1.021, 3.021, 10.333, 22.00 : Introduction to Modeling and Simulation : Spring 2012

Part II – Quantum Mechanical Methods : Lecture 10

Solar PV

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Part II Topics

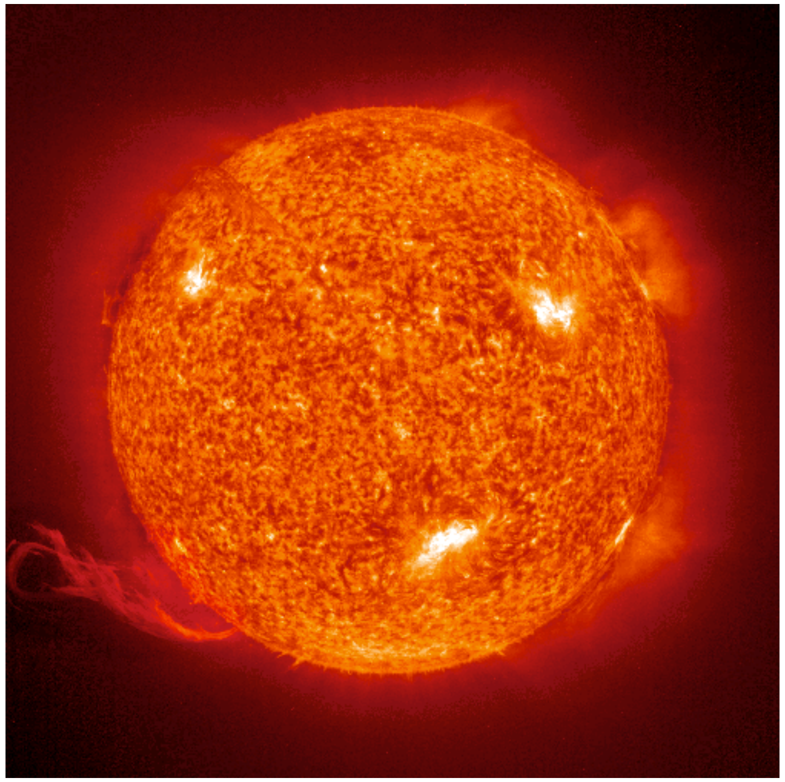
1. It's a Quantum World: The Theory of Quantum Mechanics
2. Quantum Mechanics: Practice Makes Perfect
3. From Many-Body to Single-Particle; Quantum Modeling of Molecules
4. Application of Quantum Modeling of Molecules: Solar Thermal Fuels
5. Application of Quantum Modeling of Molecules: Hydrogen Storage
6. From Atoms to Solids
7. Quantum Modeling of Solids: Basic Properties
8. Advanced Prop. of Materials: What else can we do?
9. Application of Quantum Modeling of Solids: Solar Cells Part I
10. Application of Quantum Modeling of Solids: Solar Cells Part II
11. Application of Quantum Modeling of Solids: Nanotechnology

Summary

- A bit of discussion of PSET 6
- Solar PV - More Motivation
- Solar PV - the viewpoint of the electron!
- How computational quantum mechanics can impact solar PV

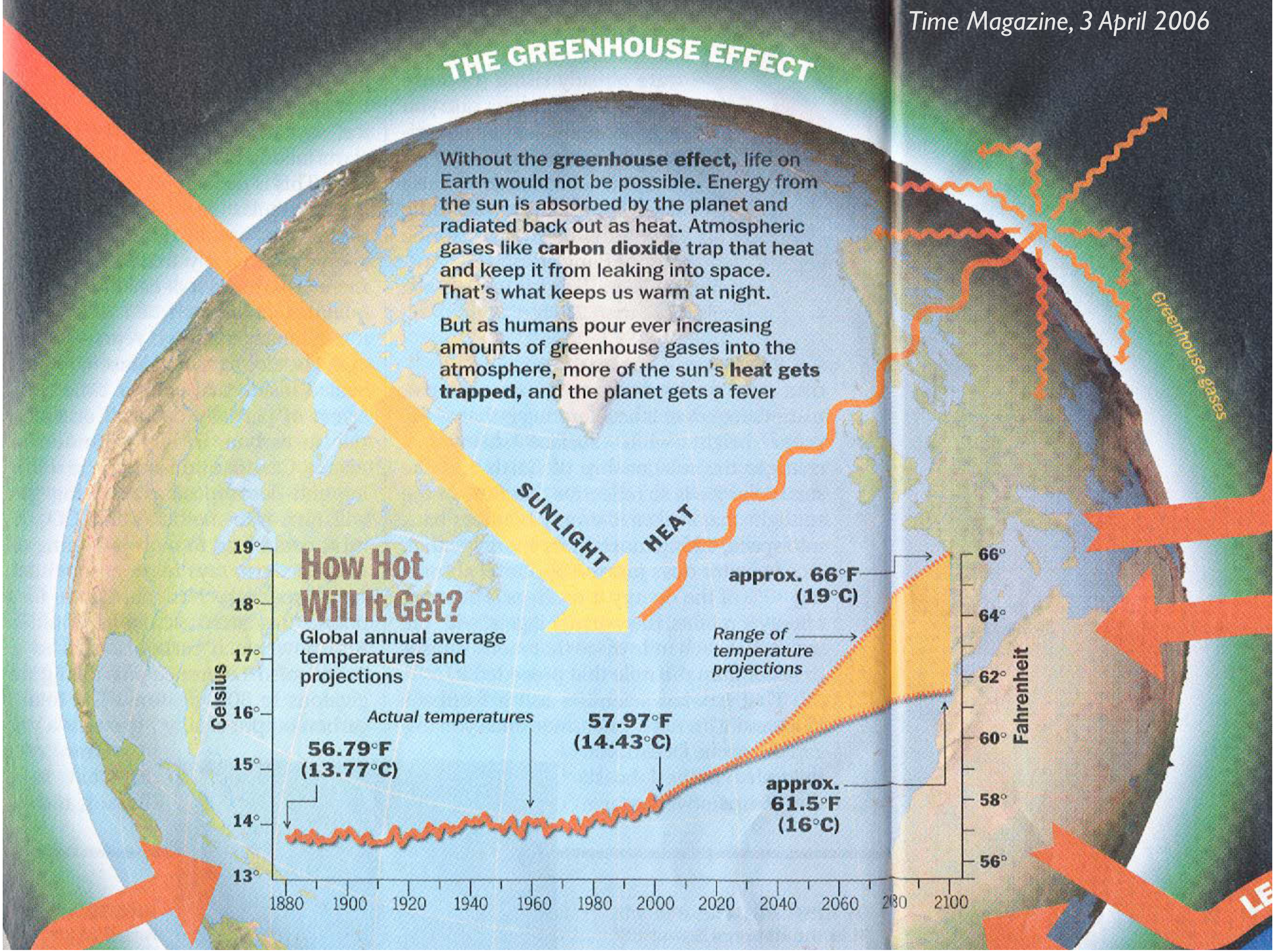
Energy from the Sun

- Energy released by an earthquake of magnitude 8 (10^{17} J):
  - the sun delivers this in one second
- Energy humans use annually (10^{20} J):
  - sun delivers this in one hour
- Earth’s total resources of oil (3 trillion barrels, 10^{22} J):
  - the sun delivers this in two days



Courtesy of SOHO/EIT (ESA & NASA) consortium.

Time Magazine, 3 April 2006



Cost of Inaction?

Grinell Glacier and Grinnell Lake, Glacier National Park, 1910-1997

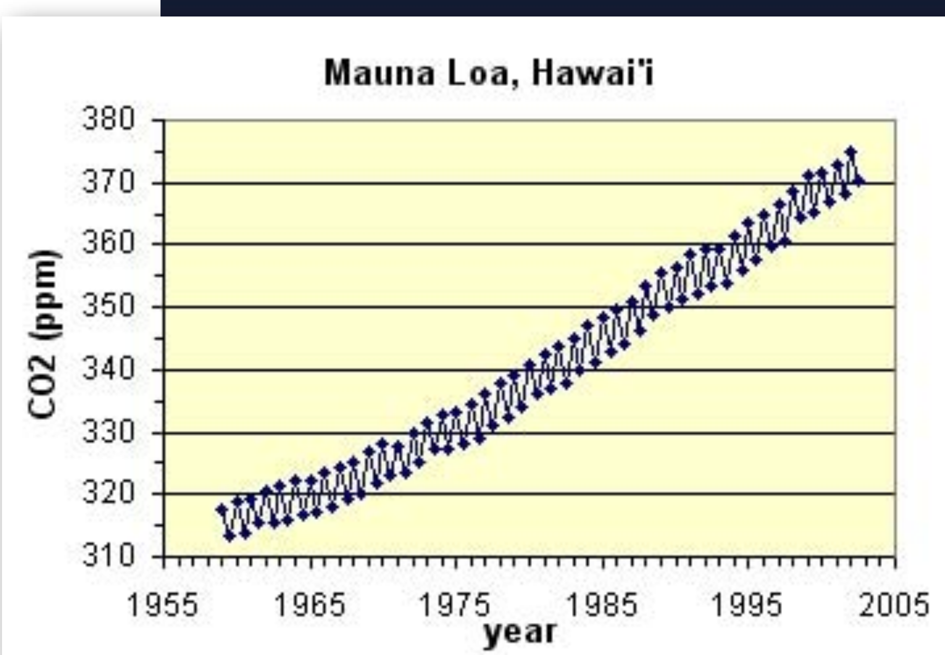
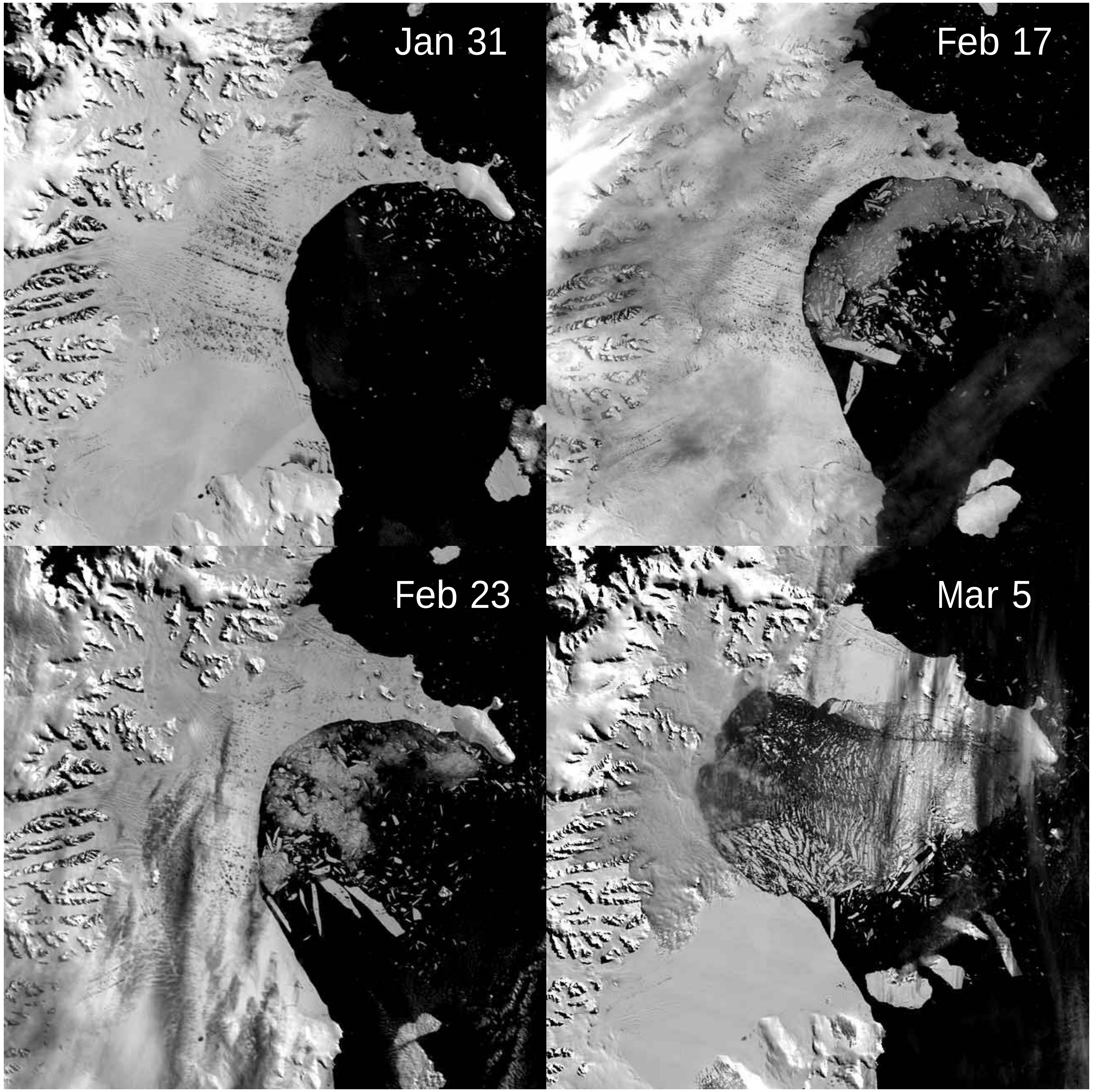


Image by Dr. Pieter Tans, NOAA/ESRL and Dr. Ralph Keeling, Scripps Institute of Oceanography.

