1.021, 3.021, 10.333, 22.00 : Introduction to Modeling and Simulation : Spring 2011

Part II – Quantum Mechanical Methods : Lecture 8

Applications in Energy: Introduction and Solar PV

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“The purpose of computing is insight, not numbers.”

— Richard Hamming

“What are the most important problems in your field? Are you working on one of them? Why not?”

“It is better to solve the right problem the wrong way than to solve the wrong problem the right way.”

“In research, if you know what you are doing, then you shouldn't be doing it.”

“Machines should work. People should think.”

...and related: “With great power comes great responsibility.” (Spiderman’s Uncle)

Part II Outline

theory & practice

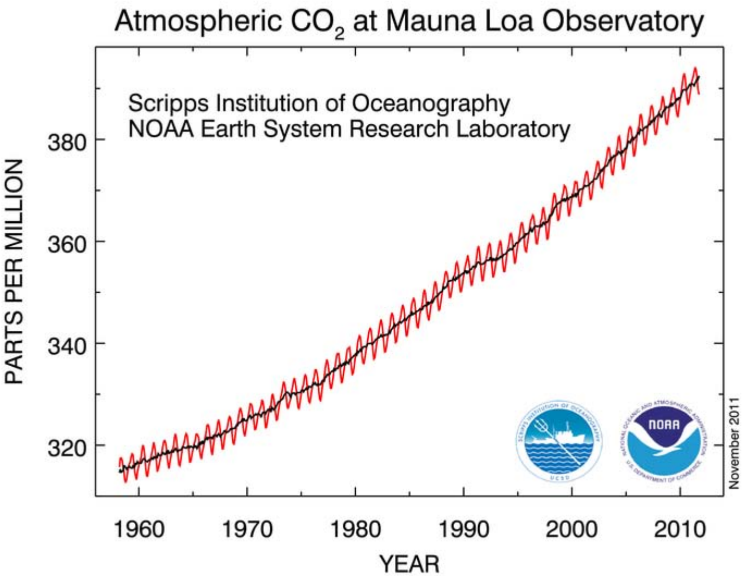
1. It's A Quantum World: The Theory of Quantum Mechanics
2. Quantum Mechanics: Practice Makes Perfect
3. From Many-Body to Single-Particle; Quantum Modeling of Molecules
4. From Atoms to Solids
5. Quantum Modeling of Solids: Basic Properties
6. More on Band Structures and Modeling of Solids
7. Advanced Prop. of Materials: What else can we do?'

example applications

8. Solar Photovoltaics: Converting Photons into Electrons
9. Solar Fuels: Pushing Electrons up a Hill
10. Hydrogen Storage: the Strength of Weak Interactions
11. A bit of review for the quiz
12. Summary, concluding remarks, and free PIZZA!

Cost of Inaction?

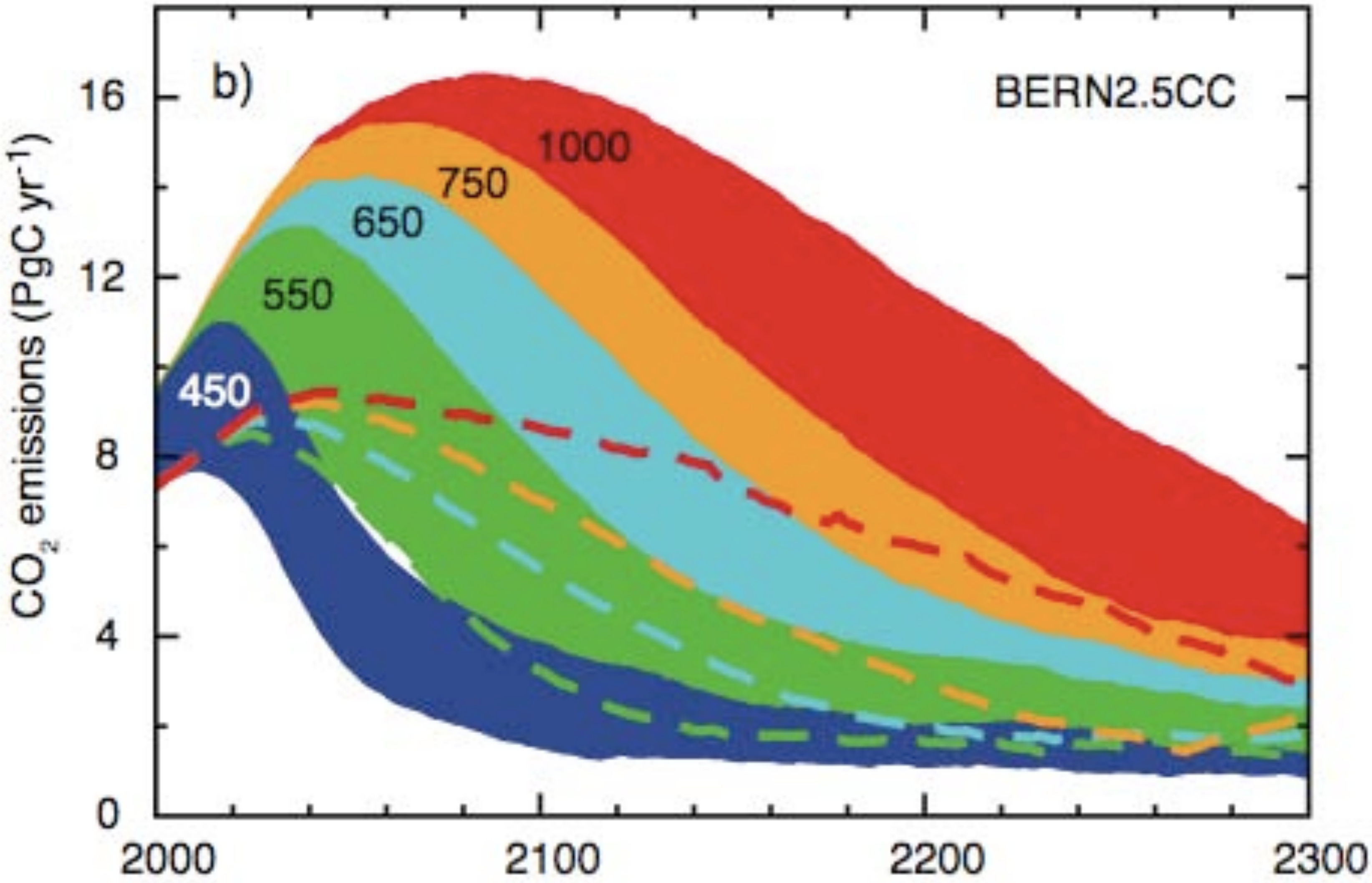
Grinell Glacier and Grinnell Lake, Glacier National Park, 1910-1997



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

Photos by Fred Kiser, Glacier National Park Archives, and Daniel Fagre, USGS.

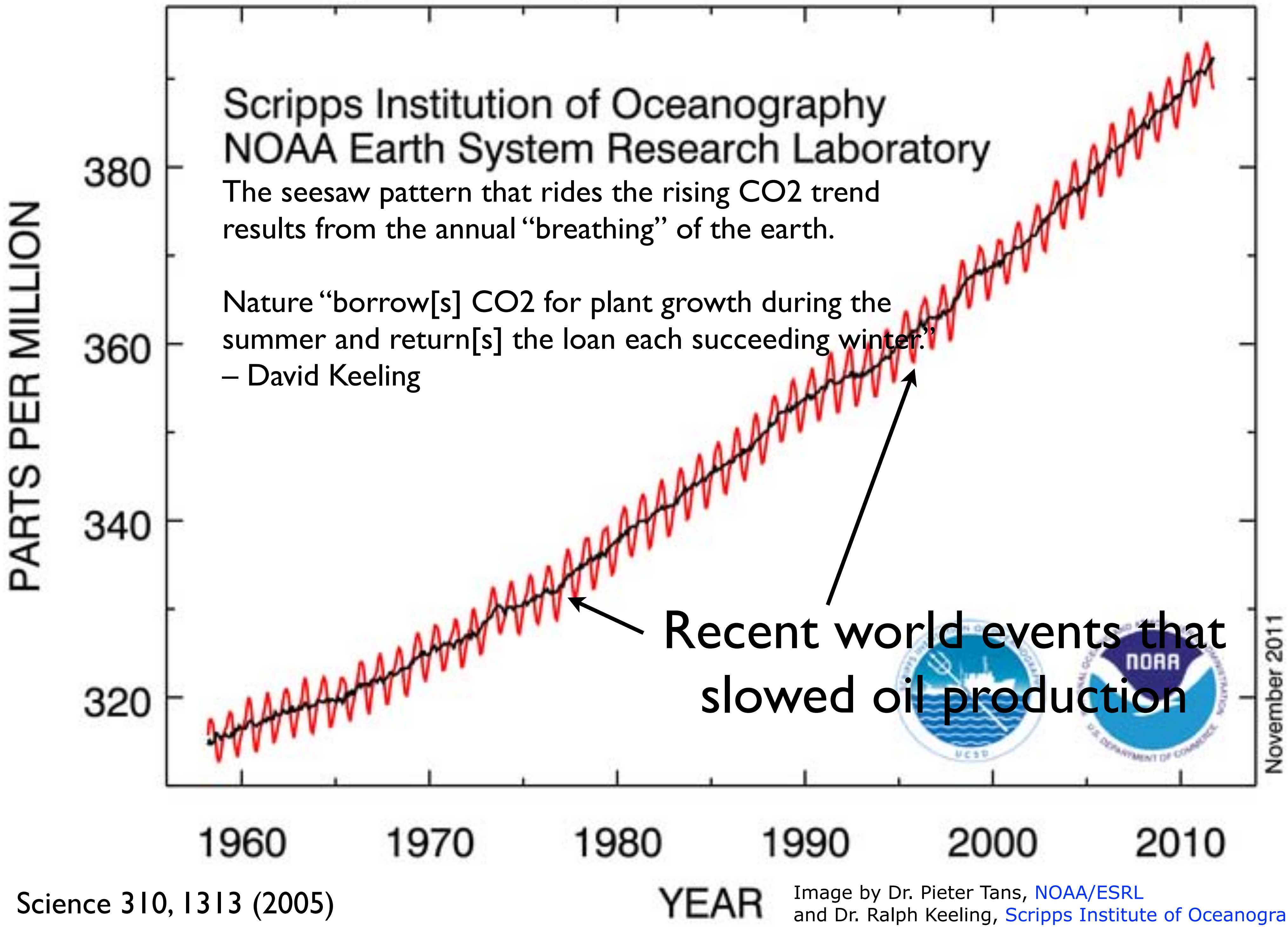
CO_2 Projections



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.

