

First in a Series  
OSTP presents  
*Hot Topics in Science and Technology*

# Nanotechnology: Energizing Our Future

Wednesday, August 10<sup>th</sup>

10 am – noon

EEOB 476

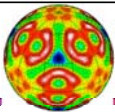
## Web Coverage

[http://www.sc.doe.gov/bes/presentations/archives\\_10AUG05.html](http://www.sc.doe.gov/bes/presentations/archives_10AUG05.html)

A panel of distinguished speakers will describe for a general audience how nanotechnology could revolutionize our homes, vehicles, and energy sources.

- 10:00 **Introductory Remarks**  
Richard Russell, Deputy Director of Technology, OSTP
- 10:10 **Energy Needs: The Big Picture**  
Patricia Dehmer, Director, Basic Energy Sciences,  
Office of Science, DOE
- 10:30 **Nanotechnology 101**  
Paul Alivisatos, Lawrence Berkeley National Laboratory
- 10:50 **Nanotechnology for the Hydrogen Economy**  
George Crabtree, Argonne National Laboratory
- 11:10 **Nanotechnology for Solar Energy**  
Prof. Nathan Lewis, California Institute of Technology
- 11:30 **Nanotechnology for Solid-State Lighting**  
Harriet Kung, Director, Materials Sciences Division,  
Basic Energy Sciences, Office of Science, DOE
- 11:50 **Wrap-up**

*Hors d'oeuvres will be served before and after the event  
in the Indian Treaty Room.*



# Some Energy Facts ...

... and their implications for R&D needed to assure a secure energy future

OSTP Series  
Hot Topics in Science and Technology  
Nanotechnology: Energizing Our Future

Patricia M. Dehmer  
Director, Office of Basic Energy Sciences  
Office of Science, U.S. Department of Energy  
10 August 2005



## Contents

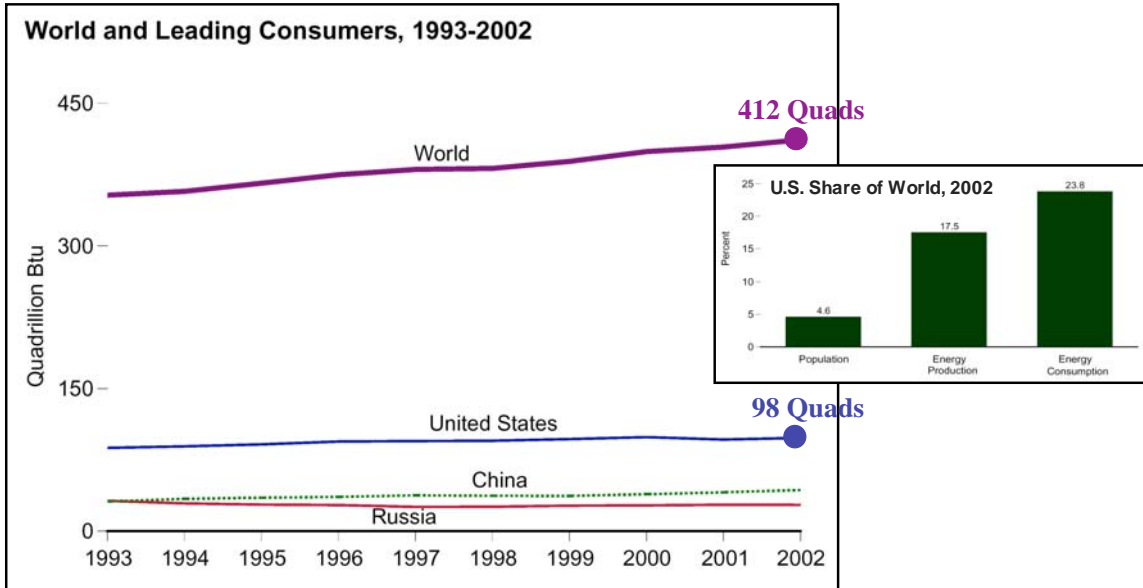
1. Energy consumption today and through the 21<sup>st</sup> century
2. Energy flow diagrams for the U.S.
3. Energy reserves
4. Renewable energy today with speculations on the future
5. Energy and the environment
6. A summary “boxology” of energy R&D areas
7. Why nanoscience and nanotechnology?



