

Energy Long Island, 2007 Conference
Farmingdale State College, New York
October 25, 2007

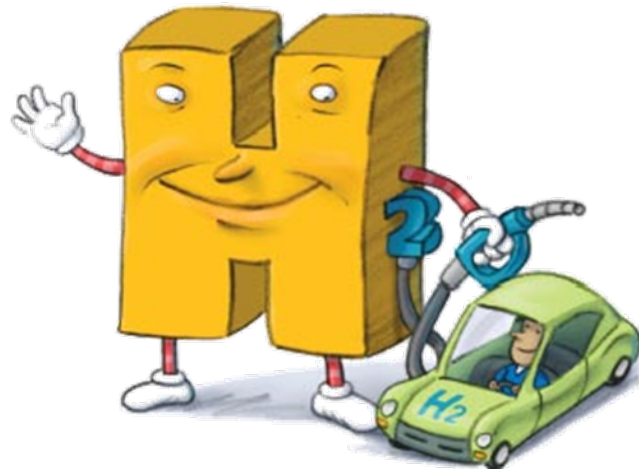
**Energy Research:
Forefront and Challenges**

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Cambridge, MA

Collaborator

George Crabtree, ANL



Energy Research: Forefront and Challenges

Outline

- Introduction – the energy challenge
- Energy alternatives and the materials challenge
- Think big, go small
- Science and Policy Perspectives

Energy: A National Initiative

The hydrogen project

“Tonight I'm proposing \$1.2 billion in research funding so that America can lead the world in developing clean, hydrogen-powered automobiles... With a new national commitment, our scientists and engineers will overcome obstacles to taking these cars from laboratory to showroom, so that the first car driven by a child born today could be powered by hydrogen, and pollution-free.”

**President Bush, State-of the-Union Address,
January 28, 2003**

"America is addicted to oil, which is often imported from unstable parts of the world,"

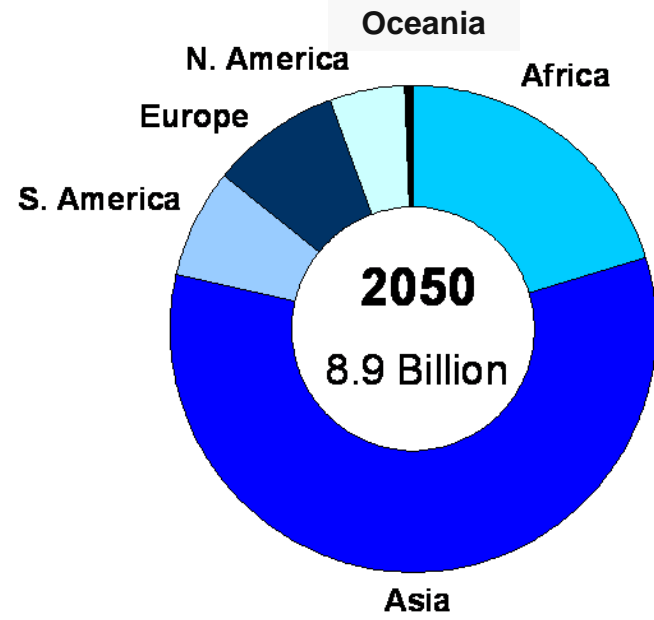
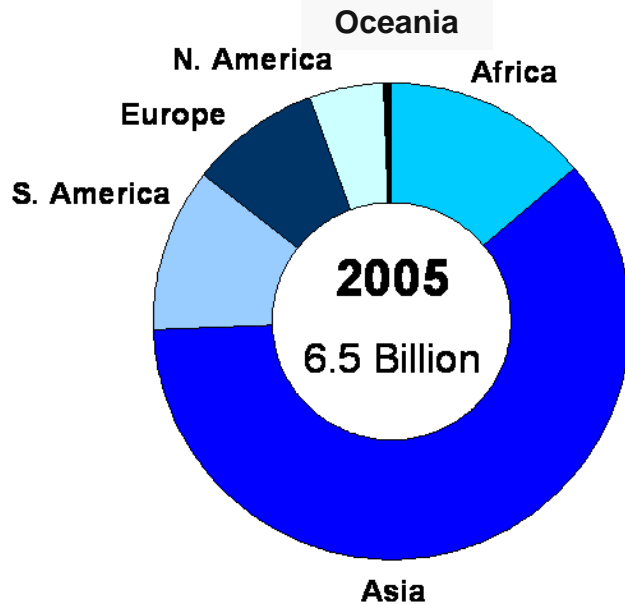
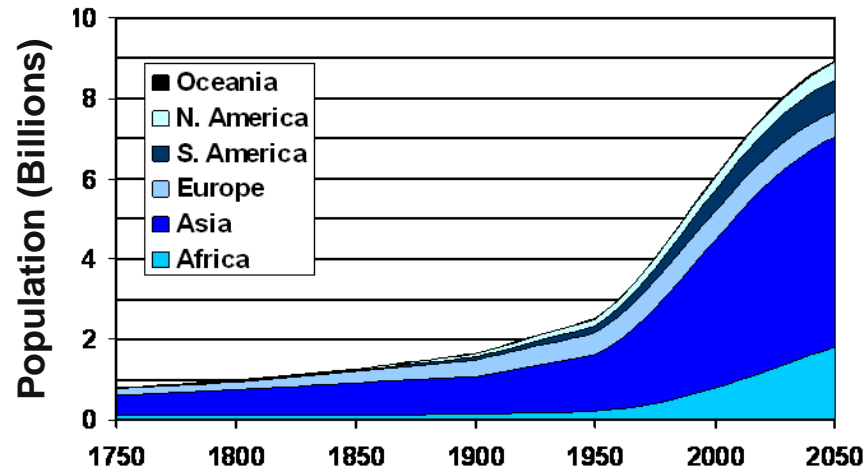
“The best way to break this addiction is through technology..”

“..better batteries for hybrid and electric cars, and in pollution-free cars that run on hydrogen’

**President Bush, State-of the-Union Address,
January 31, 2006**



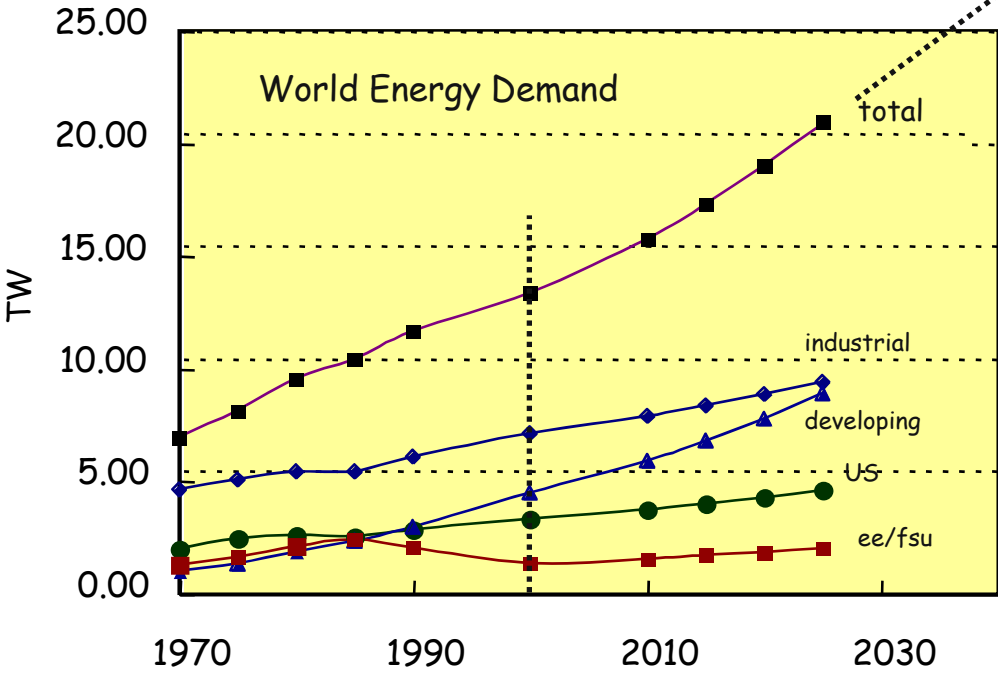
Demographic Expansion



The World Energy Demand Challenge

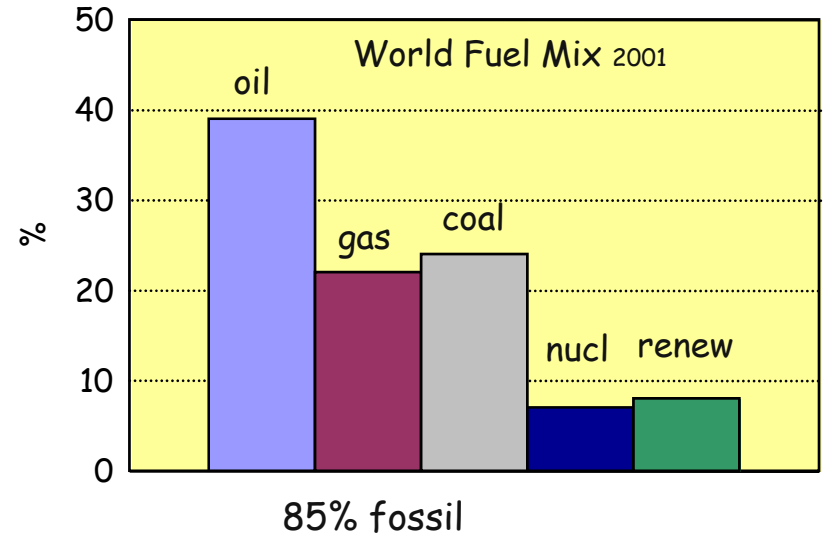


2100: 40-50 TW
 2050: 25-30 TW
 2000: 13 TW



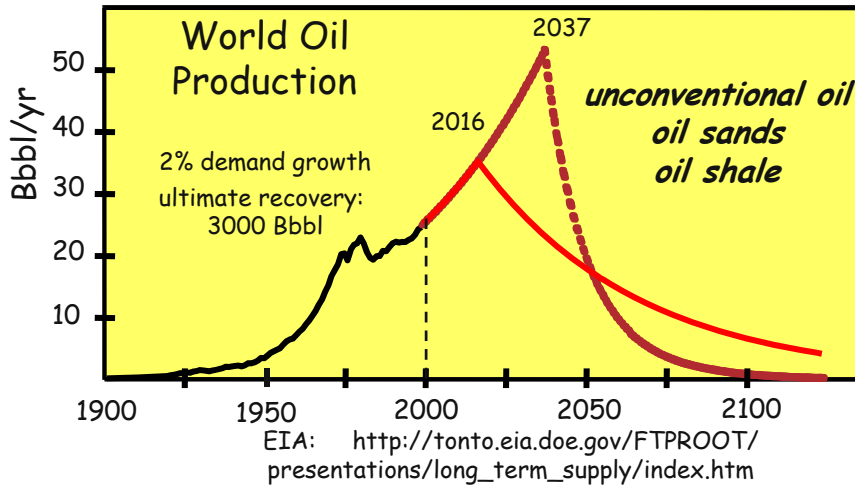
EIA Intl Energy Outlook 2004
<http://www.eia.doe.gov/oiaf/ieo/index.html>
 Hoffert et al Nature 395, 883,1998

energy gap
 ~ 14 TW by 2050
 ~ 33 TW by 2100



The Challenge of Fossil Fuel Supply and Security

When Will Production Peak?



