Modeling Organic Photovoltaics

IMA Interdisciplinary REU project
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Goals

- Develop understanding of the basic physical process in power generation
- Model power generation under various assumptions
- Compare, evaluate, and validate models

Expectations

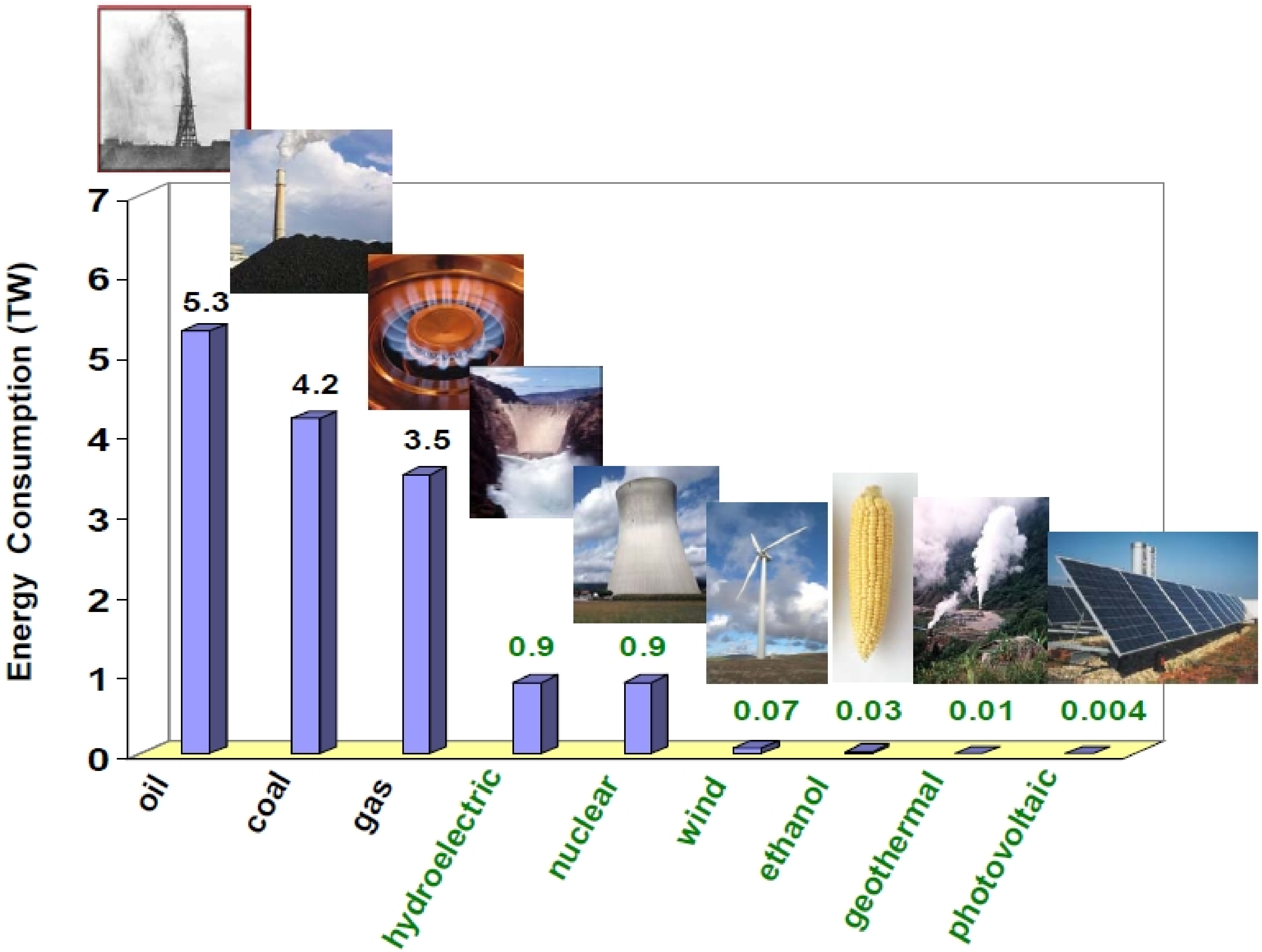
- Learn a whole lot as a team
- Make good progress
- Prepare a poster for presentation
- Write a technical report (10 pages, LaTeX)
- Make presentation on findings
- *Have fun!*