Atmospheric CO_2 at Mauna Loa Observatory

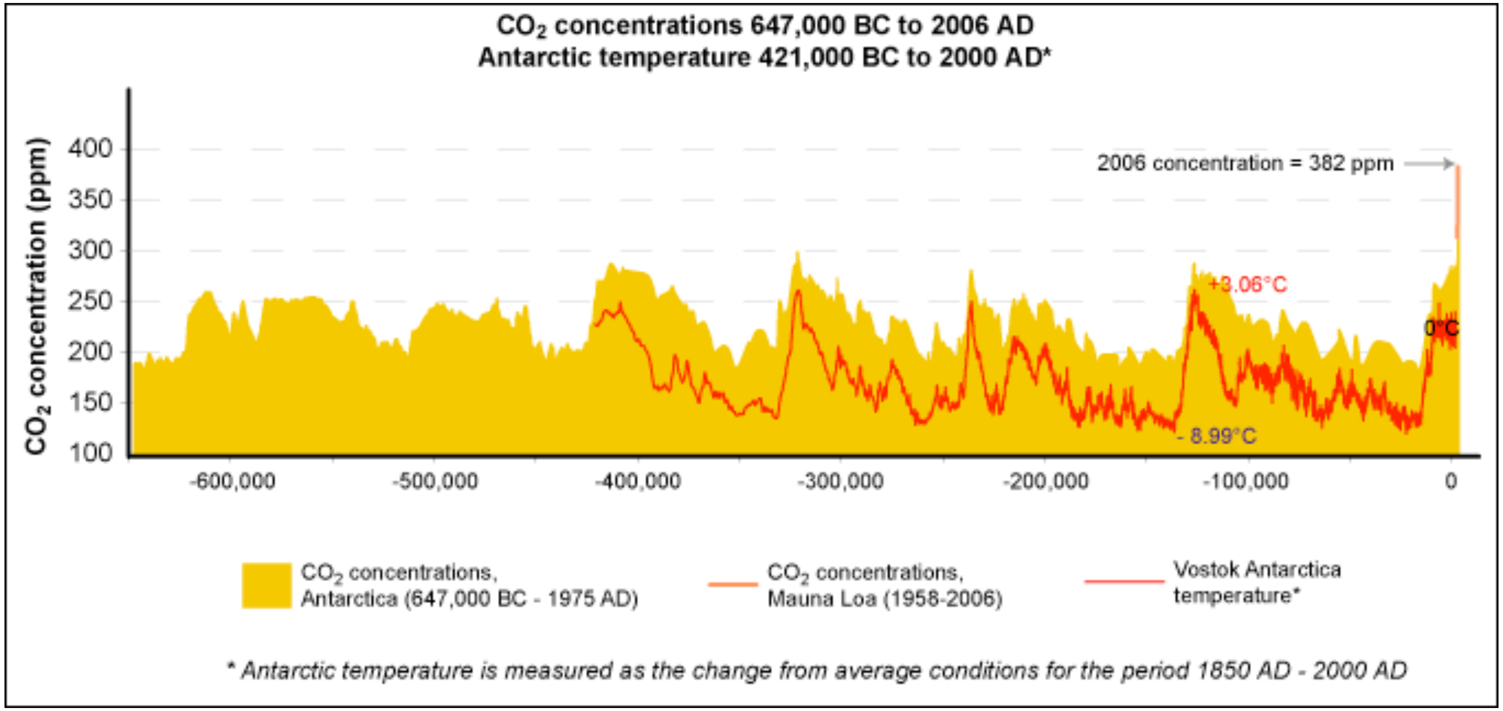


Science 310, 1313 (2005)

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

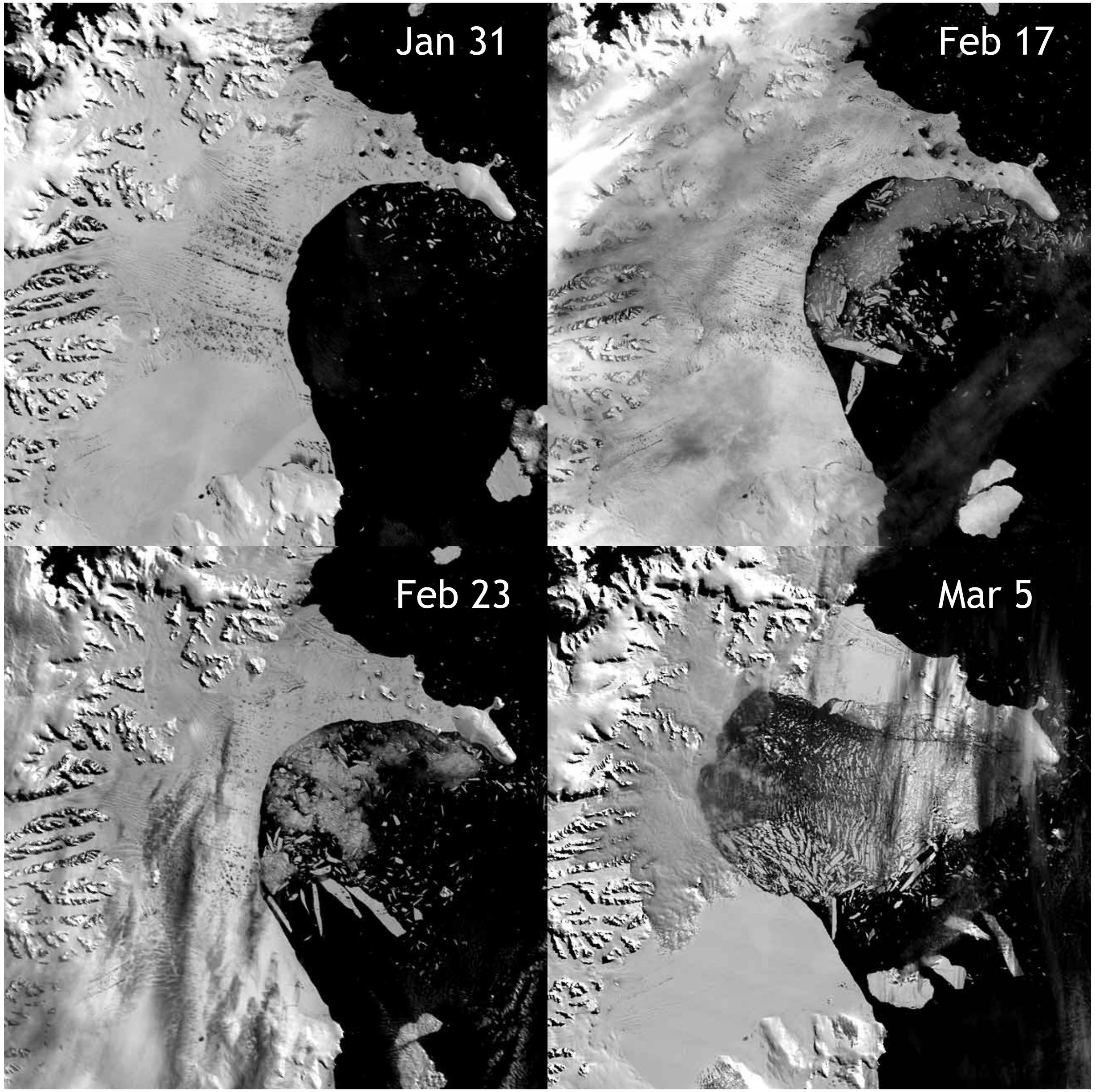
Temperature inferred from isotope ratios in the Vostok ice core

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



Images by U.S. Environmental Protection Agency.

Warming is Real and Has Real Effects



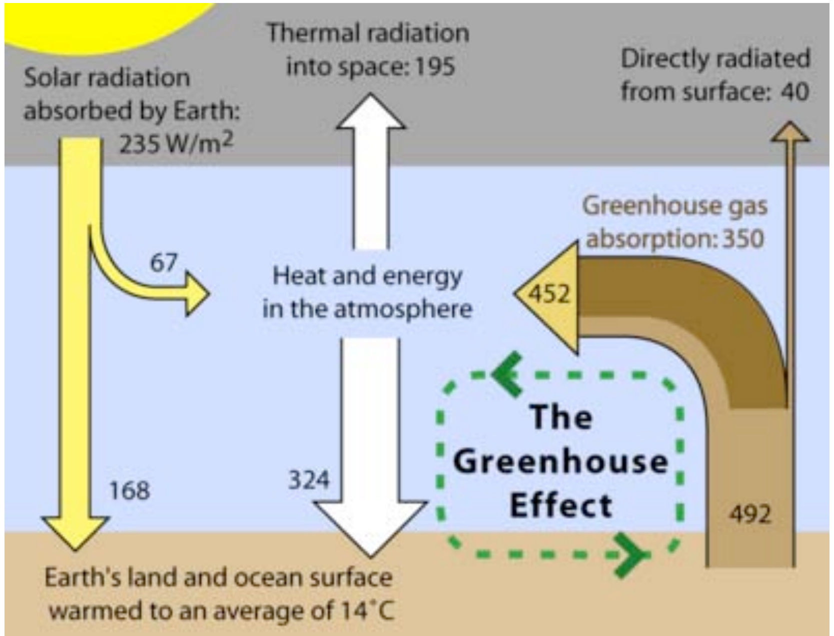
Images by NASA/Goddard Space Flight Center and
National Snow and Ice Data Center, University of Colorado-Boulder.

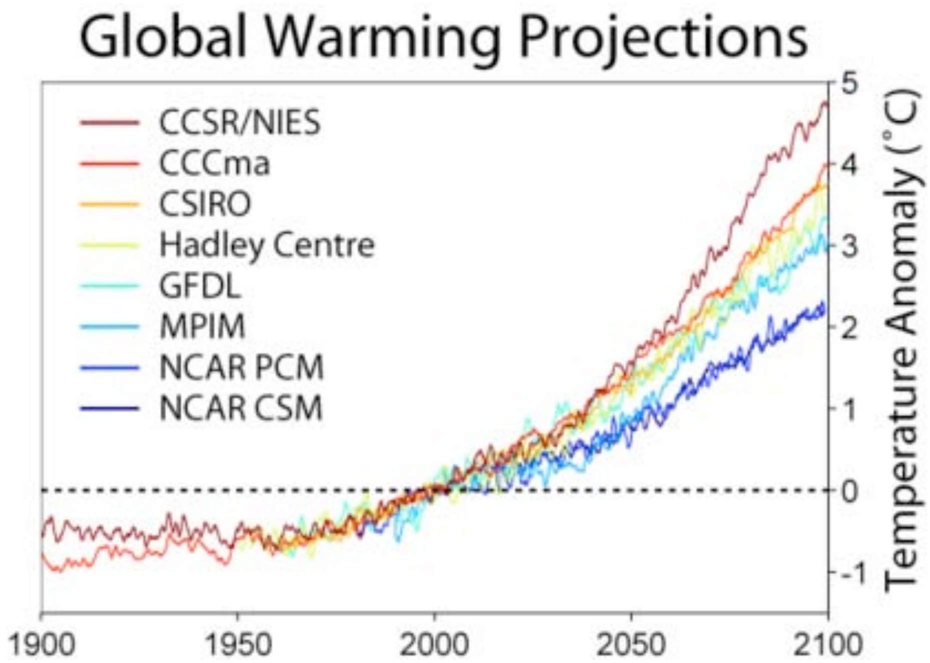
Between Jan 31, 2002 and March 5, 2002 a chunk of the Larsen B ice shelf the size of Rhode Island disintegrated.