Grinnel Glacier: 1910 photo by Fred Kiser (top); 1997 photo by Dan Fagre (bottom). Courtesy of GNP archives.

Warming is Real and Has Real Effects



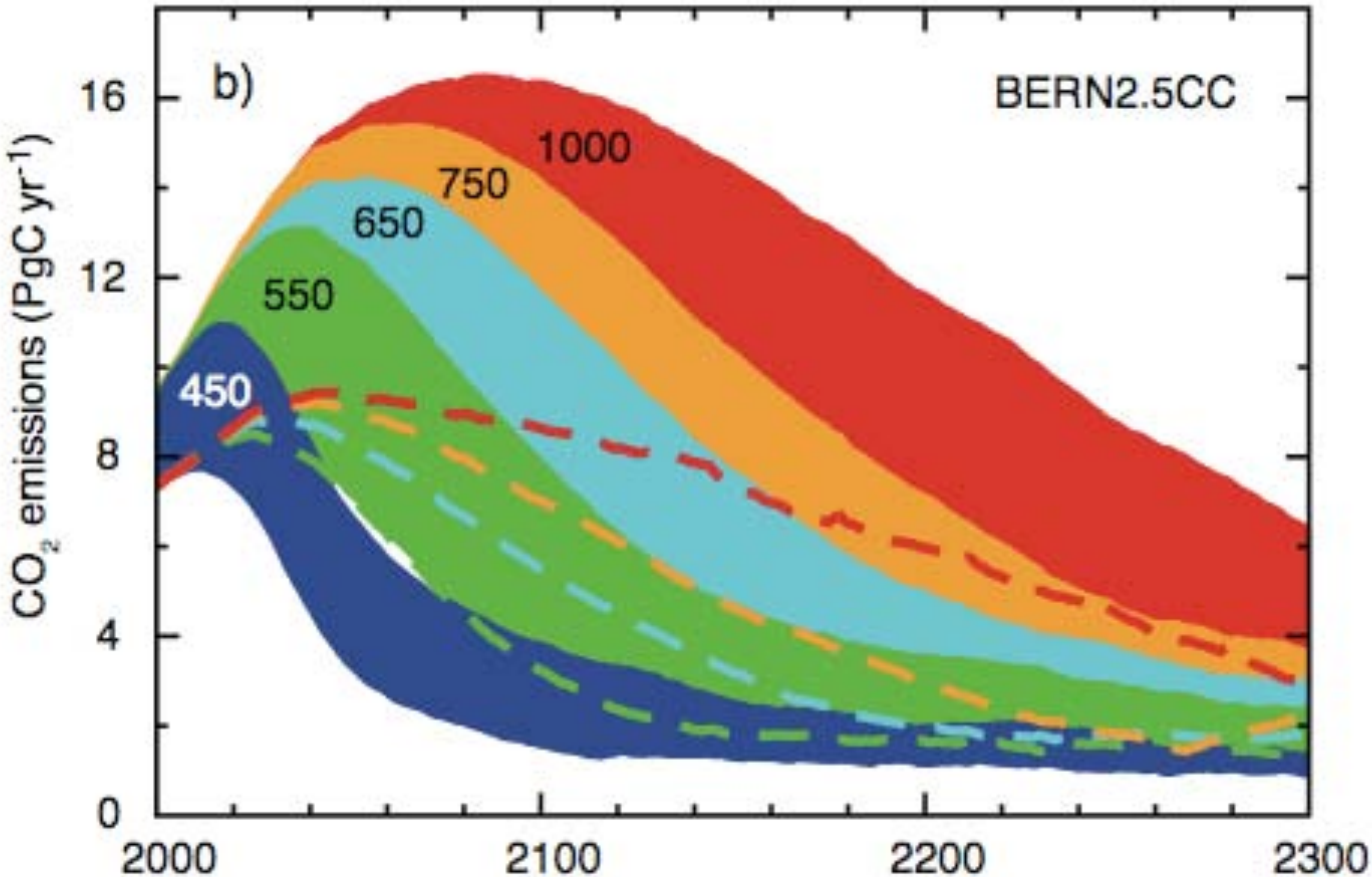
MODIS images from NASA's Terra satellite courtesy of Ted Scambos, National Snow and Ice Data Center, University of Colorado, Boulder.

Between Jan 31, 2002 and March 5, 2002 a chunk of the Larsen B ice shelf the size of Rhode Island disintegrated.

Images from NASA's Terra satellite, National Snow and Ice Data Center, University of Colorado, Boulder.

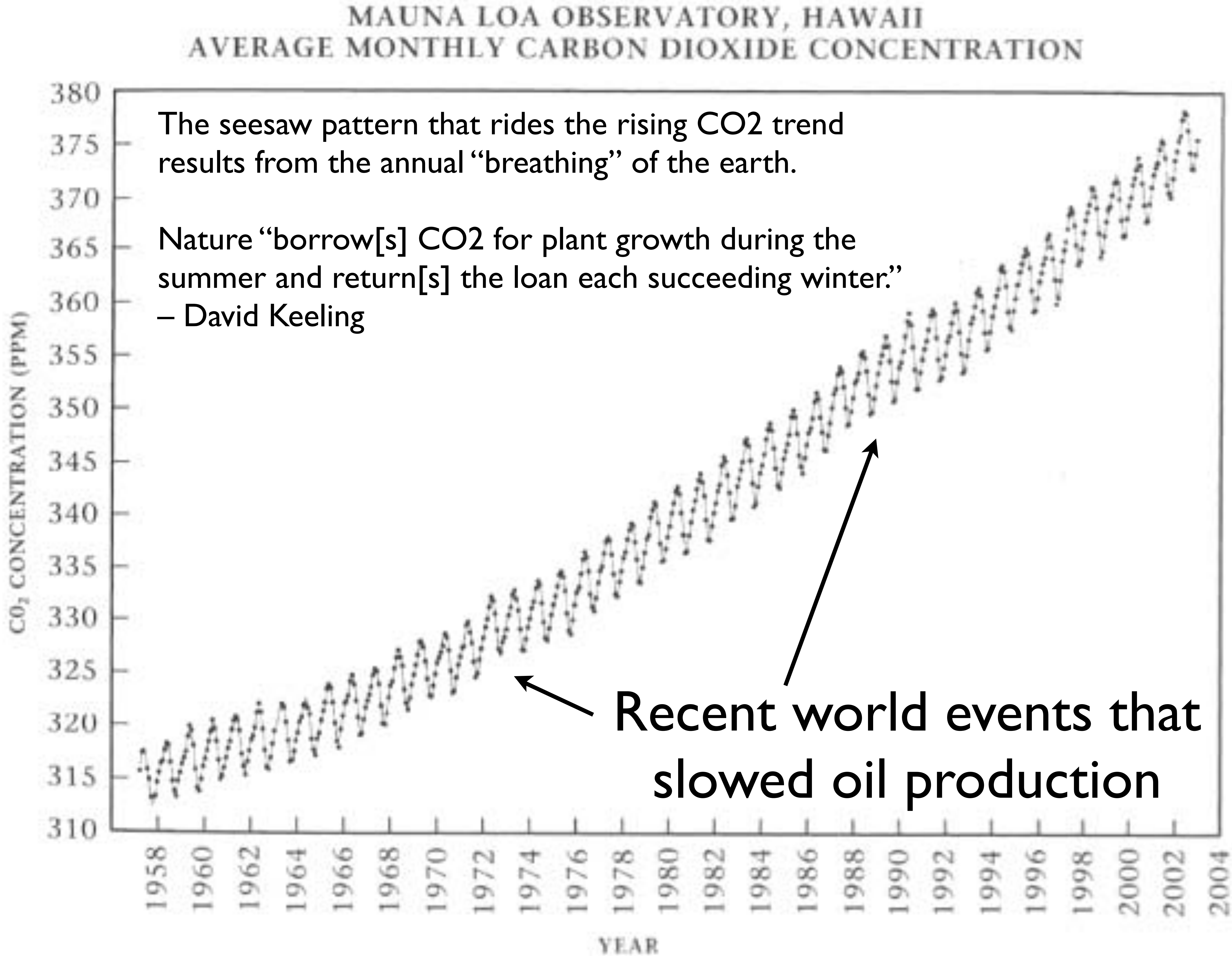

Surveys show the mountain pine beetle has infested 21 million acres and killed 411 million cubic feet of trees -- double the annual take by all the loggers in Canada. In seven years or sooner, the Forest Service predicts, that kill will nearly triple and 80 percent of the pines in the central British Columbia forest will be dead.
The Washington Post, March 1, 2006

CO_2 Projections



Source: Climate Change 2007: The Physical Science Basis. Contribution of Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change

Climate Change 2007: The Physical Science Basis. Working Group I Contribution to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change, Figure 10.22 (b). Cambridge University Press.



The seesaw pattern that rides the rising CO2 trend results from the annual "breathing" of the earth.

Nature "borrow[s] CO2 for plant growth during the summer and return[s] the loan each succeeding winter." – David Keeling

Recent world events that slowed oil production

Image by Dr. Pieter Tans, NOAA/ESRL and Dr. Ralph Keeling, Scripps Institute of Oceanography.

Science 310, 1313 (2005)