Resources

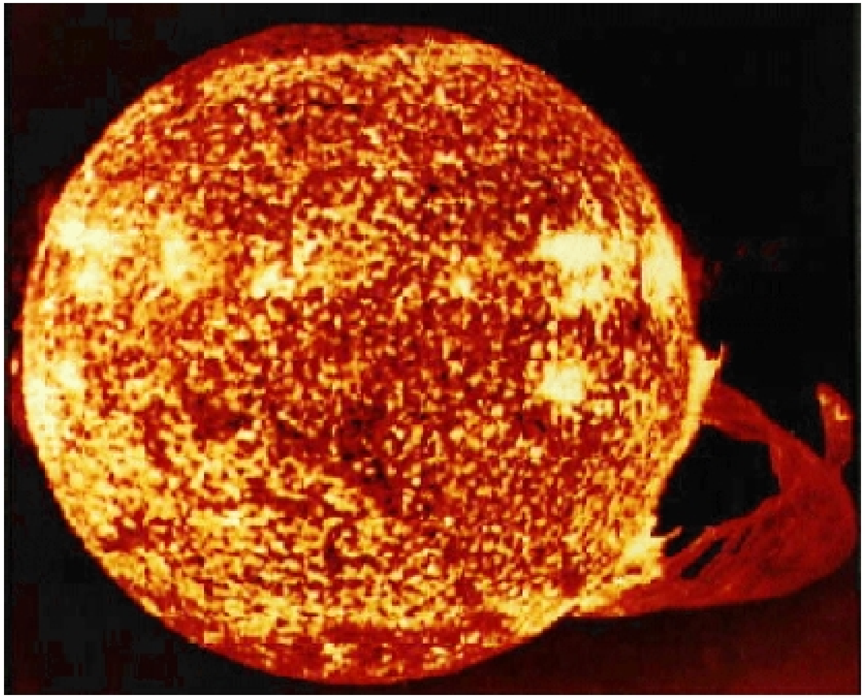
- Russell Holmes, local expert
- Papers, books, web
- Computing tools – Matlab, Mathematica, Maple, Comsol
- *We got brain power!*

The Energy Challenge

Find ways to provide clean energy to ~ 10 billion people.