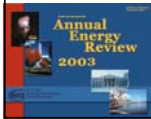
References  
are given in  
the corner

Notes are provided in the blue boxes.

## U.S. and World Energy Consumption Today

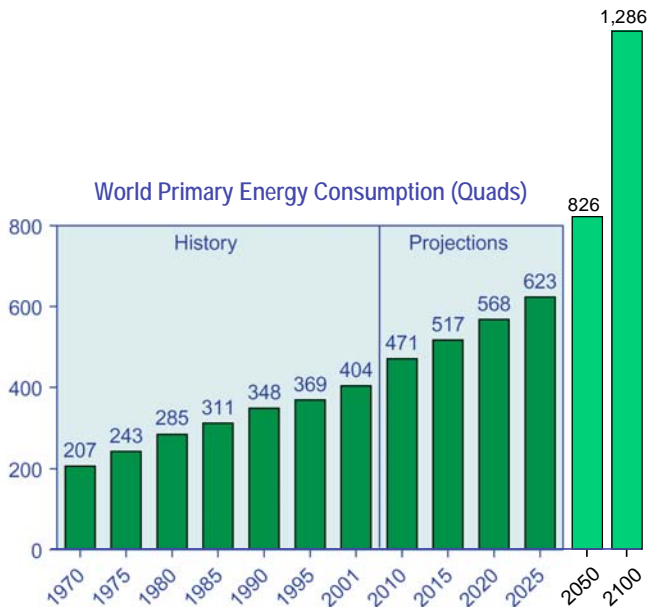


Some equivalent ways of referring to the energy used by the U.S. in 1 year (approx. 100 Quads)



- |   |  |
|---|--|
| 100.0 quadrillion British Thermal Units (Quads) | U.S. & British unit of energy                          |
| 105.5 exa Joules (EJ)                           | Metric unit of energy                                  |
| 3,346 terawatt-years (TW-yr)                    | Metric unit of power (energy/sec)x(#seconds in a year) |