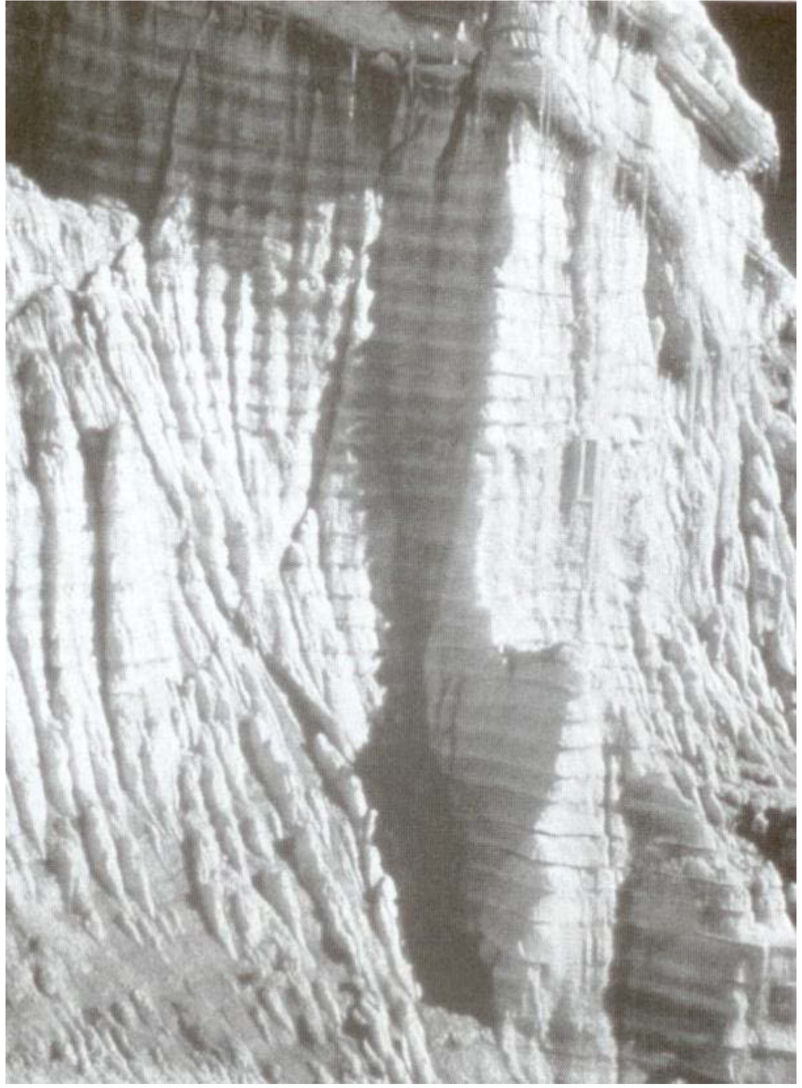


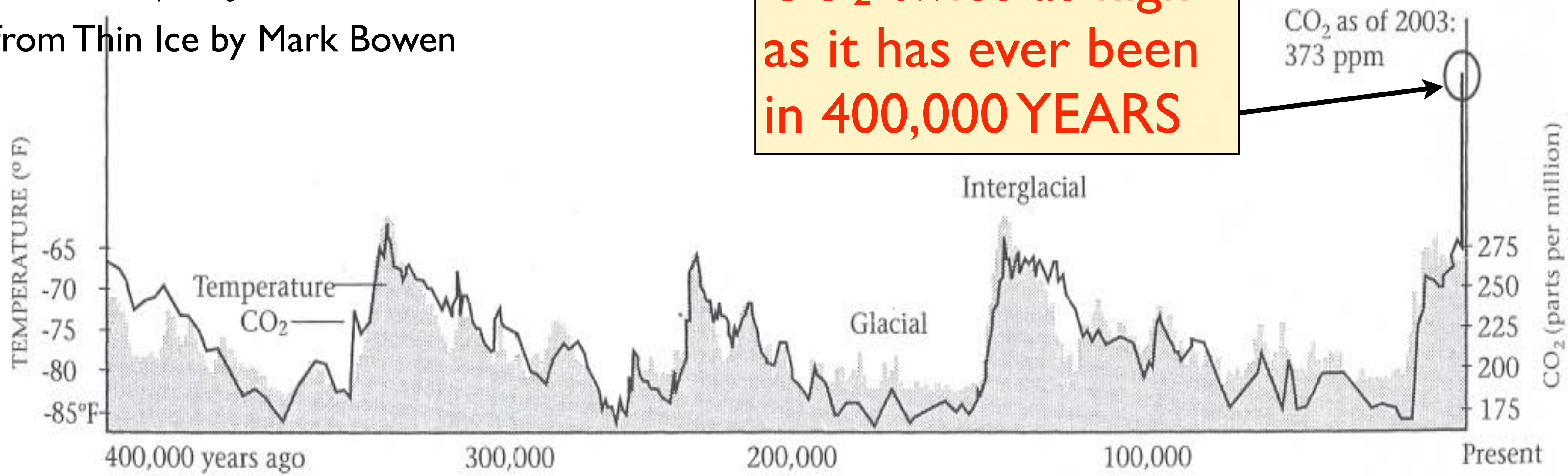
Photo by Lonnie Thompson, Courtesy of Ohio State University. All rights reserved.

from Thin Ice by Mark Bowen

Temperature inferred from isotope ratios in the Vostok ice core

Carbon dioxide levels measured in the trapped air bubbles in the same core

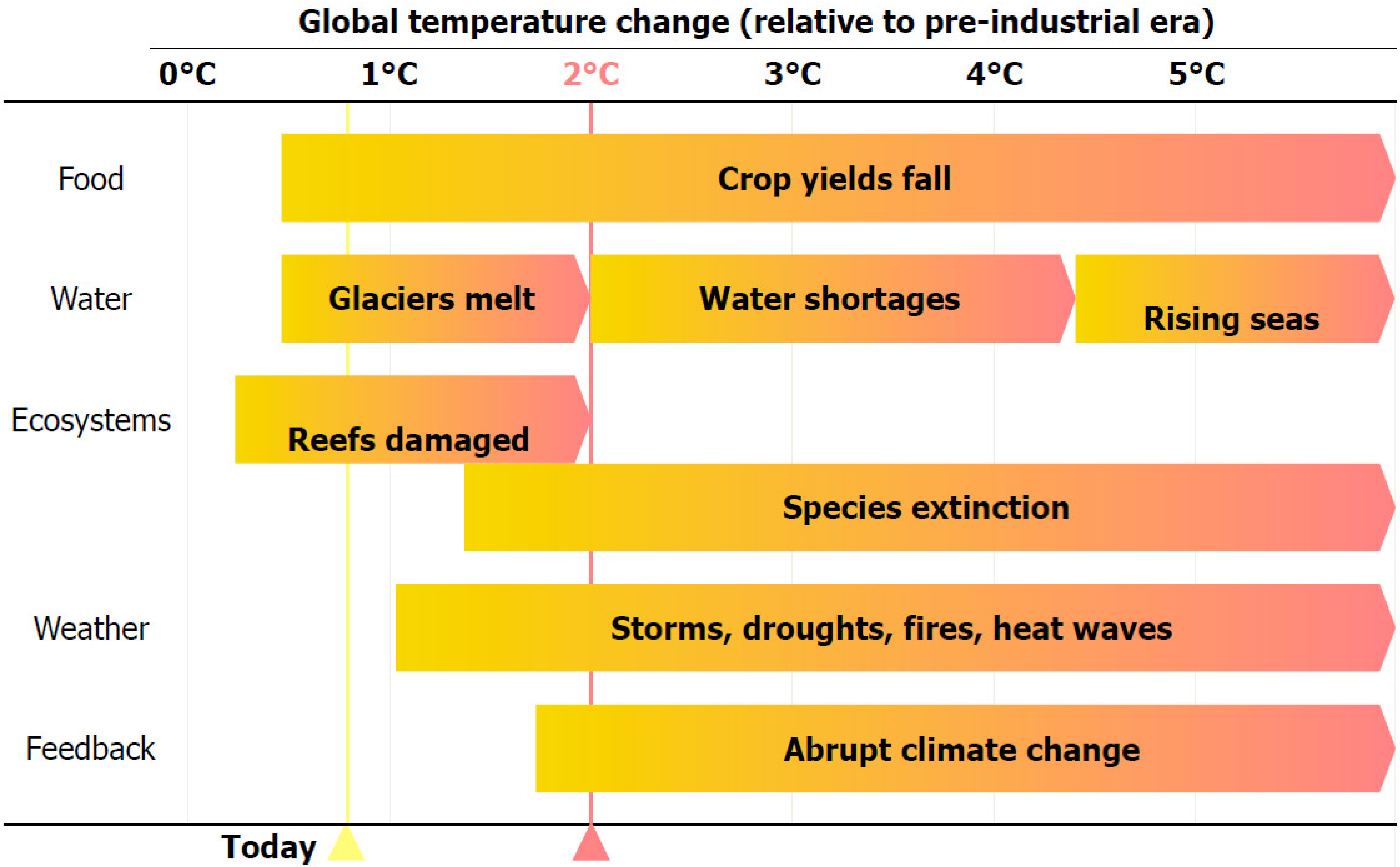
CO_2 twice as high as it has ever been in 400,000 YEARS



"I can get eight professors from MIT on both sides of this issue and no one in this room will walk away understanding what they said about climate change."

□Charlie Baker, Former Candidate for Massachusetts Governor

If warming exceeds 2°C, negative effects increase and catastrophic changes become more likely



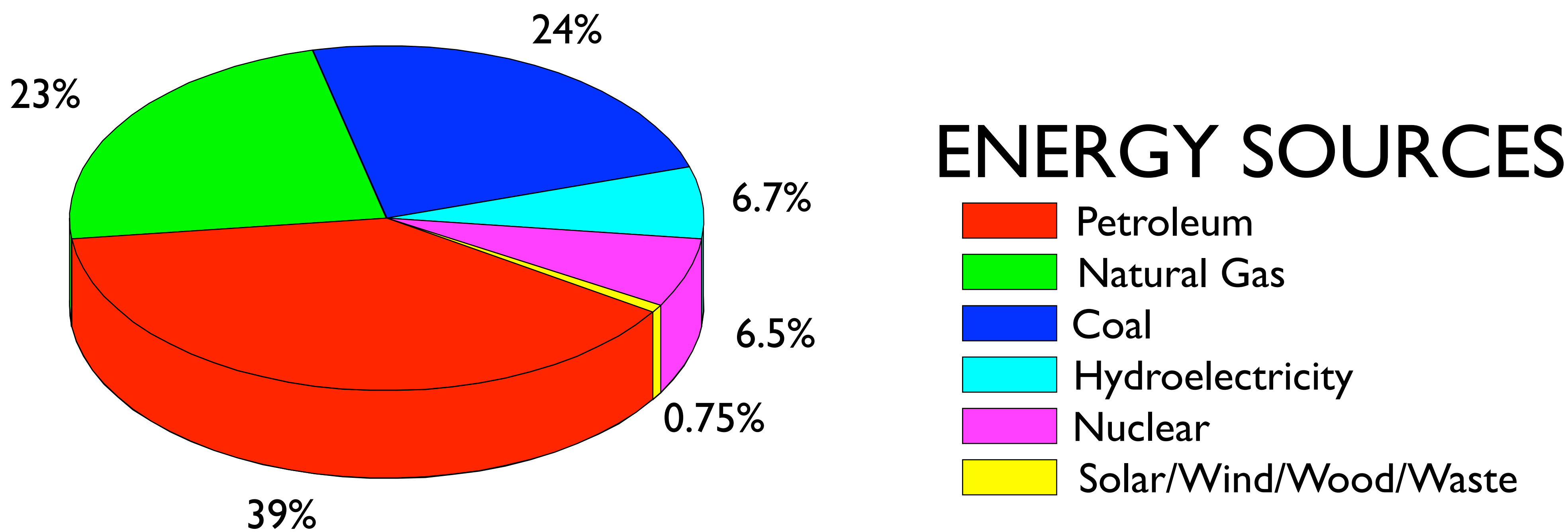
Courtesy of Hal Harvey. Used with permission.

Courtesy: Hal Harvey (Climate Works)

Abundance of Solar Energy

Average solar power incident on Earth ~ 130,000 TW
Global energy consumption (2001) ~ 13.5 TW

Source: DOE



If ~2% of the continental United States is covered with PV systems with a net efficiency of 10% we would be able to supply all the US energy needs (0.3% land coverage to meet just electricity needs)

(Land area requirement is comparable to area occupied by interstate highways)

Note: 40% of our land is allocated to producing food

Nuclear power equivalent is 3,300 x 1 GW nuclear power plants.
(1 for every 10 miles of coastline or major waterway)

Solar Across Scales

Moscone Center: 675,000 W

Residential home: 2400 W

Kenyan PV market:

Average system: 18W

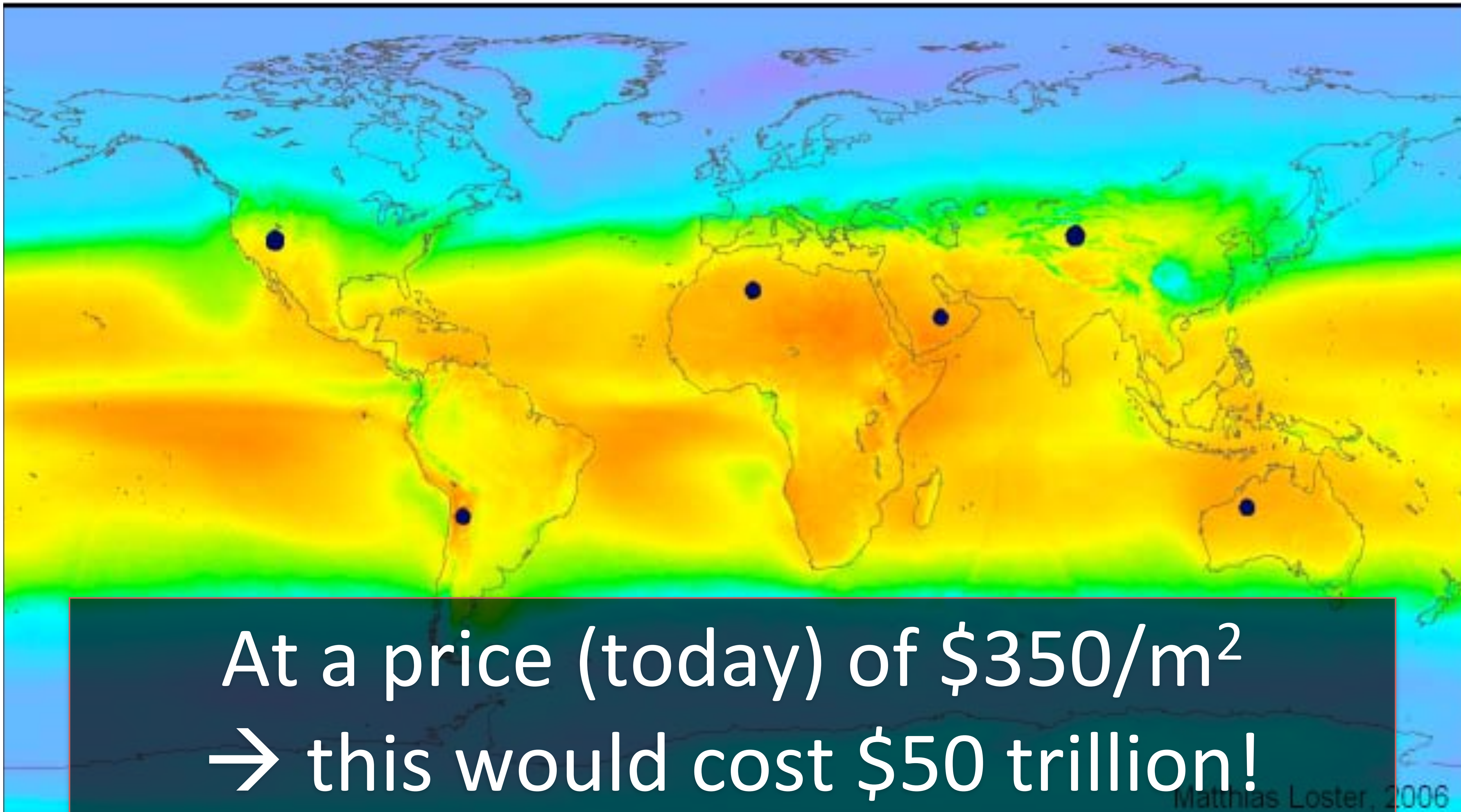
Solar Land Area Requirements

150 Km^2 solar panels in Nevada would power the U.S. (15% efficient)

J.A. Turner, *Science* 285 1999, p. 687.