R. Kerr, Science 310, 1106 (2005)

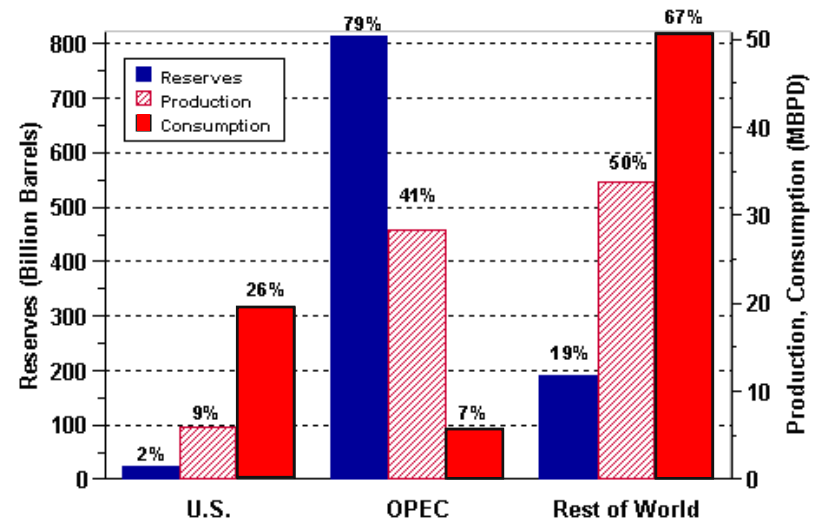
gas: beyond oil
coal: > 200 yrs



beyond the peak
new geopolitical relationships
alternative fuels
unconventional oil
break even ~ \$30-40 / bbl
50% more CO₂/gallon gasoline

World Oil Reserves/Consumption 2001

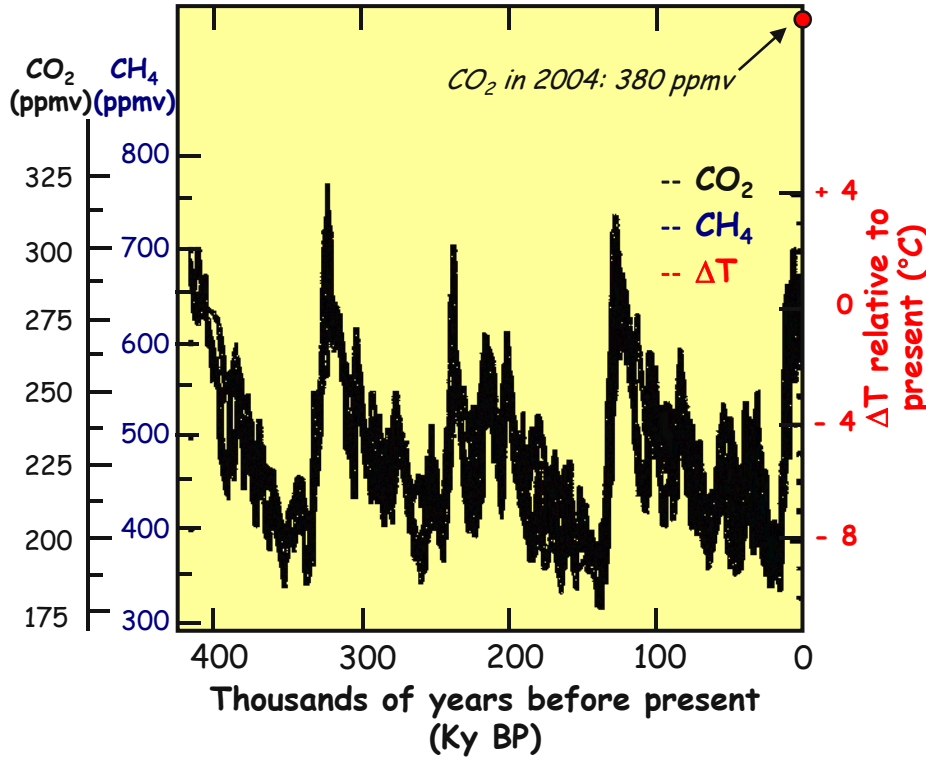
uneven distribution
⇒ insecure access



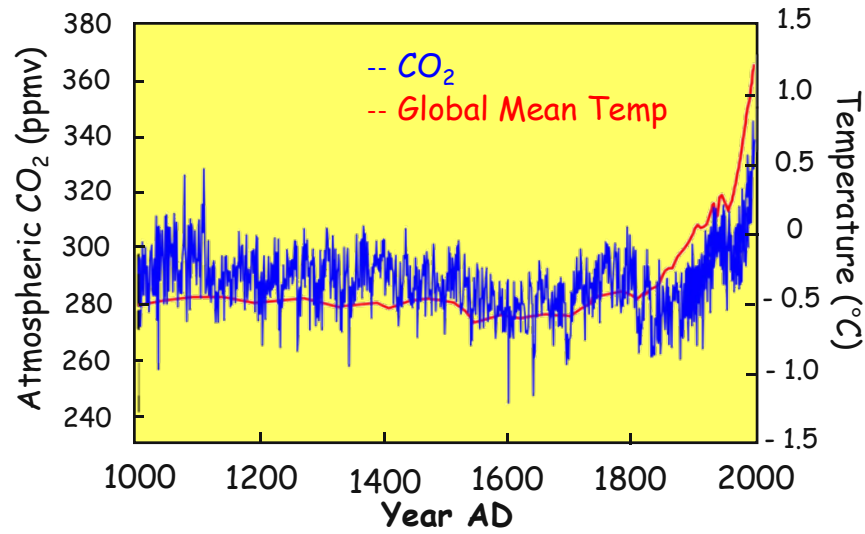
OPEC: Venezuela, Iran, Iraq, Kuwait, Qatar, Saudi Arabia, United Arab Emirates, Algeria, Libya, Nigeria, and Indonesia

http://www.eere.energy.gov/vehiclesandfuels/facts/2004/fcvt_fotw336.shtml

The Challenge of Fossil Fuel Related Climate Change



*Relaxation time
transport of CO₂ or heat to deep
ocean: 400 - 1000 years*



Climate Change 2001: The Scientific Basis, Fig 2.22

J. R. Petit et al, Nature 399, 429, 1999
Intergovernmental Panel on Climate Change, 2001
<http://www.ipcc.ch>

N. Oreskes, Science 306, 1686, 2004
D. A. Stainforth et al, Nature 433, 403, 2005

The Energy Alternatives

Fossil

Nuclear

Renewable

Fusion

solar, wind, hydroelectric
ocean tides and currents
biomass, geothermal

energy gap
~ 14 TW by 2050
~ 33 TW by 2100



10 TW = 10,000 1 GW power plants
1 new power plant/day for 27 years

China: 1 GW / week

no single solution
diversity of energy sources
required

Assessing Energy Futures

Energy Source: Solar
electricity - fuel- heat

Energy Carrier: Electricity

Energy Carrier: Hydrogen



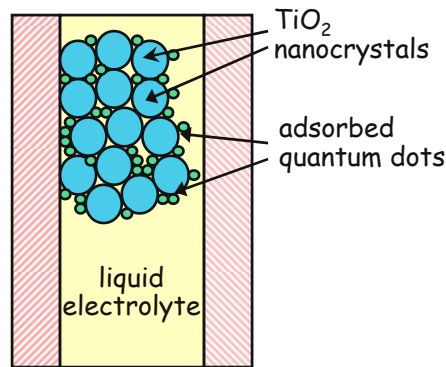
State of the art today

Future potential

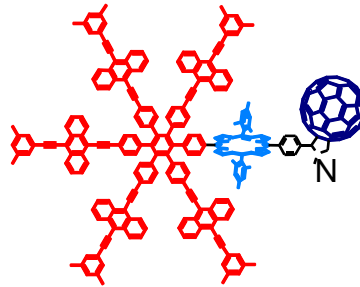
Science challenges

New Materials and Nanoscience will play a role

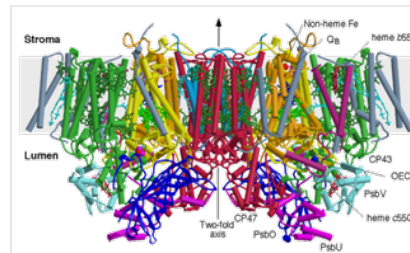
manipulation of photons, electrons, and molecules



quantum dot solar cells



artificial
photosynthesis



natural
photosynthesis



nanostructured
thermoelectrics

nanoscale architectures

top-down lithography
bottom-up self-assembly
multi-scale integration

characterization

scanning probes
electrons, neutrons, x-rays
smaller length and time scales

theory and modeling

multi-node computer clusters
density functional theory
10 000 atom assemblies

Solar energy requires interdisciplinary nanoscience research

Why Nanostructural materials are important for energy-based applications

- New desirable properties are available at the nanoscale but not found in conventional 3D materials e.g., higher diffusion coefficient to promote hydrogen release
- Higher surface area to promote catalytic interactions
- Independent control of nanomaterials parameters which depend on each other for 3D materials.