Solar power

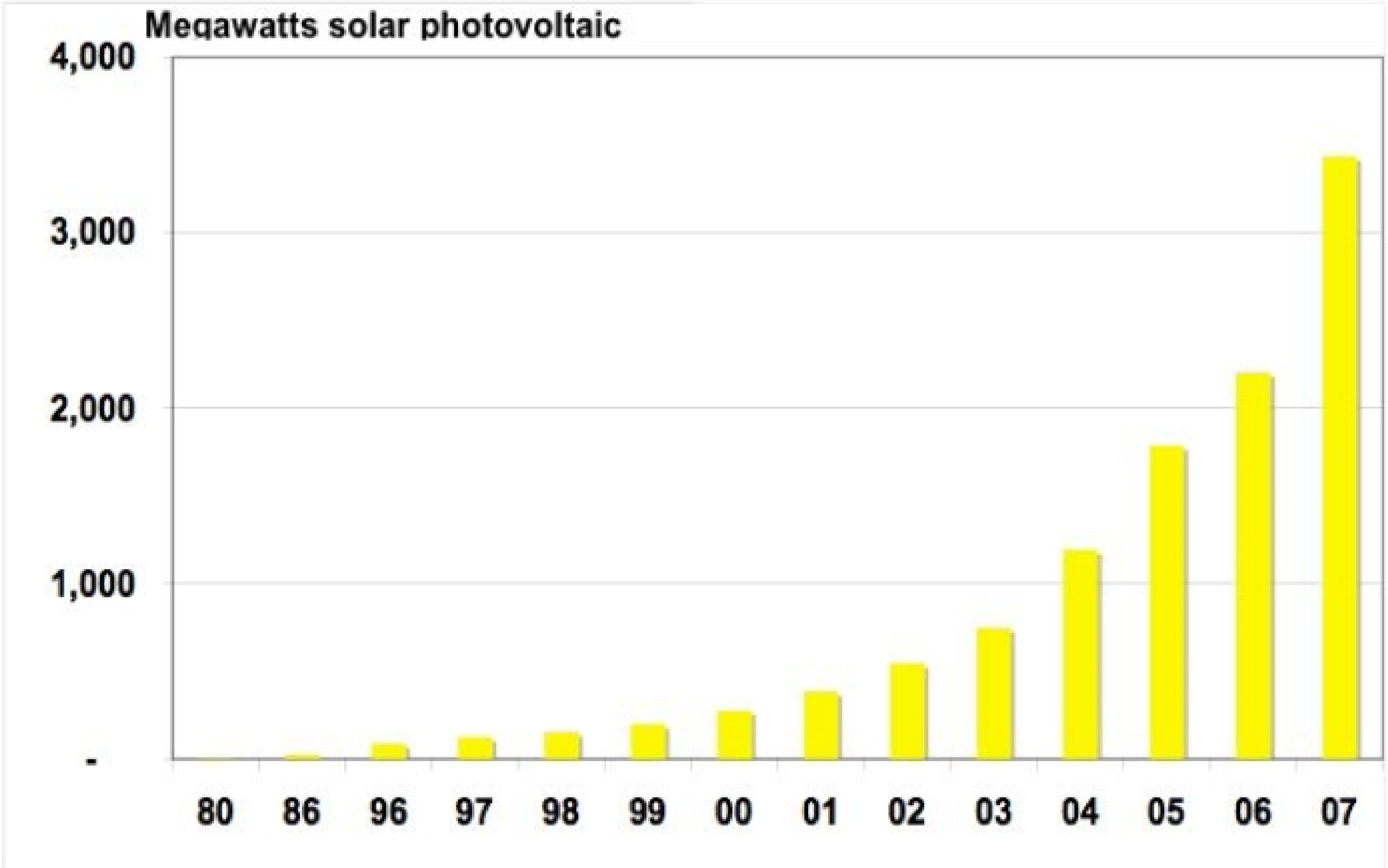


World demand ~ 15 TW

Sun ~ 120,000 TW

Covering 0.125 % of earth's surface with 10% efficient solar cells would produce enough energy to supply the annual global demand.

