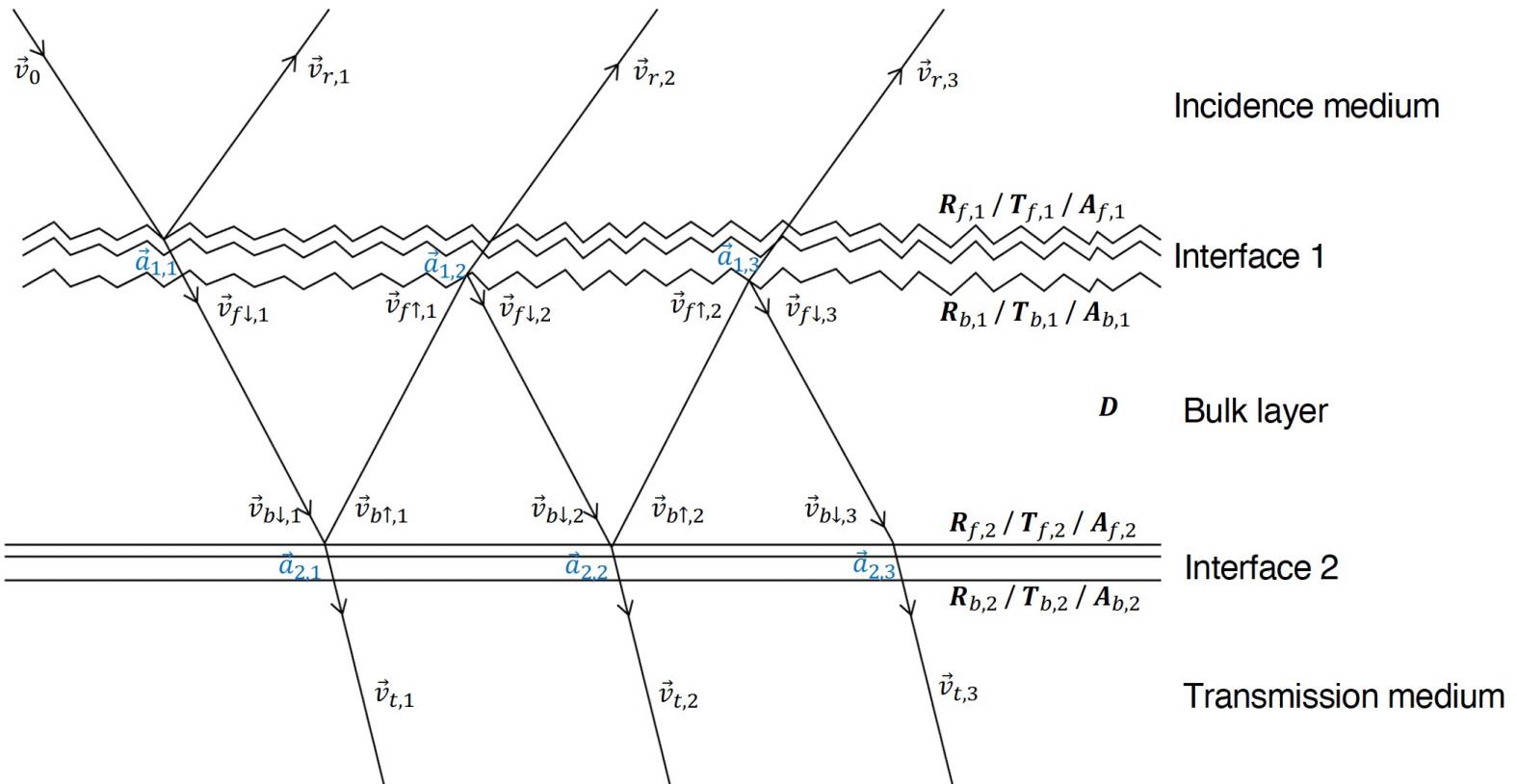
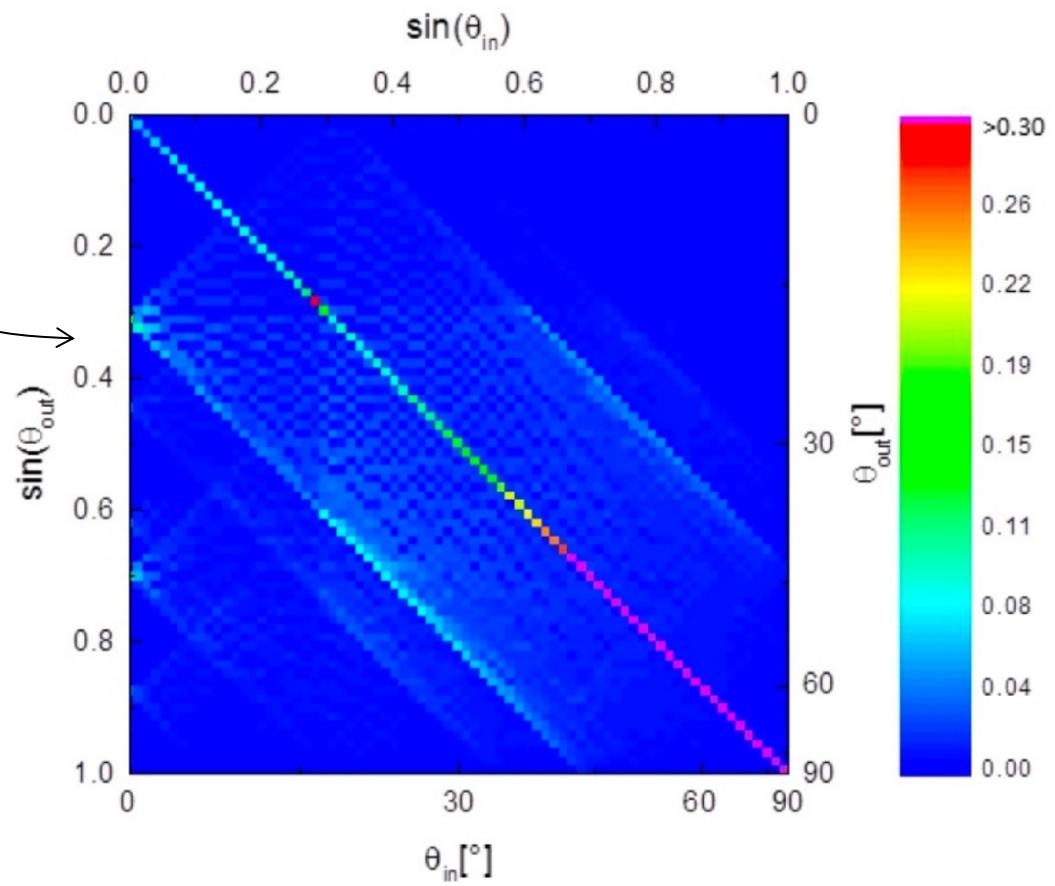