Energy Research: Forefront and Challenges

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The Energy in Sunlight

1.2×10^5 TW delivered to Earth
36,000 TW on land (world)
2,200 TW on land (US)



San Francisco Earthquake
(1906)

magnitude 7.8

10^{17} Joules

1 second of sunlight

Earth's
Ultimate Recoverable Resource
of oil

3 Trillion (=Tera) Barrels

1.7×10^{22} Joules

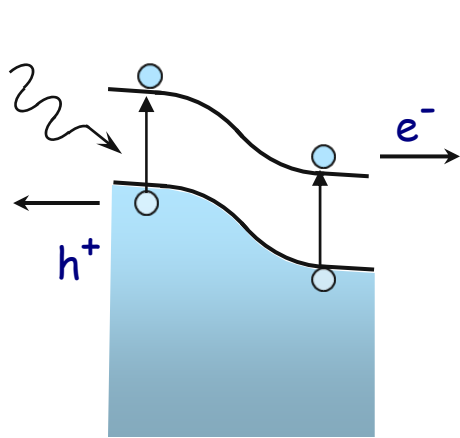
1.5 days of sunlight

Annual Human Production of Energy

4.6×10^{20} Joules

1 hour of sunlight

Solar Energy Utilization

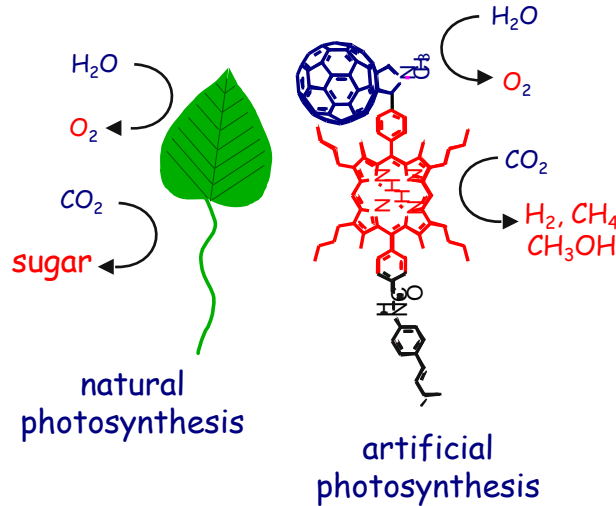


Solar Electric

.0002 TW PV (world)
 .00003 TW PV (US)
 \$0.30/kWh w/o storage



1.5 TW electricity (world)
 \$0.03-\$0.06/kWh (fossil)



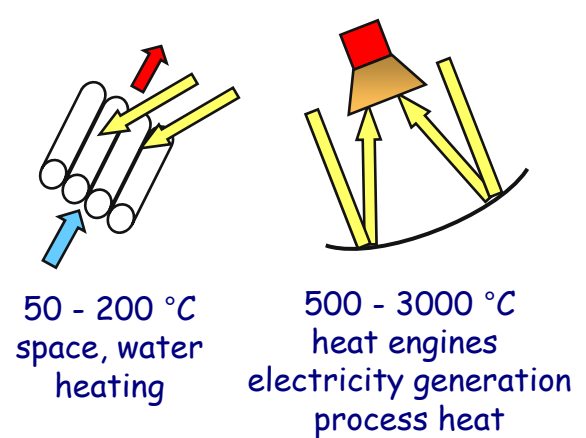
Solar Fuel

1.4 TW biomass (world)
 0.2 TW biomass sustainable (world)



11 TW fossil fuel
 (present use)

~ 14 TW additional energy by 2050



Solar Thermal

0.006 TW (world)



2 TW
 space and water
 heating (world)

Basic Research Needs for Solar Energy

- *The Sun is a singular solution to our future energy needs*

- capacity dwarfs fossil, nuclear, wind . . .
- sunlight delivers more energy in one hour than earth inhabitants use in one year
- free of greenhouse gases and pollutants
- secure from geo-political constraints

- *Enormous gap between our tiny use of solar energy and its immense potential*

- Incremental advances in today's technology will not bridge the gap
- Conceptual breakthroughs are needed that come only from high risk-high payoff basic research

- *Interdisciplinary research is required*

physics, chemistry, biology, materials, nanoscience

- *Basic and applied science should couple seamlessly*

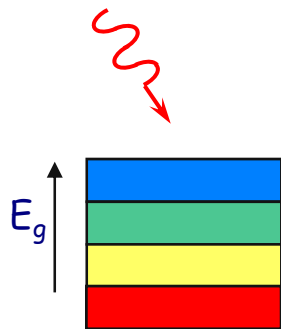
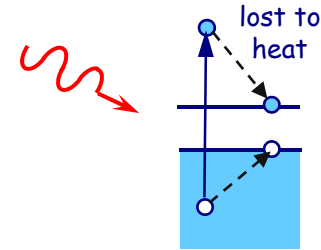


<http://www.sc.doe.gov/bes/reports/abstracts.html#SEU>

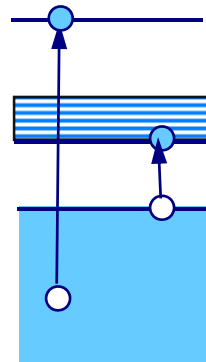
Revolutionary Photovoltaics: 50% Efficient Solar Cells

present technology: 32% limit for

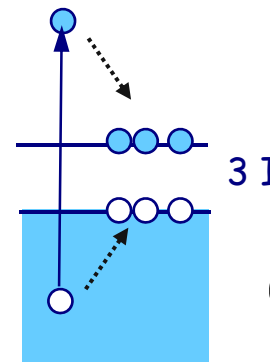
- single junction
- one exciton per photon
- relaxation to band edge



multiple junctions

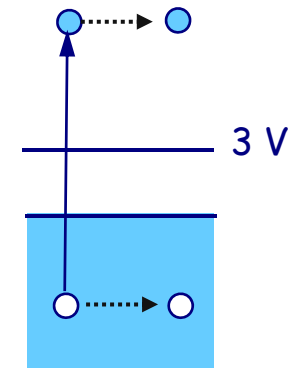


multiple gaps



multiple excitons per photon

nanoscale formats



hot carriers

rich variety of new physical phenomena
challenge: understand and implement

Solar Electric

- Despite 30-40% growth rate in installation, photovoltaics generate
 - less* than 0.02% of world electricity (2001)
 - less* than 0.002% of world total energy (2001)
- Decrease *cost/watt* by a factor 10 - 25 to be competitive with fossil electricity (without storage)
- Find effective method for *storage* of photovoltaic-generated electricity

Leveraging Photosynthesis for Efficient Energy Production

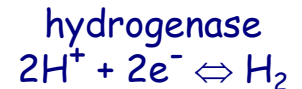
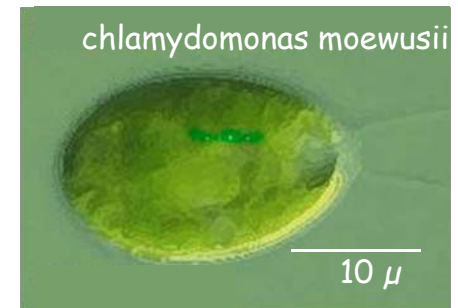
- photosynthesis converts ~ 100 TW of sunlight to sugars: nature's fuel
- low efficiency (< 0.3%) requires too much land area



switchgrass

Modify the biochemistry of plants and bacteria

- improve efficiency by a factor of 5-10
- produce a convenient fuel
methanol, ethanol, H₂, CH₄



Scientific Challenges

- understand and modify genetically controlled biochemistry that limits growth
- elucidate plant cell wall structure and its efficient conversion to ethanol or other fuels
- capture high efficiency early steps of photosynthesis to produce fuels like ethanol and H₂
- modify bacteria to more efficiently produce fuels
- improved catalysts for biofuels production

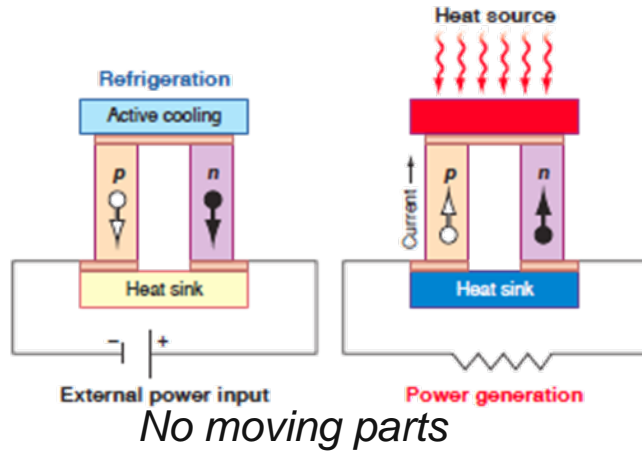
Solar Fuels: Solving the Storage Problem

- Biomass < 0.3% efficient: too much land area
Increase efficiency 5 - 10 times
- Designer plants and bacteria for designer fuels:
H₂, CH₄, methanol and ethanol
- Develop artificial photosynthesis

Energy Conversion Efficiency

| <i>conversion</i> | <i>efficiency</i> | <i>practical target</i> |
|--|--------------------------|-------------------------|
| chemical bonds \Rightarrow electrons | 30% (fossil electricity) | > 60% |
| chemical bonds \Rightarrow motion | 28% (gasoline engine) | > 60% |
| <i>photovoltaics</i> photons \Rightarrow electrons | 18% (market) / 28% (lab) | > 60% |
| <i>photosynthesis</i> photons \Rightarrow chemical bonds | 0.3% (biomass) | > 20% |
| <i>solid state lighting</i> electrons \Rightarrow photons | 5-25% | > 50% |

Thermoelectric Conversion



thermal gradient \Leftrightarrow electricity

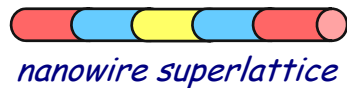
figure of merit: $ZT \sim (S^2\sigma/\kappa) T$

$ZT \sim 1$ (today)

