Hybrid solar energy conversion

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theoretical chemistry & spectroscopy

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Outline

1) Photovoltaic energy conversion
2) Organic solar cells
3) Perovskite solar cells

Outline

1) Photovoltaic energy conversion

   - Basics
   - Motivation for emerging PV

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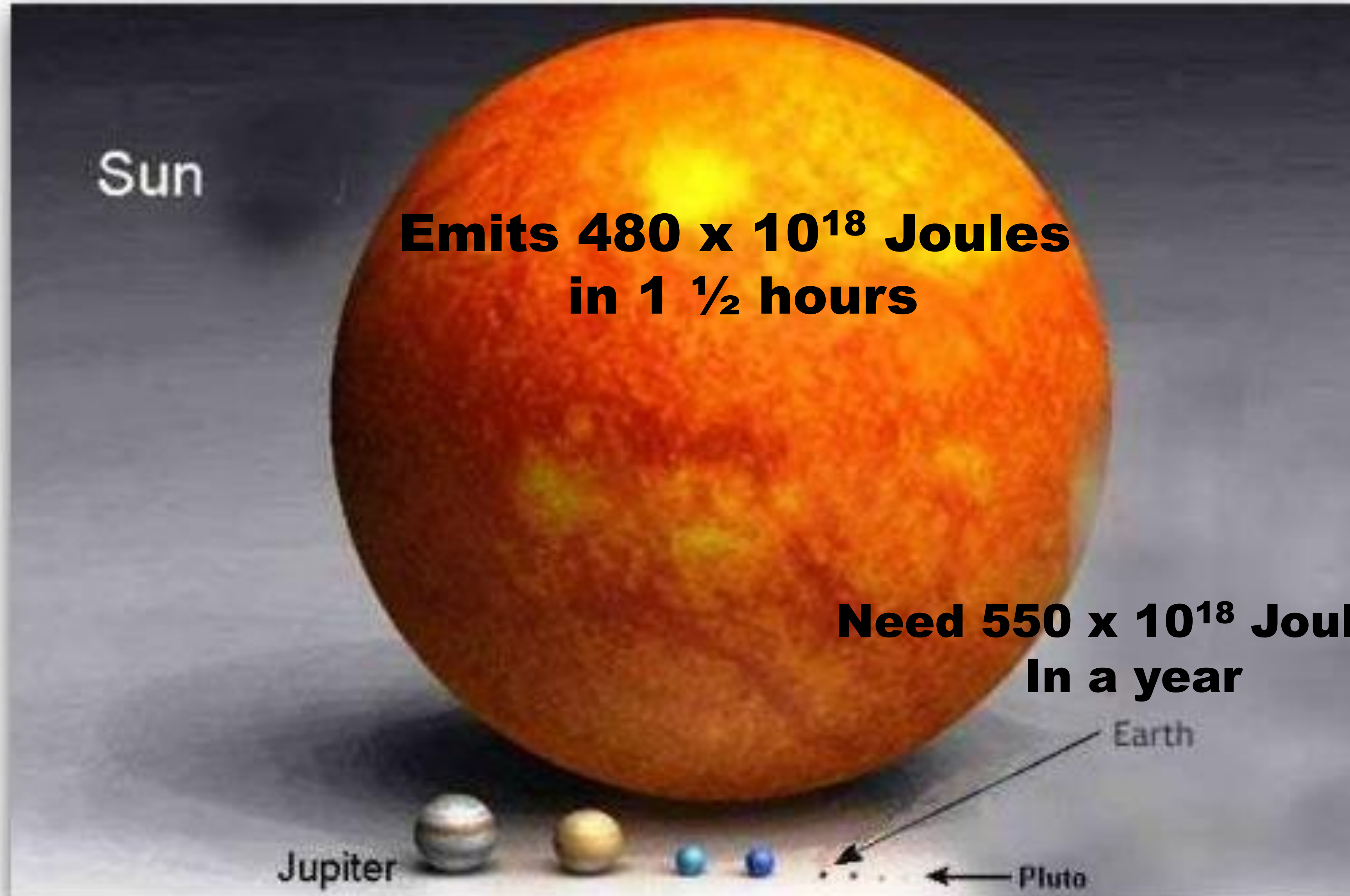
1) Photovoltaic energy conversion

   - Basics
   - Motivation for emerging PV

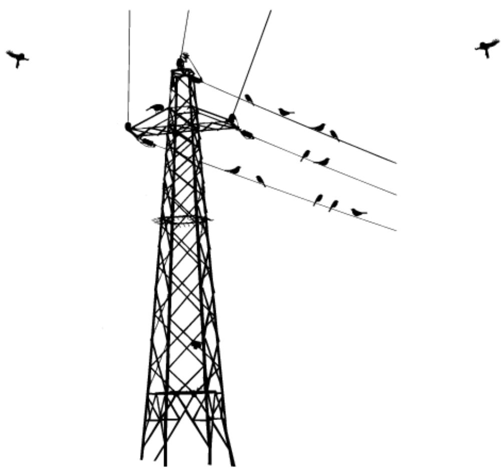
Motivation


Sun
Emits 480 x 10^{18} Joules
in 1 ½ hours
Need 550 x 10^{18} Joules
In a year
Earth
Jupiter
Pluto