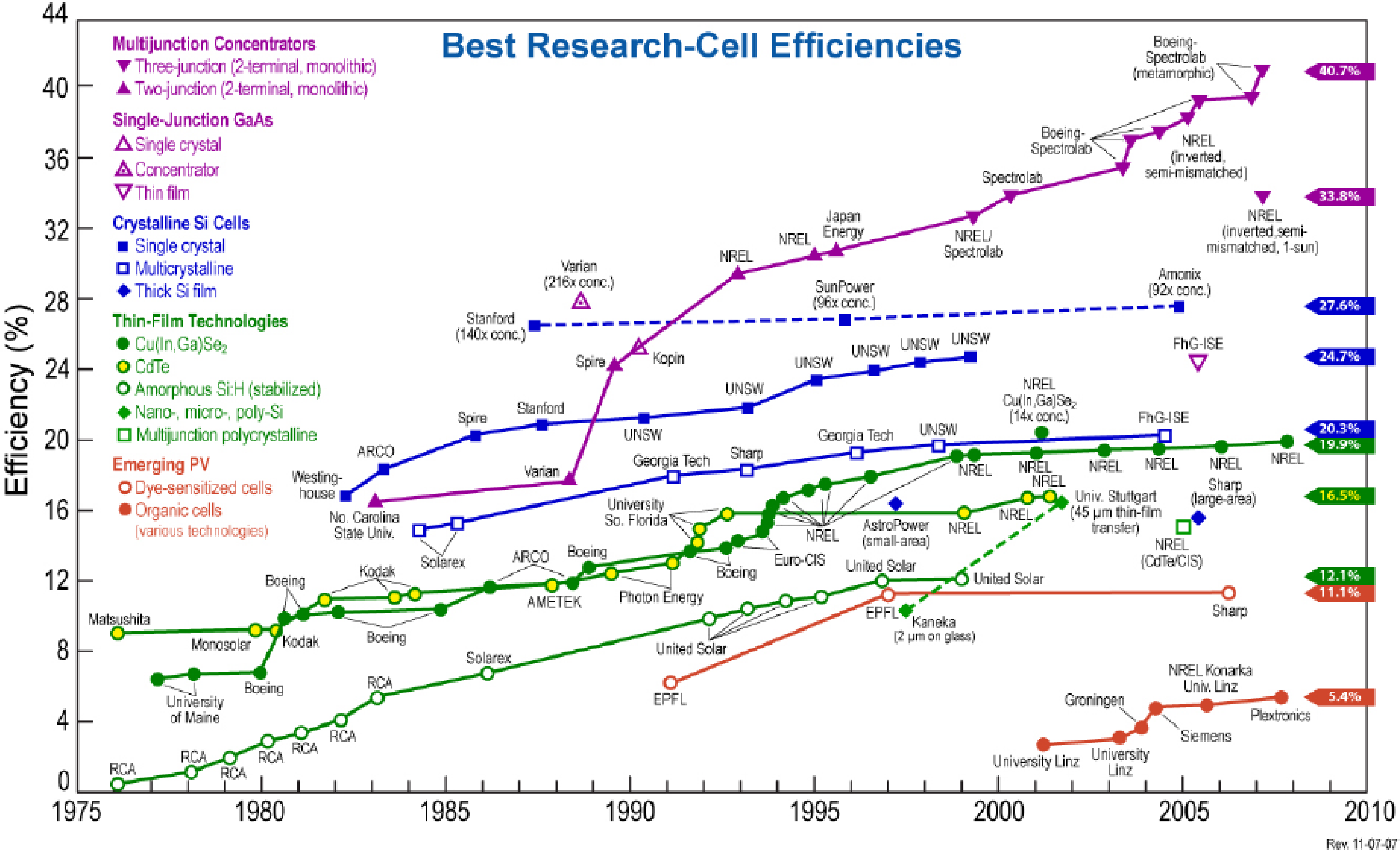
Global solar PV production



Source: O'Meara, Prometheus Institute, Solarbuzz

- ~30-50% growth
- At 35% growth rate we will reach 1 TW in ~ 20 Years

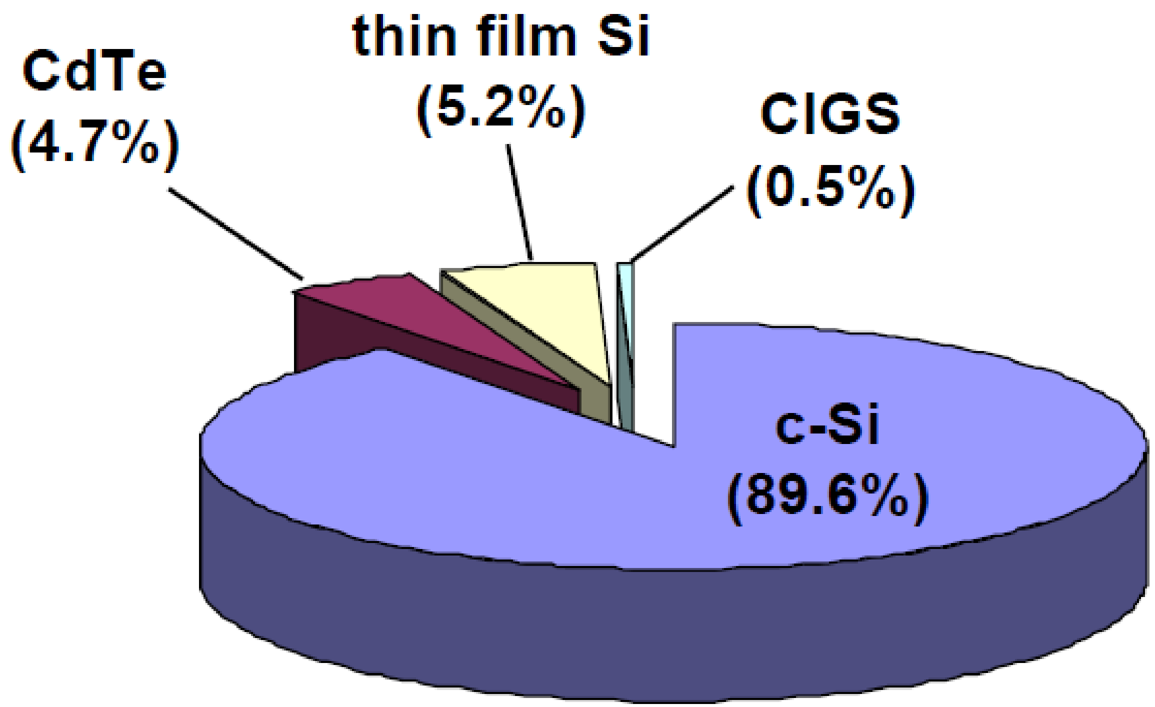
State-of-the-art in solar cells



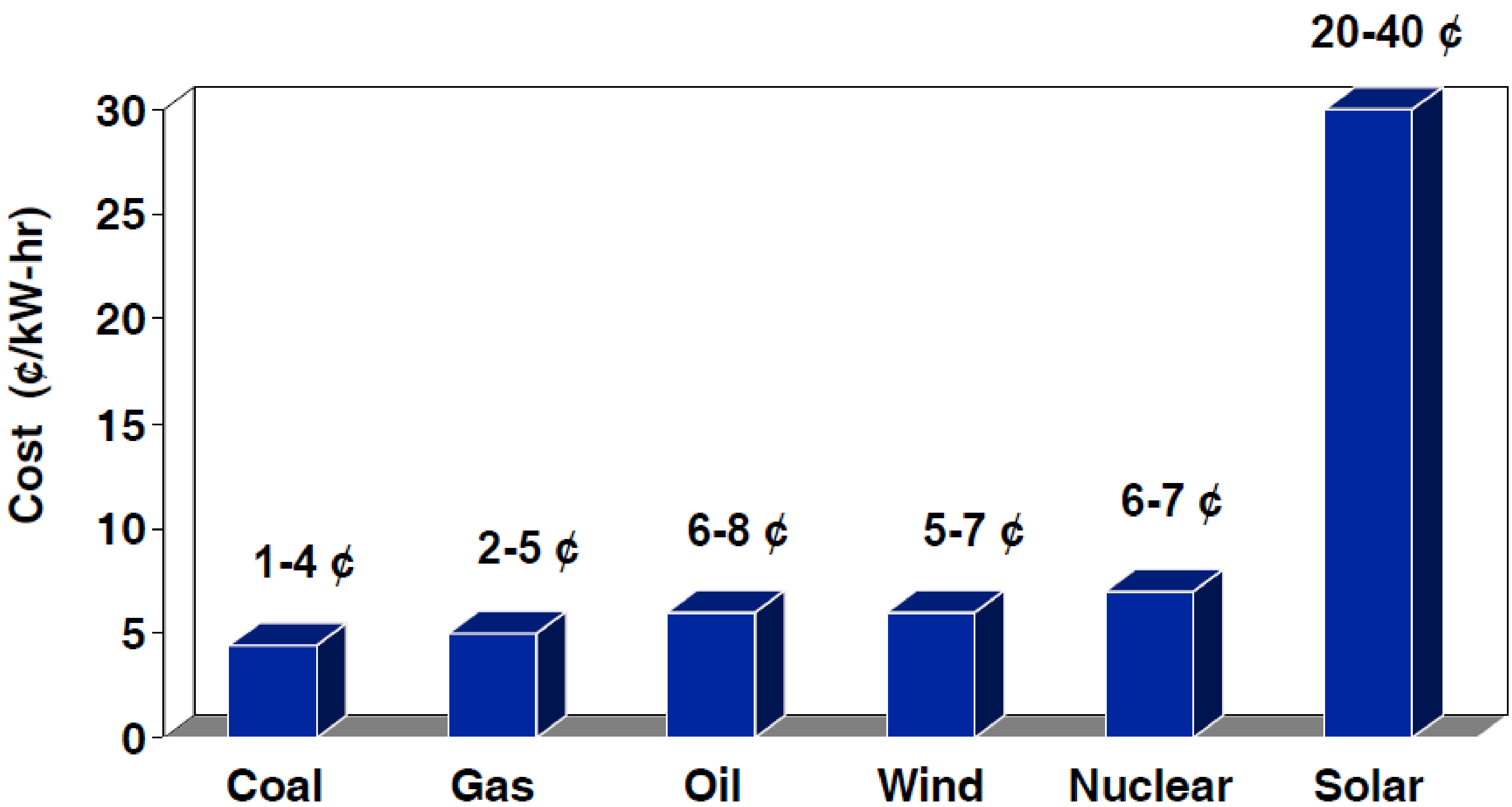
Module efficiency ~ 0.5 - 0.8 × lab efficiencies

United States Department of Energy Report on the Basic Energy Sciences