Challenge: use nanostructures to achieve $ZT \sim 2-3$

Scientific Challenges

increase electrical conductivity
decrease thermal conductivity

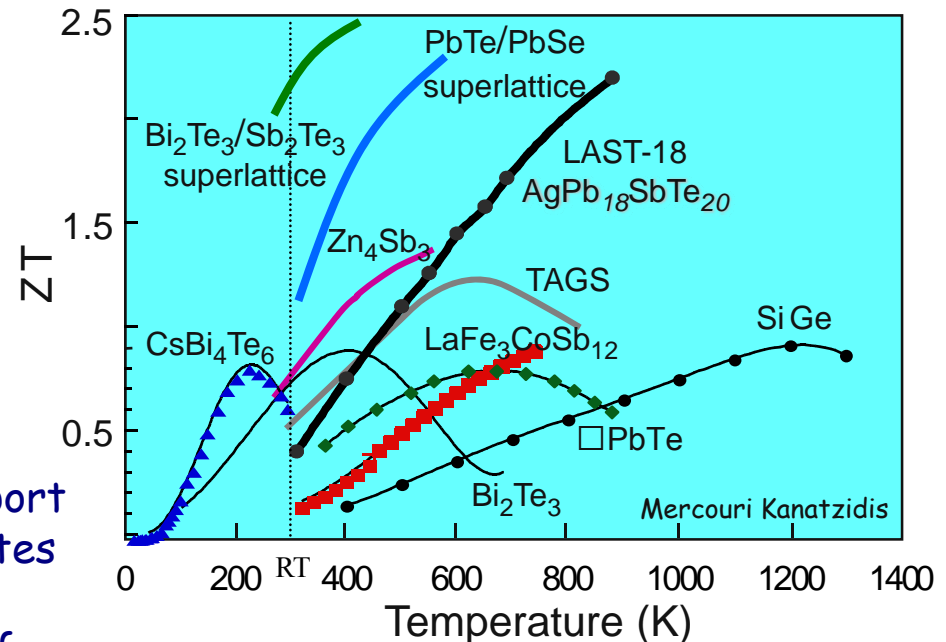


nanoscale architectures

Interfaces preferentially block heat transport
Quantum confinement tunes density of states
doping adjusts Fermi level

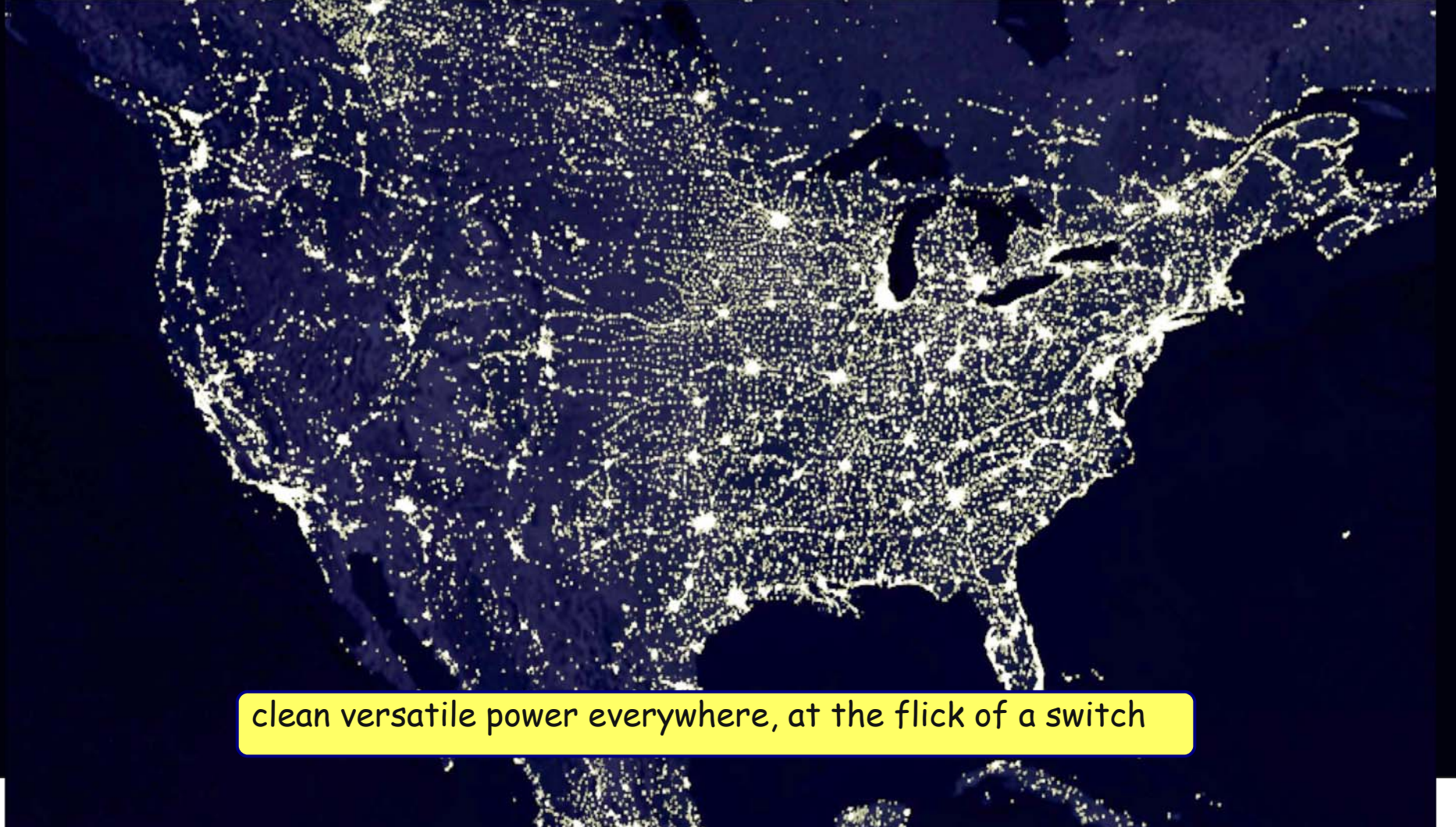
Thermoelectrics industry is now taking off.

One million cooling/heating devices based on waste heat conversion in autos were sold in 2007



The Grid - the Triumph of 20th Century Engineering

electricity is our dominant energy carrier



clean versatile power everywhere, at the flick of a switch

The 21st Century: A Different Set of Challenges

capacity

growing use of electricity
growing cities and suburbs
high people / power density
urban power bottleneck



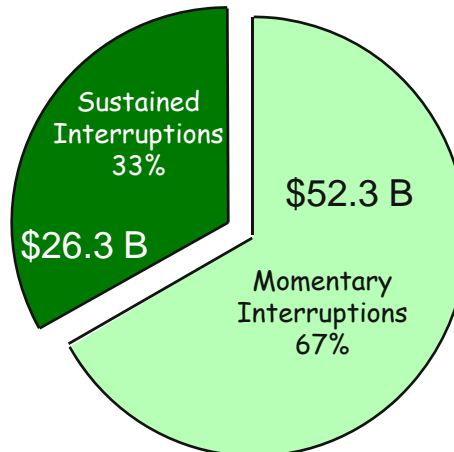
2030

50% demand growth (US)
100% demand growth (world)

reliability power quality

average
power loss/customer
(min/yr)

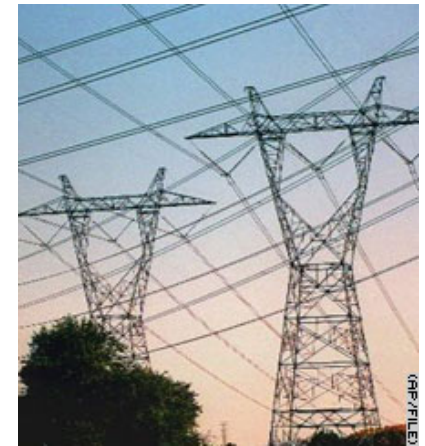
| | |
|--------|-----|
| US | 214 |
| France | 53 |
| Japan | 6 |



\$79 B economic loss (US)

LaCommare & Eto, Energy 31, 1845 (2006)

efficiency lost energy



62% energy lost in
production / delivery
8-10% lost in grid
40 GW lost (US)
~ 40 power plants
2030: 60 GW lost (US)
340 Mtons CO₂

Superconductivity for the 21st Century Grid

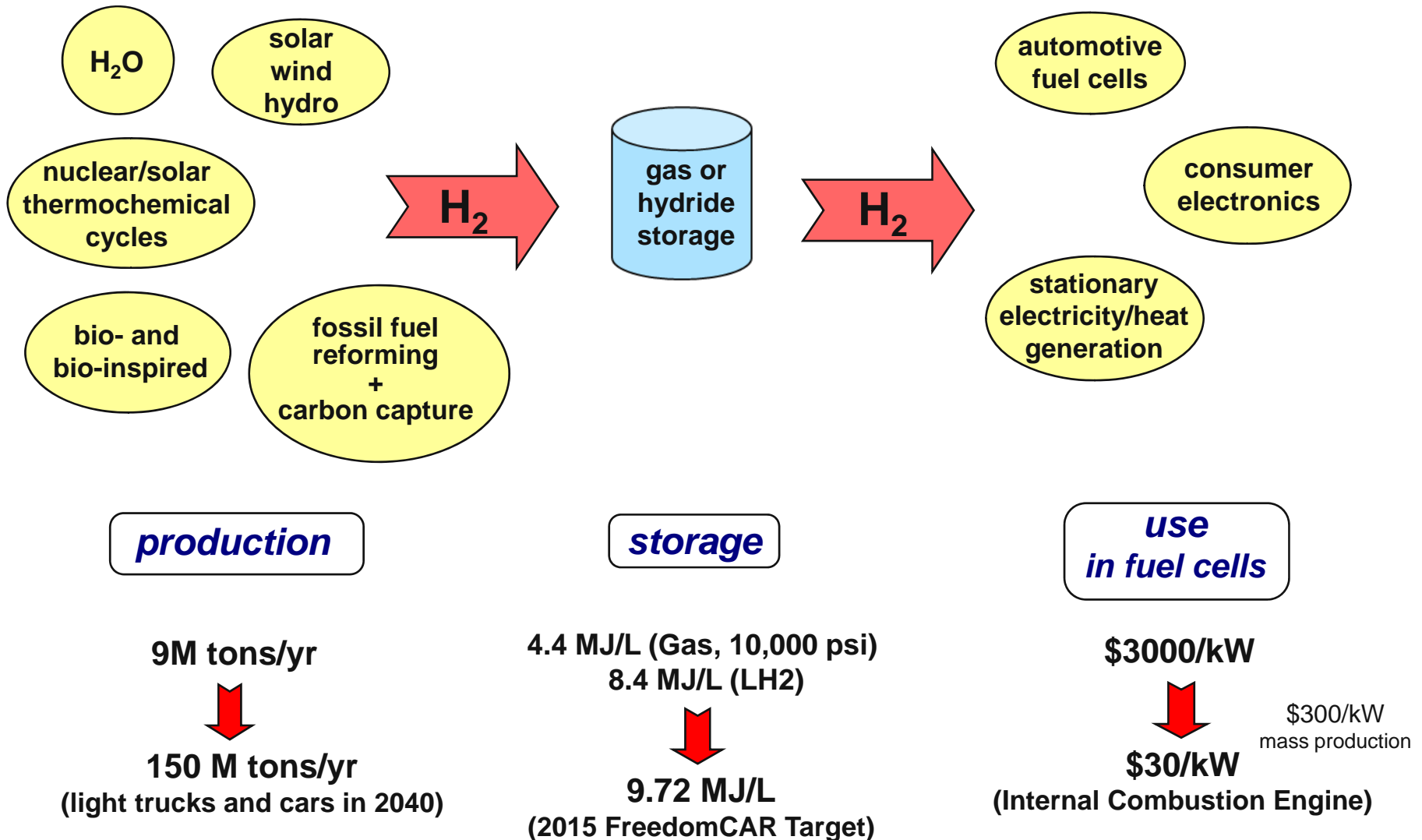
*Superconductors carry electrical current
without resistance or energy loss*