Motivation

Flexible, large area, mobile, low maintenance

Large scale



Mobility

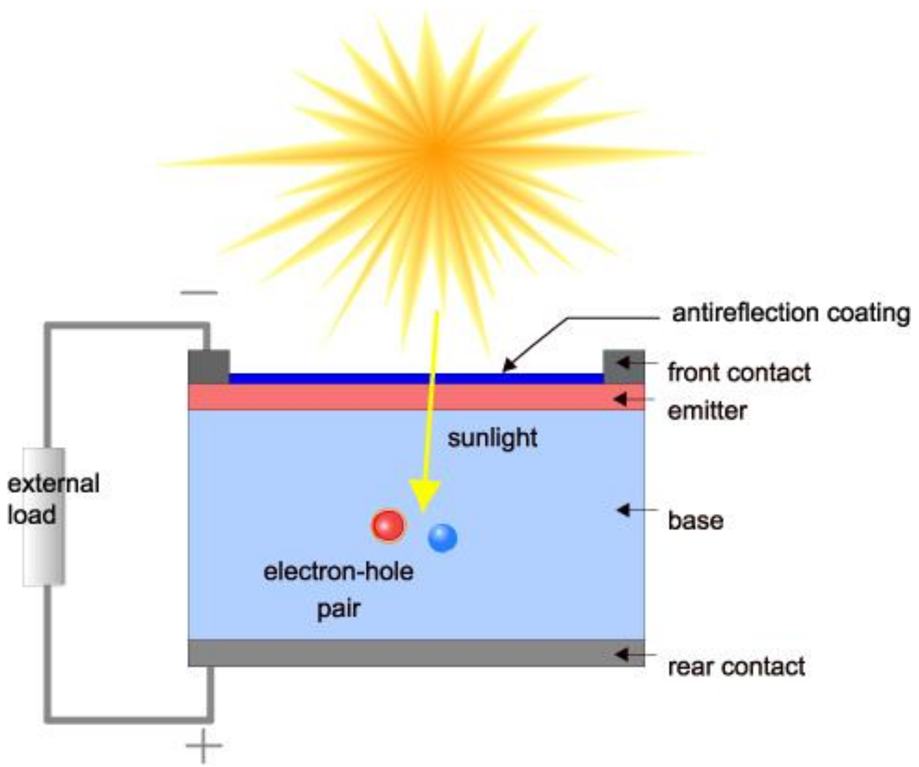
Transportation

Challenges

Converting to a useful form

Meeting versatile energy demands

Photovoltaics

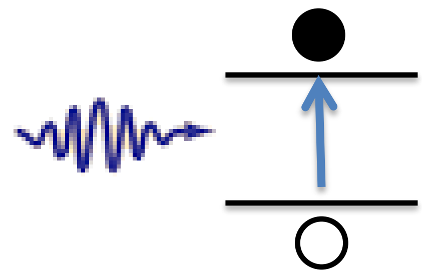


Conversion of light to electricity

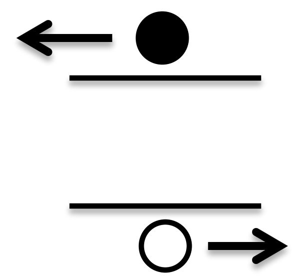
Current x Voltage = power

Photovoltaics

1. Light absorption

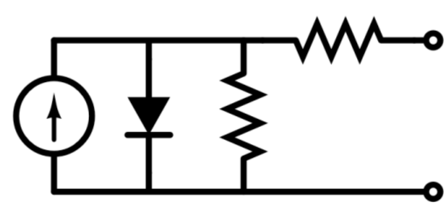


2. Charge separation



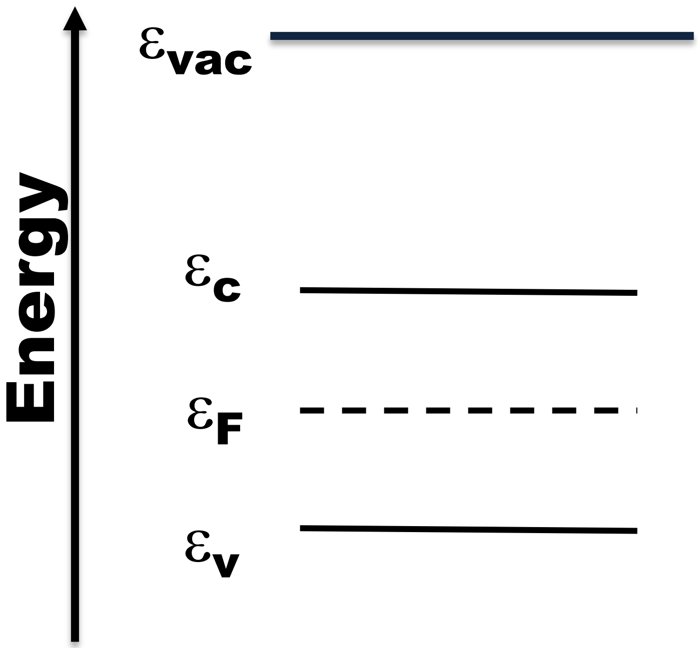
3. Charge transport

4. Charge collection



Example: silicon

In the dark



Carrier density n_i

n = density of free electrons

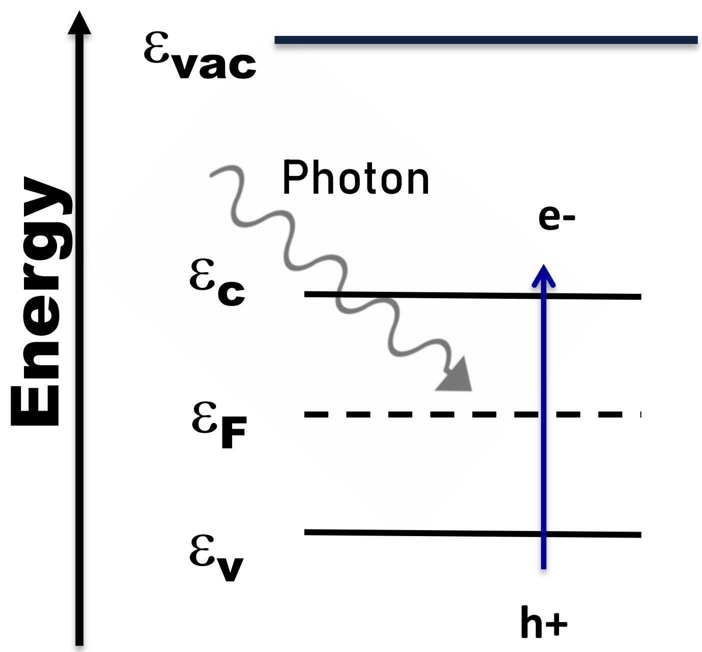
p = density of free holes

ni = total intrinsic carrier density

$$n_i{}^2 = np$$

Example: silicon

Under illumination



1. Photon with energy $E \geq E_g$
2. Electron-hole pair created
3. Radiative recombination

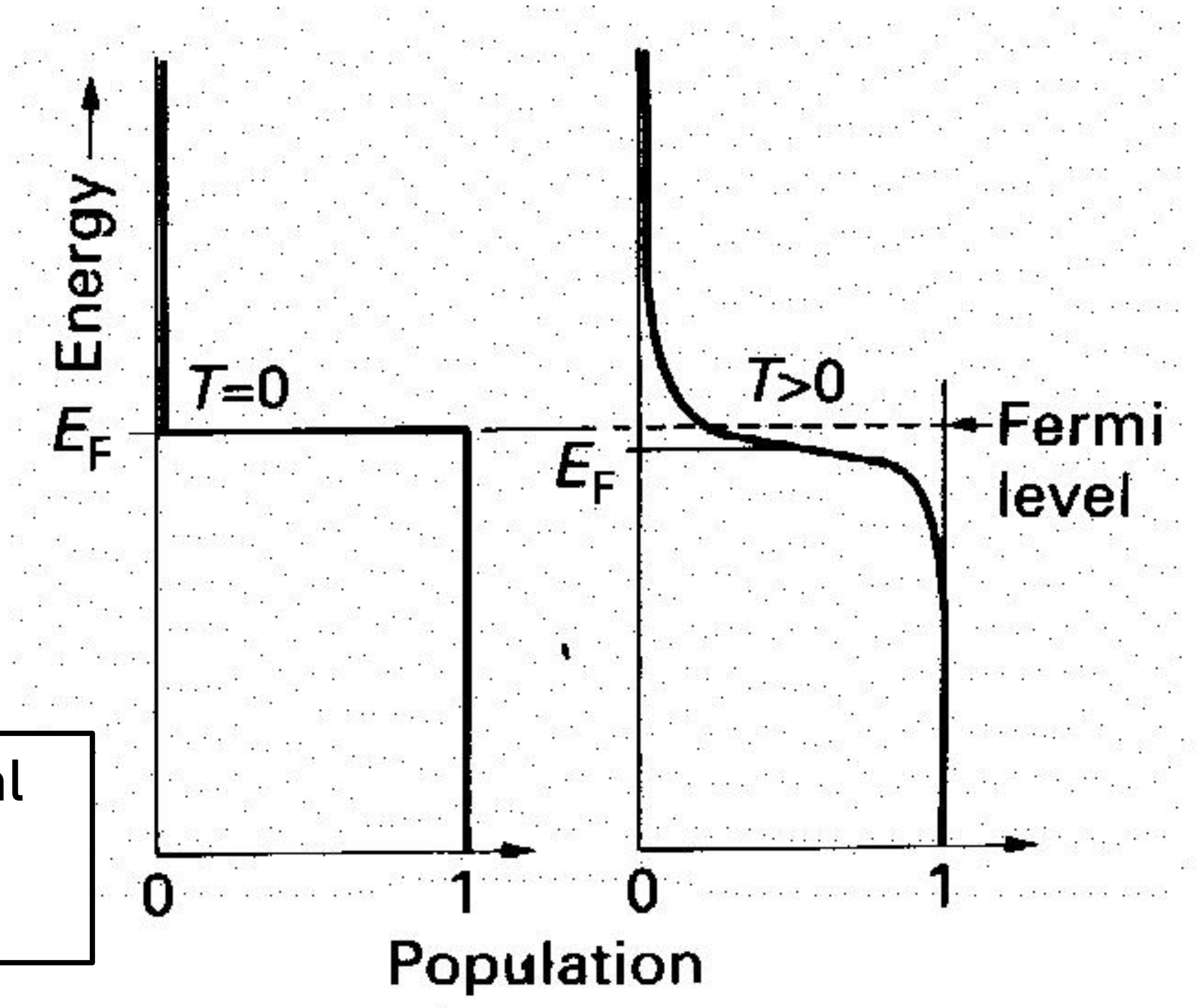
Fermi-dirac distribution

The energetic distribution of a system of electrons

$$f(E) = \frac{1}{\exp(\frac{E-\mu}{kT})}$$

$\mu = E_F$ at T = 0K

μ is the chemical potential of the free charge in the semiconductor



Fermi-dirac distribution

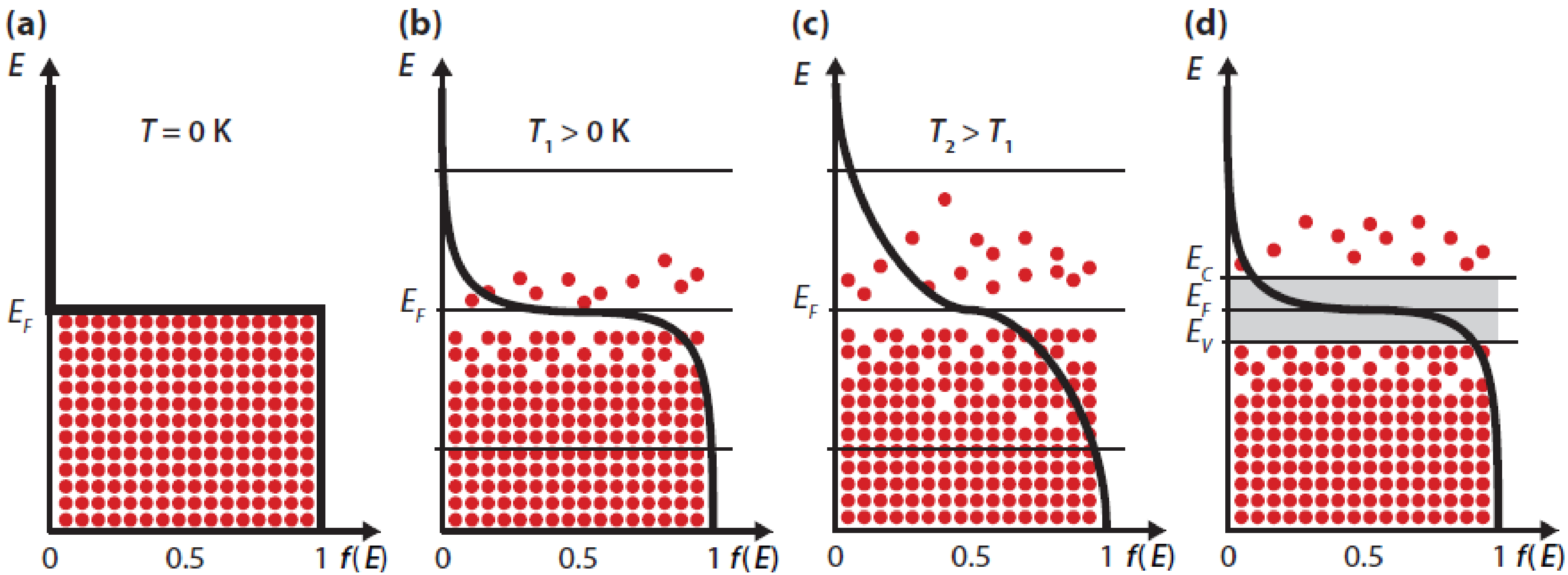
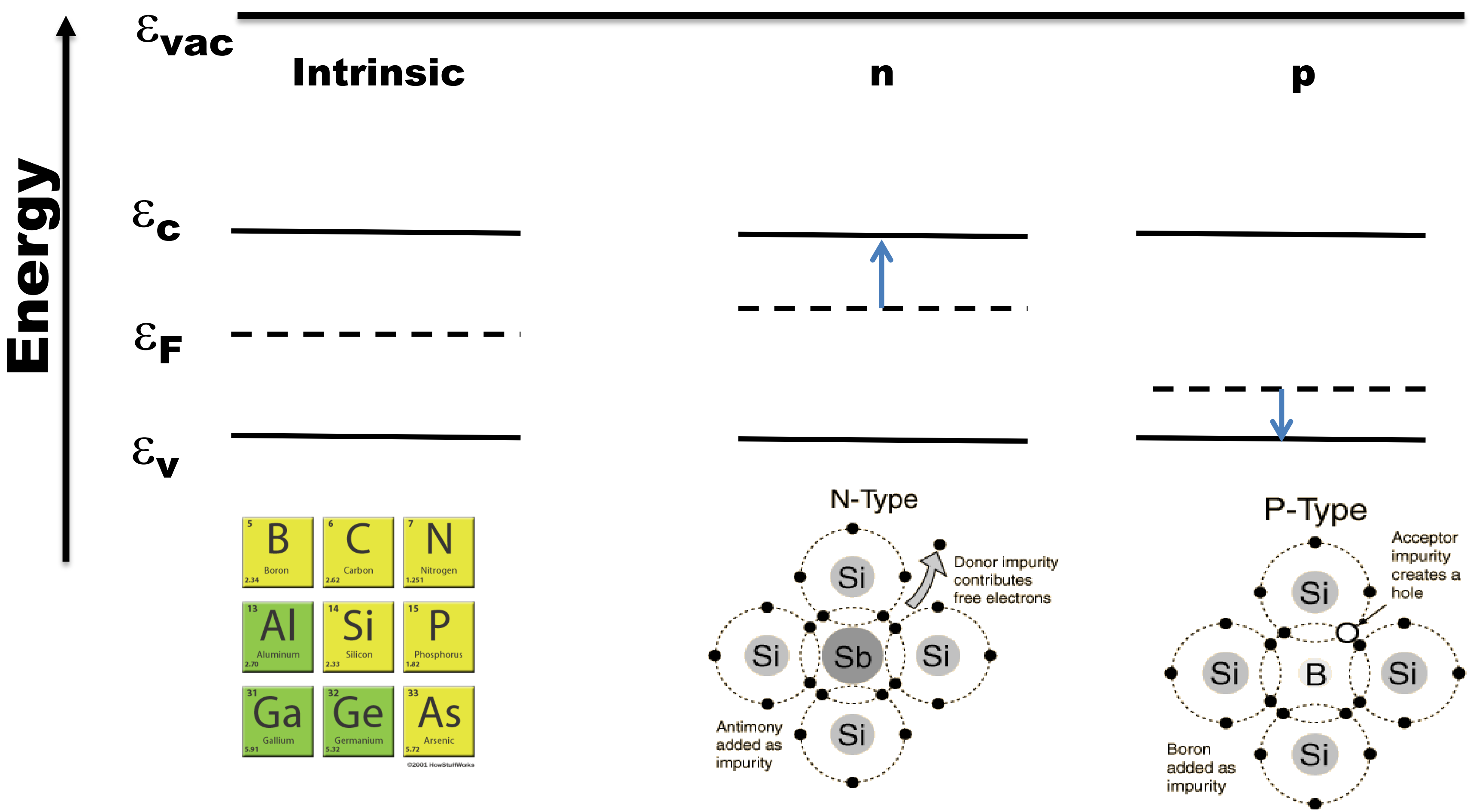


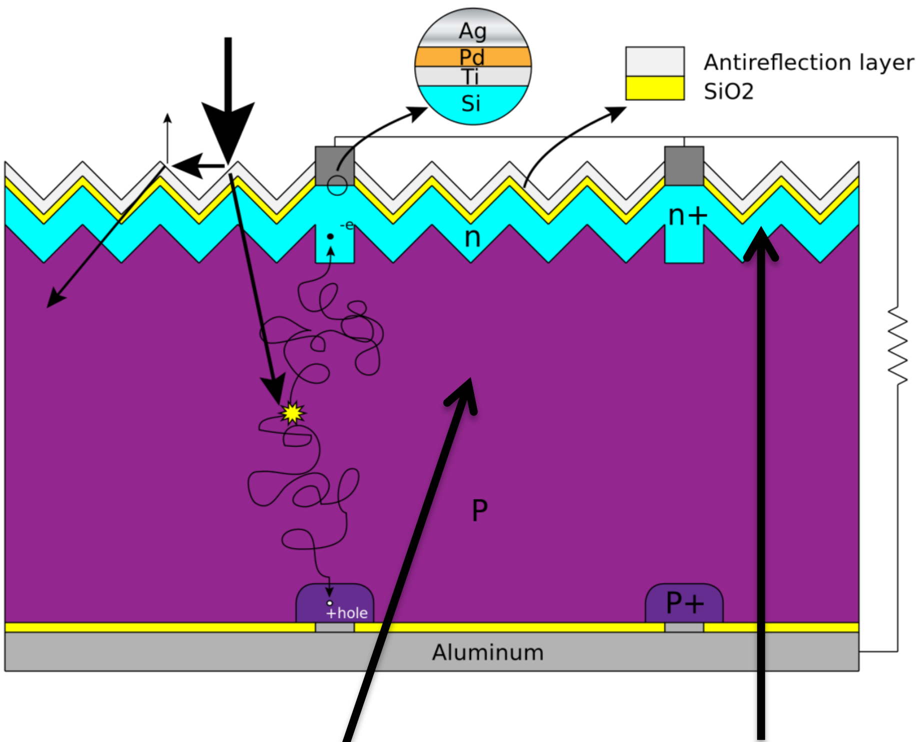
Figure 6.6: The Fermi–Dirac distribution function. (a) For $T = 0$ K, all allowed states below the Fermi level are occupied by two electrons. (b, c) At $T > 0$ K not all states below the Fermi level are occupied and there are some states above the Fermi level that are occupied. (d) In an energy gap between bands no electrons are present.