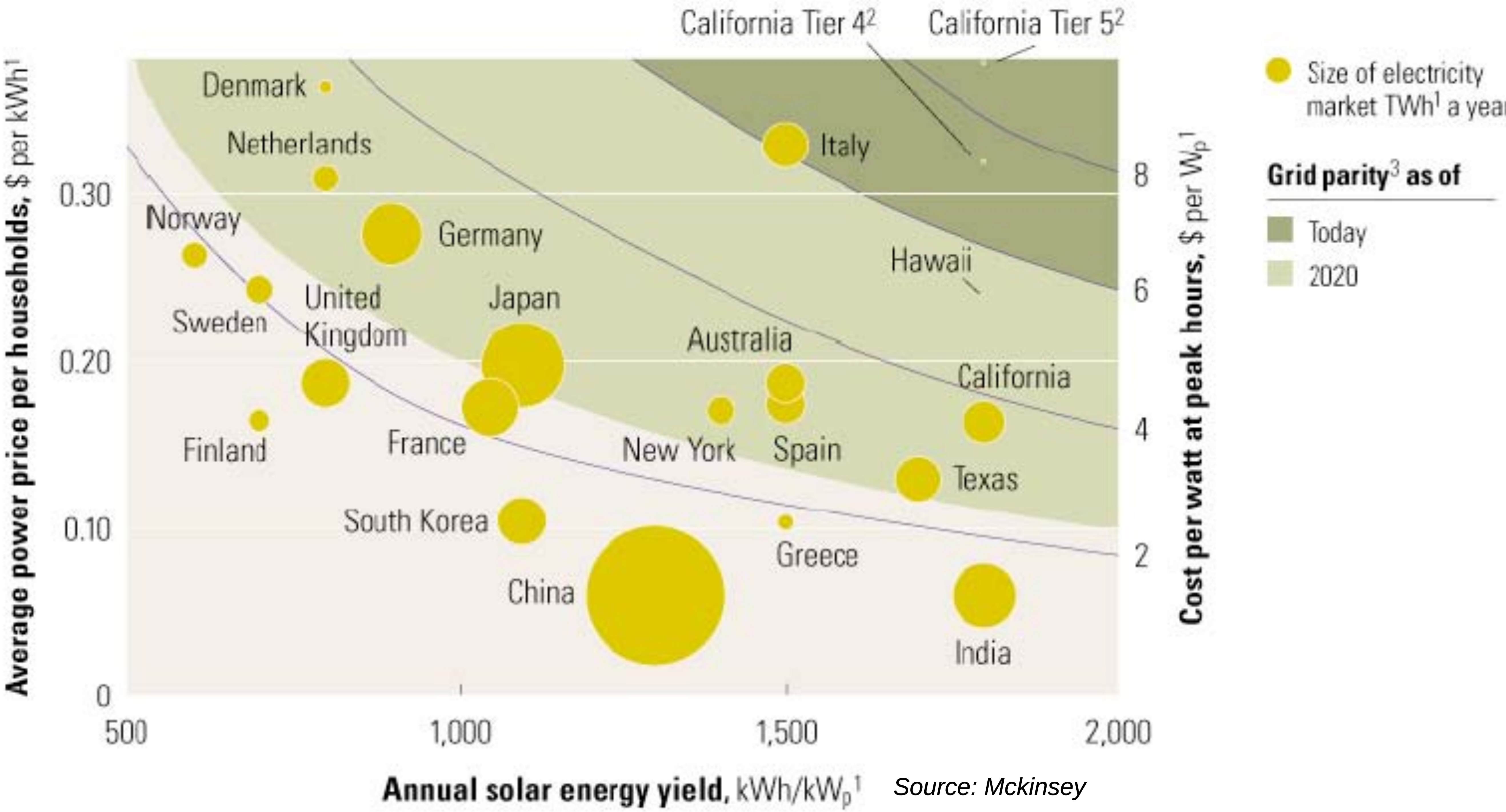
Image by the United States Geological Survey is in the public domain.

Solar Land Area Requirements for ~20TW



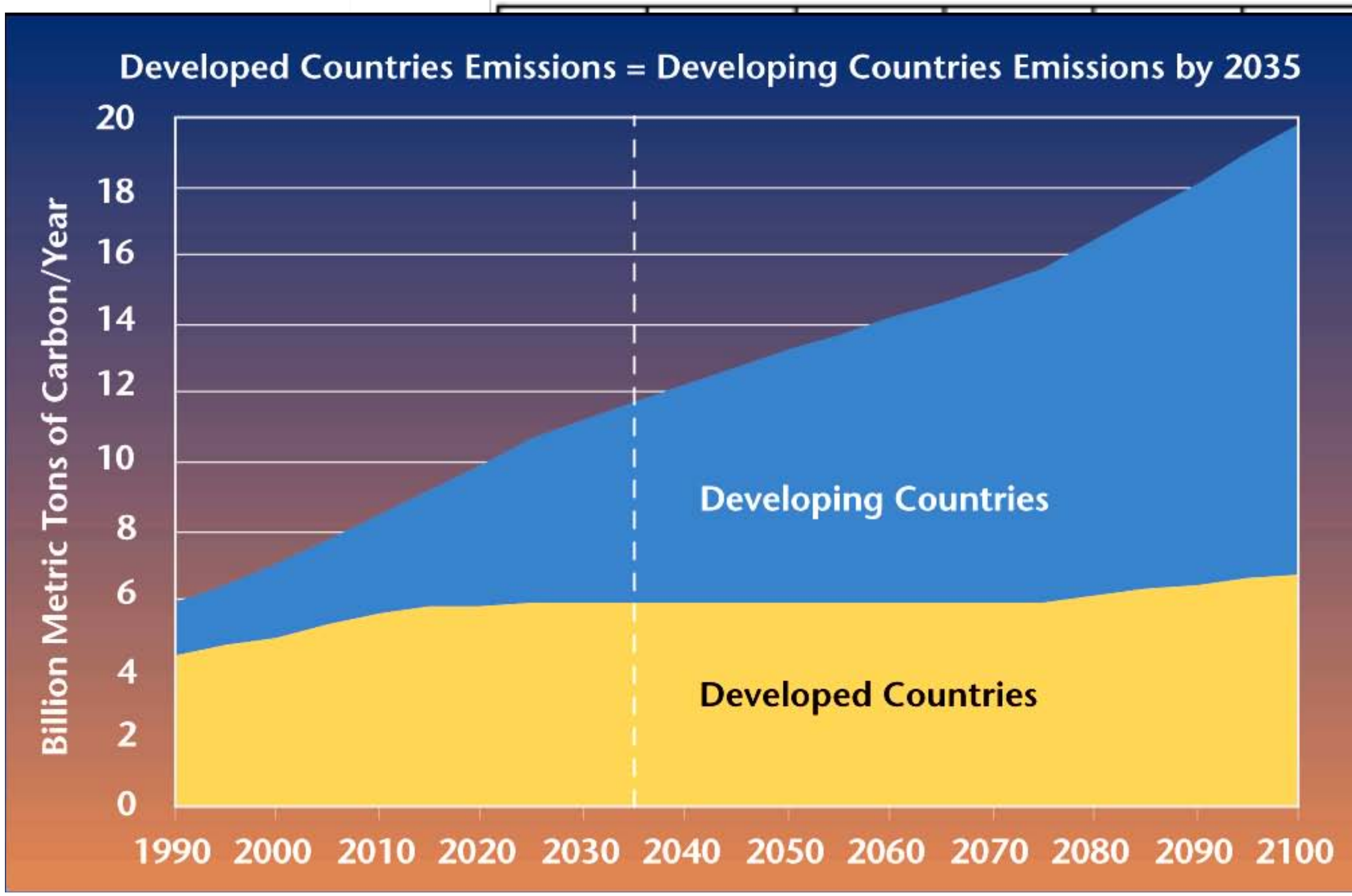
At a price (today) of $\$350/m^2$
→ this would cost $50 trillion!

Solar PV: Grid Parity



Source: Mckinsey

Aim: capture 10% of electrical generation with PV



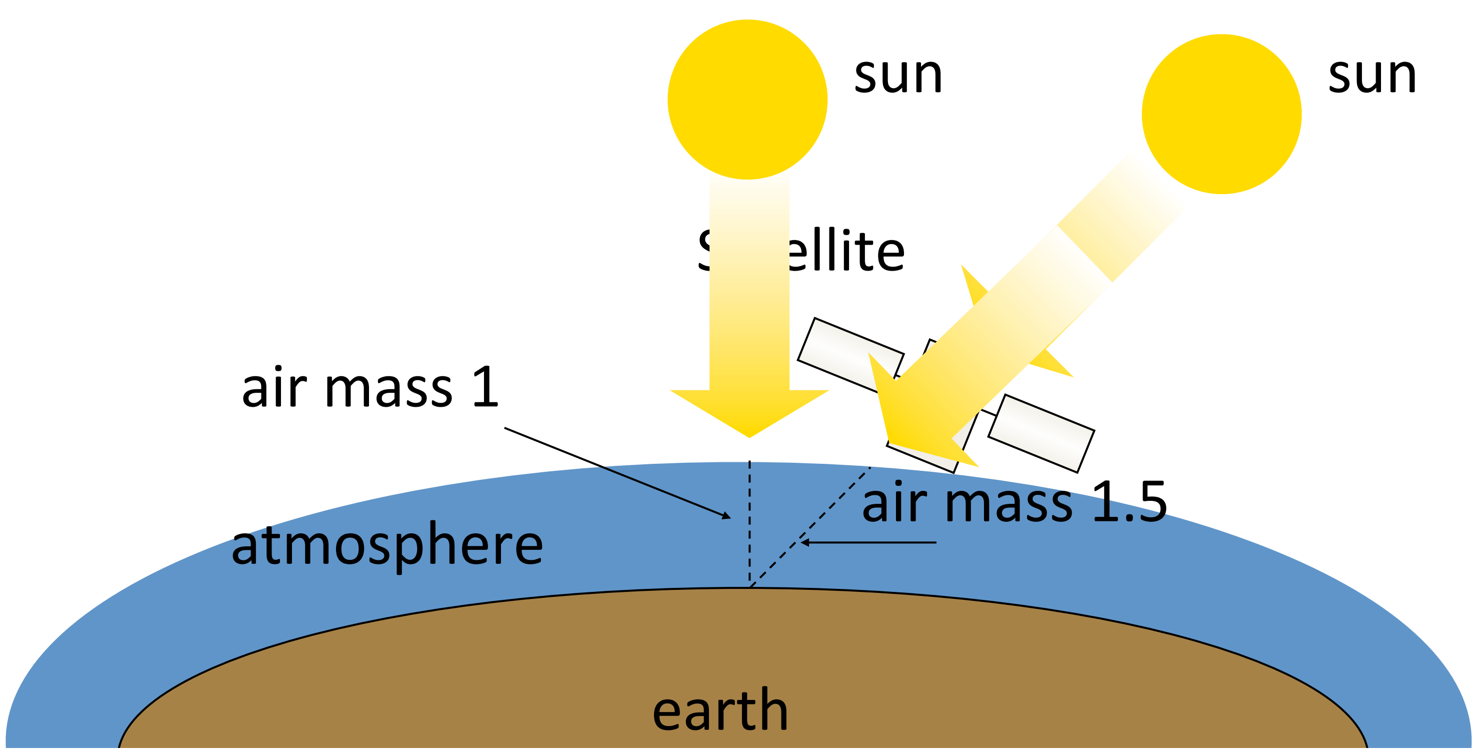
Side note: replacing fossil fuels in the developing world will become much more important in the near future.

At 14¢ per kW_eh, PV could cost-effectively replace 10% of electrical energy used in U.S.

No storage needed.

Could be deployed by 2022, with 0.04% land use.

SOLAR INTENSITY:
HOW MUCH AREA IS REQUIRED TO GENERATE POWER?