capacity \Rightarrow high current / low voltage

reliability / quality \Rightarrow smart, self-healing power control

efficiency \Rightarrow zero resistance (DC)
100 times lower than copper (AC)

Hydrogen as an Energy Carrier

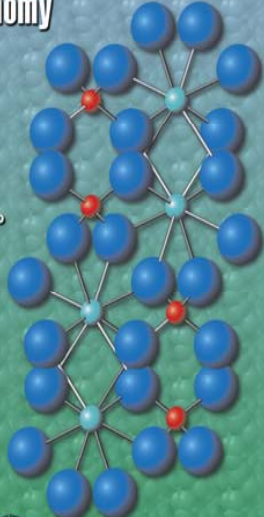


Hydrogen Studies

Basic Research Needs for the Hydrogen Economy

Report of the
Basic Energy
Sciences Workshop
on Hydrogen
Production,
Storage, and Use

May 13-15, 2003



Basic Energy Sciences
Department of Energy
July 2003/February 2004

<http://www.sc.doe.gov/bes/hydrogen.pdf>

All emphasize:

- Necessity for basic research
- Collaborations between basic and applied research, multidisciplinary

THE HYDROGEN ECONOMY: OPPORTUNITIES, COSTS, BARRIERS AND R&D NEEDS

Committee on Alternatives and Strategies
for Future Hydrogen Production and Use

Board on Energy and Environmental Systems
Division on Engineering and Physical Sciences

NATIONAL RESEARCH COUNCIL

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Washington, D.C.

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National Research Council
National Academy of Sciences
February 2004

<http://www.nap.edu/catalog/10922.html>

PHYSICS TODAY December 2004 The Hydrogen Economy

If the fuel cell is to become the modern steam engine, basic research must provide breakthroughs in understanding materials, and design to make a hydrogen-based energy system a vibrant and competitive force.

George W. Crabtree, Mildred S. Dresselhaus, and Michelle V. Buchanan

Since the industrial revolution began in the 18th century, fossil fuels in the form of coal, oil, and natural gas have powered the technology and transportation networks that drive society. But continuing to power the world from fossil fuels threatens our energy supply and puts enormous strains on the environment. The world's demand for energy is projected to double by 2050 in response to population growth and the industrialization of developing countries. The supply of fossil fuels is limited, with restrictive shortages of oil and gas projected to occur within our lifetimes (see the article by Paul Weisz in *PHYSICS TODAY*, July 2004, page 47). Global oil and gas reserves are concentrated in a few regions of the world, while demand is growing everywhere; as a result, a secure supply is increasingly difficult to assure. Moreover, the use of fossil fuels puts our own health at risk through the chemical and particulate pollution it creates. Carbon dioxide and other greenhouse gas emissions that are associated with global warming threaten the stability of Earth's climate.

A replacement for fossil fuels will not appear overnight. Extensive R&D is required before alternative sources can supply energy in quantities and at costs competitive with fossil fuels, and making those alternative sources available commercially will itself require developing the proper economic infrastructure. Each of those steps takes time, but greater global investment in R&D will most likely hasten the pace of economic change. Although it is impossible to predict when the fossil fuel supply will fall short of demand or when global warming will become acute, the present trend of yearly increases in fossil fuel use shortens our window of opportunity for a managed transition to alternative energy sources.

Hydrogen as energy carrier

One promising alternative to fossil fuels is hydrogen^{1,2} (see the article by Jean Ogden, *PHYSICS TODAY*, April 2002, page 69). Through its reaction with oxygen, hydrogen re-

George Crabtree is a physicist in the materials science division of Argonne National Laboratory in Illinois. Mildred Dresselhaus is a professor in the department of physics and the department of electrical engineering and computer science at the Massachusetts Institute of Technology in Cambridge. Michelle Buchanan is a chemist in the chemical sciences division at Oak Ridge National Laboratory in Tennessee.

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leases energy explosively in heat engines or quietly in fuel cells to produce water as its only byproduct. Hydrogen is abundant and generously distributed throughout the world without regard for national boundaries; using it to create a hydrogen economy—a future energy system based on hydrogen and electricity—only requires technology, not political access.

Although in many ways hydrogen is an attractive replacement for fossil fuels, it does not occur in nature as the fuel H₂. Rather, it occurs in chemical compounds like water or hydrocarbons that must be chemically transformed to yield H₂. Hydrogen, like electricity, is a carrier of energy; and like electricity, it must be produced from a natural resource. At present, most of the world's hydrogen is produced from natural gas by a process called steam reforming. However, producing hydrogen from fossil fuels would rob the hydrogen economy of much of its reason d'être. Steam reforming does not reduce the use of fossil fuels but rather shifts them from end use to an earlier production step, and it still releases carbon to the environment in the form of CO₂. Thus, to achieve the benefits of the hydrogen economy, we must ultimately produce hydrogen from non-fossil resources, such as water, using a renewable energy source.

Figure 1 depicts the hydrogen economy as a network composed of three functional steps: production, storage, and use. There are basic technical reasons to achieve each of these steps, but none of them can yet compete with fossil fuels in cost, performance, or reliability. Even when using the cheapest production method—steam reforming of methane—hydrogen is still four times the cost of gasoline for the equivalent amount of energy. And production from methane does not reduce fossil fuel use or CO₂ emission. Hydrogen can be stored in pressurized gas containers or as a liquid in cryogenic containers, but not in densities that would allow for practical applications—driving a car up to 500 kilometers on a single tank, for example. Hydrogen can be converted to electricity in fuel cells, but the production cost of prototype fuel cells remains high: \$3000 per kilowatt of power produced for prototype fuel cells (mass production could reduce this cost by a factor of 10 or more), compared with \$30 per kilowatt for gasoline engines.

The gap between the present state of the art in hydrogen production, storage, and use and that needed for a competitive hydrogen economy is too wide to bridge in incremental advances. It will take fundamental breakthroughs of the kind that come only from basic research.

Beyond reforming

The US Department of Energy estimates that by 2040 cars and light trucks powered by fuel cells will require about 150 megajoules per year of hydrogen.³ The US currently produces about 9 megajoules per year, almost all of it by reforming natural gas. The challenge is to find inexpensive

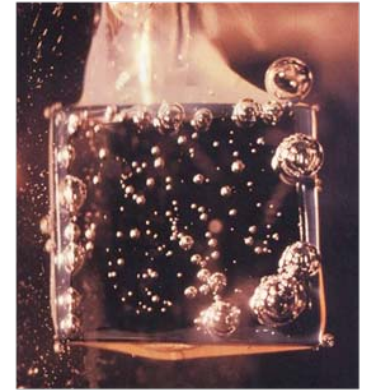
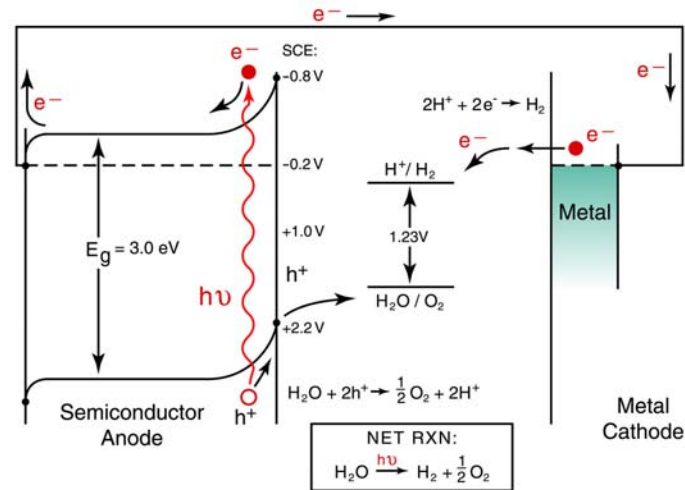
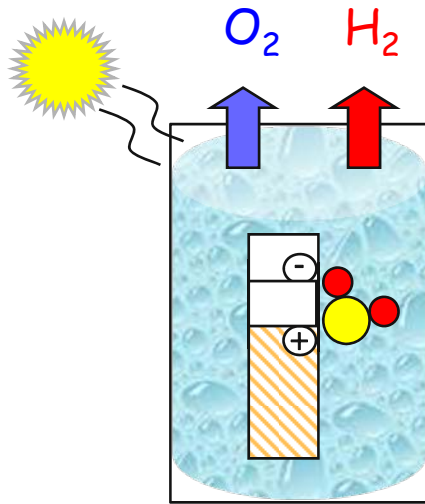
December 2004 Physics Today 39