Doping



Impurities that donate (n-type) or accept (p-type) electrons

Silicon pn junction



Base

1 µm

Emitter

<< 1 µm

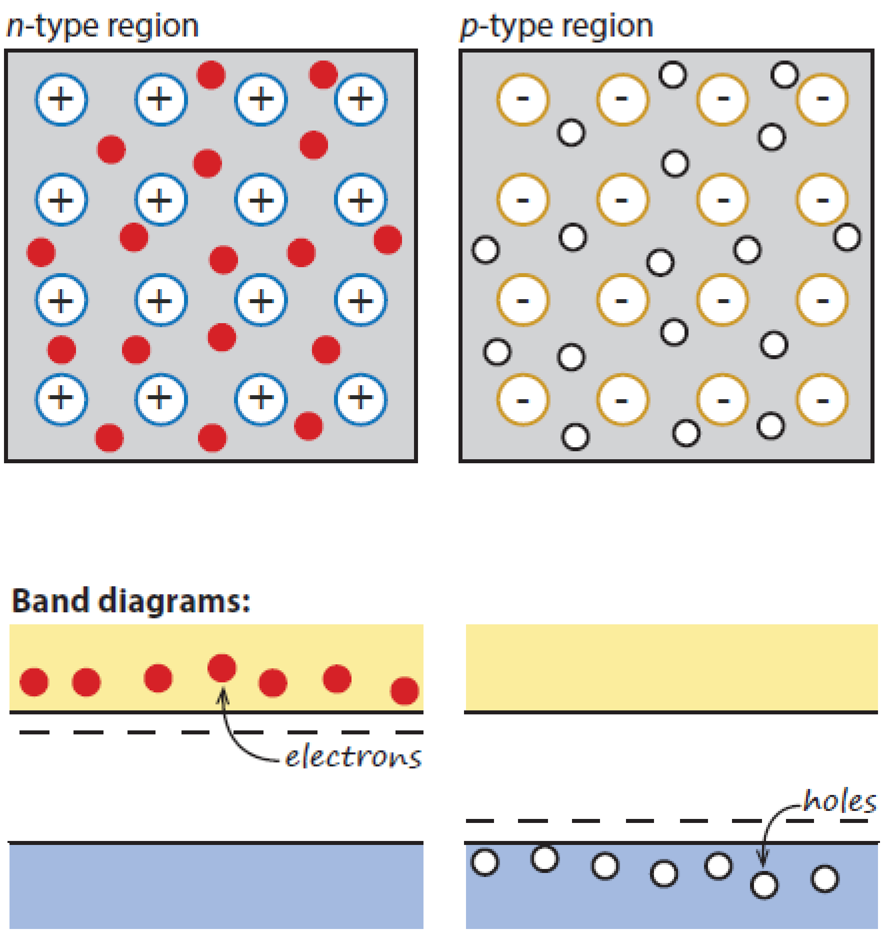
Silicon solar cells, typical parameters

$n = 1.5 \times 10^{10}$ @ 300k

$N_A = 10^{16}$
$N_D = 10^{18}$

Thickness of wafer = 10^{-6} m
Depletion region $W = 3 \times 10^{-7}$ m

Silicon pn junction



Isolated doped semiconductors

Charge neutrality guaranteed by free charge + ionised atoms

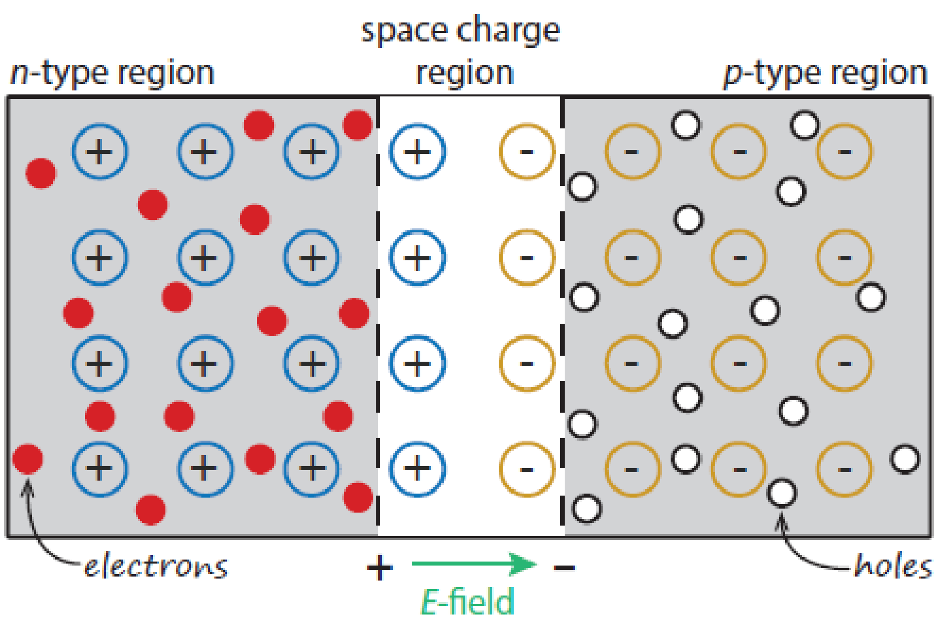
n-type semiconductor

Density of free electrons equal to density of donor atoms

p-type semiconductor

Density of free holes equal to density of acceptor atoms

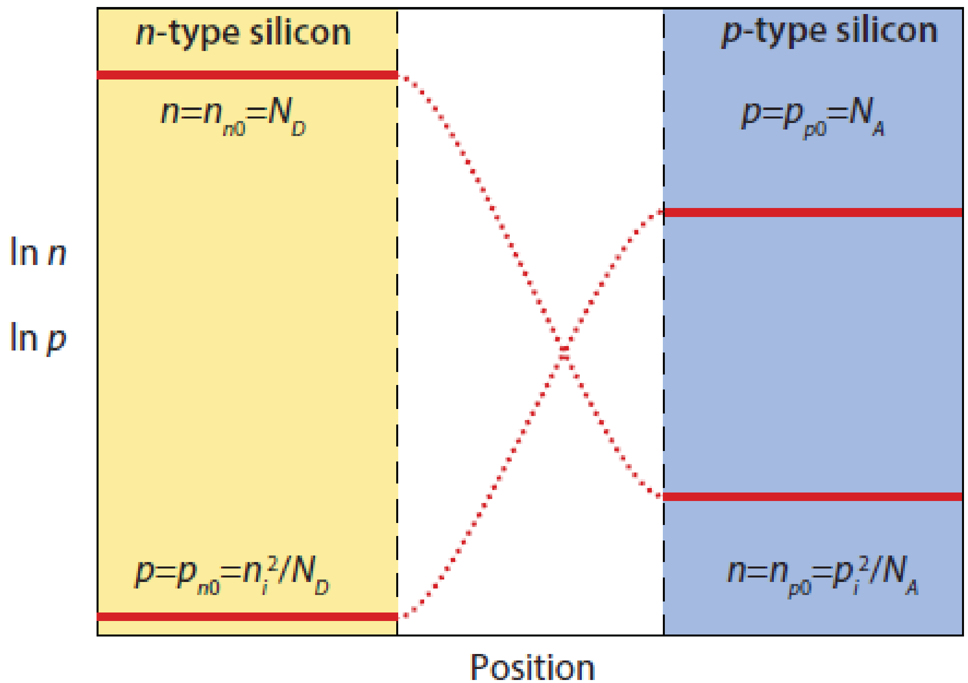
Silicon pn junction



- Diffusion and recombination of carriers at the junction
- Depletion of free charge in the *space charge region* or *depletion zone*
- Charge neutrality not preserved at the junction
- Electric field across the junction

No current flows

Silicon pn junction

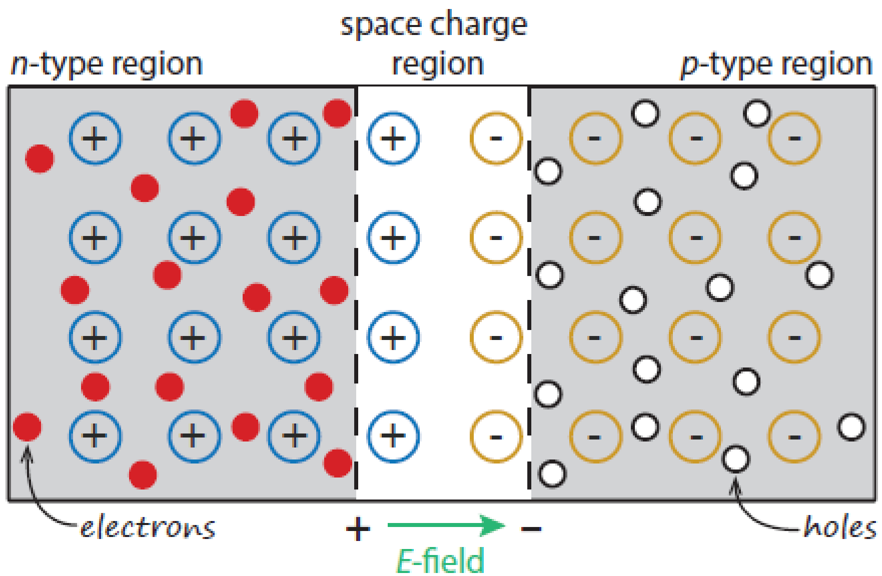


Equilibrium

<u>Charge concentration profile</u>

- ❑ Rapid decrease in n and p in the depletion region
- ❑ Charge profiles unchanged outside of depletion region
- ❑ Junction determines current flow

pn junction - dark



drift and diffusion currents

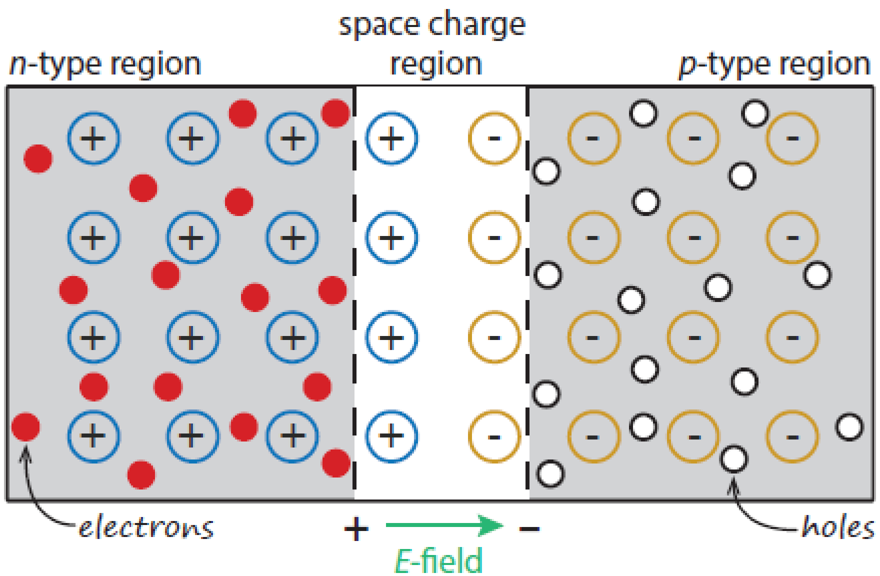
Drift – current due to an electric field