Workshop on Solar Energy Utilization by N. S. Lewis et al. (2005) and from *J. Crystal Growth* 275, 292 (2005) by T. Surek.

2007 market share for various technologies



~ × 5 more expensive than other sources



Residential	~ 40 ¢
Commercial	~ 30 ¢
Industrial	~ 22 ¢

Why organic?

Pros:

Lightweight, flexible
High-throughput processing
Cheap

Cons:

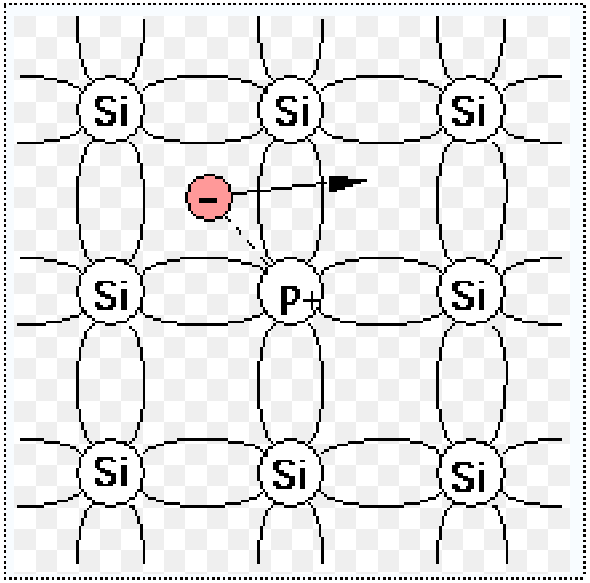
Low efficiency
Basic questions still open