G. W. Crabtree, M. S. Dresselhaus,
M. V. Buchanan

Physics Today 57(12), 39-44, 2004

<http://www.physicstoday.org/vol-57/iss-12/p39.html>

Efficient Solar Water Splitting



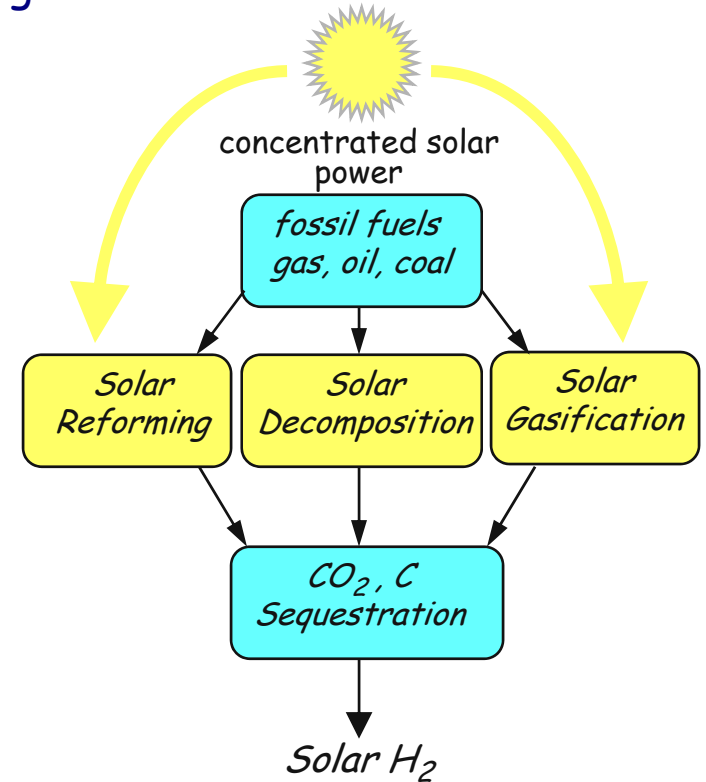
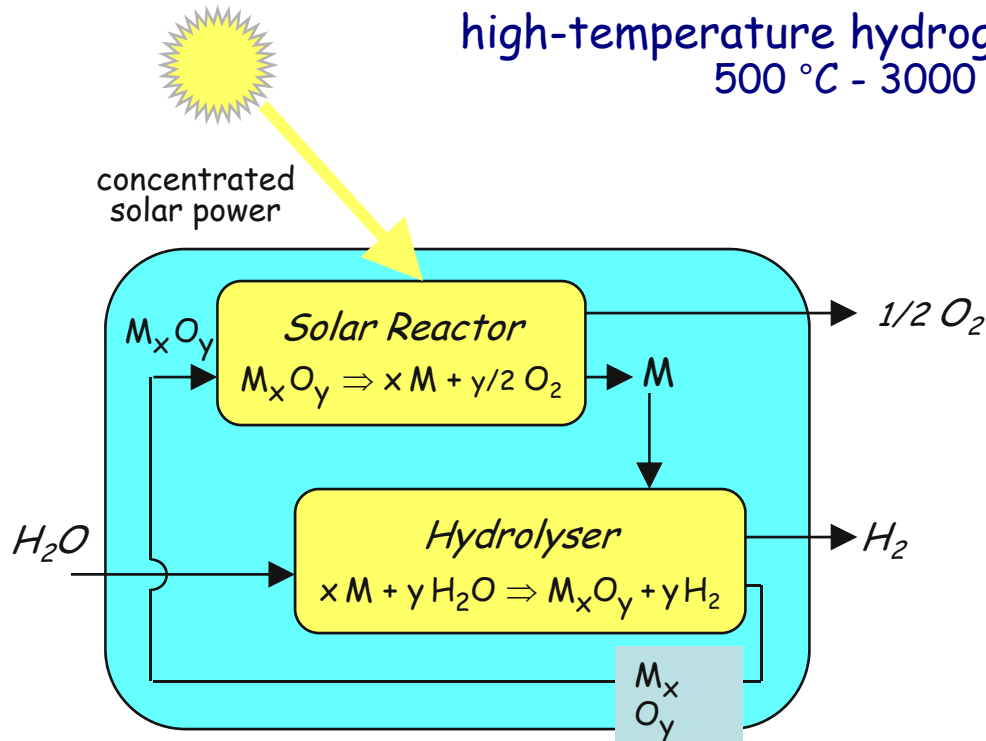
demonstrated efficiencies 10% in laboratory

Scientific Challenges

- cheap electrode materials that are robust in water
- catalysts for the redox reactions at each electrode
- nanoscale architecture for electron excitation \Rightarrow transfer \Rightarrow reaction

Solar Thermochemical Fuel Production

high-temperature hydrogen generation
500 °C - 3000 °C



Scientific Challenges
high temperature reaction kinetics of
- metal oxide decomposition
- fossil fuel chemistry
robust chemical reactor designs and materials

Energy Research: Forefront and Challenges

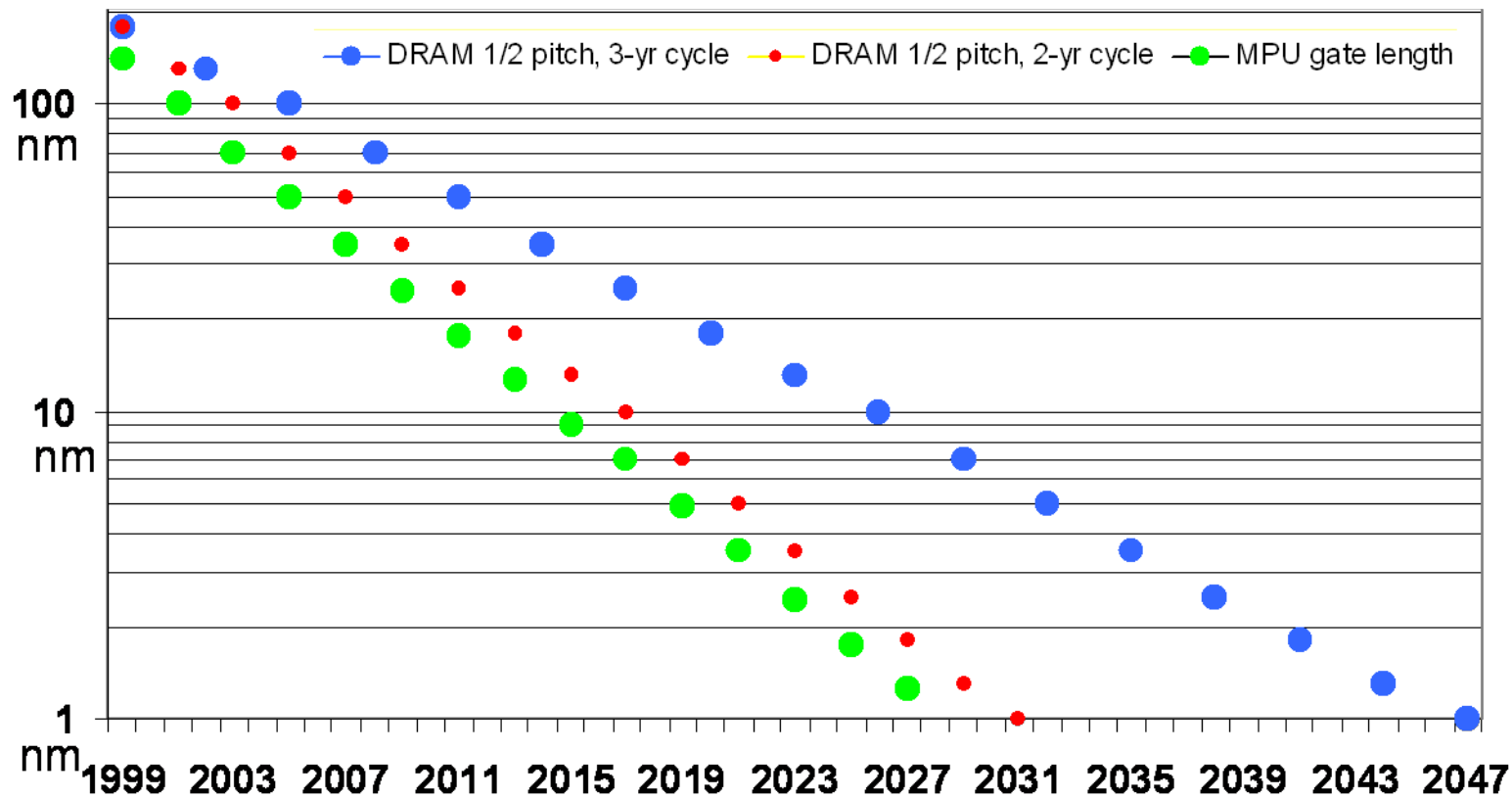
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Moore's Law for semiconductor electronics