$$I^{drift} = q(n\mu_n + p\mu_p)E_x$$

Diffusion – current due to spatial variation in carrier concentration

$$I^{diffusion} = q(D_n \frac{dn}{dx} - D_p \frac{dp}{dx})$$

pn junction - dark



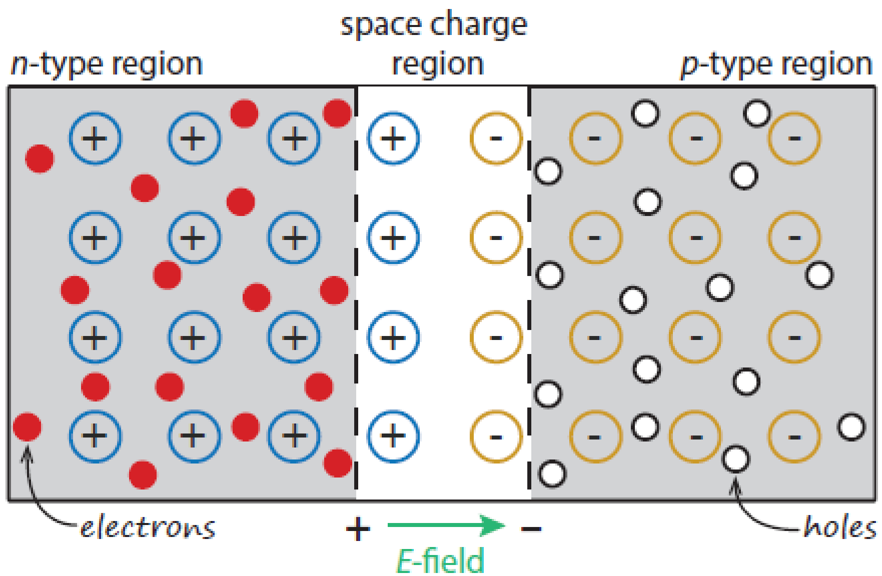
drift and diffusion currents

Relation between carrier mobility µ and diffusion coefficient D

Einstein relation

$$D_n = \frac{k_B T}{q} \mu_n$$

pn junction - dark



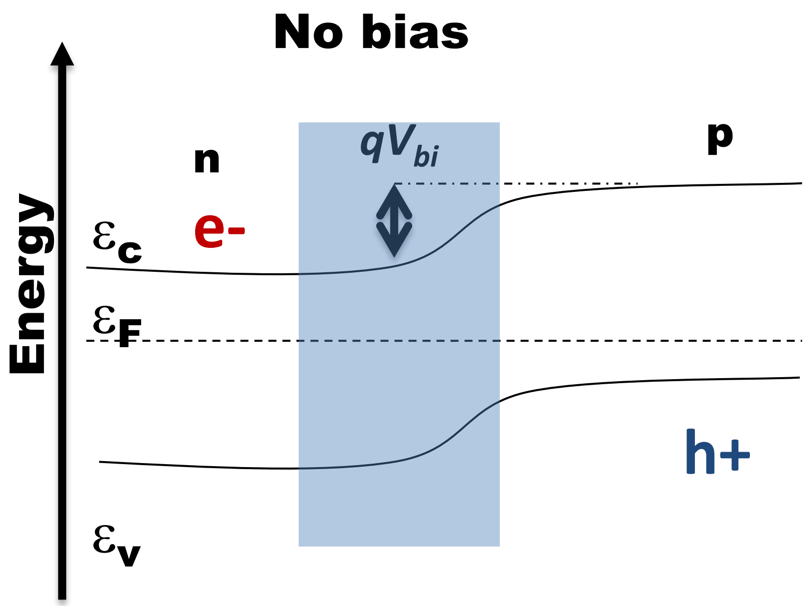
In equilibrium

Drift and Diffusion currents cancel

No net current flow

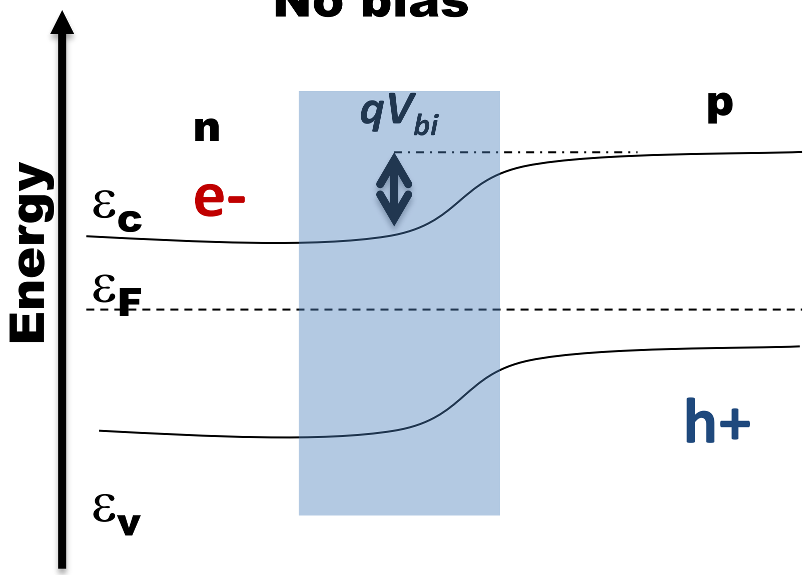
$$I = q\left(n\mu + p\mu_p + D\frac{dn}{dx} - D_p\frac{dp}{dx}\right) = 0$$

pn junction – dark, voltage



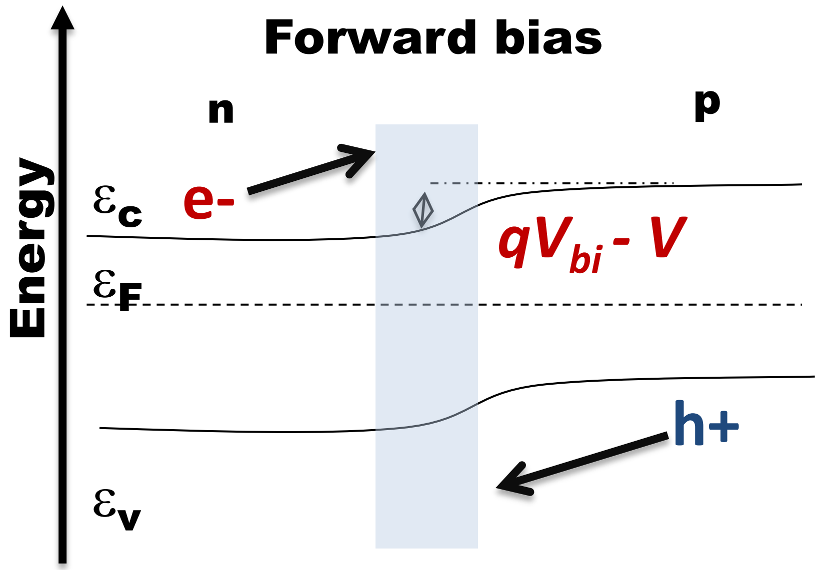
At V = 0, no current flows

pn junction – dark, voltage



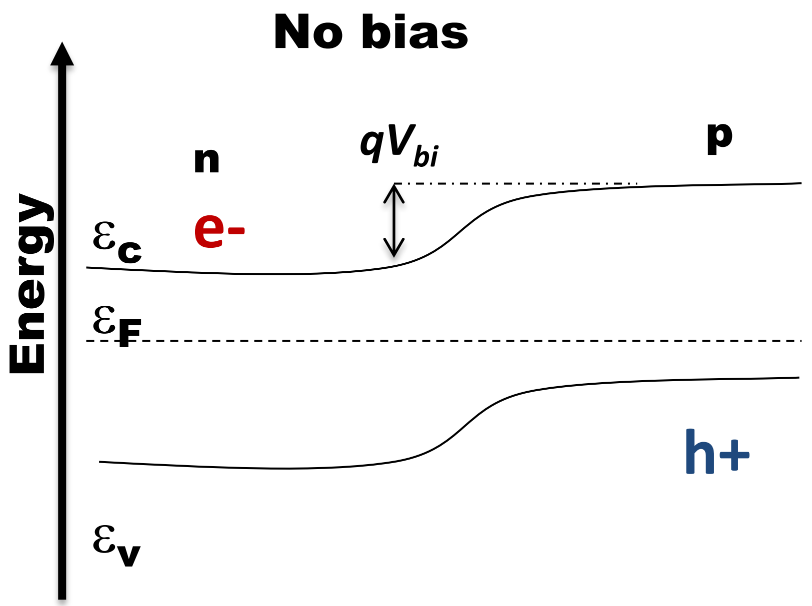
At V = 0, no current flows

At V > 0 V_{bi} is reduced and current flows across the junction



Current is due to drift

pn junction – dark, voltage



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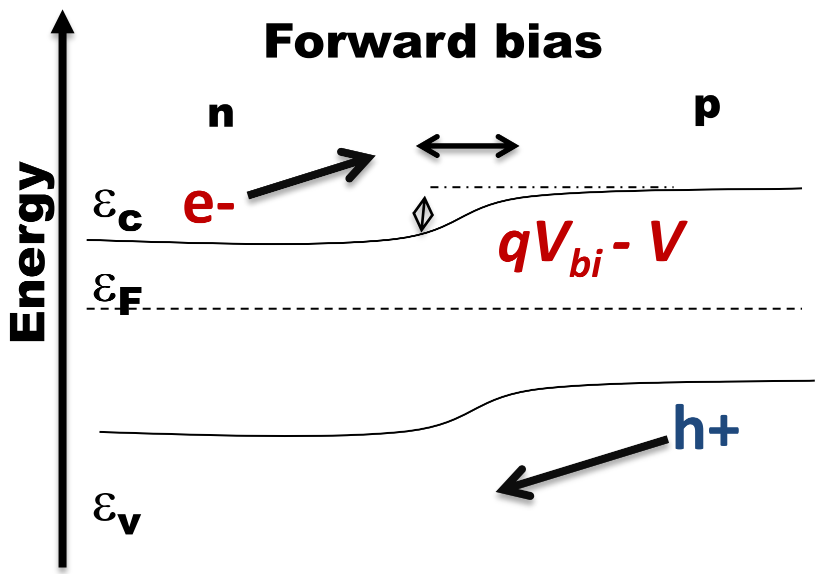
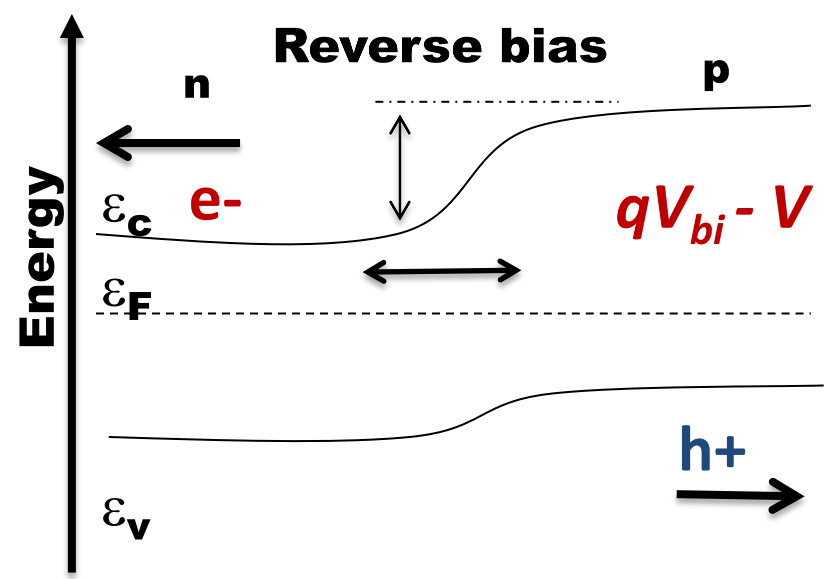
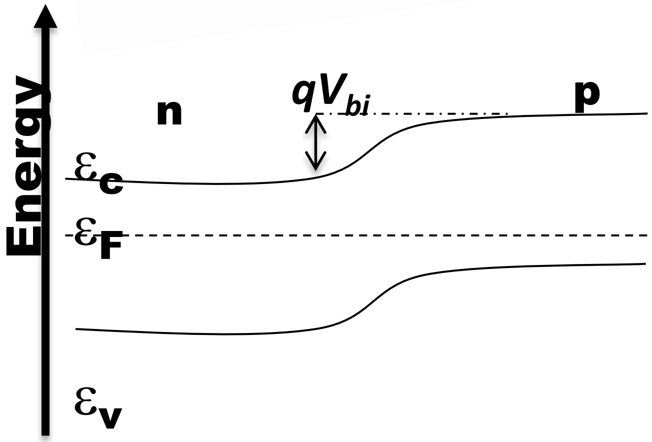
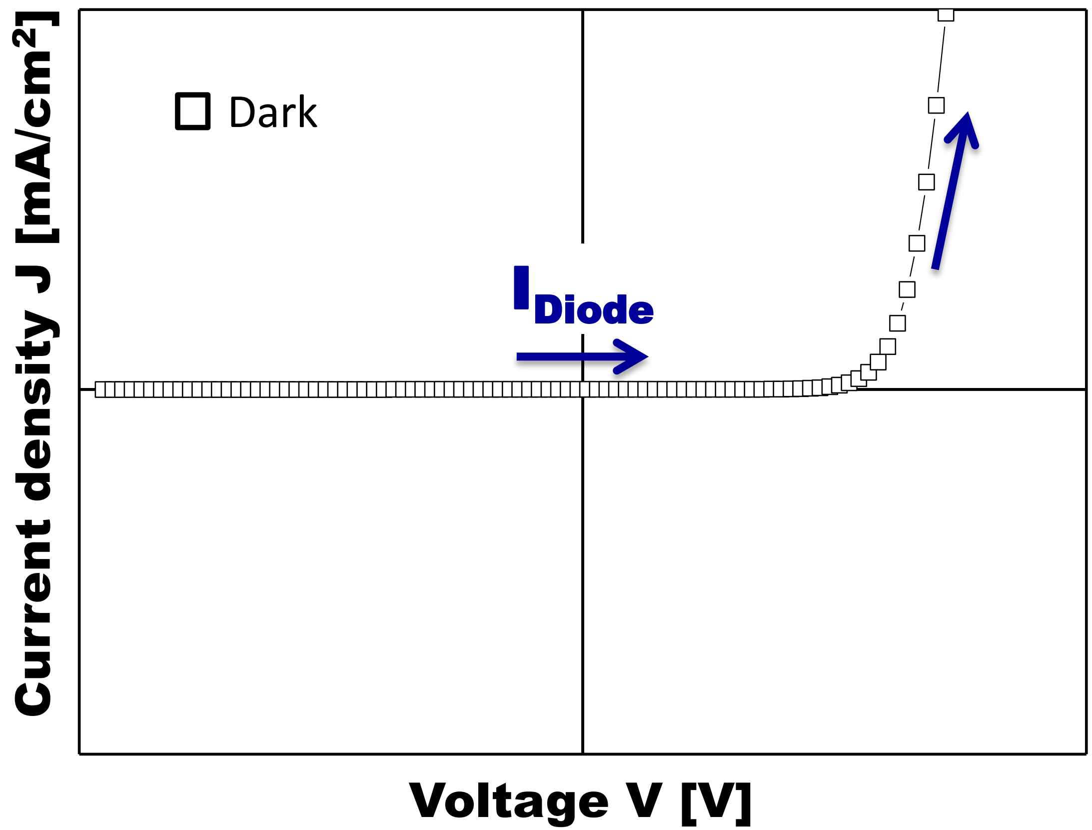