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

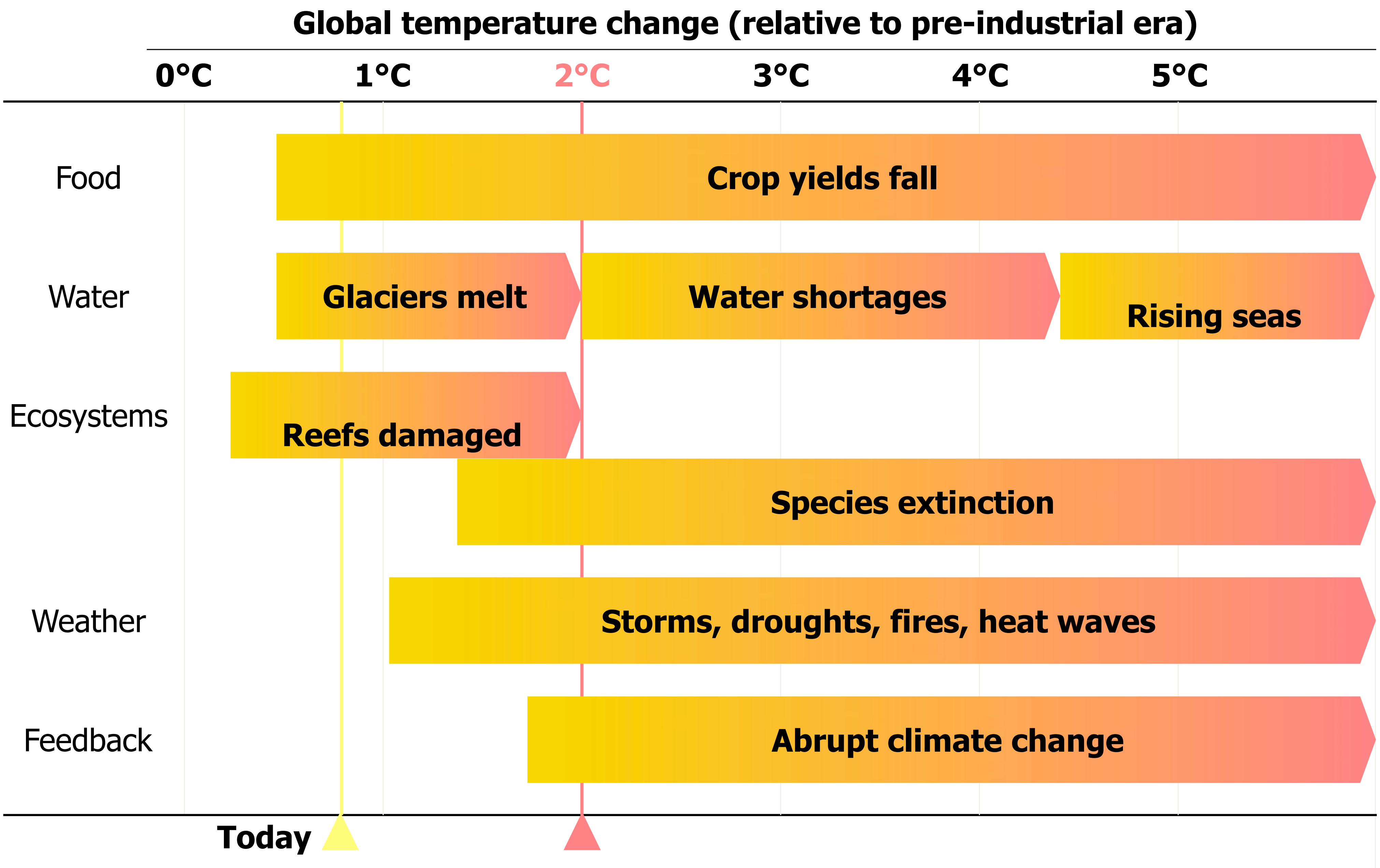

Thermal radiation into space: 195
Solar radiation absorbed by Earth: 235 W/m2
Directly radiated from surface: 40
Greenhouse gas absorption: 350
67
Heat and energy in the atmosphere
452
The Greenhouse Effect
168
324
492
Earth's land and ocean surface warmed to an average of 14˚C


Global Warming Projections
CCSR/NIES
CCCma
CSIRO
Hadley Centre
GFDL
MPIM
NCAR PCM
NCAR CSM
Temperature Anomaly (˚C)
5
4
3
2
1
0
-1
1900
1950
2000
2050
2100

"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, Candidate for Massachusetts Governor

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



It's Not *Only* About Warming: Abundance of Affordable Energy Resources Can Uplift the World

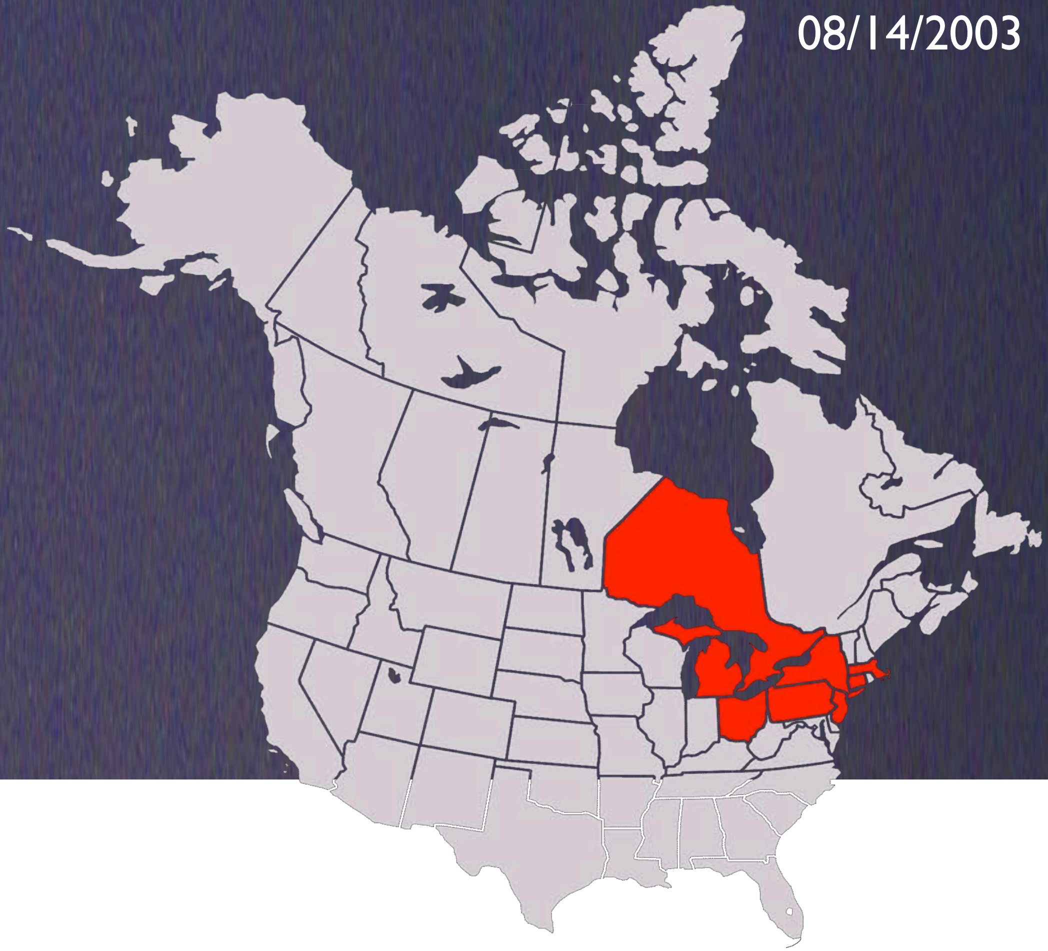
Image removed due to copyright restrictions. Please see Benka, Stephen G. "The Energy Challenge." *Physics Today* 55 (April 2002): 38-9.

HUMAN WELL-BEING INCREASES WITH INCREASED PER-CAPITA ENERGY USE

It's Not *Only* About Warming: Abundance of Affordable Energy Resources Can Uplift the World

North American Electrical Blackout

08/14/2003



… August 15 …
just 24 hours into blackout
Air Pollution was Reduced

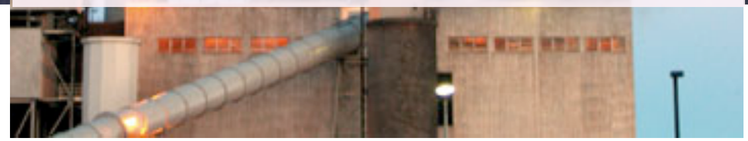
SO_2 >90%

O_3 ~50%

Light Scattering Particles ~70%

"This clean air benefit was realized over much of eastern U.S."

Marufu et al., Geophysical Research Letters 2004



Courtesy: Vladimir Bulovic

by 4:13 pm 256 power plants were off-line

Map of the World Scaled to Energy Consumption by Country

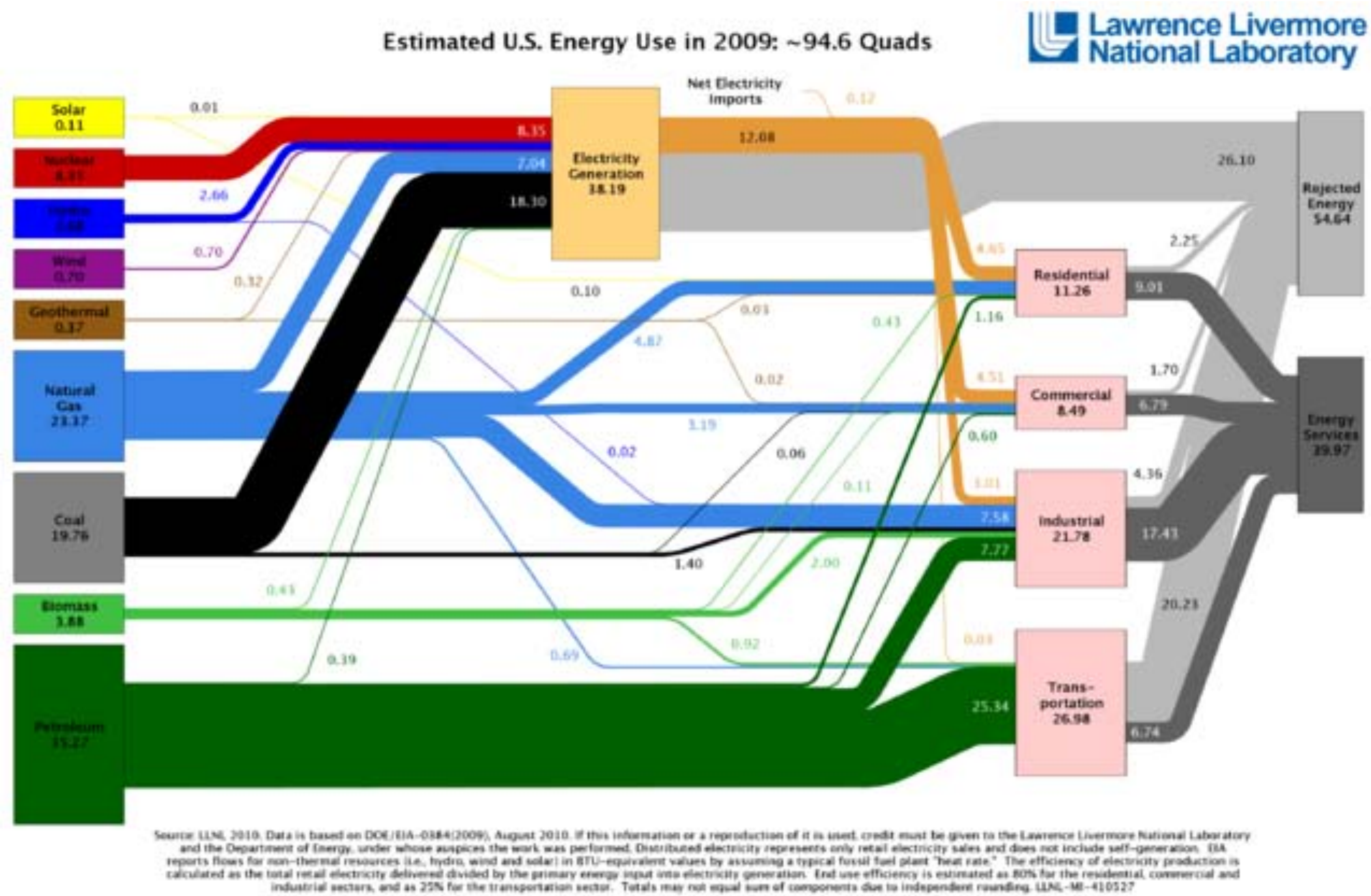
- In 2002 the world burned energy at a rate of 13.5 TW
- How fast will we burn energy in 2050?
- (assume 9 billion people)
- If we use energy like in U.S. we will need 102 TW
- Conservative estimate: 28~35 TW

Energy use estimates from Nocera, Daedalus 2006 & Lewis and Nocera, PNAS 2006

Image by Mark E. J. Newman.