## Projected World Energy Consumption in the Coming Century

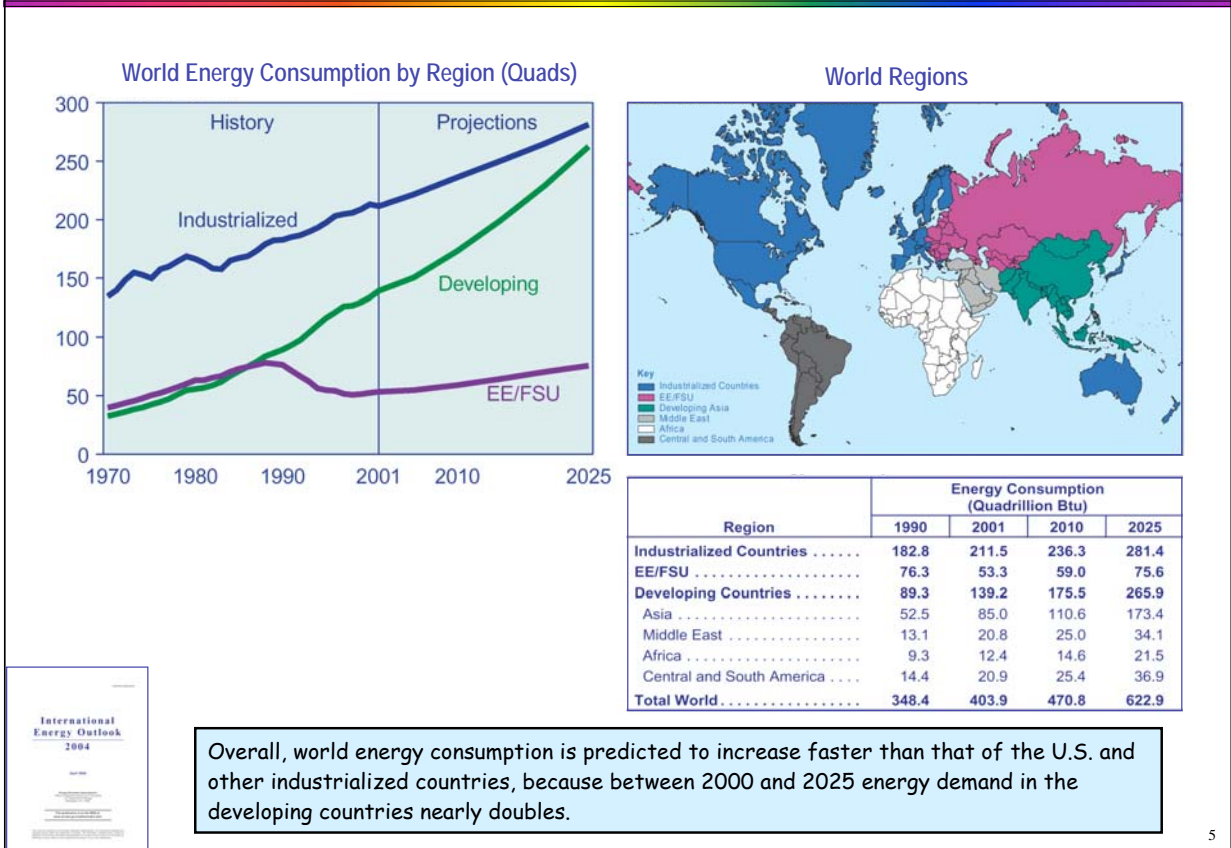


Projections to 2025 are from the Energy Information Administration, International Energy Outlook, 2004.

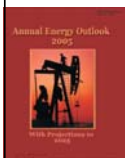
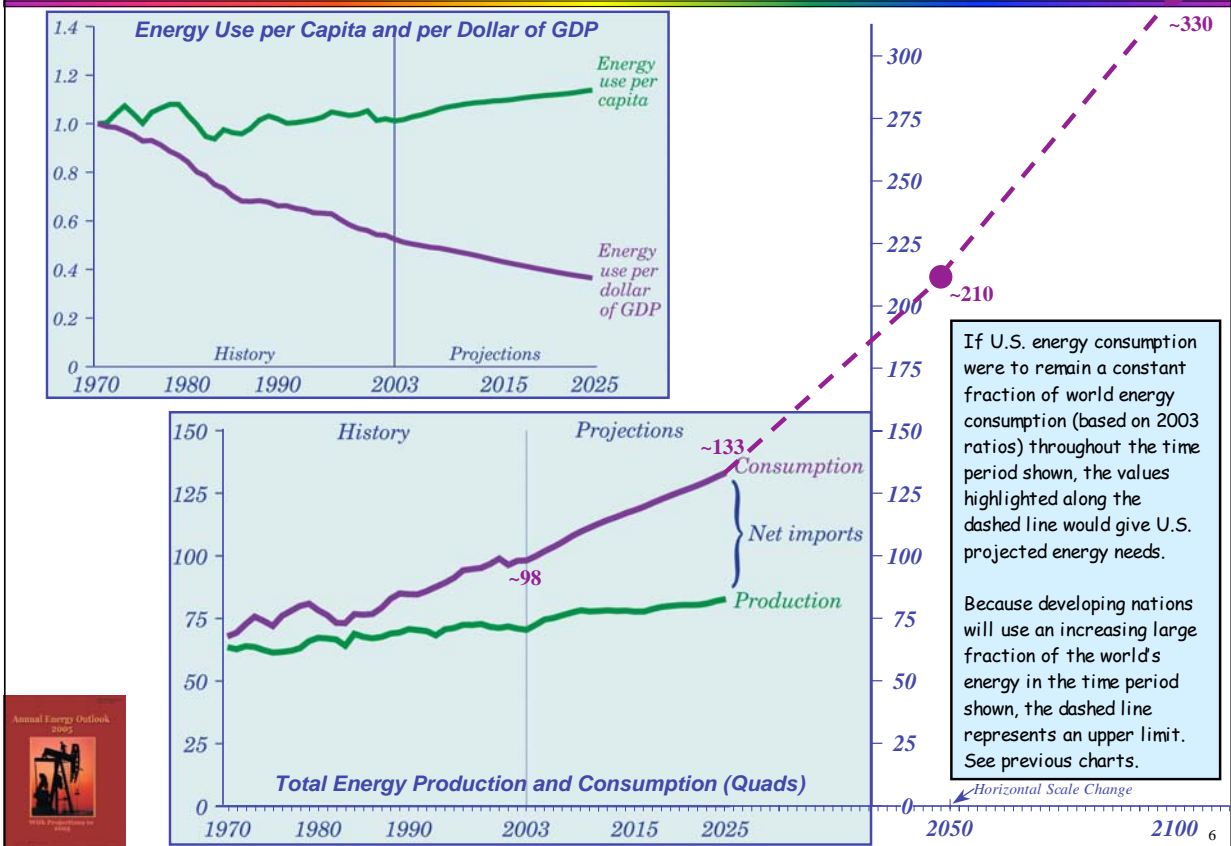
Projections for 2050 and 2100 are based on a scenario from the Intergovernmental Panel on Climate Change (IPCC), an organization jointly established in 1988 by the World Meteorological Organization and the United Nations Environment Programme. The IPCC provides comprehensive assessments of information relevant to human-induced climate change. The scenario chosen is based on "moderate" assumptions (Scenario B2) for population and economic growth and hence is neither overly conservative nor overly aggressive.