pn junction – dark, voltage

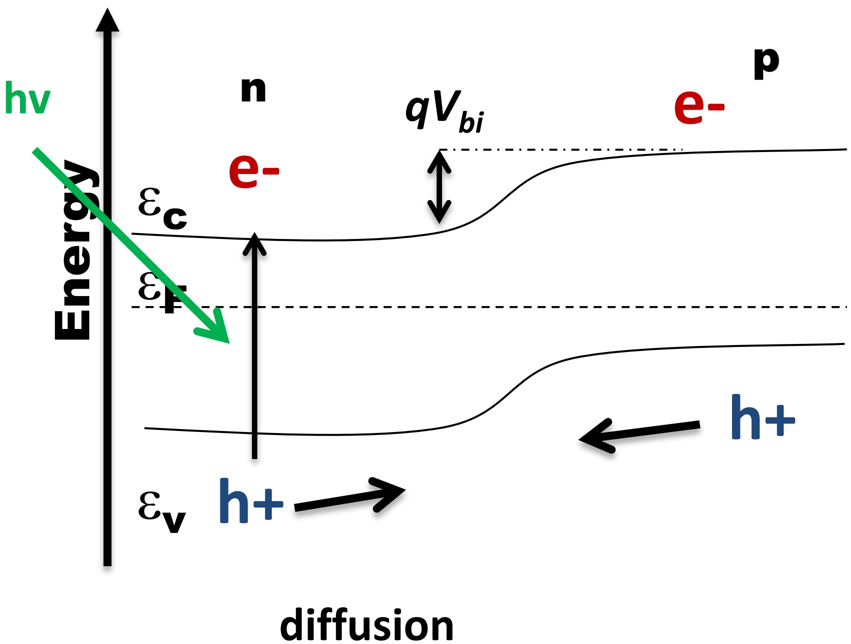


$$I^{diode} = Io\left(\exp\left(\frac{qV}{nkT}\right) - 1\right)$$



All solar cells behave as diodes in the dark

pn junction – illumination



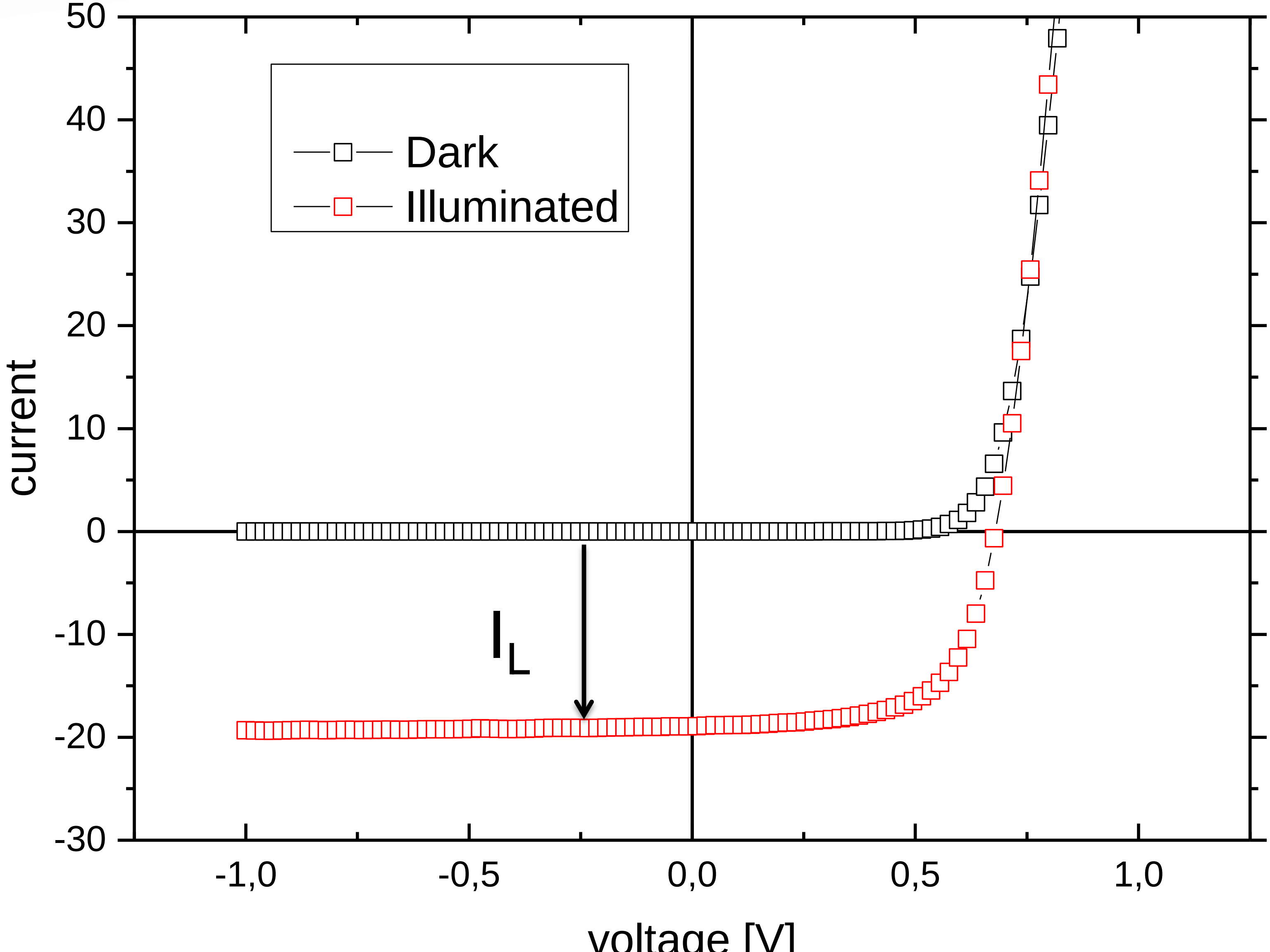
Diffusion of photogenerated carriers across junction - Photocurrent

Drift of carriers due to applied voltage

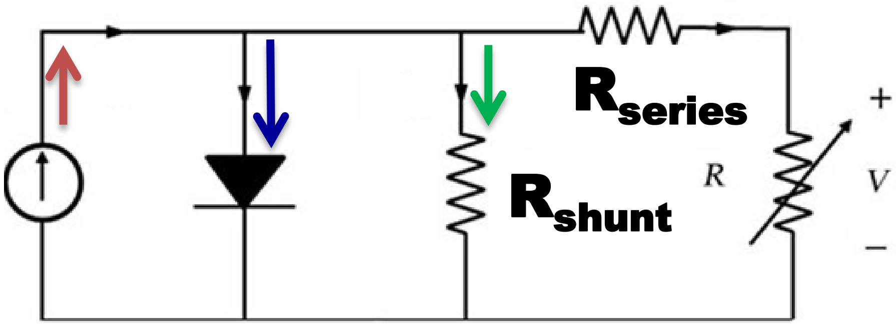
$$I^{solar\ cell} = I_L - Io\left(\exp(\frac{qV}{nkT}) - 1)\right)$$