Solar spectrum outside atmosphere:

air mass 0 (AM0) 1353 W/m^2

At earth's surface:

sun at zenith:

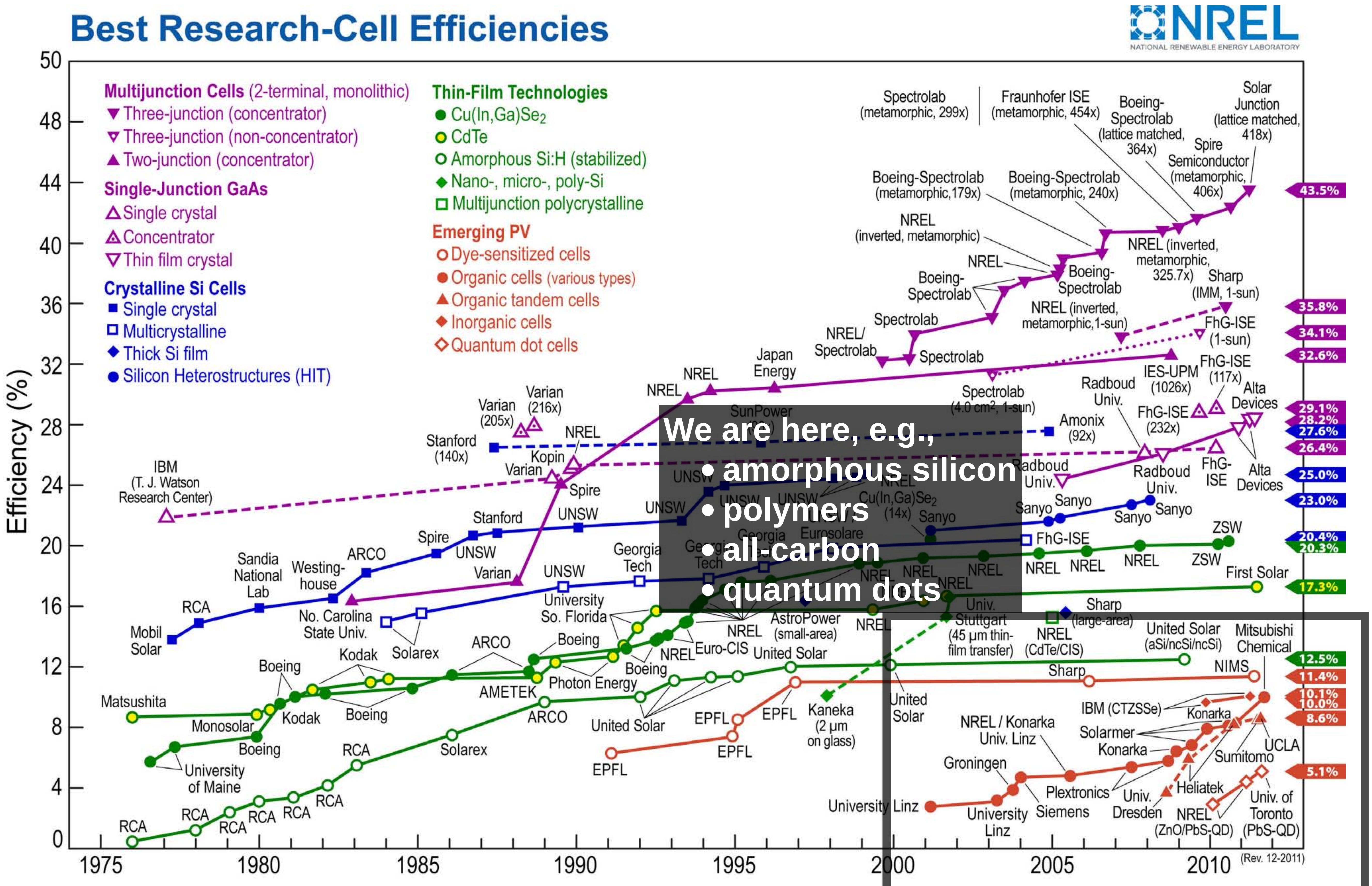
air mass 1 (AM1) 925 W/m^2

sun at 45°:

air mass 1.5 (AM1.5) 844 W/m^2

AM1.5 is terrestrial solar cell standard

Comparison of PV Technologies



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Solar PV technology landscape (2015)

- Cost/efficiency tradeoff:
- high efficiency modules have lower installation costs
- low efficiency modules have lower module costs

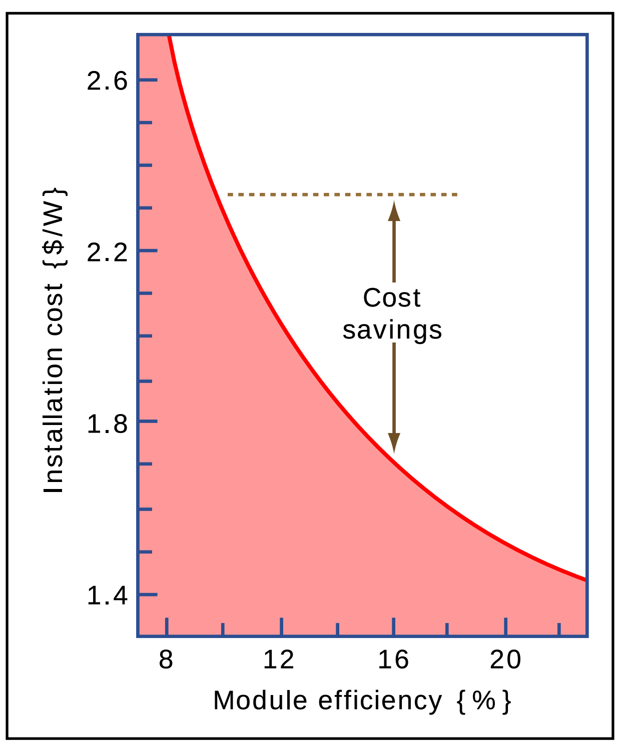
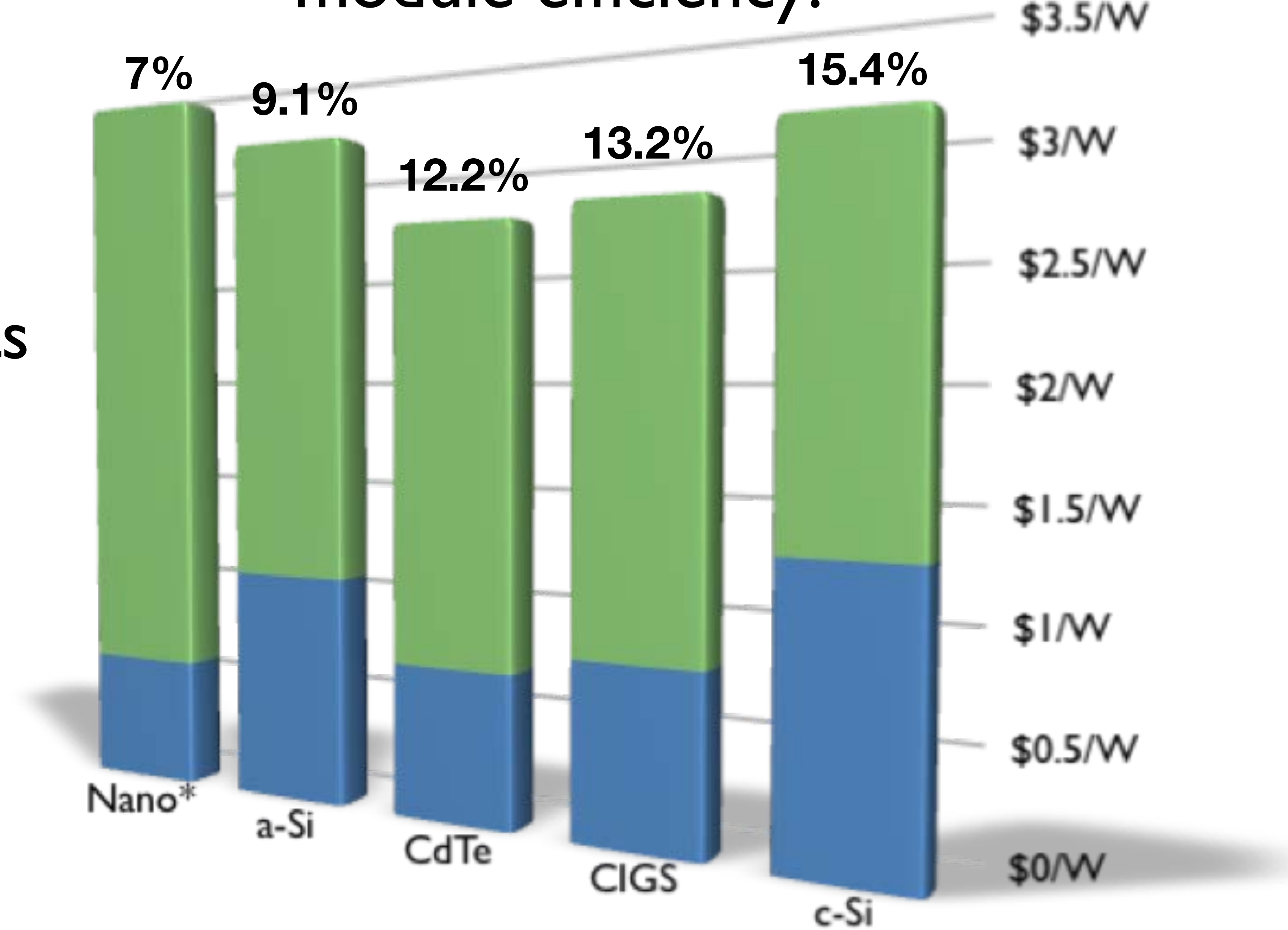
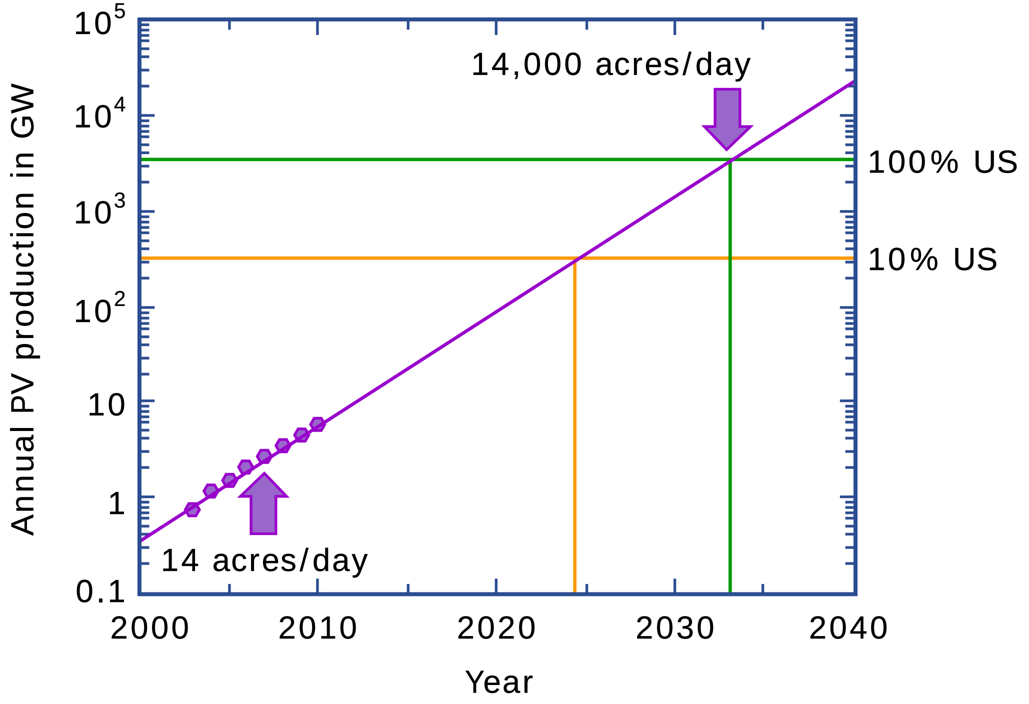


Image by MIT OpenCourseWare.

module efficiency:



How do we supply 81 kWh/day/person of solar electricity?



Expected Global Solar Cell Production.
After Mike Rogol.