Some Terminology

- **Electron hole** - the lack of an electron at a position where one could exist in an atom or atomic lattice
- **Electron-hole pair** - a Coulomb bound pair of a negative and a positive polarons, situated on different molecules
- **Exciton** - an excited quasiparticle in a solid, which is formed by a Coulomb-bound electron-hole pair

Some Terminology

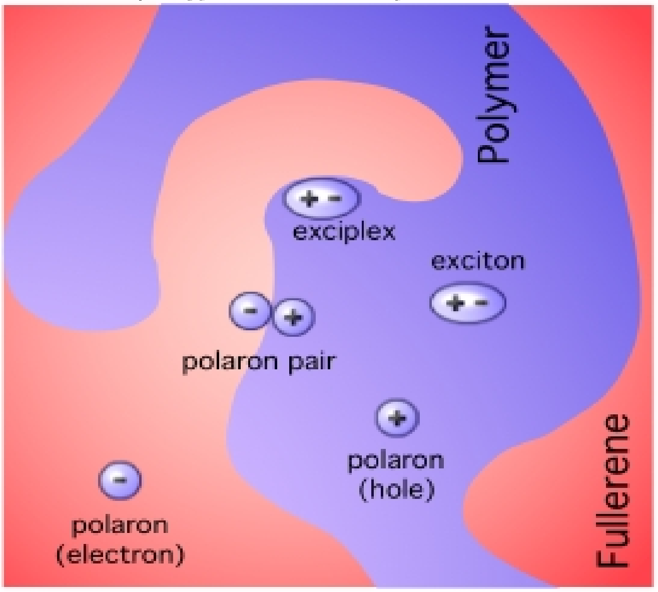
- **Donor** - a dopant atom that added to a semiconductor can form n-type regions
- **Acceptor** - a dopant atom that added to a semiconductor can form p-type regions



- Si, doped as a n-type semiconductor, using P (acting as a donor).

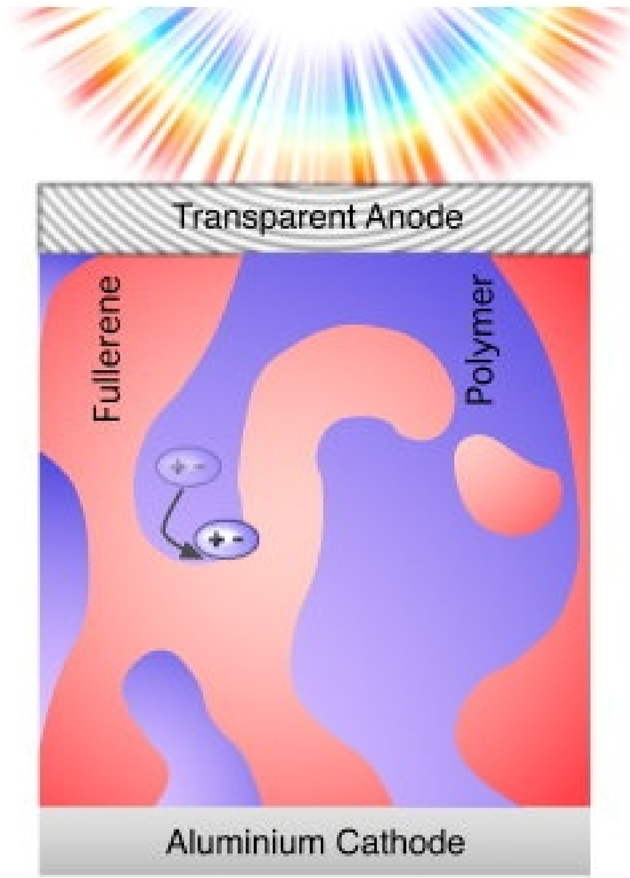
Some Terminology

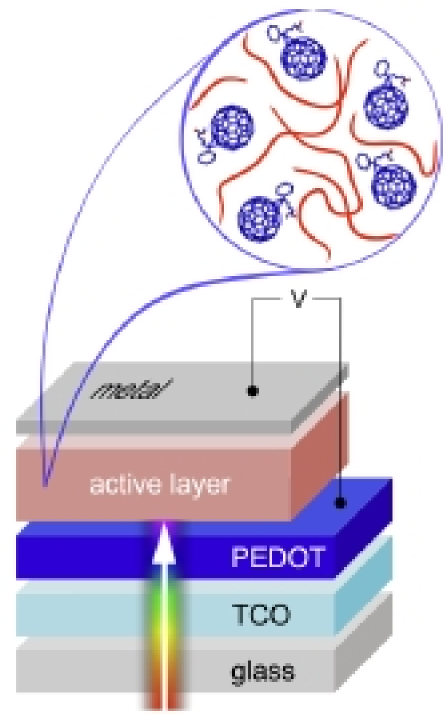
- **heterojunction** - the interface that occurs between two layers or regions of dissimilar crystalline semiconductors