I_L – photogenerated current

pn junction – illumination



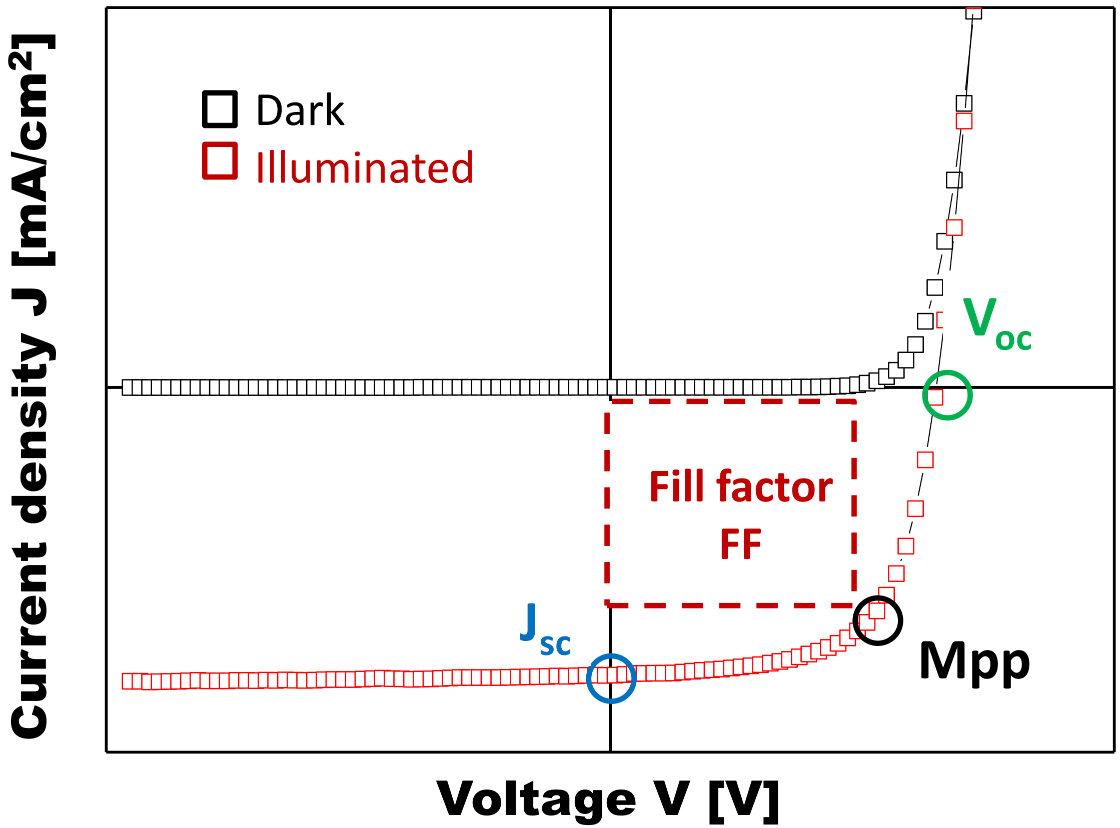
Solar cell parameters



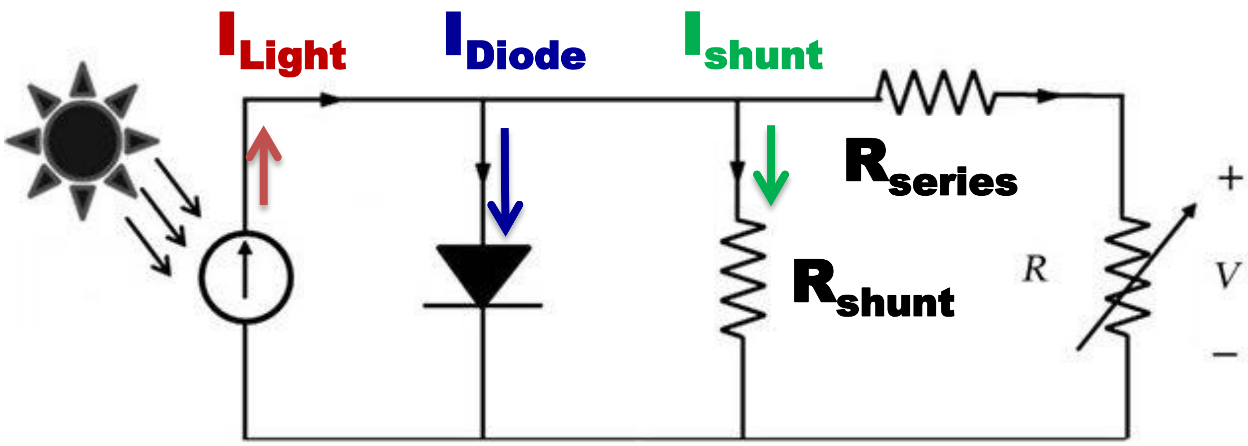
Efficiency & MPP

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

$$FF = \frac{M_{pp}}{J_{sc} V_{oc}}$$

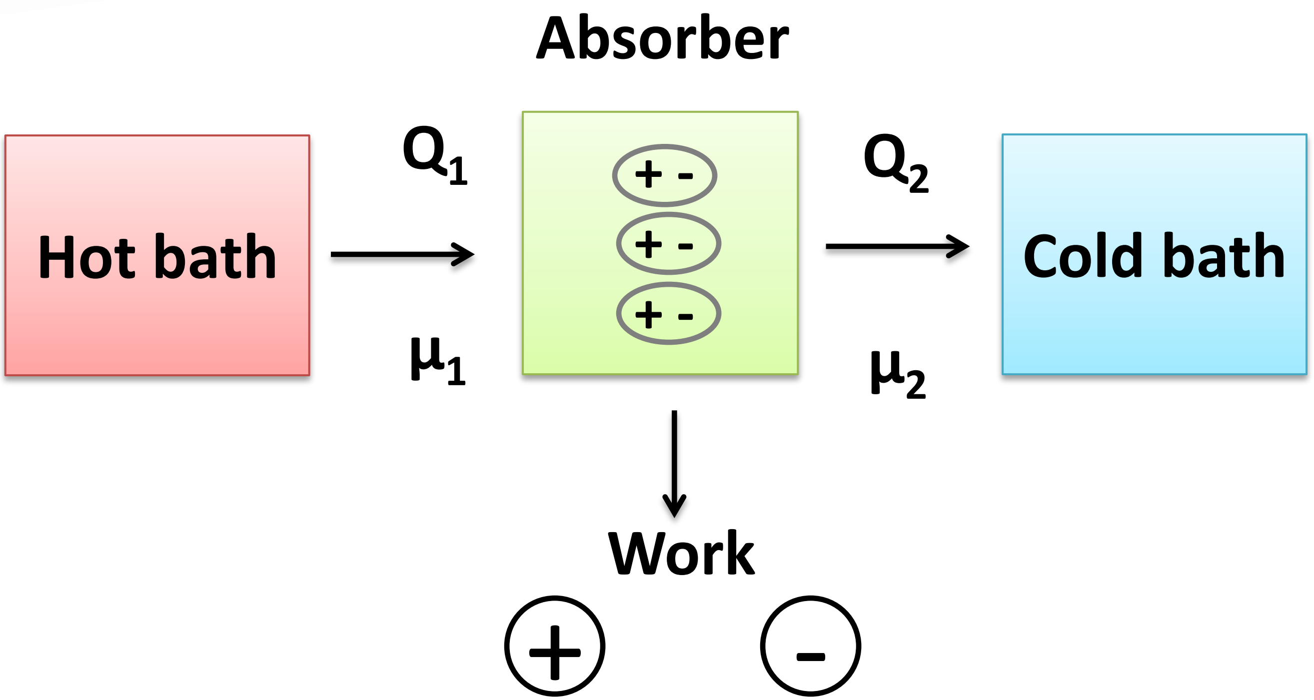


Solar cell – equivalent circuit



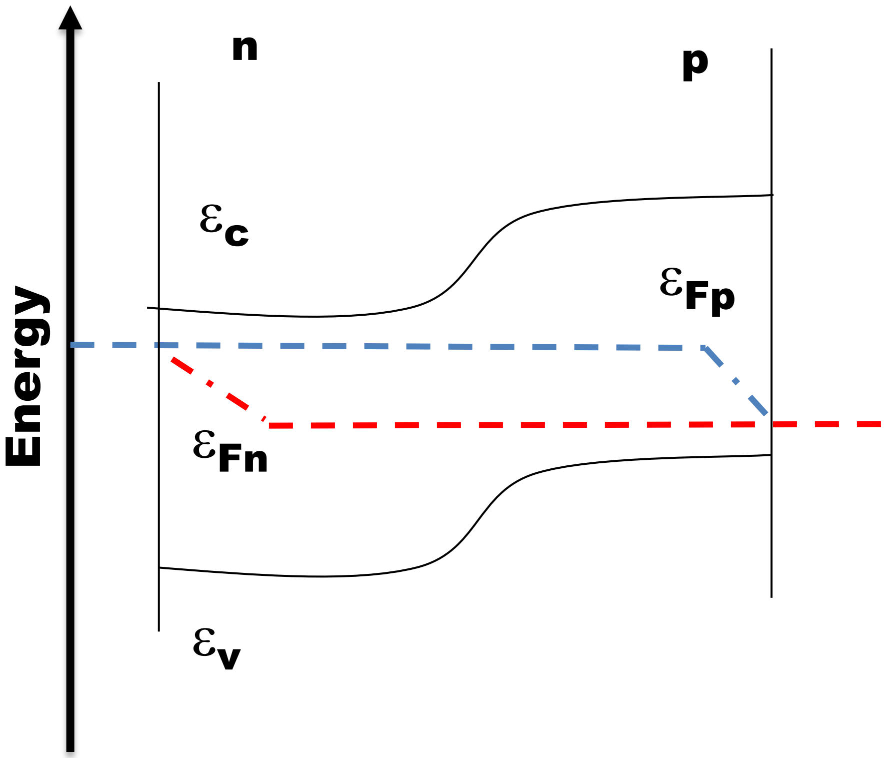
$$I_{solar\ cell} = I_{diode} + I_{shunt} - I_{Light}$$

Photovoltaics



Heat engine/chemical engine
Work = charge separation + transport (voltage + current)
Open circuit (V = 0 V) – Carnot bound

Open circuit voltage V_{oc}



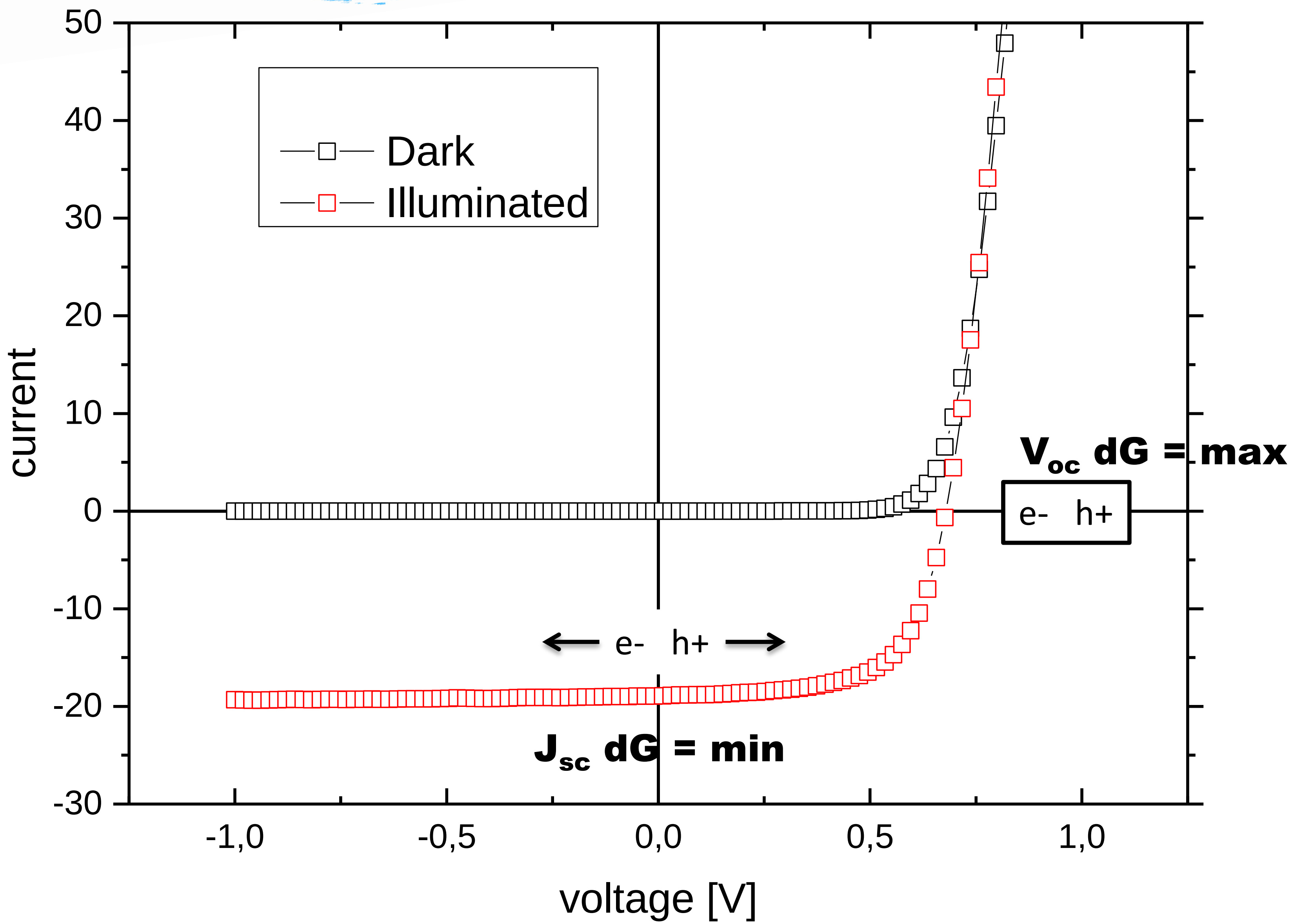
Generation = recombination

No work is done

Potential to do work is determined by chemical potential of photocharge

$dG = (\mu_e - \mu_h)dN$

Solar cell current-voltage curve



Thermodynamics of PV energy conversion

Detailed balance limit of efficiency of pn junction solar cells, W. Schockley and H. J. Queisser, J. Appl. Phys. 1961 (Schockley-Queisser Limit)

Physics of solar cells, Peter Würfel

From steam engine to solar cells: can thermodynamics guide the development of future generations of photovoltaics, T. Markvart, WIREs Energy Environ 2016, 5: 543–569.