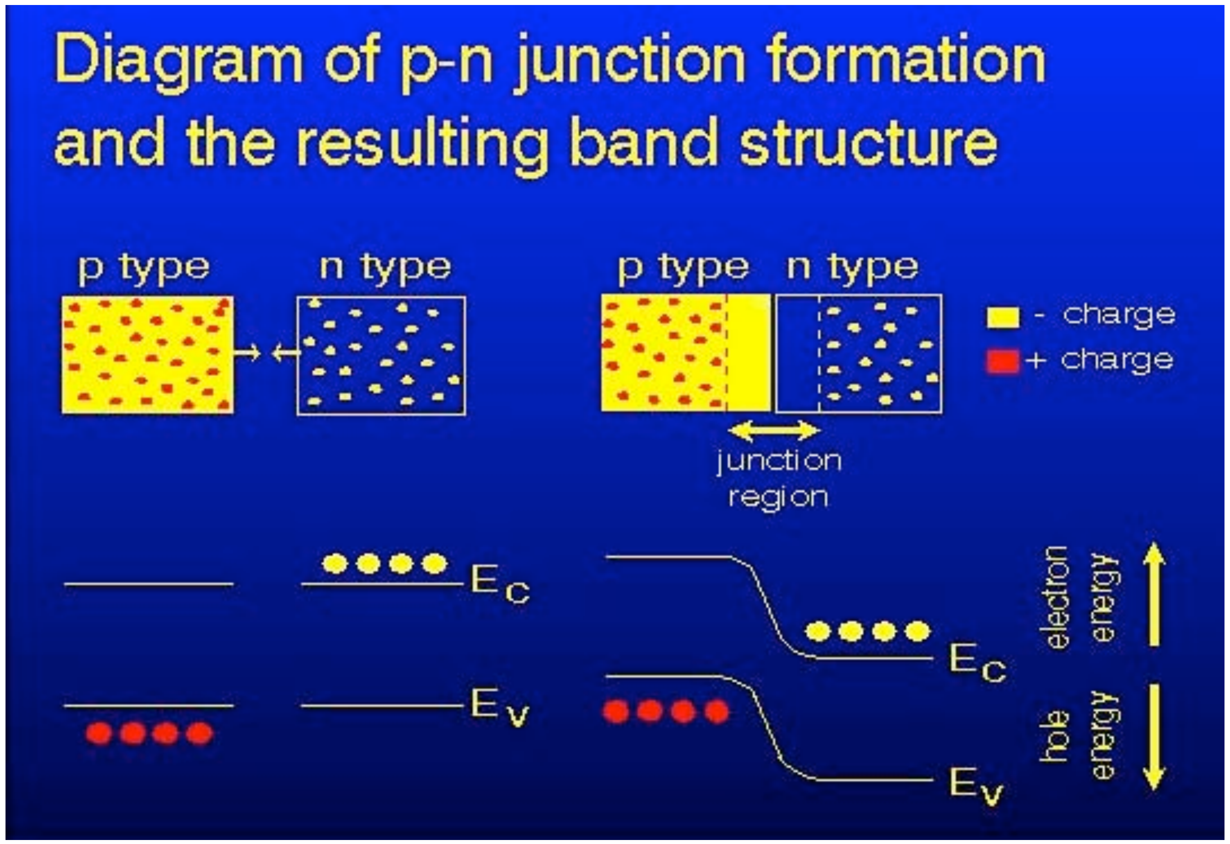
Image by MIT OpenCourseWare.

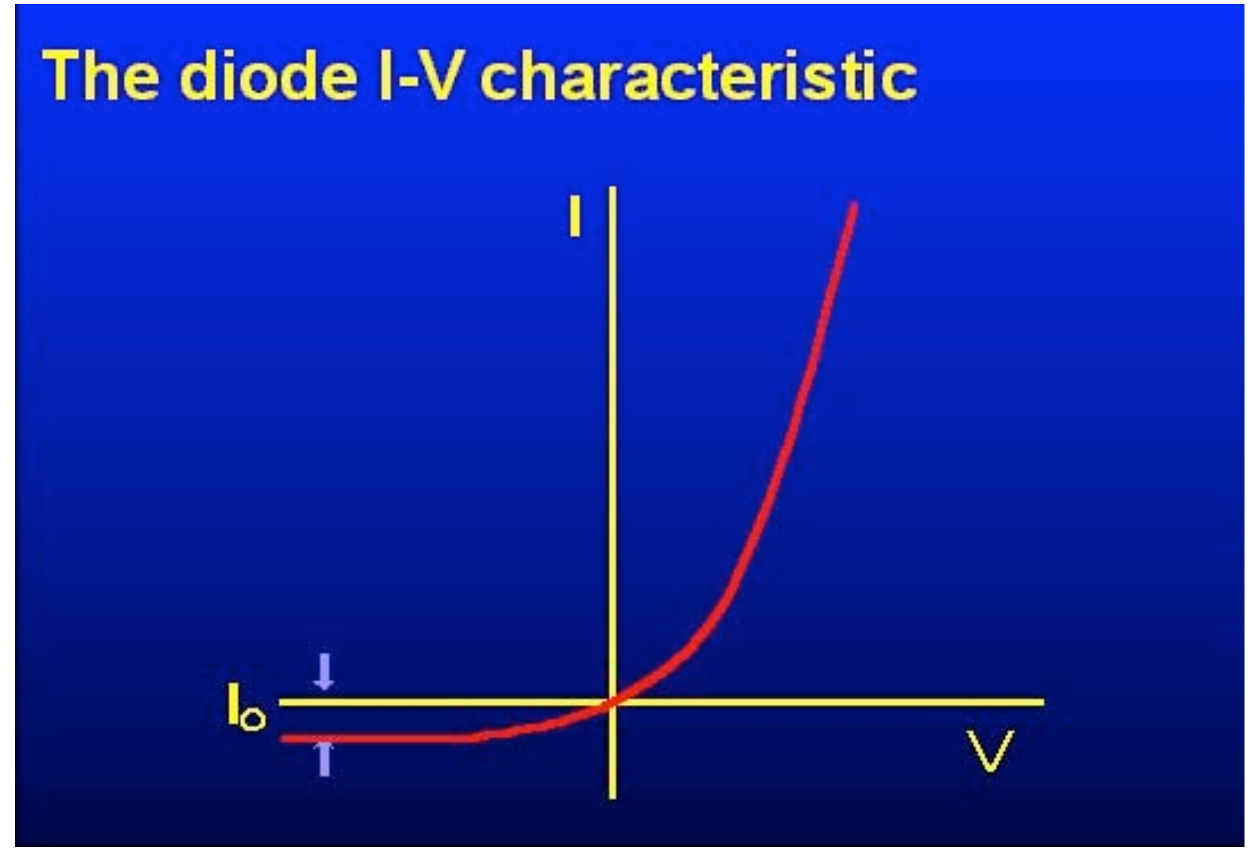
2006: Solar Cell Production Rate: 14 acres / day

2035: Required Solar Cell Production Rate: 14,000 acres / day

To survive, any new technology needs to:
- ACCELEREATE OVER THE Si-PRODUCTION
- REACH HIGHER EFFICIENCIES and/or LOWER INSTALLATION COSTS

PN Junction (brief review)





Equilibrium in a p-n junction is still "dynamic" and there are four kinds of currents contributing to the net zero flow of charge.

(1)Majority Hole Current. Diffusional current from hole movement from p to n (current from p to n).

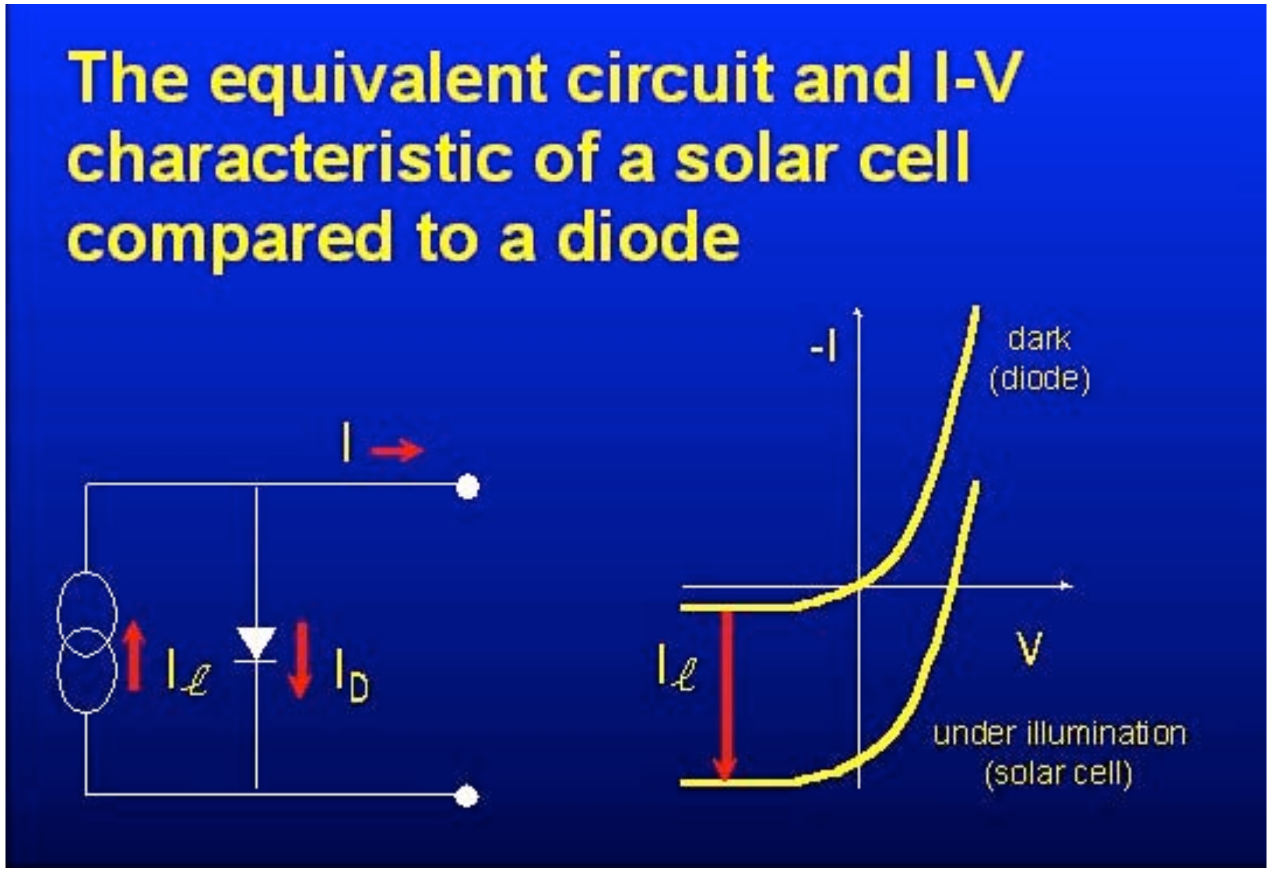
(2)Minority Hole Current. Drift current from holes moving from n to p, assisted by the electric field (current from n to p).

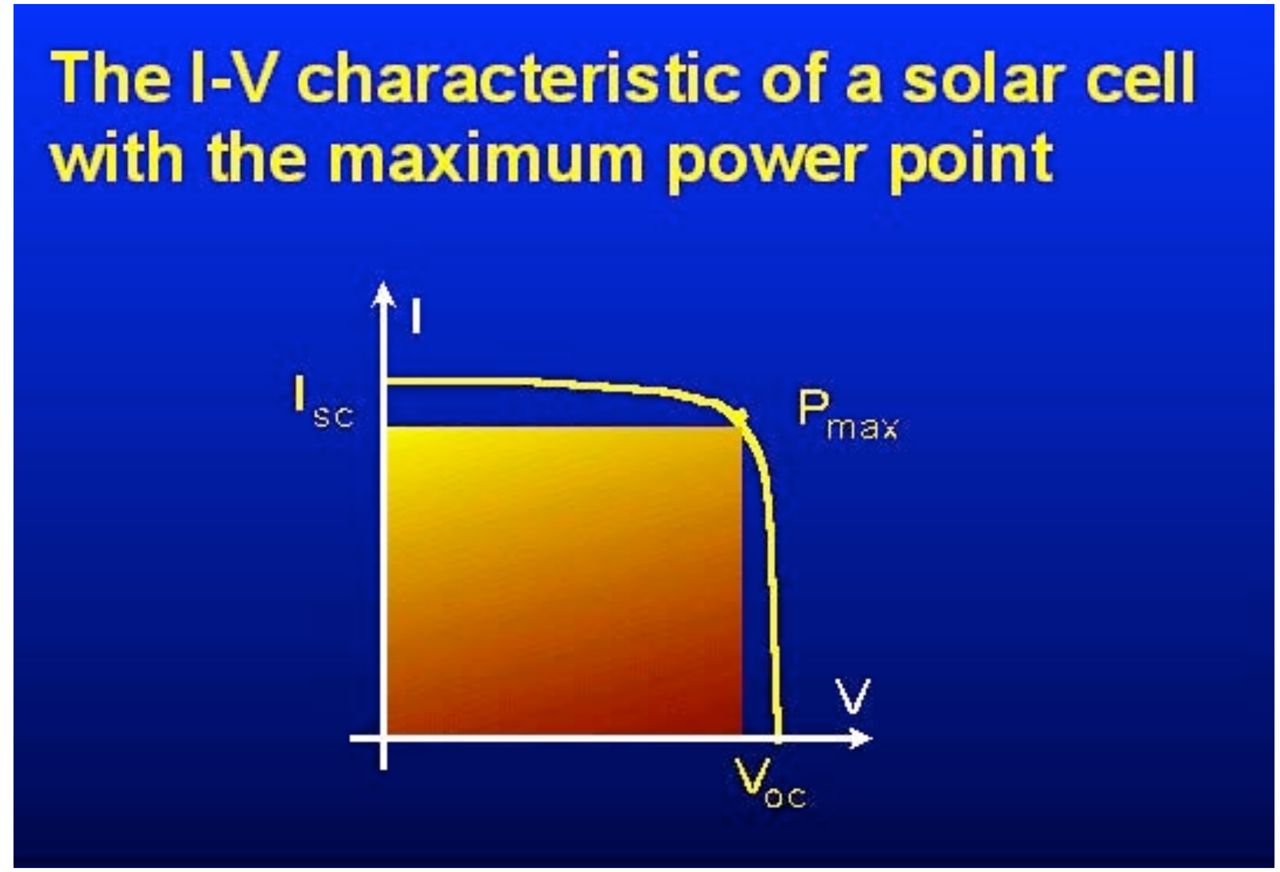
(3)Majority Electron Current. Electron diffusion from n to p from the high concentration gradient (current from p to n).