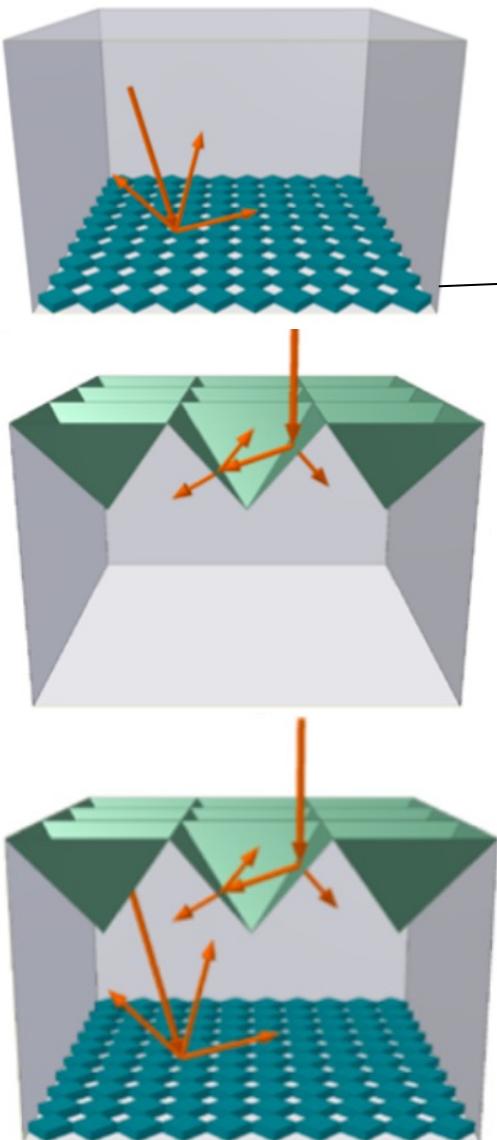