A thermodynamic cycle for the solar cell, R. Alicki, D. Gelbwasser, A. Jenkens, Annals of Physics, 378, 2017, 71-87

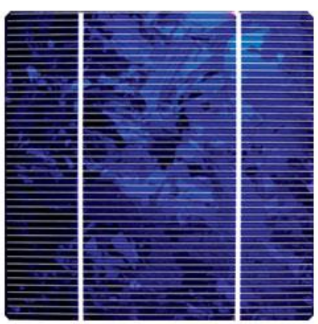
Outline

1) Photovoltaic energy conversion

   - Basics
   - Motivation for emerging PV

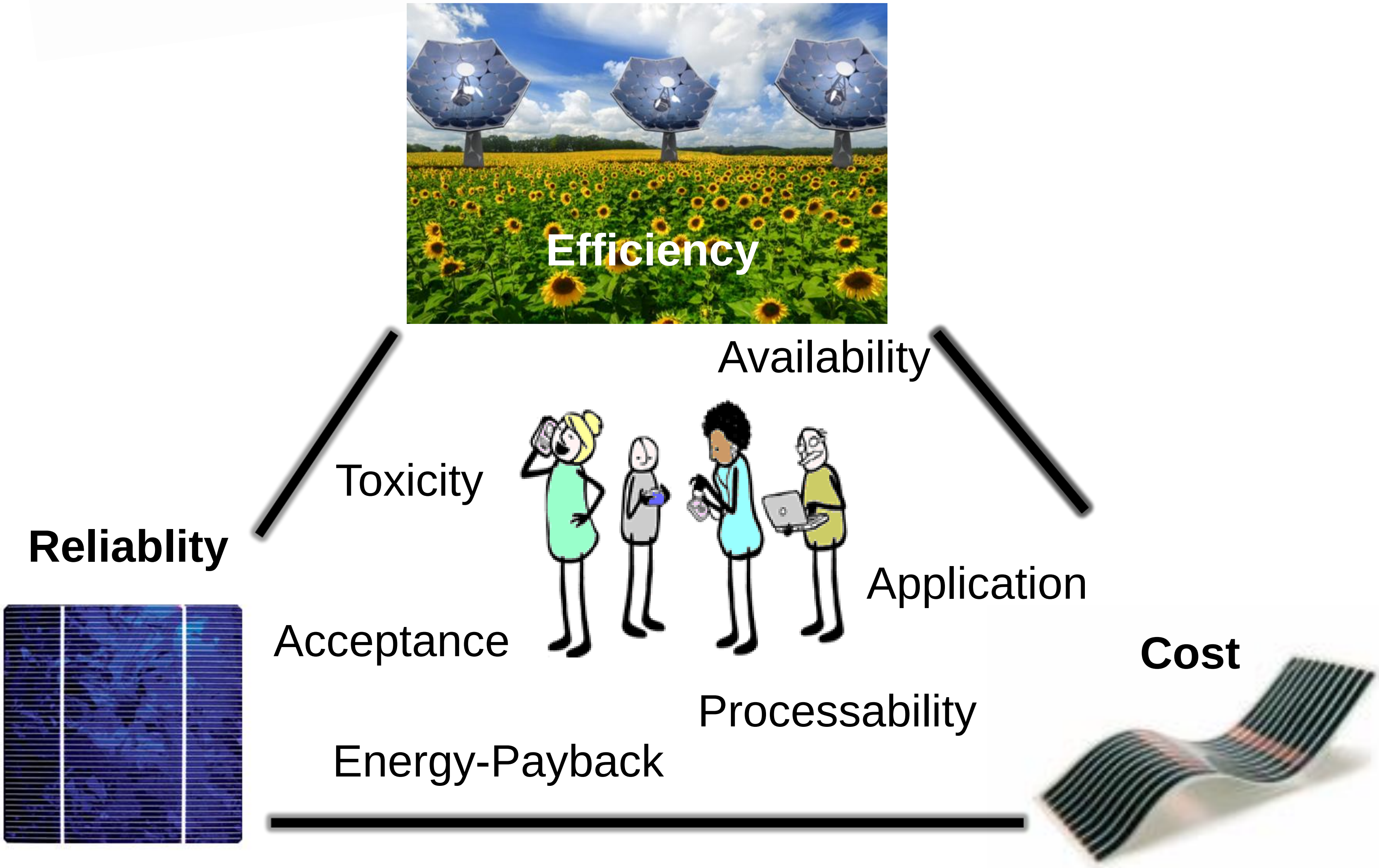
The golden triangle

Reliablity



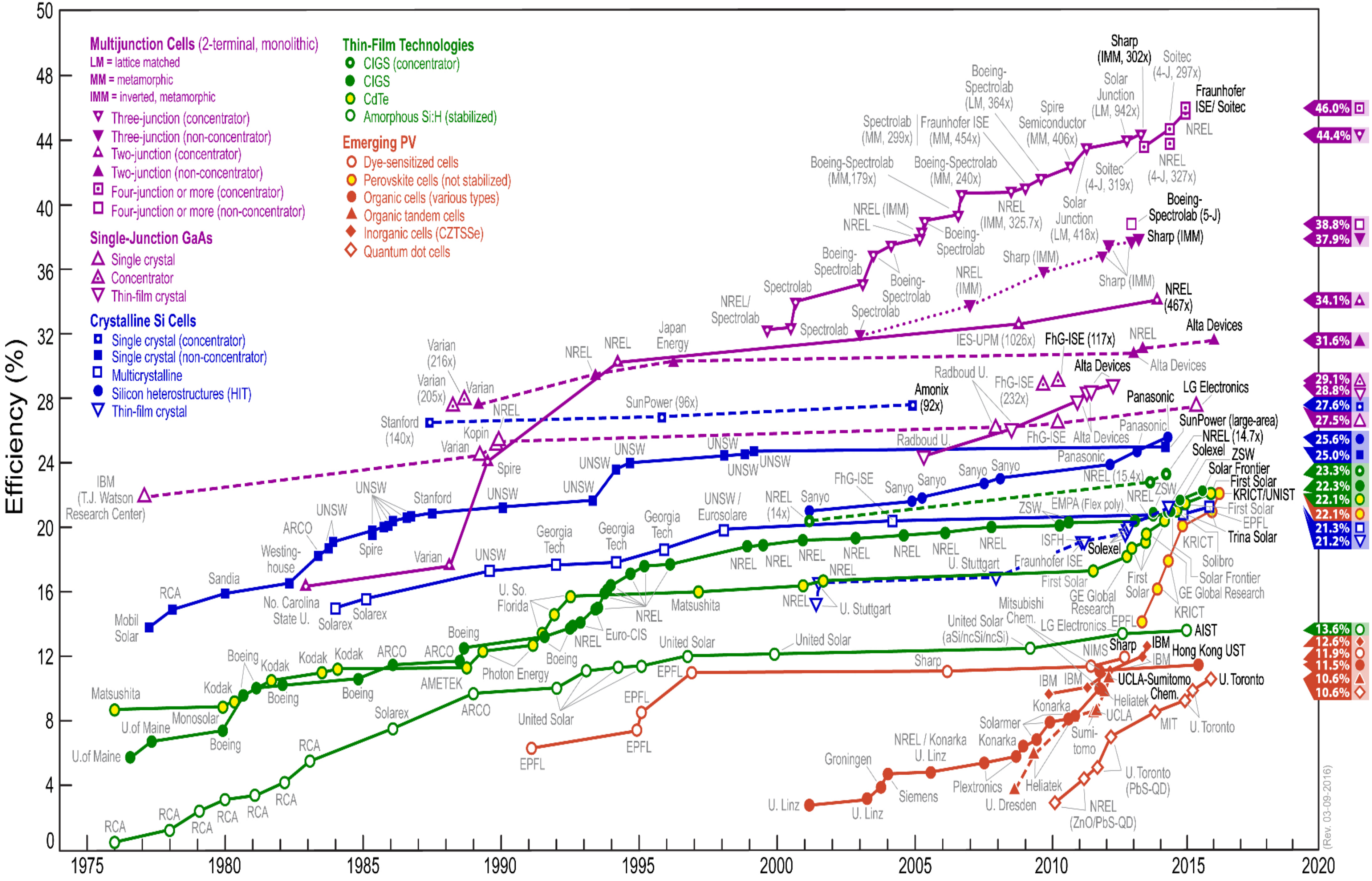
Cost

The golden triangle

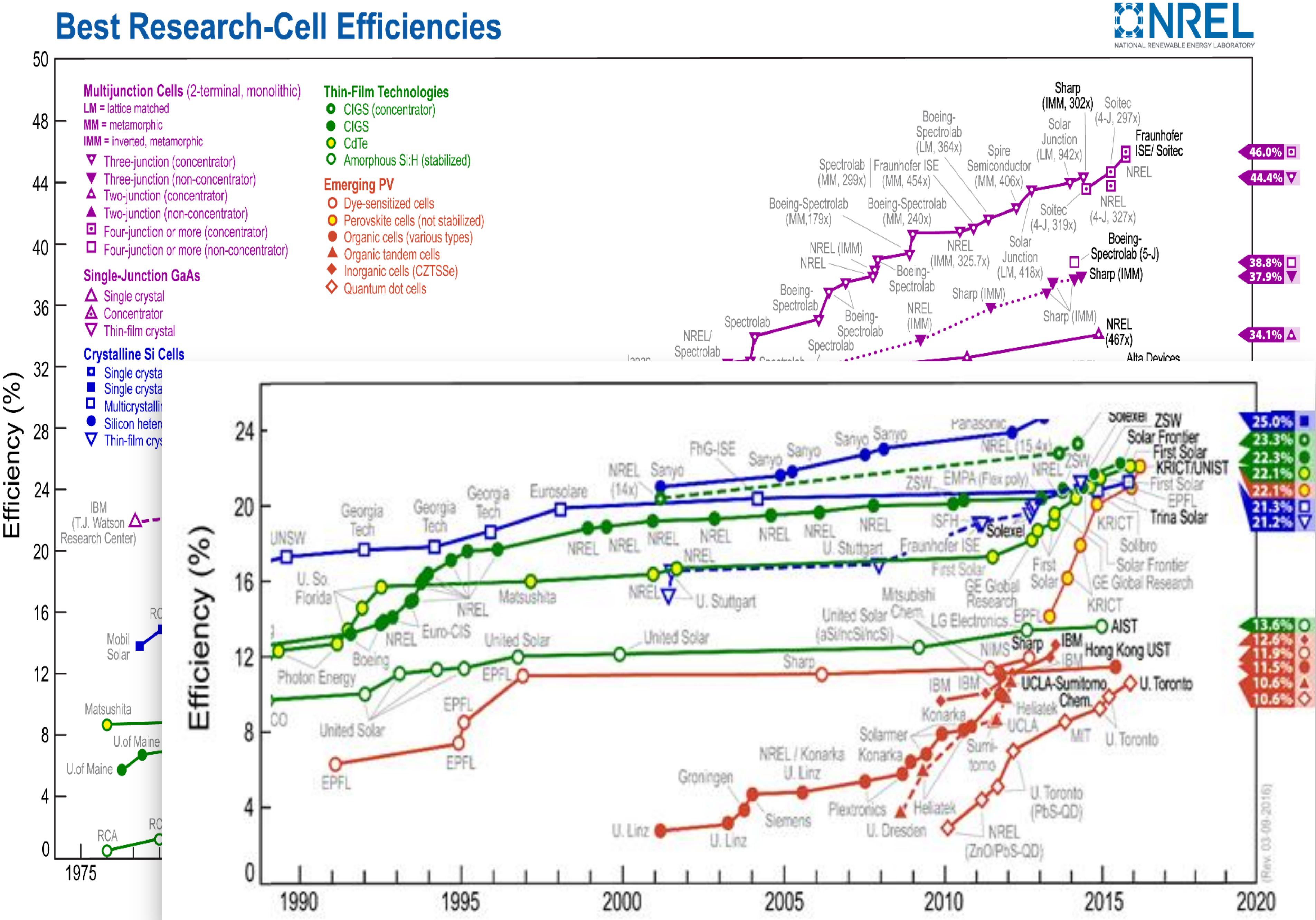


Best Research-Cell Efficiencies

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

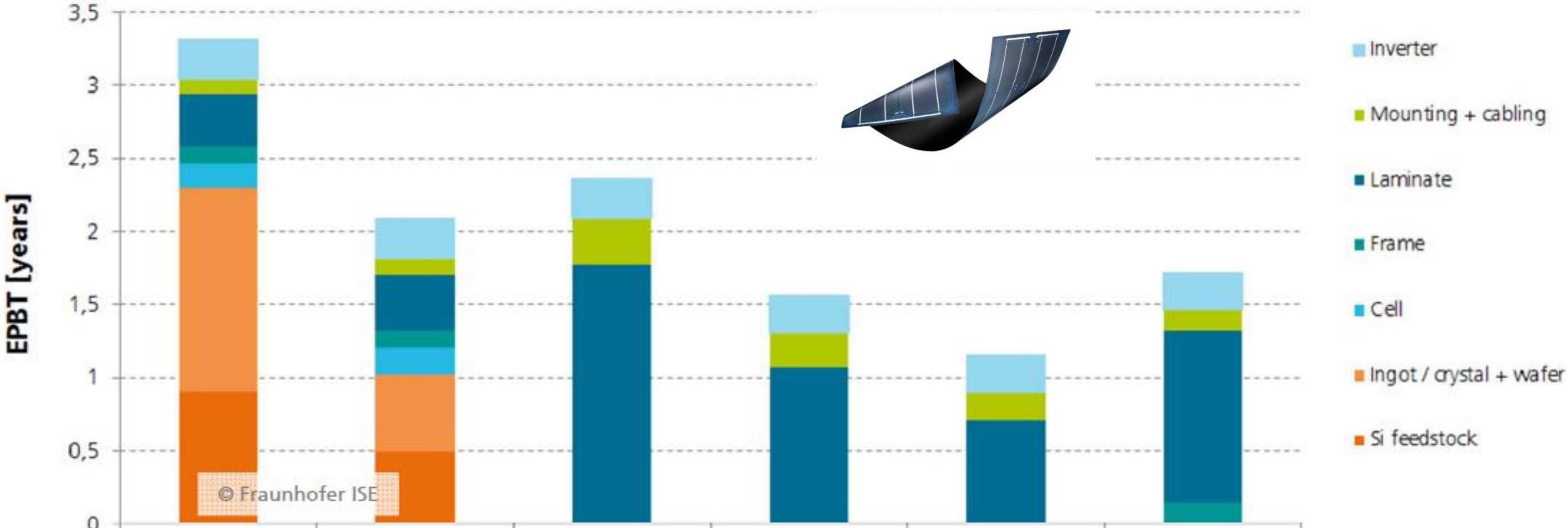


Best Research-Cell Efficiencies



Energy payback

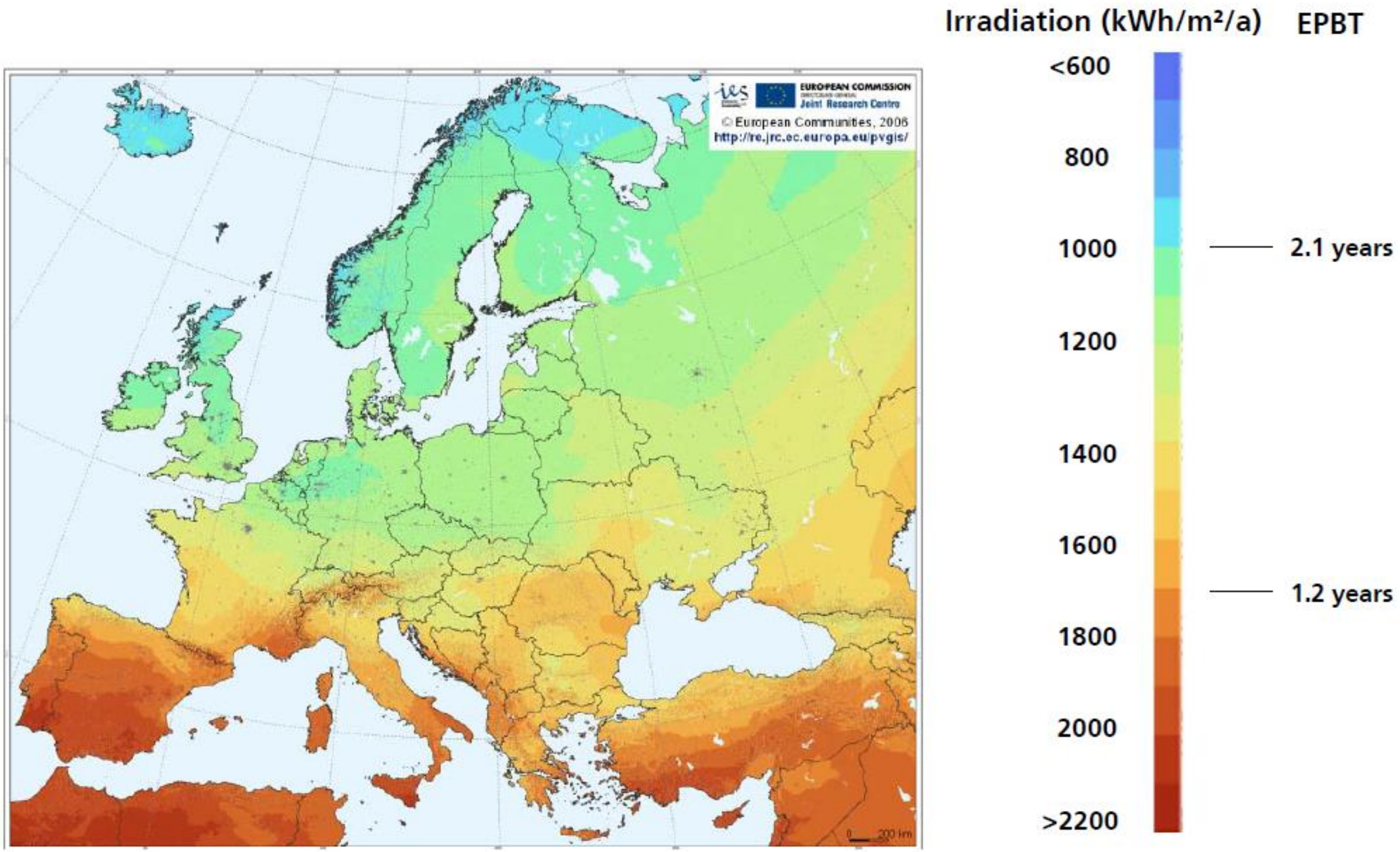
Global Irrad.: 1000 kWh/m²/yr



Mono-Si	Multi-Si	a-Si	µm-Si	CdTe	CIGS	Technology
Glass-EVA-backsheet	Glass-EVA-backsheet	Glass-PVB-glass	Glass-EVA-glass	Glass-EVA-glass	Glass-Eva or PVB-glass	Module composition
2011	2011	2008-2011	2013 estimate	2010-2111	2011	Status
14,8%	14,1%	7,0%	10,0%	11,9%	11,7%	Efficiency
~300 MWp	~300 MWp	33-45 MWp	120 MWp	963 MWp	20-66 MWp	Scale of production

Data: M.J. de Wild-Scholten 2013. Graph: PSE AG 20

Energy payback



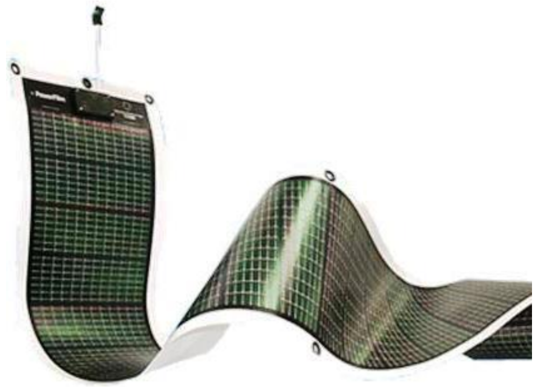
Data: M.J. de Wild-Scholten 2013. Image: JRC European Commision. Graph: PSE AG 2014 (Modified scale with updated data from PSE AG and Fraunhofe