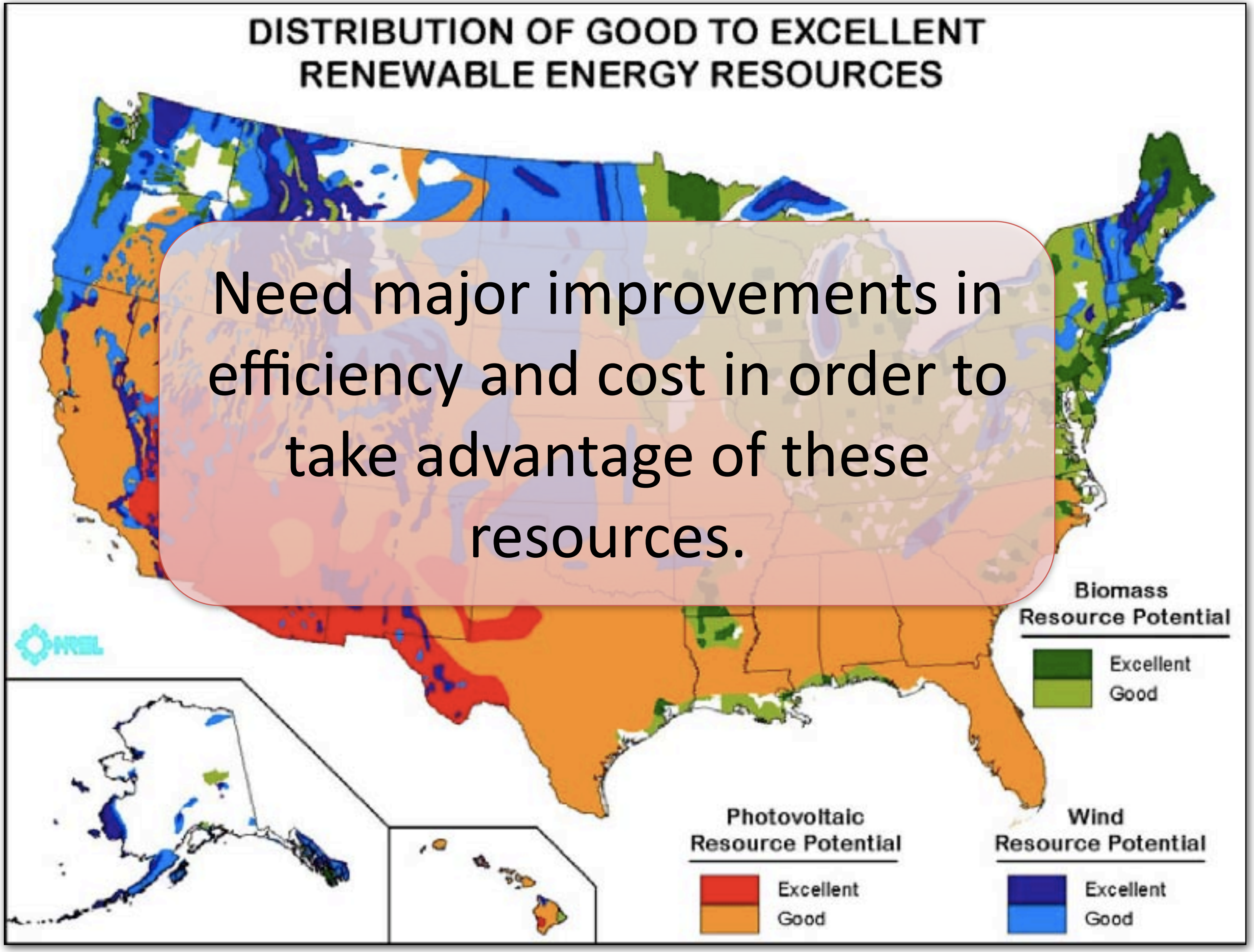
U.S. Energy Consumption

Goal: consume half of our electricity through renewable sources by the year 2050.



Public domain image.

U.S. Resources



Need major improvements in efficiency and cost in order to take advantage of these resources.

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

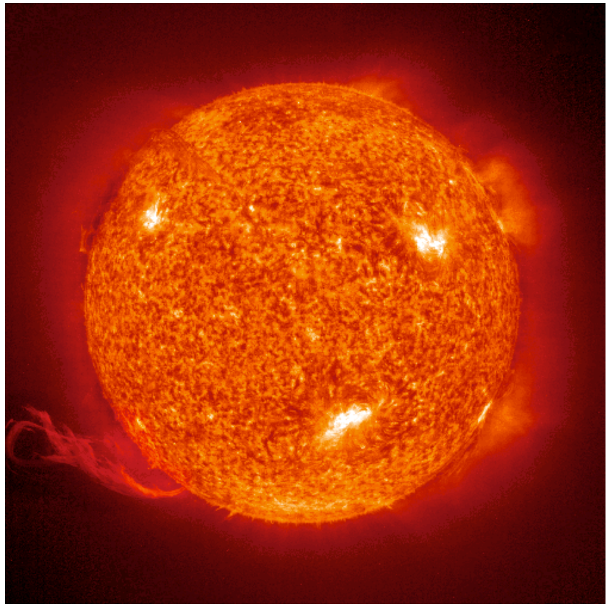


Image by NASA/Goddard Space Flight Center.

Solar Across Scales

Moscone Center: 675,000 W

Residential home: 2400 W

Photos by Mark H. Anbinder on Flickr, Pujanak on Wikimedia Commons.

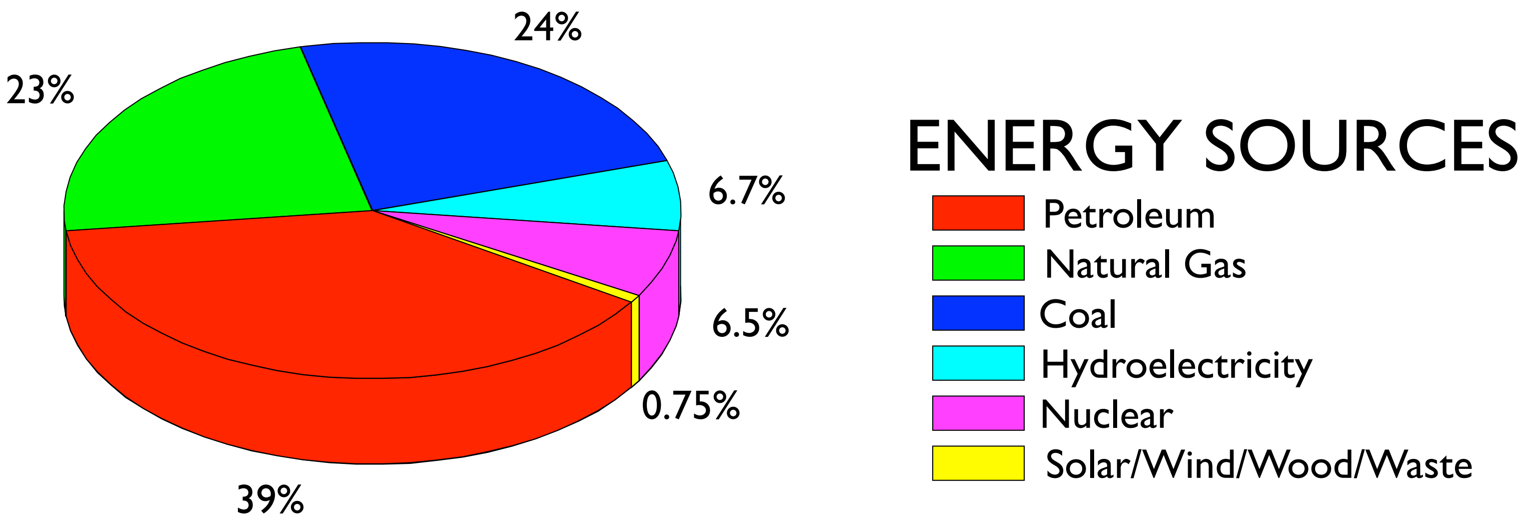
Kenyan PV market:

Average system: 18W

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)

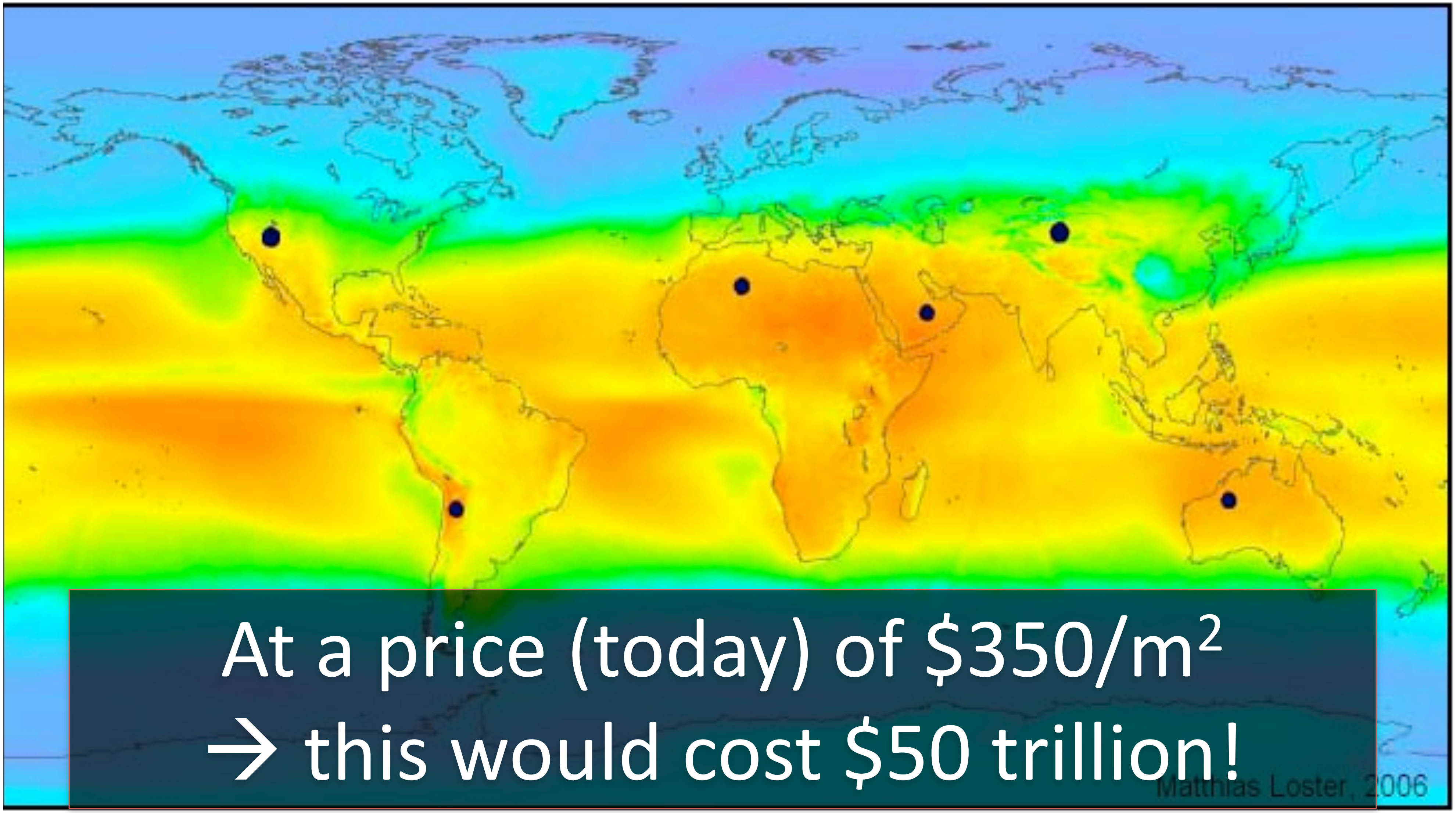
Solar Land Area Requirements

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

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

Image from National Atlas of the United States,
U.S. Geological Survey/Department of the Interior.