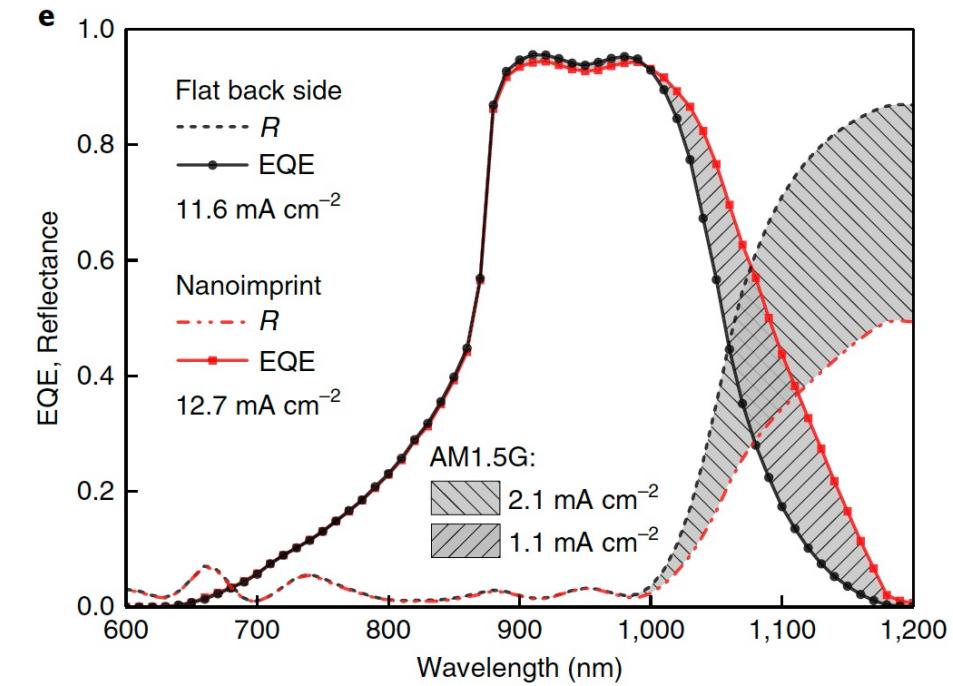
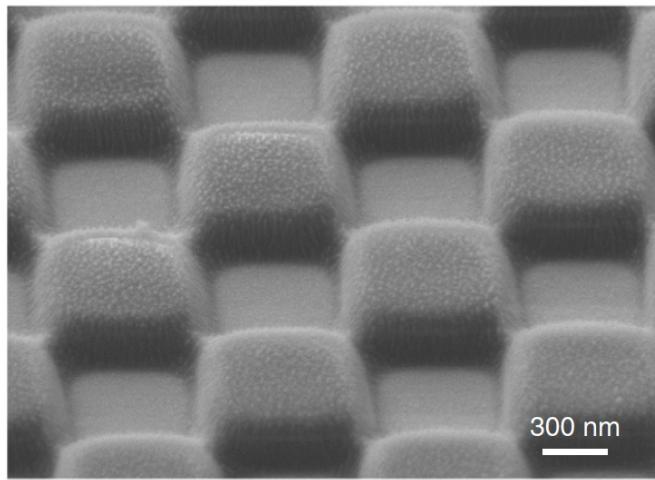
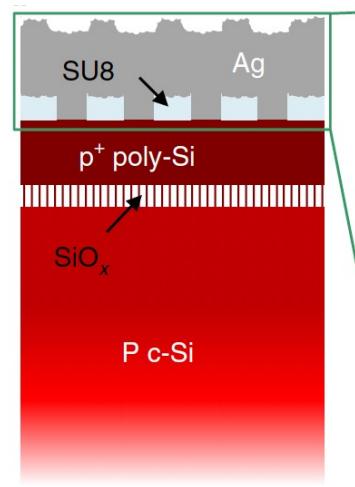
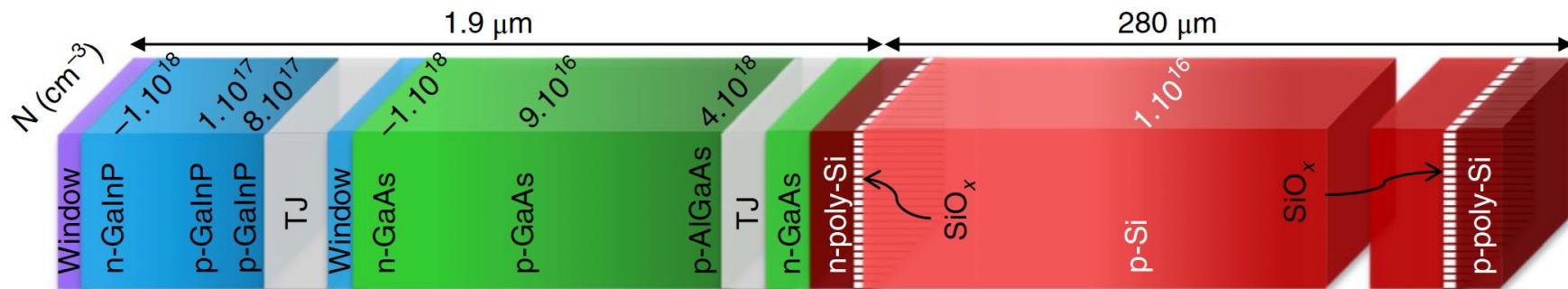
Image from [1]

[1] N. Tucher *et al.*, *Optics Express*, vol. 23, no. 24, p. A1720, 2015, doi: [10.1364/OE.23.0A1720](https://doi.org/10.1364/OE.23.0A1720).

8. Textured Si: pyramids/grating



9a. III-V on Si, planar vs. rear grating



9b. III-V on Si, planar vs. pyramidal Si texture

Use same III-V layer stack as previous example, but assume Si is pyramidally textured on both sides, and epoxy/glass is used to mechanically connect the III-V layers to the Si.



10. Conformal perovskite on pyramidal Si texture