Three generations of PV

I Crystalline silicon

- Wafer based
- Price determined by solar cell + module
- Max theoretical efficiency 30%

II Thin film



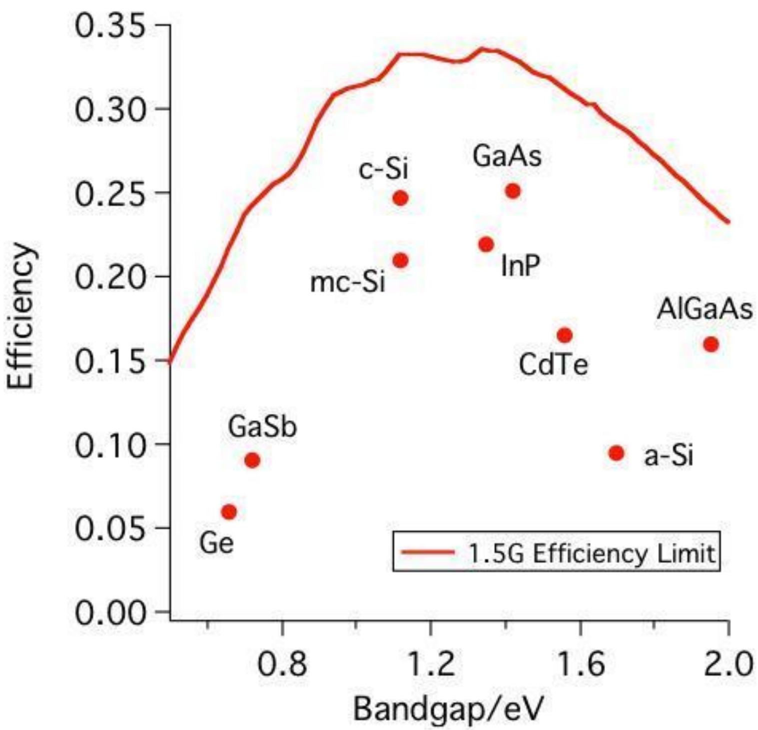
- Substrate based
- Price determined by processing
- Max theoretical efficiency depends on material (> 30%)

III Beyond the Shockley Queisser limit

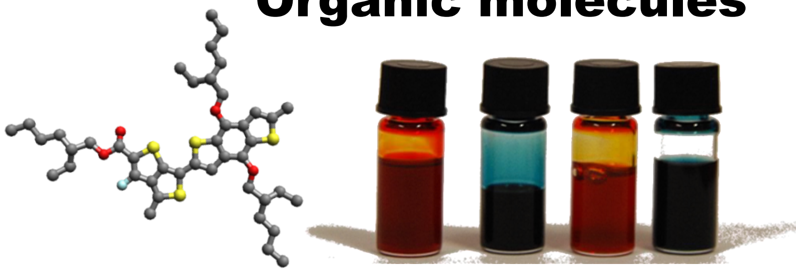
- New concepts in energy conversion
- Fundamentally different than pn junction photovoltaics
- Max theoretical efficiency ???

Beyond thermodynamic limits

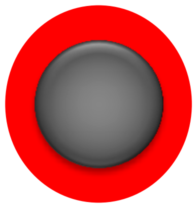
Thermodynamic limit single junction solar cells

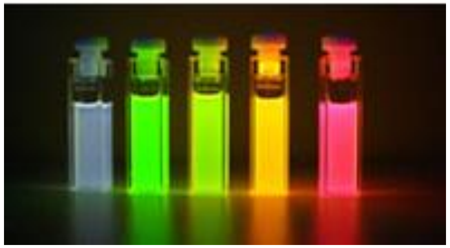


Organic molecules

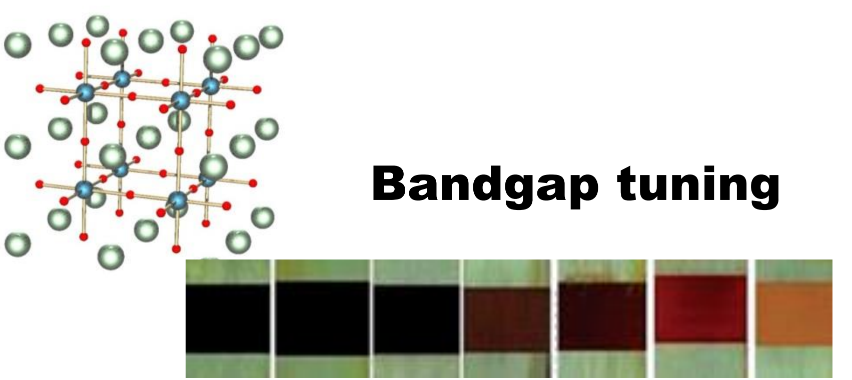


Nanostructures





Bandgap tuning



Research topics

- Material abundancy, processing & upscaling
- Increasing kWh/m^2 (efficiency, cost & space)
- Increasing throughput
- Going beyond thermodynamic limits
- Breakthroughs with interdisciplinary research

Outline

1) Photovoltaic energy conversion
   - Basics
   - Motivation for new technologies

2) Organic solar cells
   - Charge separation
   - Charge transport
   - State of the art and open questions

3) Perovskite solar cells
   - Structure
   - Performance