soon, all microchips will be nanoscale devices



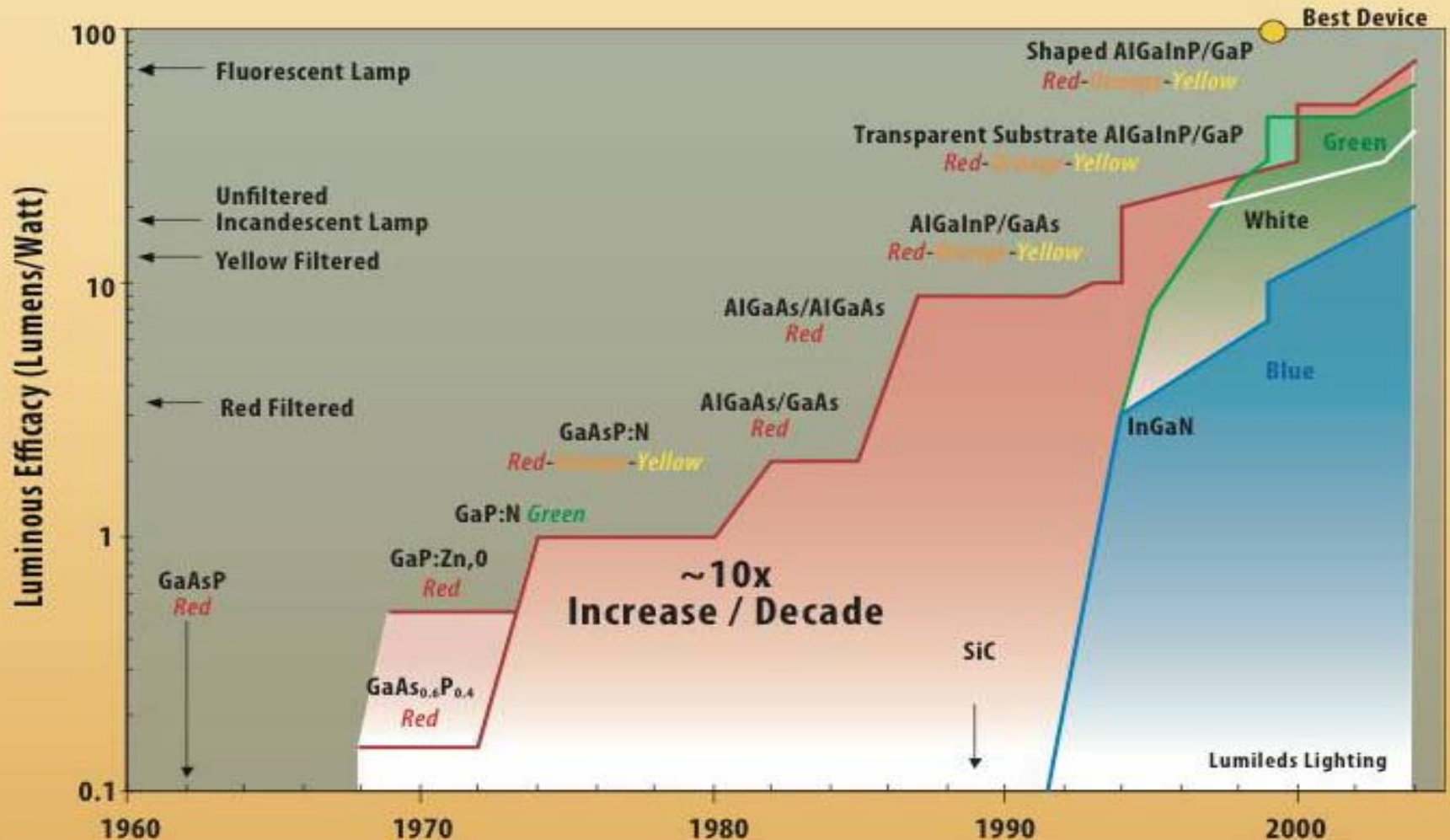
CONCLUSION: Moore's law continues for this decade regarding future size, device performance and cost for semiconductor electronics industry.

Extension of Moore's Law to the Energy Industry

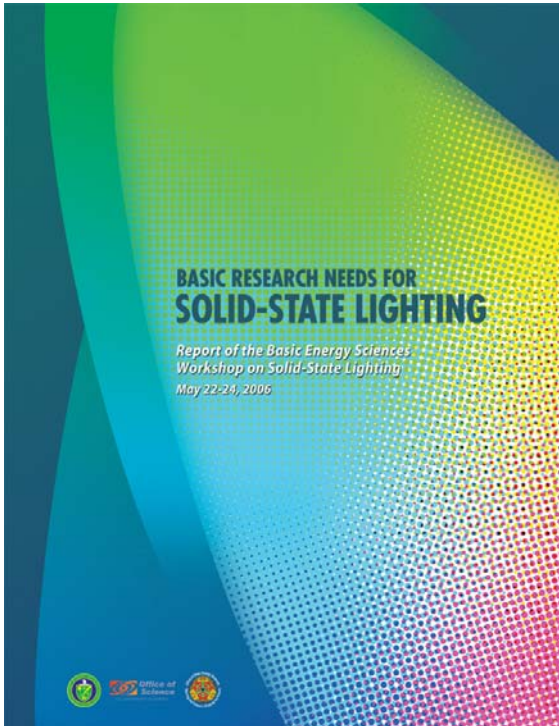
- Moore's law has for many years been working to set goals for the electronics, opto-electronics, and magnetics industries.
- We now need to apply Moore's law to set goals for the energy industry.

Moore's law for Solid-State Lighting at Half the Energy Consumption as for Conventional Lighting

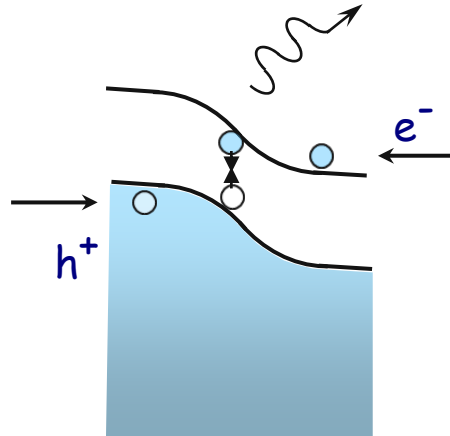
Evolution of LED Efficiency



Electricity Use: Solid State Lighting



<http://www.sc.doe.gov/bes/reports/abstracts.html#SSL>

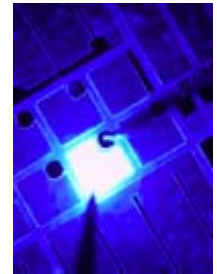


wide bandgap
compound semiconductors
GaN InGaN AlGaN
color: control bandgap
efficiency: control defects
white light: mix 3 or 4 colors

Lighting ~ 22%
of electricity use



incandescent
~ 5% efficient



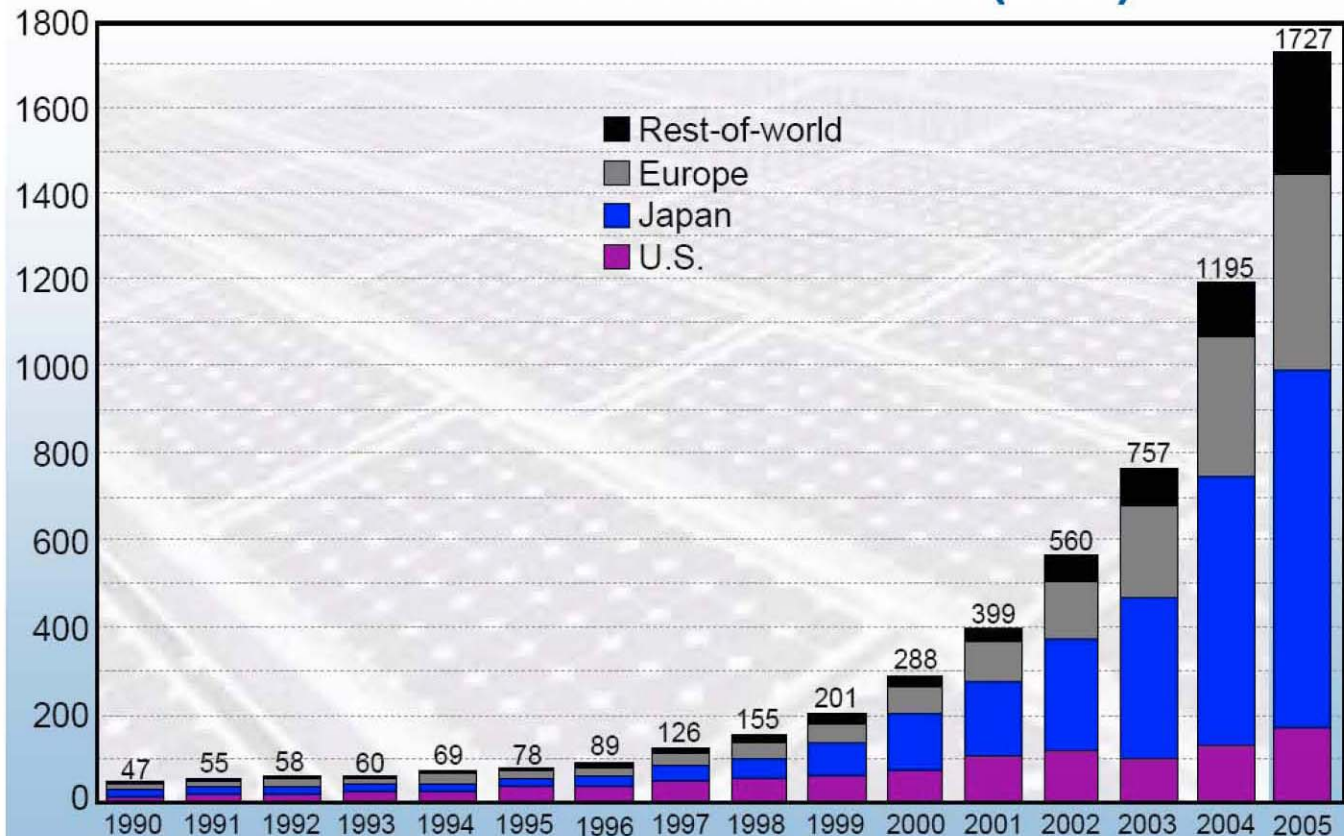
Solid state
> 50% efficient



Research Challenges
new materials
doping and defect control
white light at 50% efficiency
cut cost

Example of Moore's law

World PV Cell Production (MW)



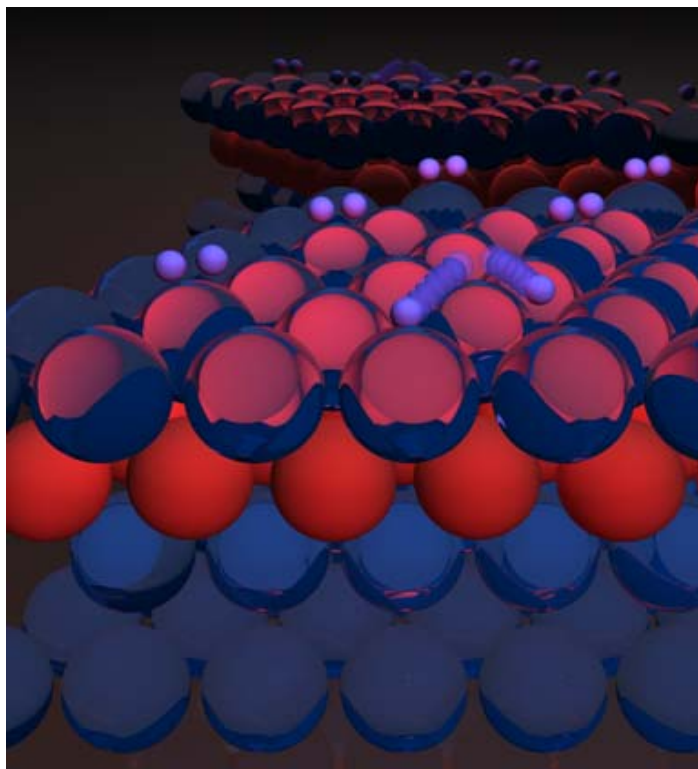
Source: Paul Maycock, PV News, March 2006