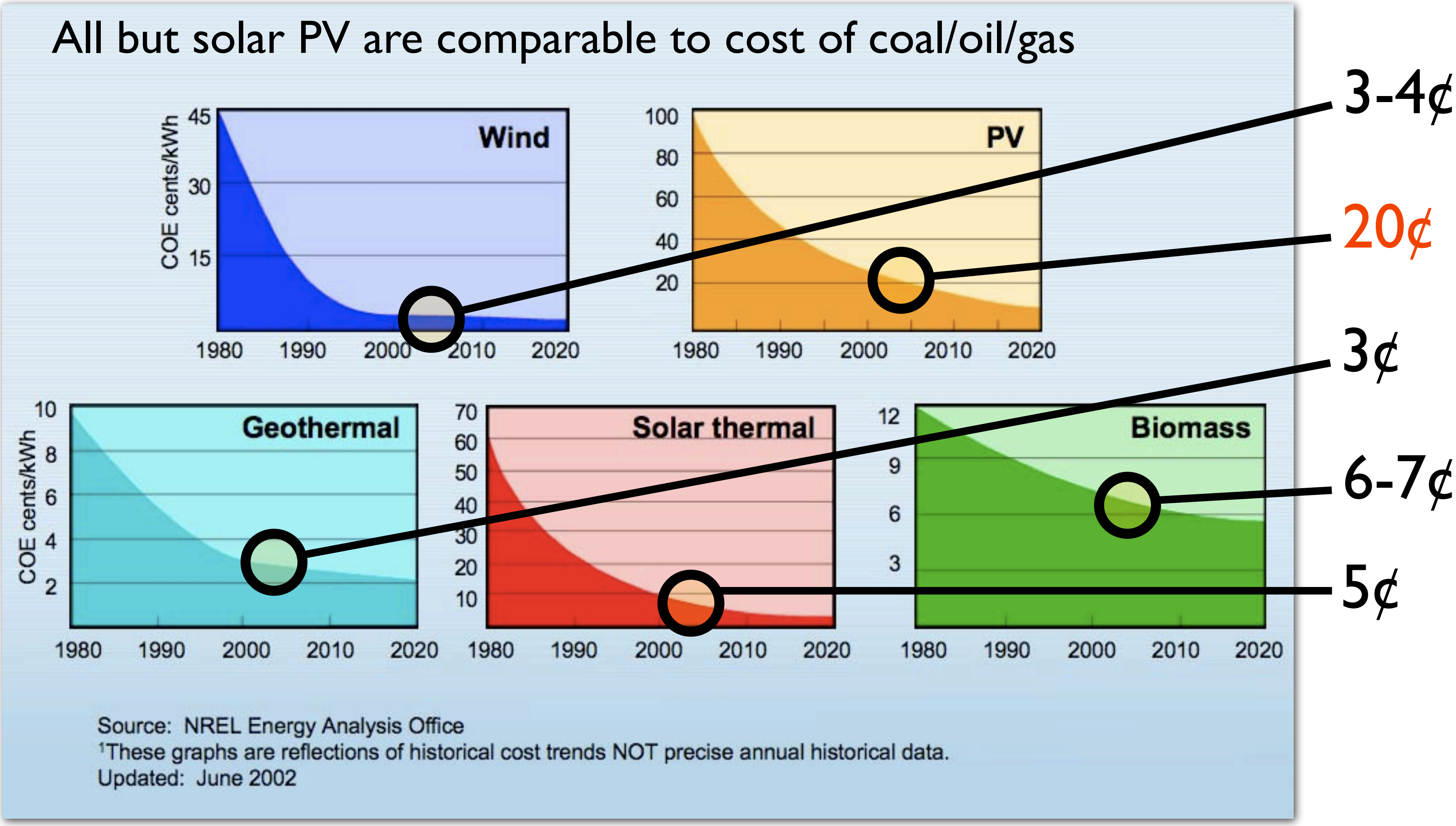
Solar Land Area Requirements for ~20TW



At a price (today) of $\$350/m^2$

→ this would cost \$50 trillion!

A Challenge with Solar PV

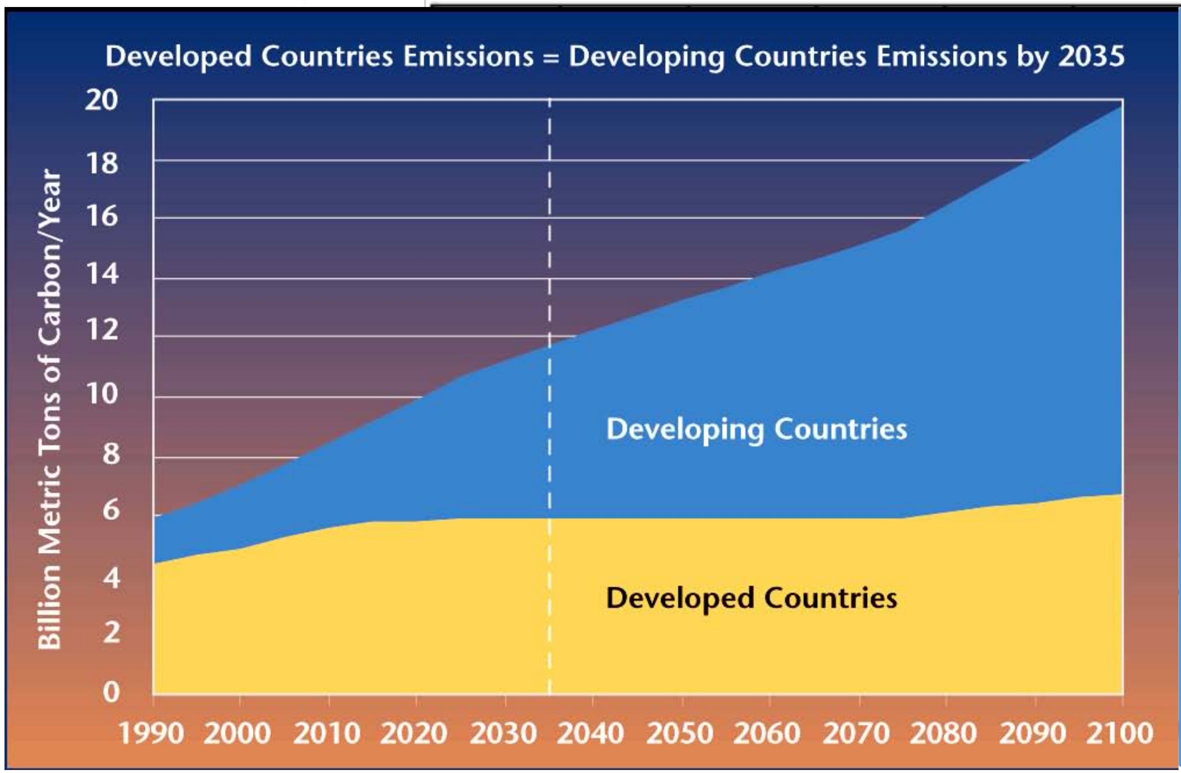


Solar PV: Grid Parity

Please see Exhibit 1 from Lorenz, P., D. Pinner, and T. Seitz. "The Economics of Solar Power." *Energy, Resources, Materials*: McKinsey & Company, June 2008.

Source: Mckinsey

Aim: capture 10% of electrical generation with PV



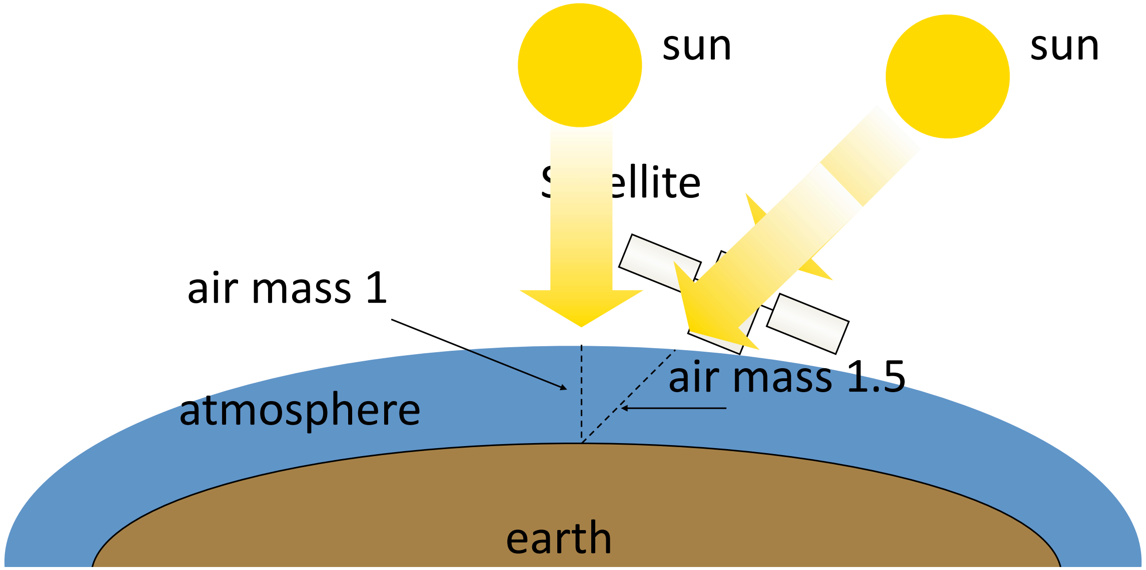
Side note: replacing fossil fuels in the developing world will become much more important in the near future.

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?



<u>Solar spectrum outside atmosphere:</u>

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

<u>At earth's surface:</u>

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

Solar PV technology landscape (2015)