(4)Minority Electron Current. Electron drift from p to n, assisted by the electric field (current from n to p).

In reverse bias ($V < 0$), the current comes from minority carriers and is due to drift. In forward bias ($V > 0$), the current arises from majority carriers and is due to diffusion.

PN Junction (brief review)





The presence of light induces a net positive change in the generation–recombination rate. Roughly speaking, for each type of current, the effect of light is:

(1)Majority Hole Current. Relatively unaffected, if generation occurs evenly on both sides.

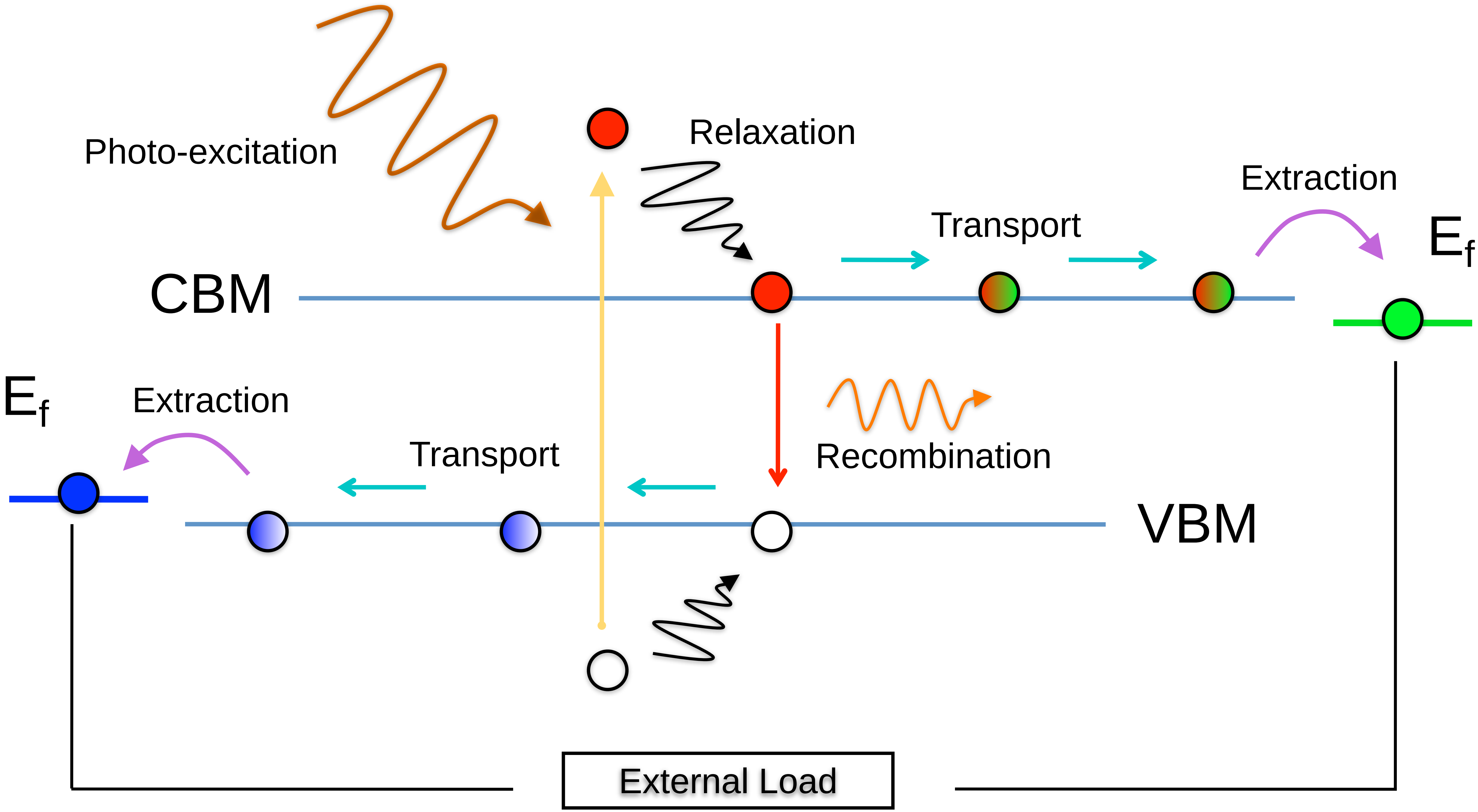
(2)Minority Hole Current. Increased, due to the additional carriers now present. The additional carriers resulting from illumination are immediately transferred across the junction in the form of a drift current.

(3)Majority Electron Current. Relatively unaffected.

(4)Minority Electron Current. Increased, due to the additional carriers now present.

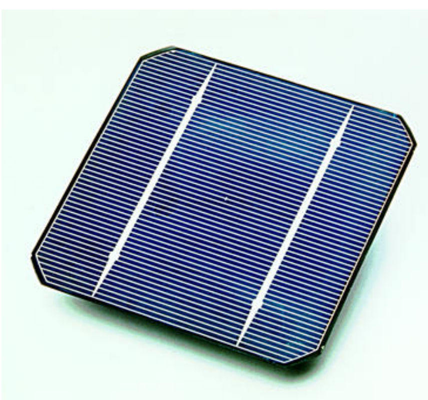
Effectively, under illumination, the IV characteristic of the PN junction is shifted downwards, by an amount that is directly determined from the photocurrent incident upon the junction.

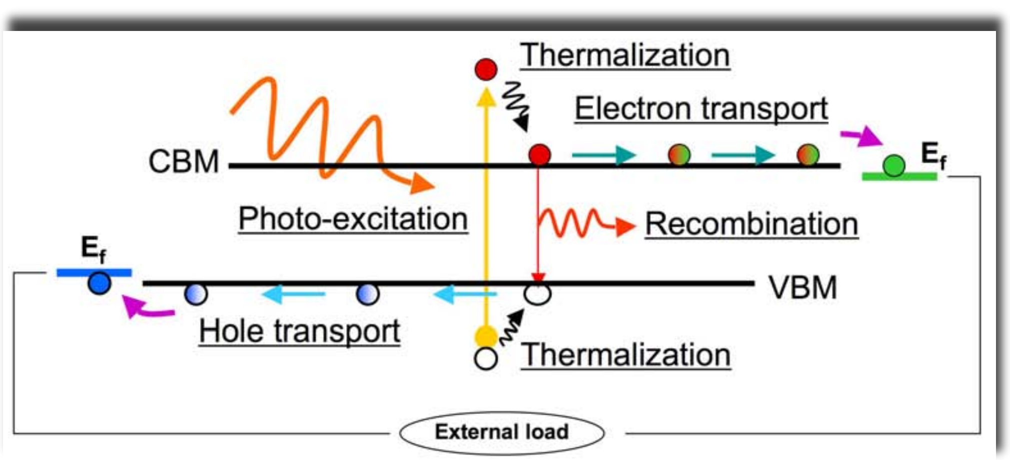
Fundamental Processes Involved in Solar Photovoltaics: Electron's View



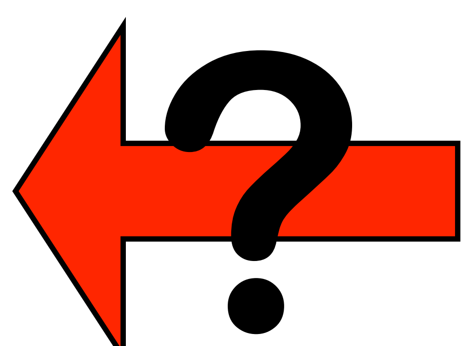
The Role of Computational Quantum Mechanics

- What do we know how to compute?
- How does it help for solar PV?





?
electrical properties

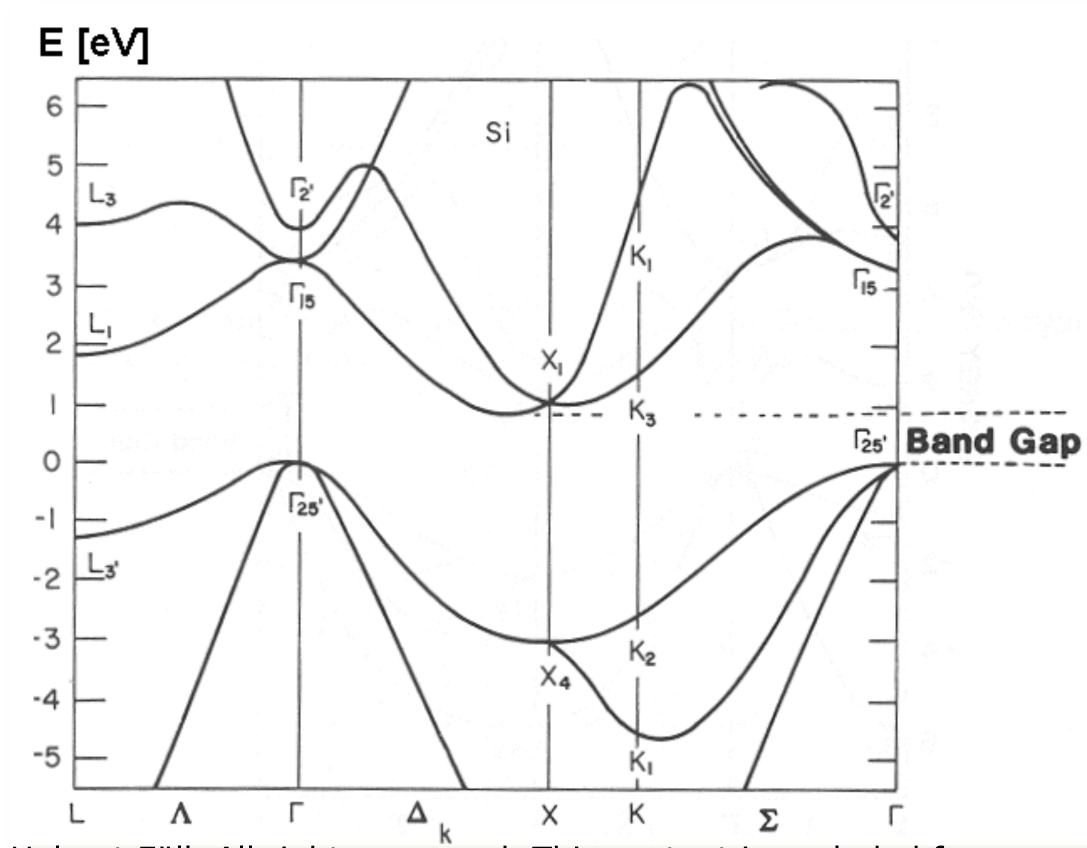


?
mechanical properties

?
optical properties

Crystalline Silicon Solar PV (80% of current market)