Annual Growth Rate > 30% For The Last Decade

Technological Advances in Solar Photovoltaics

- Multiple gap solar cell (e.g., GaInP/GaInAs/Ge) to capture solar spectrum efficiently (40.7% efficiency achieved): R.R. King et al., Appl. Phys. Lett. 90, 183516 (2007)
- Tune compositions and strain for superlattices to optimize response to solar spectrum
- Use solar concentrator (e.g., 240 suns) to drastically reduce size of active area of solar cell by factor of 1000
- Allows reduction of overall cost despite added costs for MOCVD fabrication, solar tracking and cooling
- Spectrolab is in high volume production of a system with 40% average efficiency and cost of < 0.15 \$/kw hr by 2010. This company has a roadmap for year by year increase in efficiency

Predicting Catalysts for Hydrogen Production, Storage or Fuel-Cell Utilization



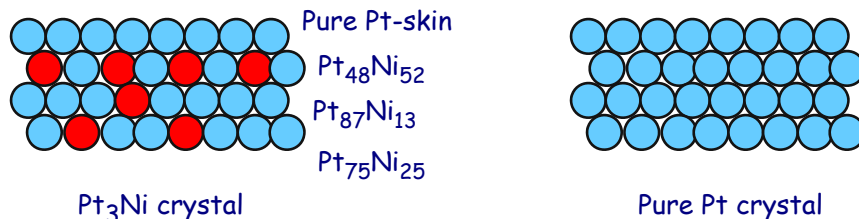
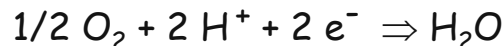
Theoretical calculation of molecular hydrogen undergoing dissociation over near-surface alloys.

- Small purple spheres: **hydrogen**
- Blue spheres: **platinum** atoms
- Red spheres: **nickel** atoms
- **Bicolor** blue and red spheres: platinum atoms whose electronic properties have been dramatically altered by the underlying nickel.

- There is a need for low-temperature, highly efficient and durable catalysts for large scale hydrogen production.
- New catalyst structures and compositions are now being predicted *a priori* using quantum chemistry and molecular dynamics.
- Single metallic layers of one metal embedded within a matrix of another metal produce low-energy hydrogen scission and recombination.
- **Nickel within platinum can attach atomic hydrogen weakly like copper and gold, while dissociating molecular hydrogen rapidly like platinum and rhodium.**
- This study may lead to breakthroughs in hydrogen production, storage and combustion in fuel cells.

Pt Catalysis: 10x Increase for Oxygen Reduction Reaction

Oxygen Reduction Reaction



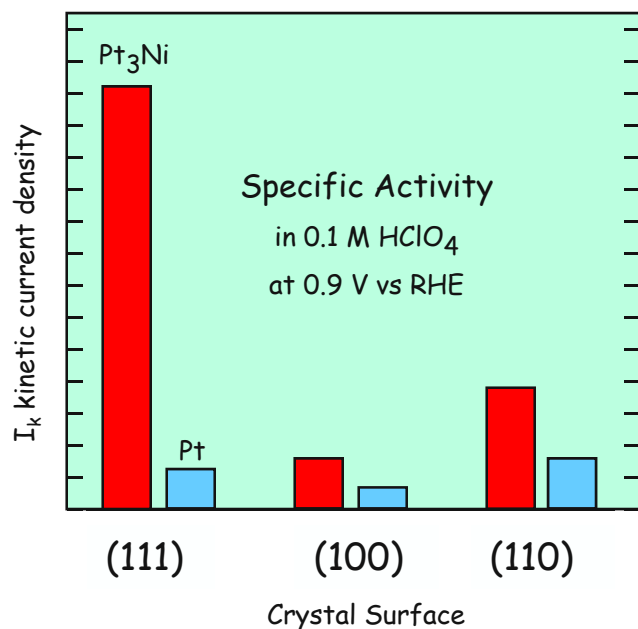
10x greater catalytic activity in Pt₃Ni with a (111) surface means
 10x less Pt
 10x higher reaction rate

Surface catalysis controlled by subsurface structure

Continuous tuning by subsurface composition

Tune surface electronic structure and bond strength

Predictable by density functional theory of the effect of d-band impurities



Other substitutions:

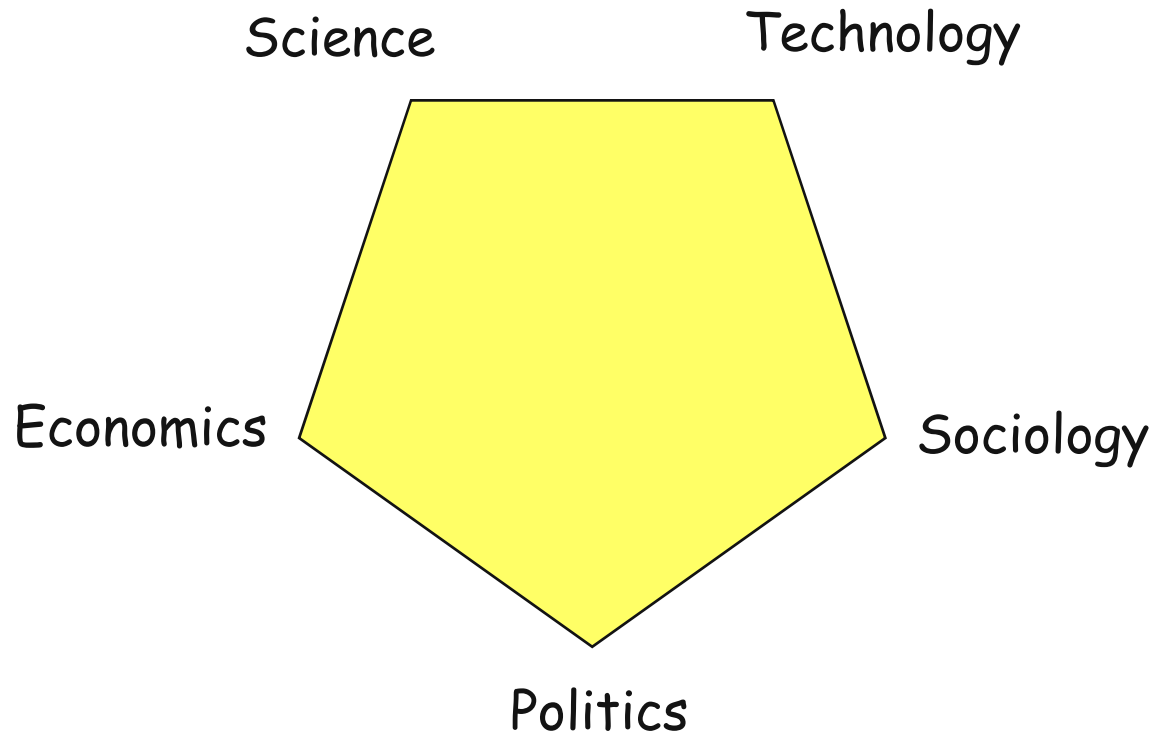
| | | | | |
|----|----|----|----|----|
| 25 | 26 | 27 | 28 | 29 |
| Mn | Fe | Co | Ni | Cu |

Energy Research: Forefront and Challenges

Outline

- Introduction – the energy challenge
- Energy alternatives and the materials challenge
- Think big, go small
- Science and Policy Perspectives

Energy: a BIG Complex System



- no one dimensional solutions will work
- transition to renewable energy requires confluence of all elements

Perspective

- Grand energy challenge
 - Double by 2050, triple by 2100
 - Supply, security, pollution, climate
 - Complex emergent system- cannot predict distant outcomes
- Efficient energy conversion is key for production, storage and use
- Materials and nanoscience are key to energy conversion
- Discovery science is needed, incremental advances not sufficient
- Basic research investments today create energy alternatives tomorrow

Summary and Policy Issues

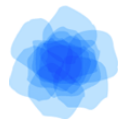
- A mix of future sustainable energy conversion technologies will be needed
- New materials and nanoscience discoveries are necessary to its development
- Strong interplay between basic and applied sciences is a key to success
- Interdisciplinary approaches, and coupling theory/experiment are vital
- Working with industry at all stages is a key factor
- The challenges and constraints are global and complementary among different countries
- International collaboration and networking must be encouraged and supported



European Commission



Lisbon 2007 Declaration
On
**International Cooperation in
Materials Research:
Key to Meeting Energy
Needs and Addressing Climate Change**
Conclusions of the
First World Materials Summit
Held under the auspices of:
Portuguese European Presidency
Lisbon
5th October 2007



PORTUGAL 2007

Materials Scientists Meet in Lisbon and Unite to Battle Climate Change

- (1) To produce internationally agreed strategic plans (“road maps”) for the development of new and improved materials and the products for future energy technologies.
- (2) To bring together leading academic, public sector and industrial scientists in a series of focused workshop meetings, to discuss important technical issues, to ensure that key problems are tackled in a swift and effective manner. Several topics have already been selected and the agenda has been prepared:
 - Transformation and recycling of CO₂ into a new raw material,
 - Hydrogen generation and storage,
 - Clean Coal Technology,
 - Nuclear energy: Fusion and Fission, in particular for hydrogen production
 - Fuel Cells Technologies (Sydney 2008)
- (3) To identify and train a new generation of young international leaders for leveraging materials science and technology for clean energy research and development.
- (4) To promote major new international collaborative materials research programs relevant to future energy technologies.
- (5) To provide information to global, regional and national policy makers, and to investment analysts in the energy sector.
- (6) To ensure that manufacturers in the energy sector, especially small and medium enterprises, have the best possible access to information related to innovative materials developments.
- (7) To interface with other key international organizations relevant to the energy sector or involved in energy-related materials research.
- (8) To stimulate public interest in, and awareness of, energy-related issues.
- (9) To attract and nurture the young generation of scientists and engineers to meet the mega challenge of clean energy sustainability and growth through providing a clear picture of the challenges, opportunities and career paths.