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

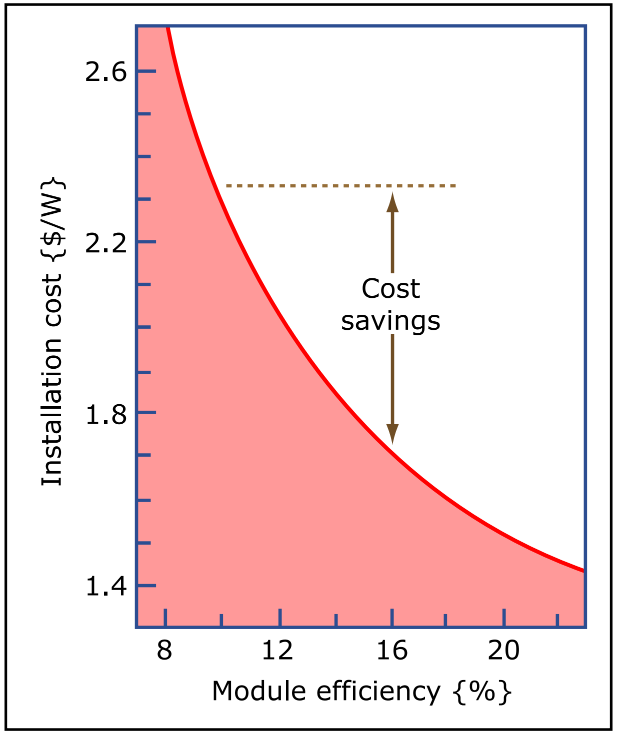
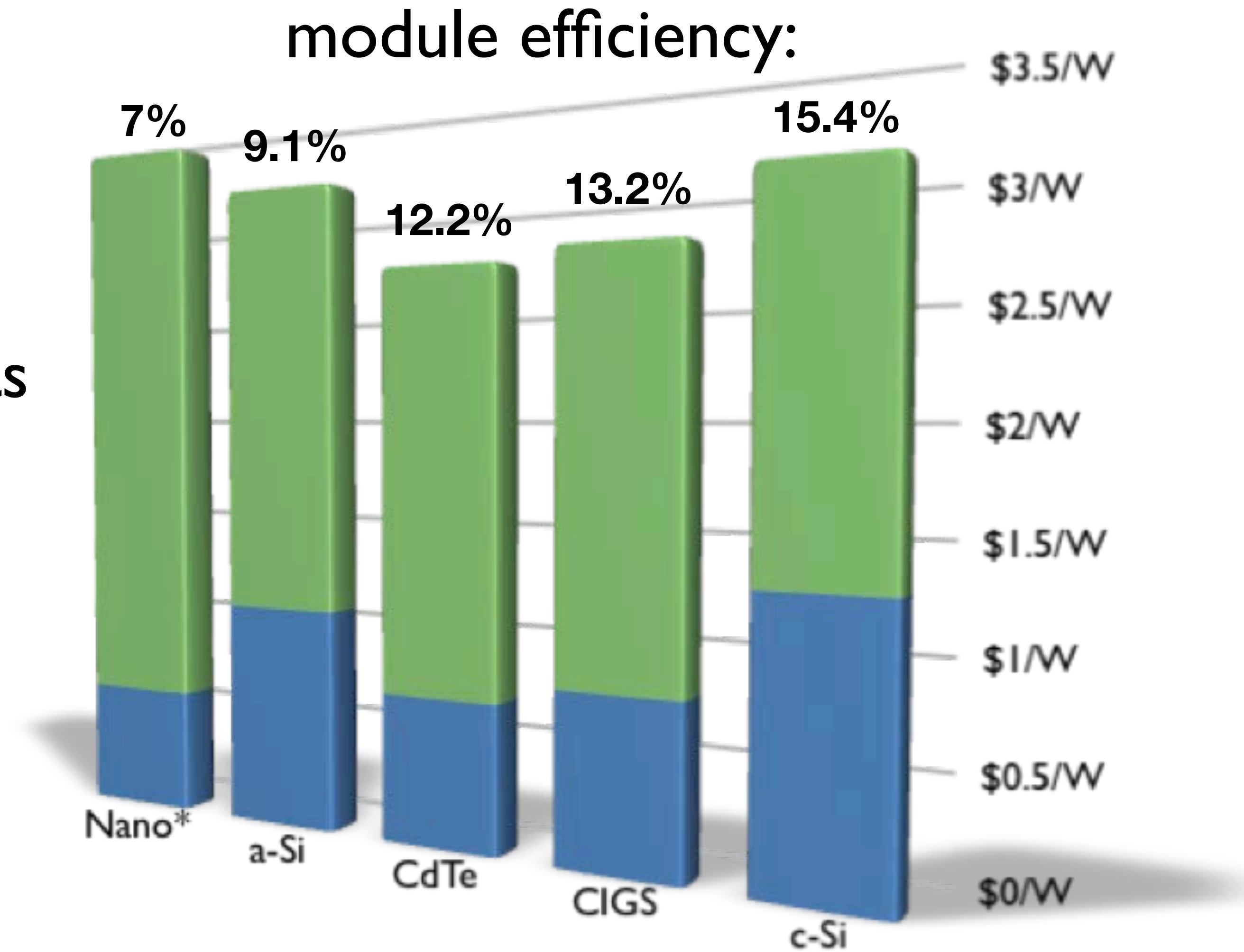


Image by MIT OpenCourseWare.



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

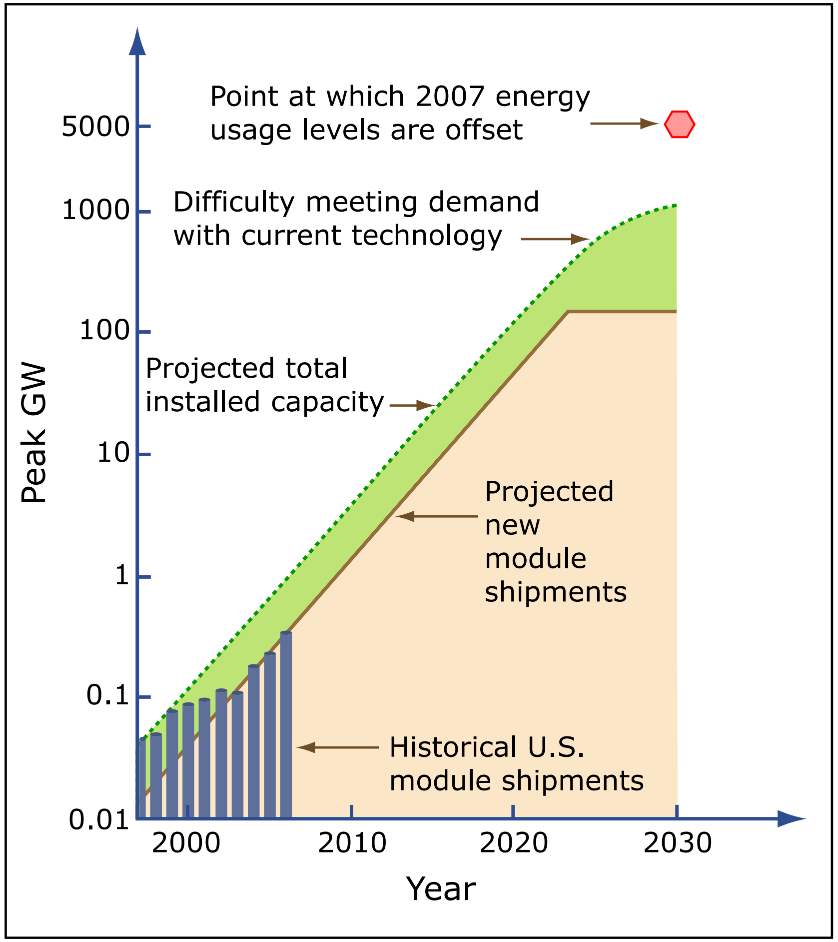
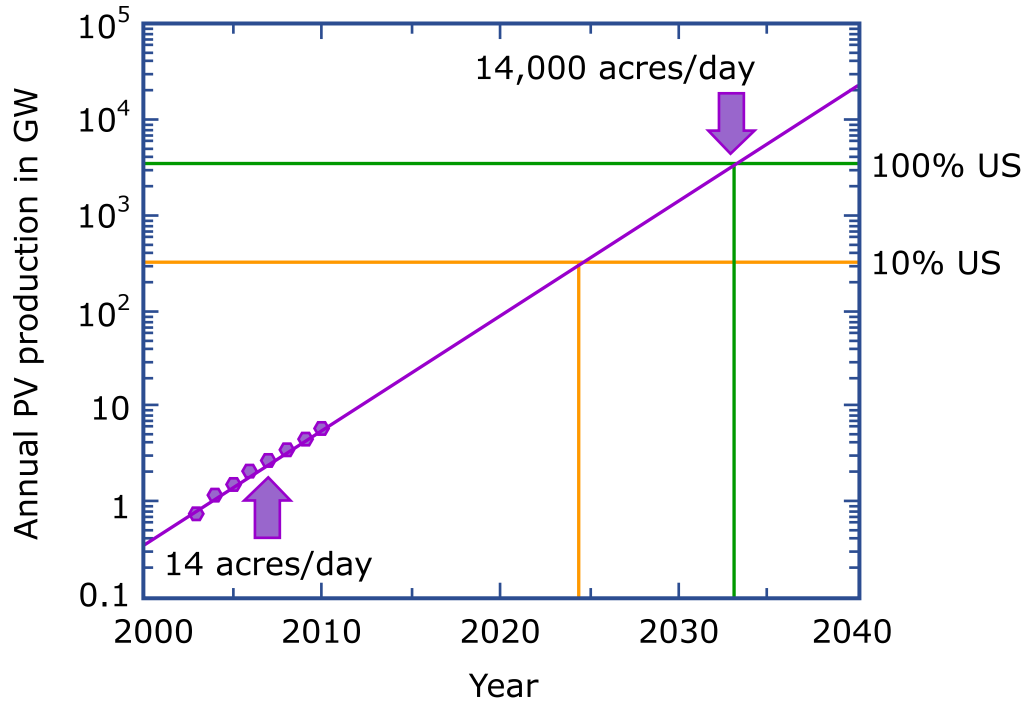


Image by MIT OpenCourseWare.

TECHNOLOGY	*BOTTLENECK*
nano	*low efficiency*
a-Si	*Si deposition*
CdTe	*tellurium availability*
CIGS	*indium availability*
c-Si	*module assembly*

At present manufacturing rates, only 10% of 2007 fuel usage will be eliminated by 2025

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



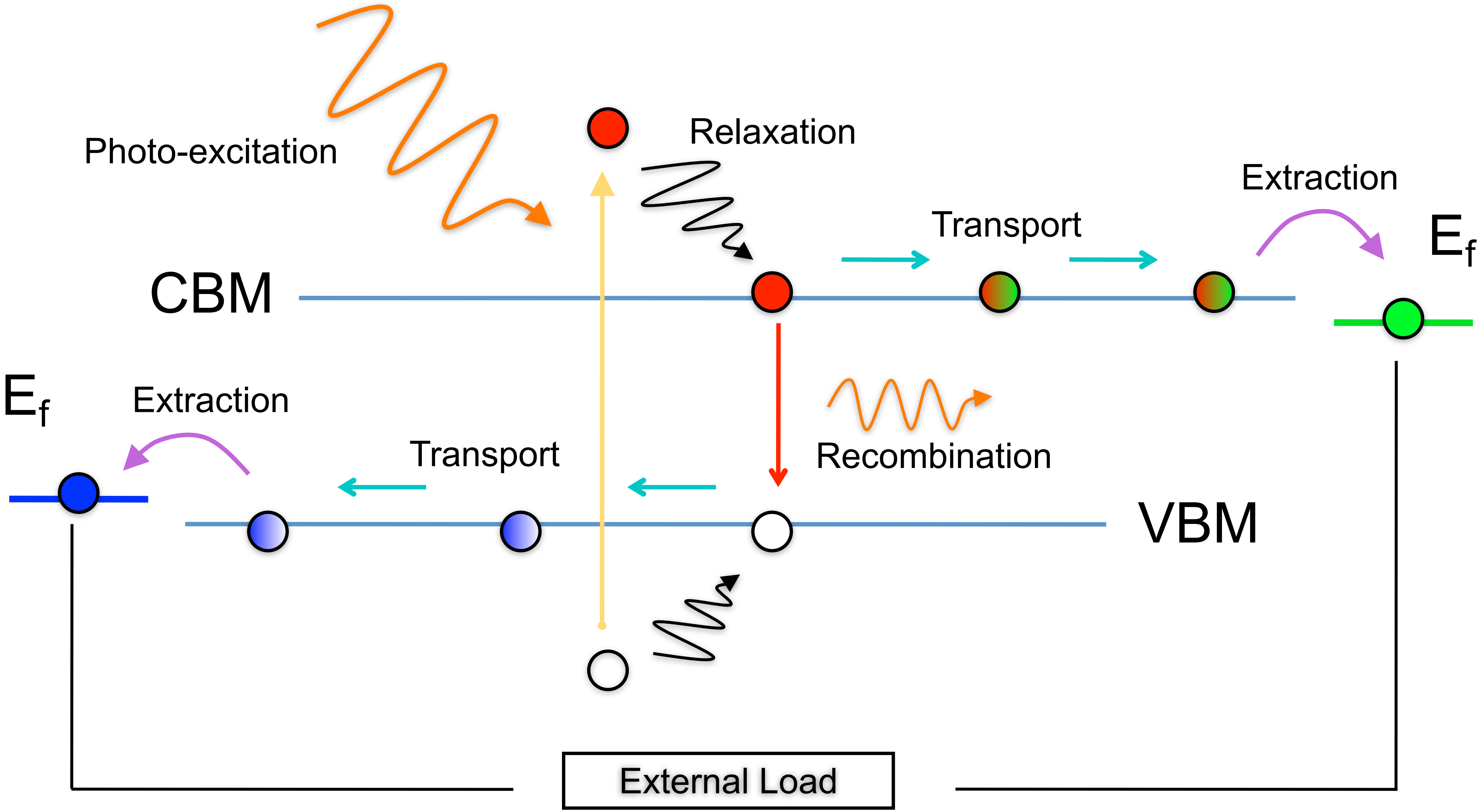
Expected Global Solar Cell Production.
After Mike Rogol.