- Light Absorption
  - Band Gap
  - Band Structure



- Electron/Hole Transport
  - Electron/Hole Mobilities

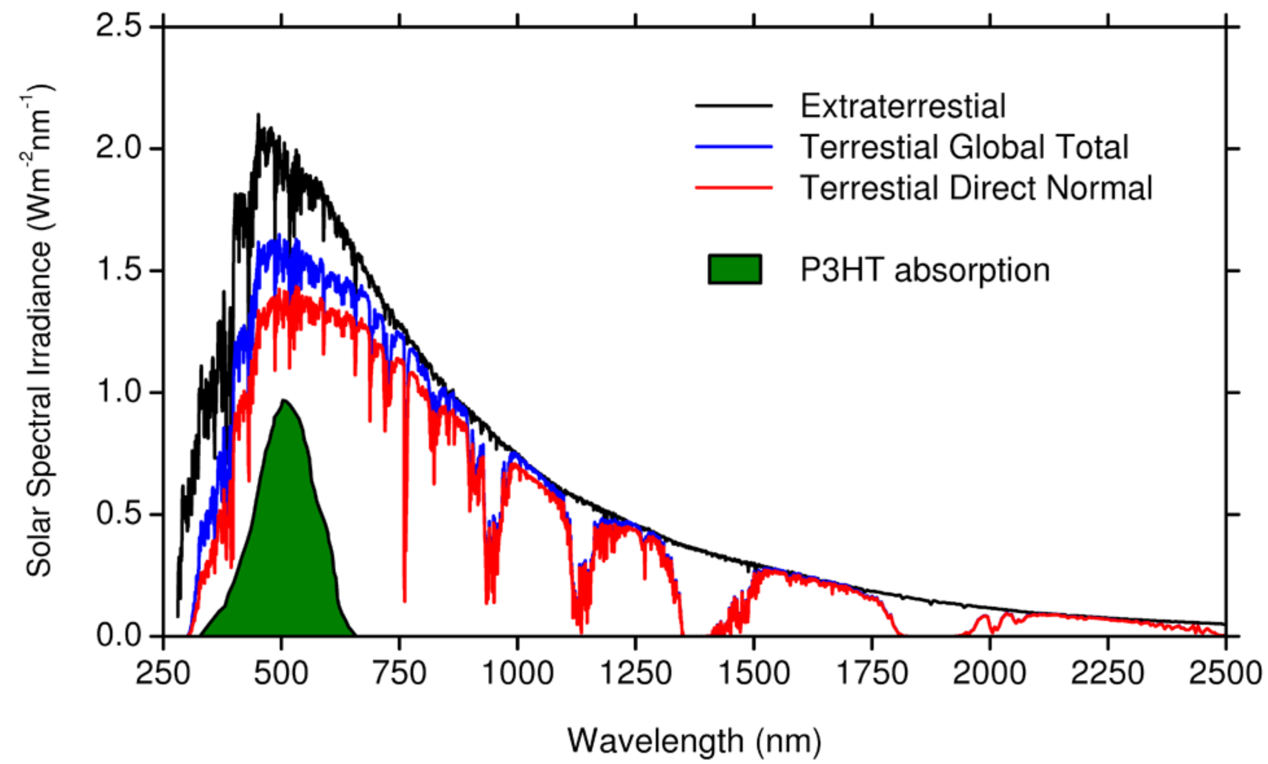
$$\sigma = e^2\tau \int \frac{d\mathbf{k}}{4\pi^3} \left(-\frac{\partial f}{\partial E}\right) \mathbf{v}(\mathbf{k})\mathbf{v}(\mathbf{k})$$

Amorphous Silicon Solar PV (3% of current market)

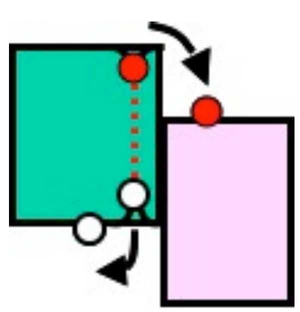
- Light Absorption (is actually pretty good)
- Electron-Hole Separation (also not a problem)
- Electron/Hole Transport (Holes are Slow!)
  - Hole Mobilities
  - Hole Traps: from total energy differences ($E_{neutral}$-$E_{charged}$)

Organic Solar PV

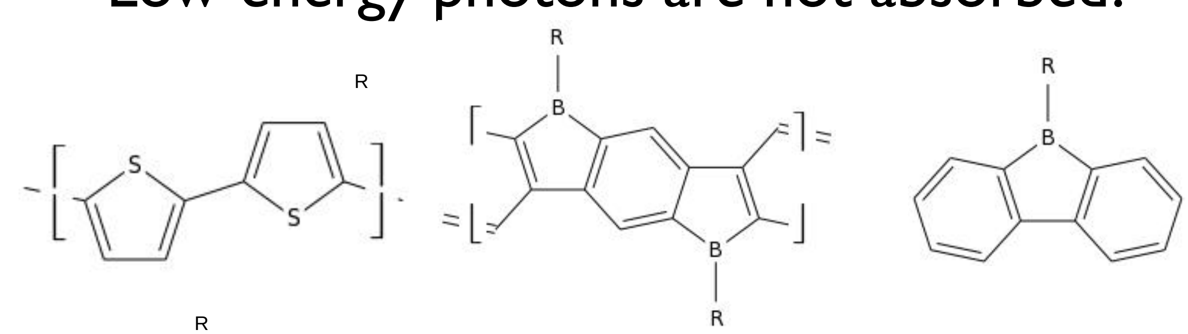
- Light Absorption (need to capture more of the solar spectrum)
  - Band gap



- Electron-Hole Separation
  - Orbital energies

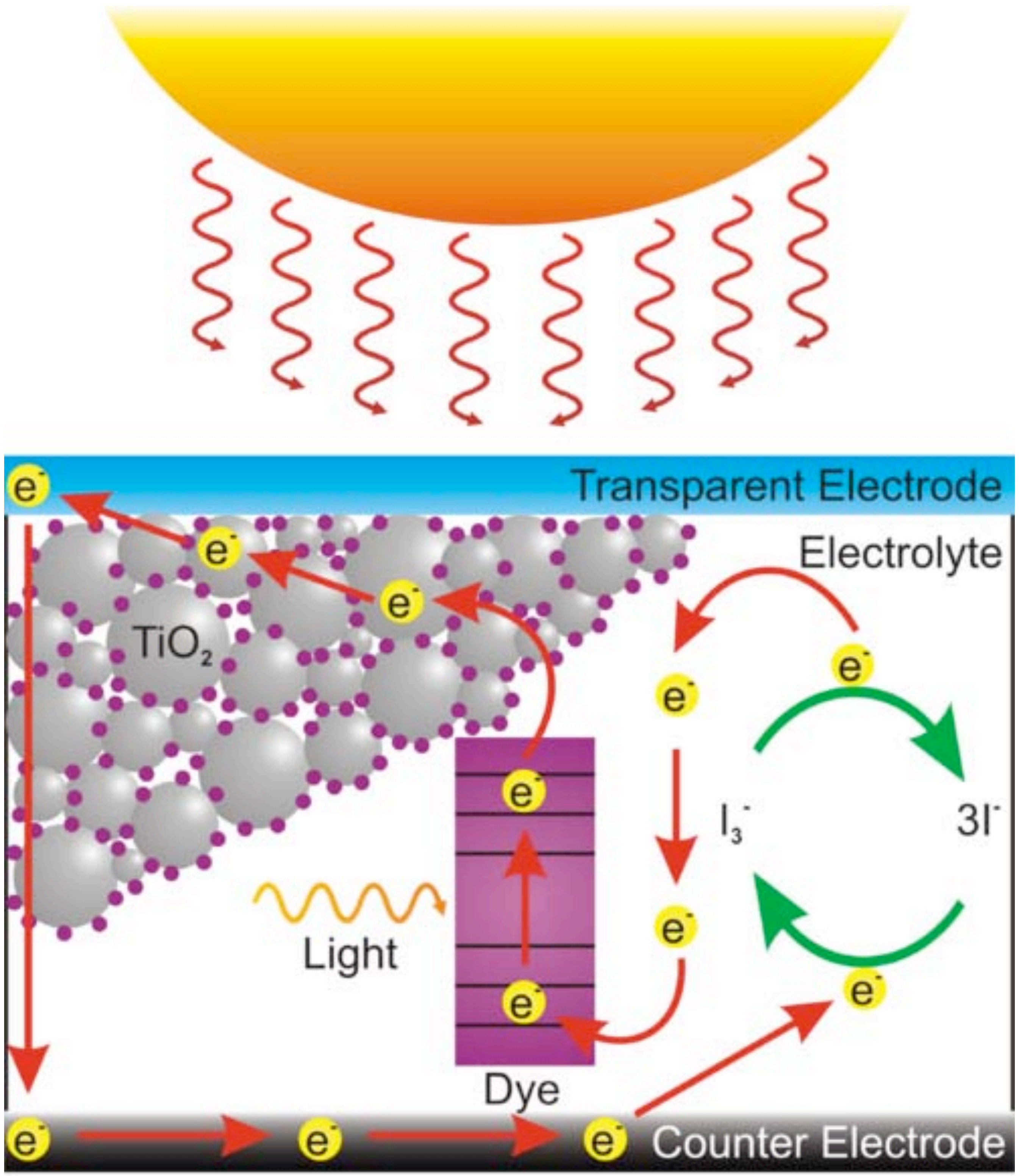


Poly(3-hexylthiophene) (P3HT): $E_{g,exp}$ = 2.1 eV
Low-energy photons are not absorbed!



Egap = Eo   Egap = 0.55Eo   Egap = 1.1Eo

Dye Sensitized Solar PV



www.energyer.com

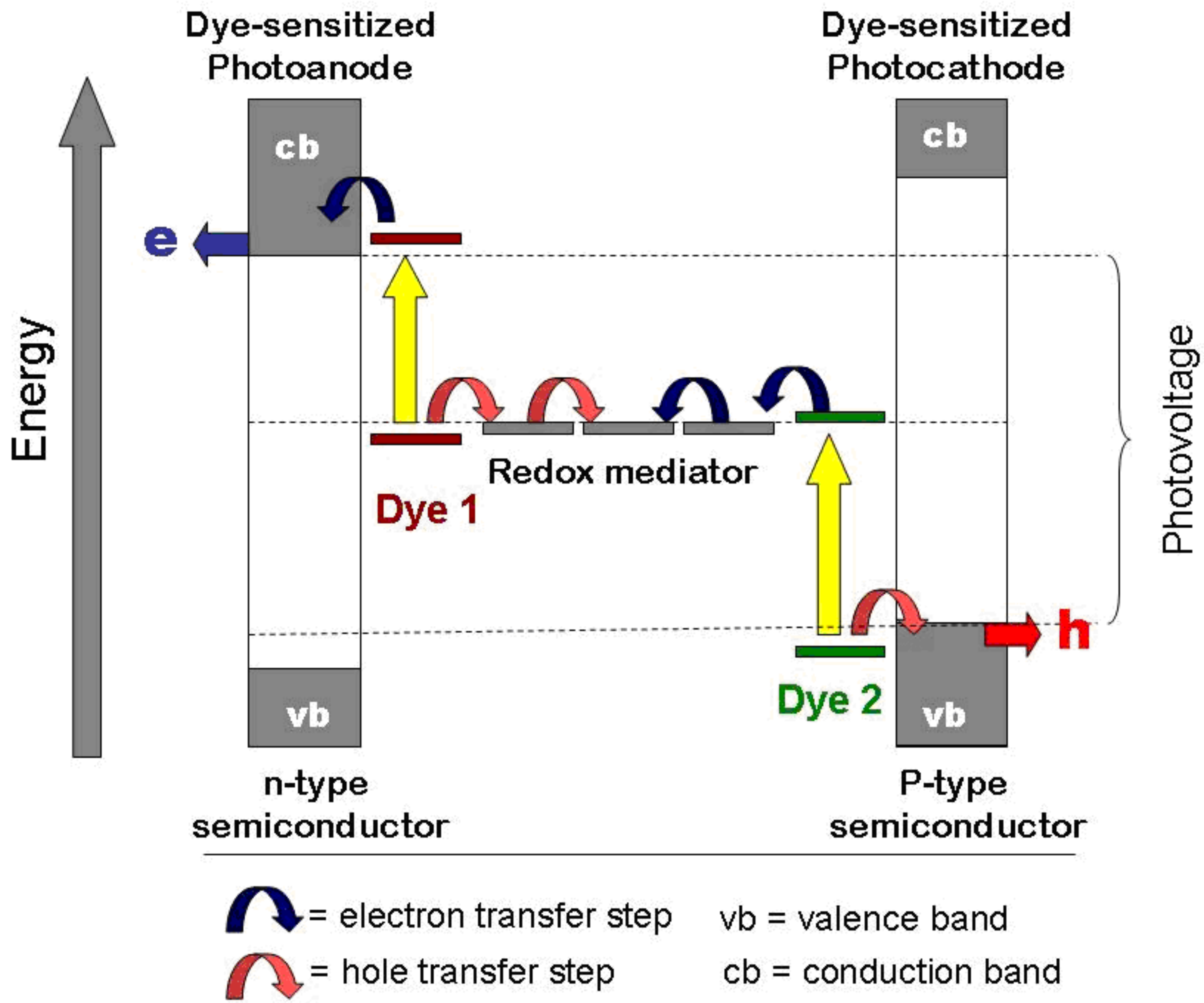
Image in the public domain. Via M. R. Jones on Wikimedia Commons.

Gratzel and O'Regan
(Nature, 1991)

Made up of 3 active materials:

- Dye absorbs light.
- TiO_2 nanoparticles with very large surface area take electron.
- Liquid electrolyte delivers new electron from cathode to dye.

Dye Sensitized Solar PV



- Biggest problem is a liquid electrolyte.
- Relative energy levels of TiO2 and dye also key.

Summary

- Energy is a Major Global Challenge
- The Sun has a Lot of it For Free but it's Too Expensive to Utilize
- Computational Quantum Mechanics can Help us Understand and Predict PV New Materials

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