How it works – a cartoon

Step 2: Exciton Diffusion => to Acceptor Interface

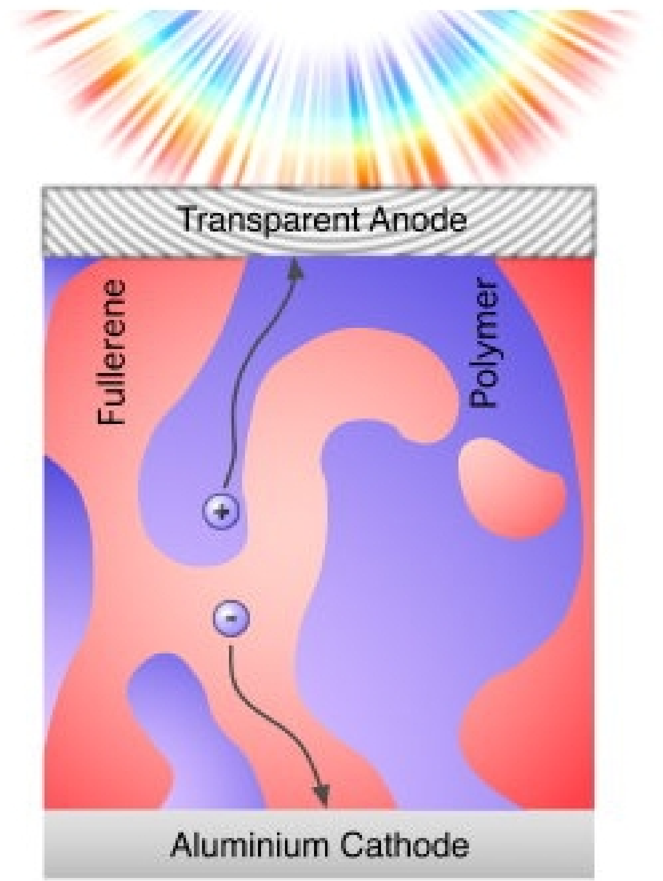




- Source: Carsten Deibel, Notes on Disordered Matter

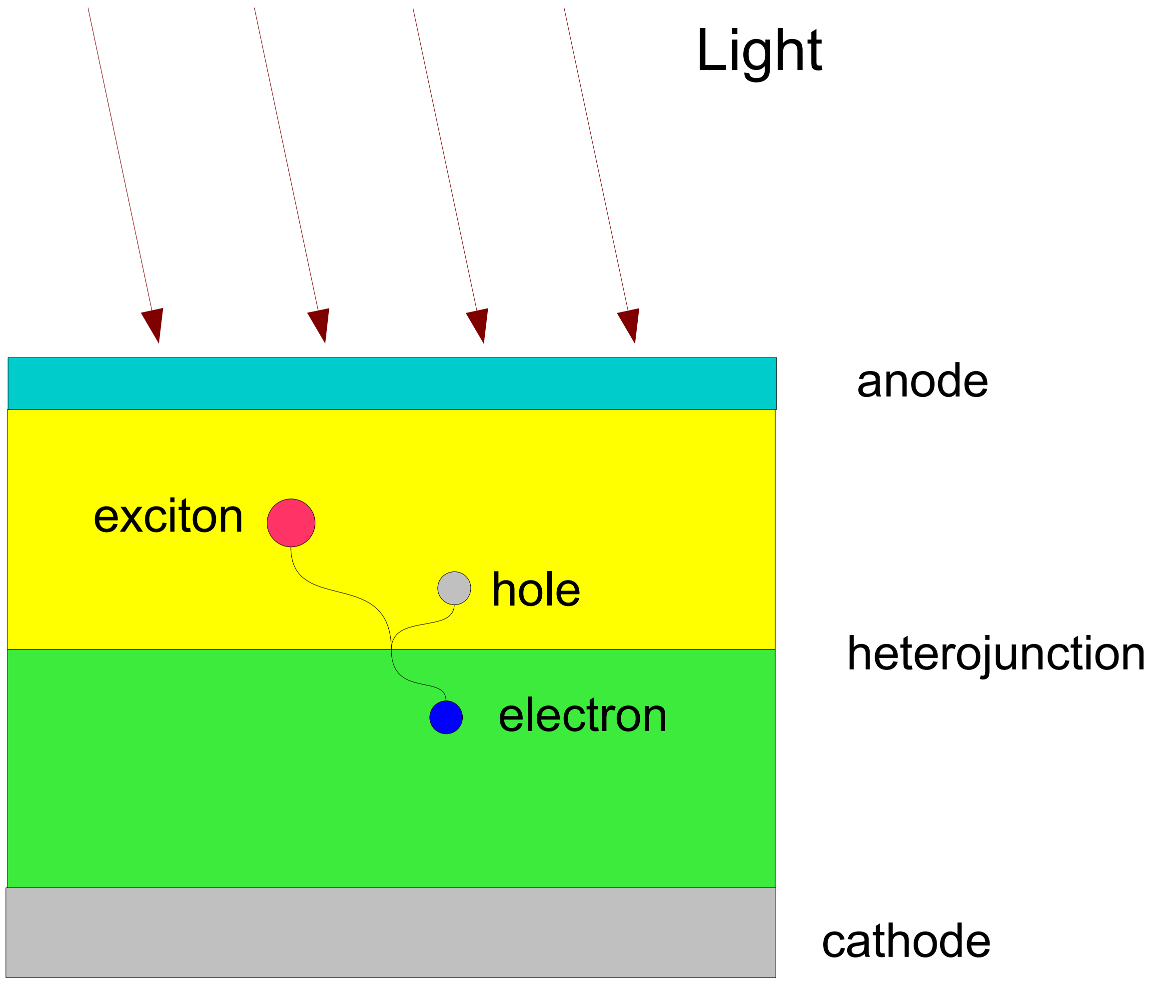
How it works – a cartoon

Step 5: Charge Transport => Photocurrent!



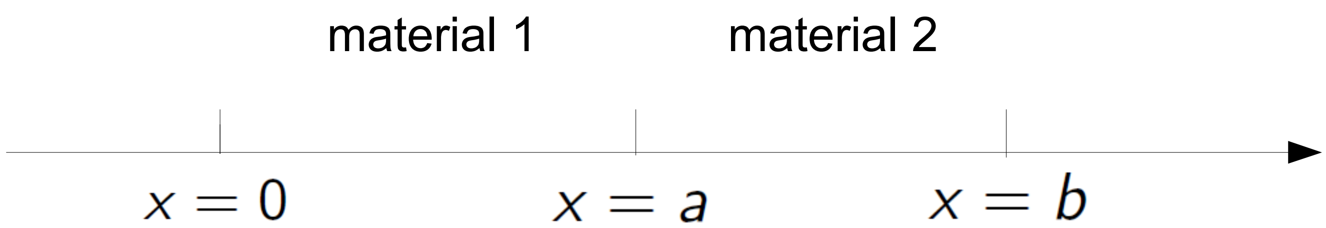
- Source: Carsten Deibel, Notes on Disordered Matter

How it works – a very simplified view



Model version 0.0

- View the process as one-dimensional
- Generation of excitons proportional to local light intensity
- Excitons move by diffusion
- All excitons at the junction get converted to electron-hole pairs
- All electrons are collected by the cathode



$$I_1 = (0, a) \text{ and } I_2 = (a, b)$$

$n_i(x)$ exciton density in material i

$Q_i(x)$ energy dissipated by light

β_i the reciprocal of the diffusion length

γ_i depends on the quantum efficiency of the exciton generation

$$\frac{d^2 n_i}{dx^2} = \beta_i^2 n_i(x) - \gamma_i Q_i(x) \qquad \text{for} \quad x \in I_i$$

Boundary conditions

All excitons dissociate at the heterojunction interface

$$n_i(a) = 0$$

No excitons can escape at the anode or cathode

$$\frac{dn_1}{dx}(0) = 0 \qquad \frac{dn_2}{dx}(b) = 0$$

Current density

Assuming that all electrons generated by dissociation of excitons are collected, the current density is proportional to the flux of excitons at the junction. You have two contributions

$$J = -D_1 \frac{dn_1}{dx}(a) + D_2 \frac{dn_2}{dx}(a)$$

Who me worry?

- How do you calculate light intensity? Doesn't that depend on how the cell is made, and the wave length and angle of incidence of the light?
  - *Fresnel equations - describe the behaviour of light when moving between media of differing refractive indices*
- What about all those constants you introduced? Do we know their values?
  - *Refractive index, diffusion length, etc.*
- How do you solve the differential equations?

Other models

- Different *boundary conditions*
  - The interfaces of the active layer act as perfect sinks $n_1(0) = n_2(b) = 0$
  - Many others...
- Various levels of complexity for modeling the *energy dissipated* $Q_i(x)$

Getting started...

- Try to reproduce some of the results in the considered papers
- Compare the different types of models
- Study the sensitivity of models to parameters (e.g. diffusion length of excitons)

If we have time...

- Consider a more general form of the heterojuncion
- ...