Image by MIT OpenCourseWare.

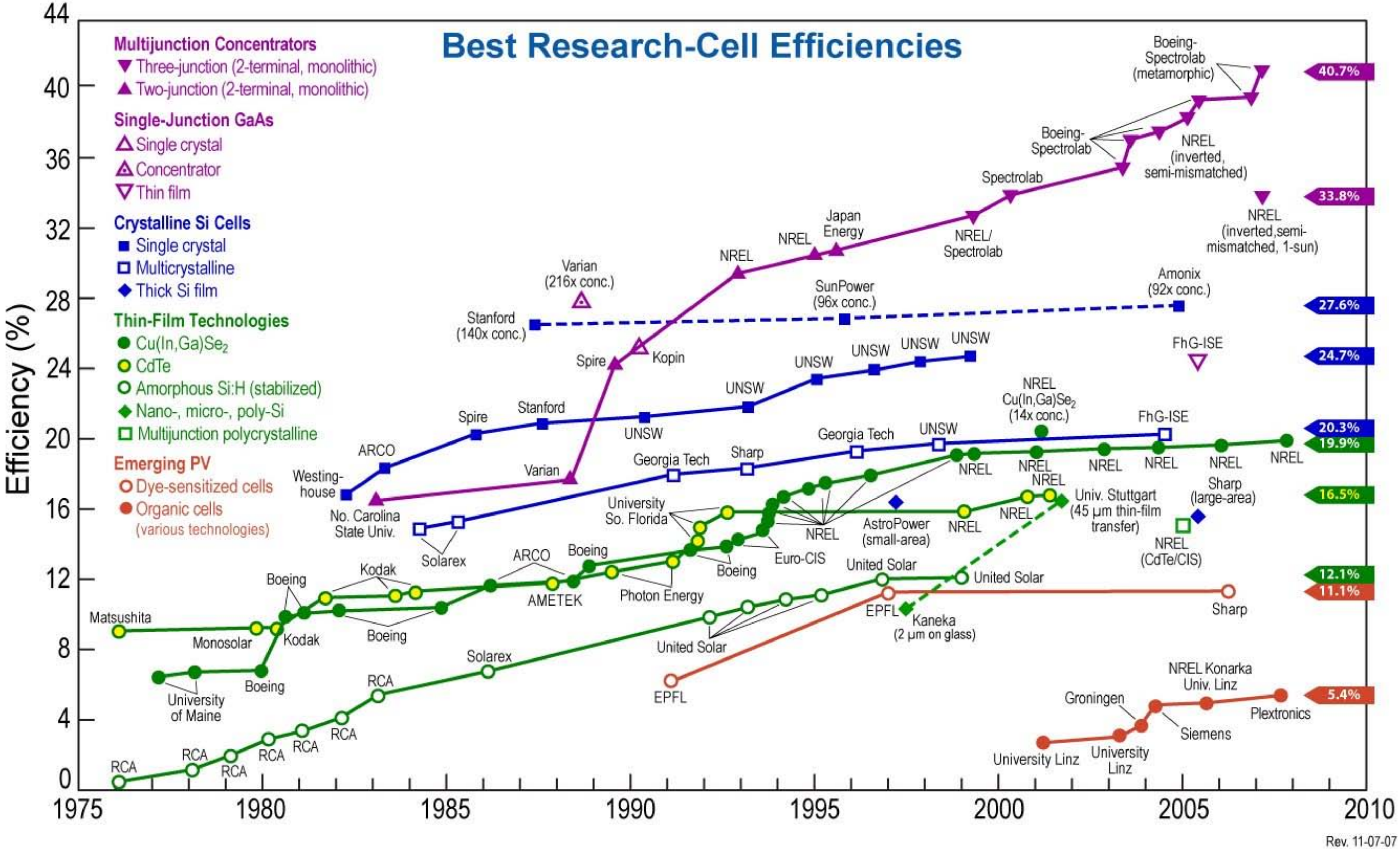
2035: Required Solar Cell Production Rate: 14,000 acres / day

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

Fundamental Processes Involved in Solar Photovoltaics: Electron's View



Many Materials for PV



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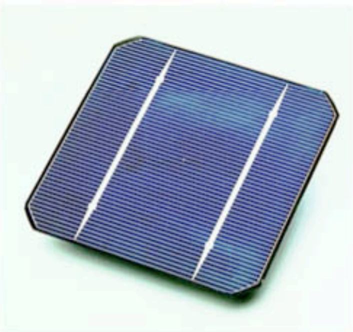
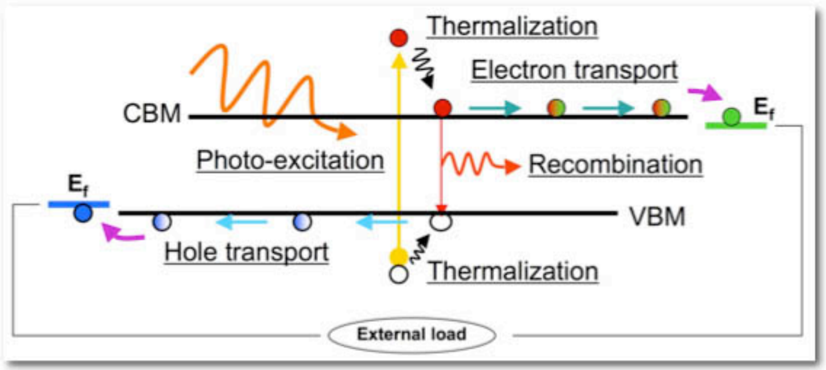
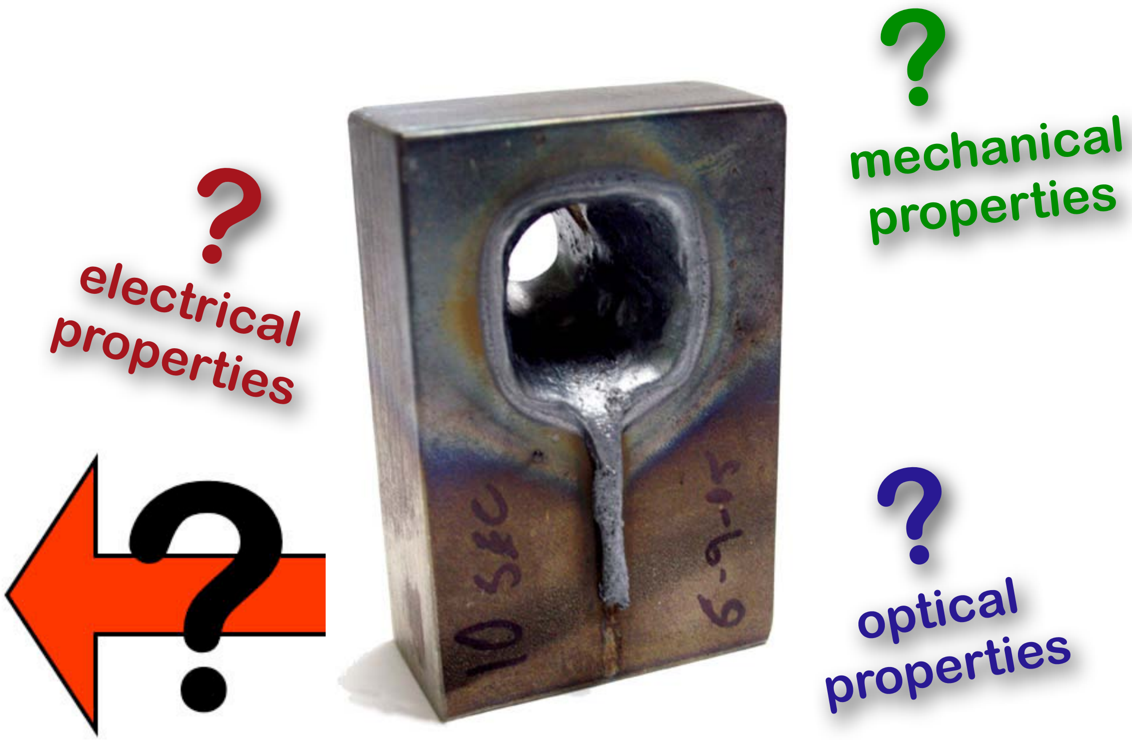
The Role of Computational Quantum Mechanics

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







Crystalline Silicon Solar PV (80-90% of current market)

- Light Absorption
  - Band Gap

Please see graph at
http://www.tf.uni-kiel.de/matwis/amat/semi_en/kap_2/illustr/si_banddiagram.gif.

  - 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

Graph of P3HT absorption removed due to copyright restrictions.

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

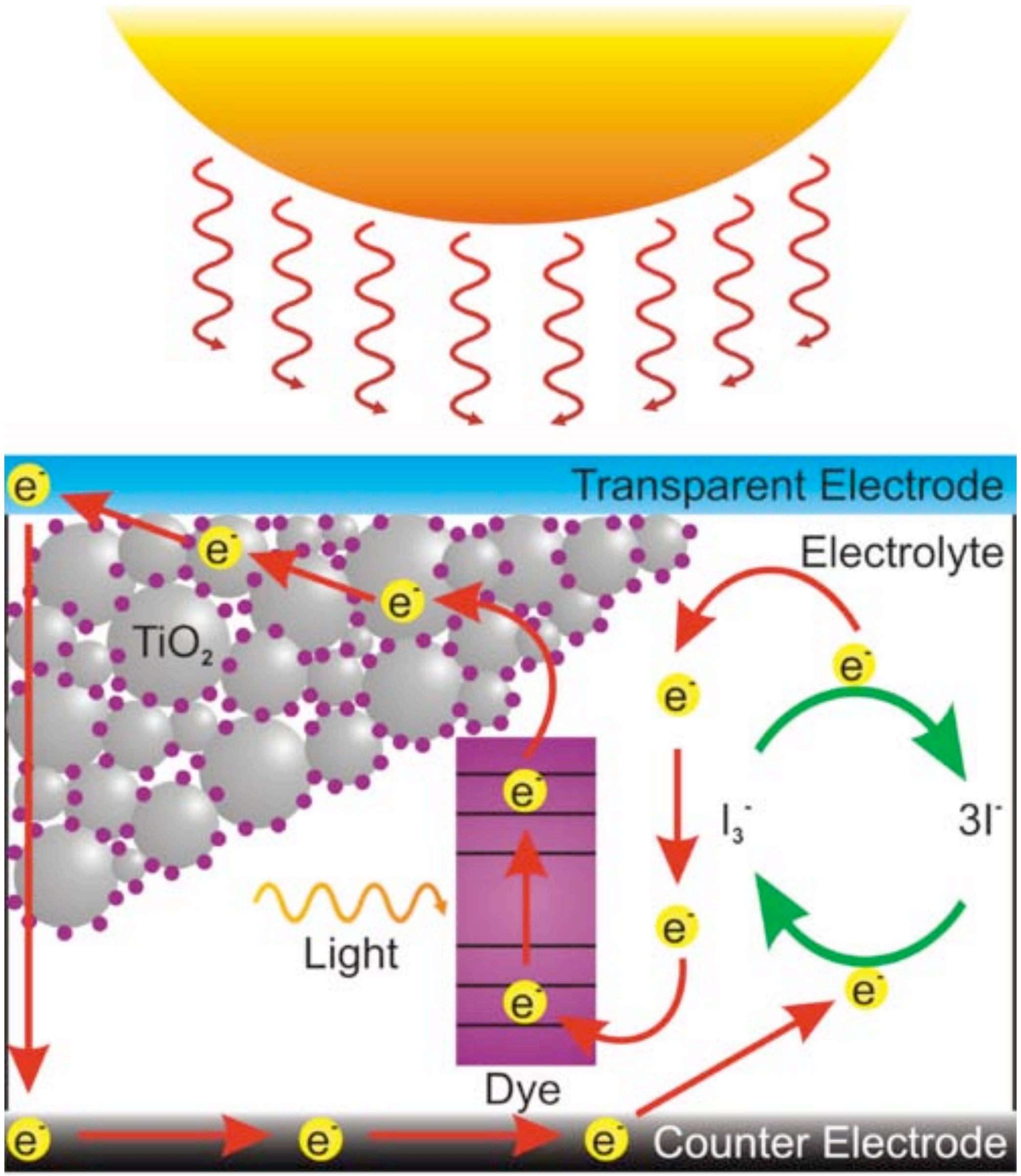


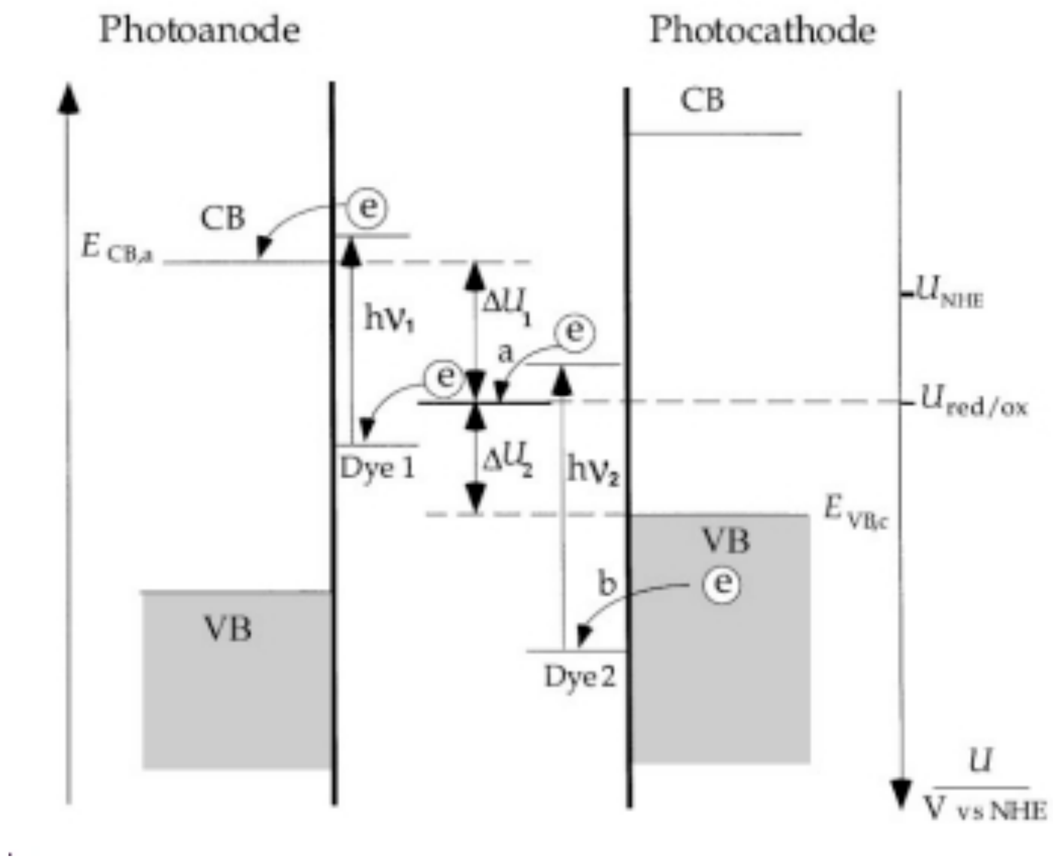
Image by M. R. Jones on Wikimedia Commons.

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.

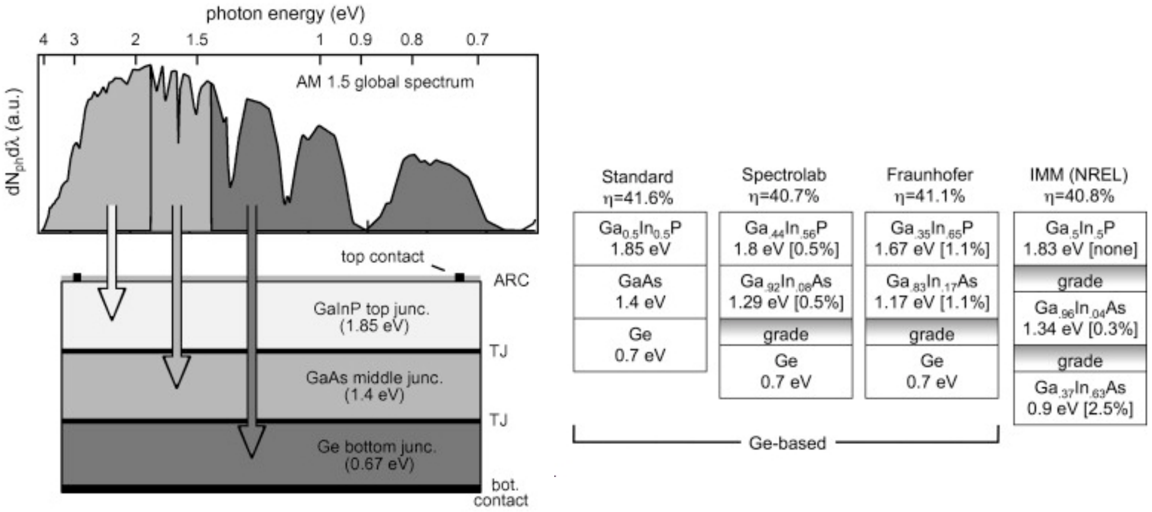
Dye Sensitized Solar PV



Courtesy of Elsevier, Inc., http://www.sciencedirect.com. Used with permission.

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

Multi-Junction Solar PV



Courtesy of Elsevier, Inc., http://www.sciencedirect.com. Used with permission.

Image removed due to copyright restrictions.
Please see the schematic of a tandem PV cell in Pentland, William. "Solar Energy's Bleeding Edge - Breakthrough PV Research Projects." *CleanBeta Blog*, June 22, 2008.

- Light Absorption
  - Band gaps
- Conductivity Across Interfaces
  - Band gaps, Band structures

Needing to Know Structure and Chemistry

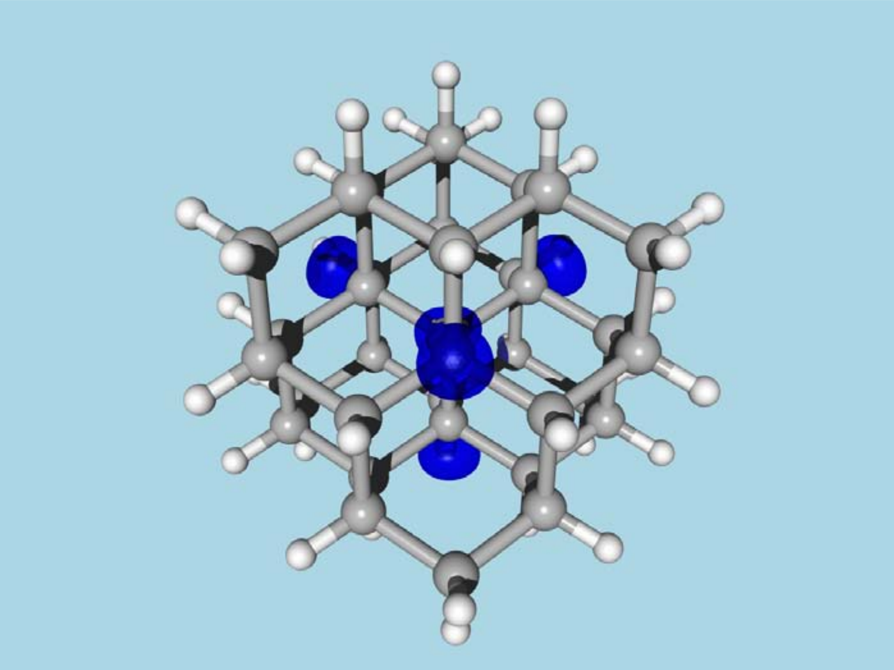
Photo by Ryne P. Raffaelle, Stephanie L. Castro, Aloysius F. Hepp, and Sheila G. Bailey, NASA Glenn Research Center.

- Structure
- Surface Chemistry
- Strain

J.P. Wilcoxon *et al.* Phys. Rev. B **60** 2704 (1999)

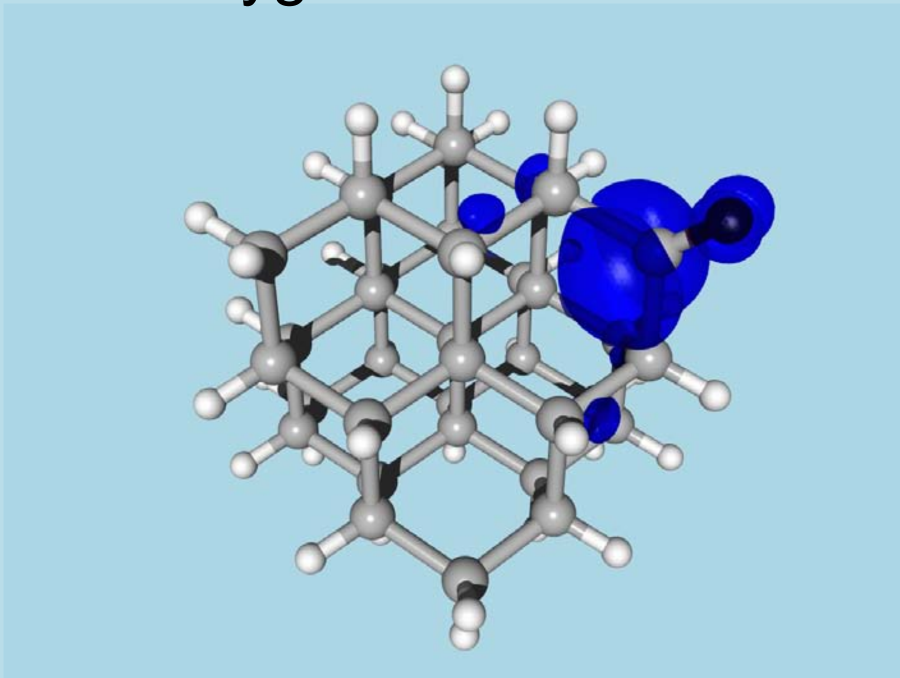
Needing to Know Structure and Chemistry

Clean Surface



Emits blue light

Oxygenated Cluster



Emits red light

A. Puzder *et al.* Physical Review Letters, **88** 097401 (2002)

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

3.021J / 1.021J / 10.333J / 18.361J / 22.00J Introduction to Modeling and Simulation
Spring 2011