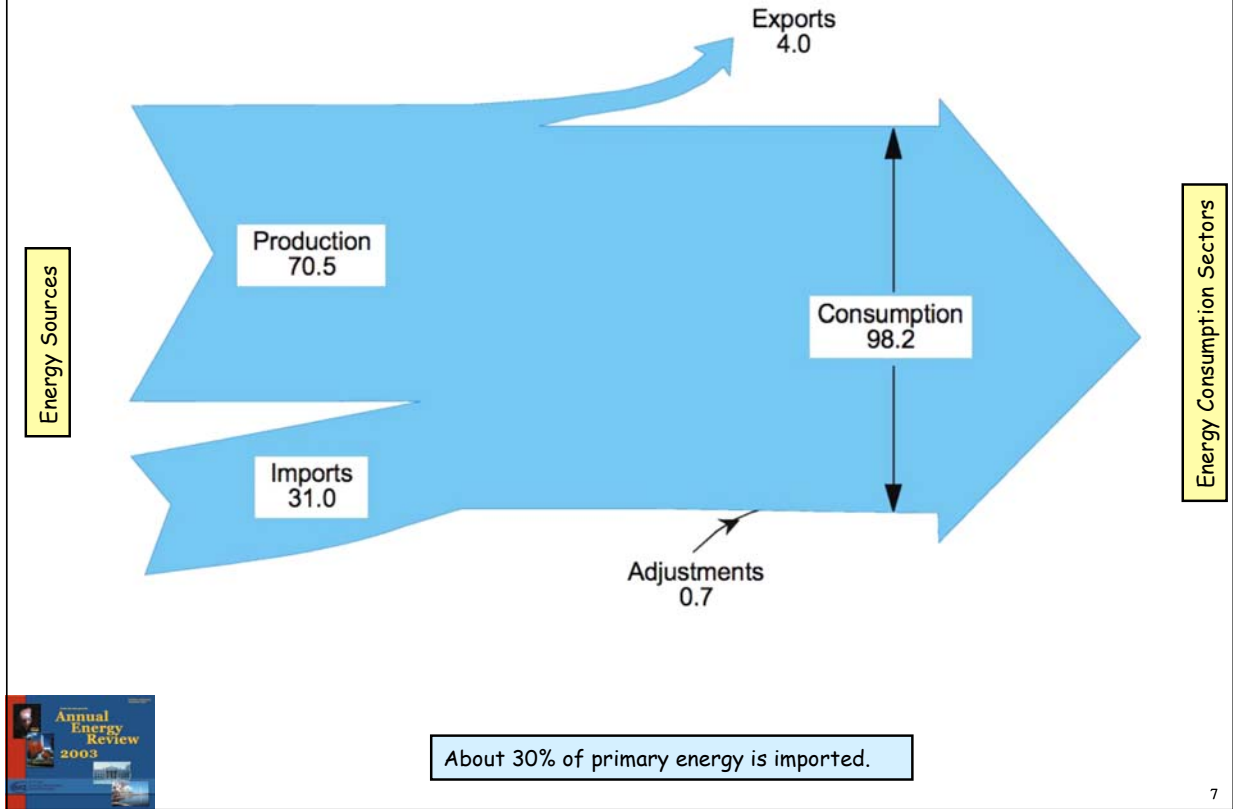
## Projected World Energy Consumption by Region



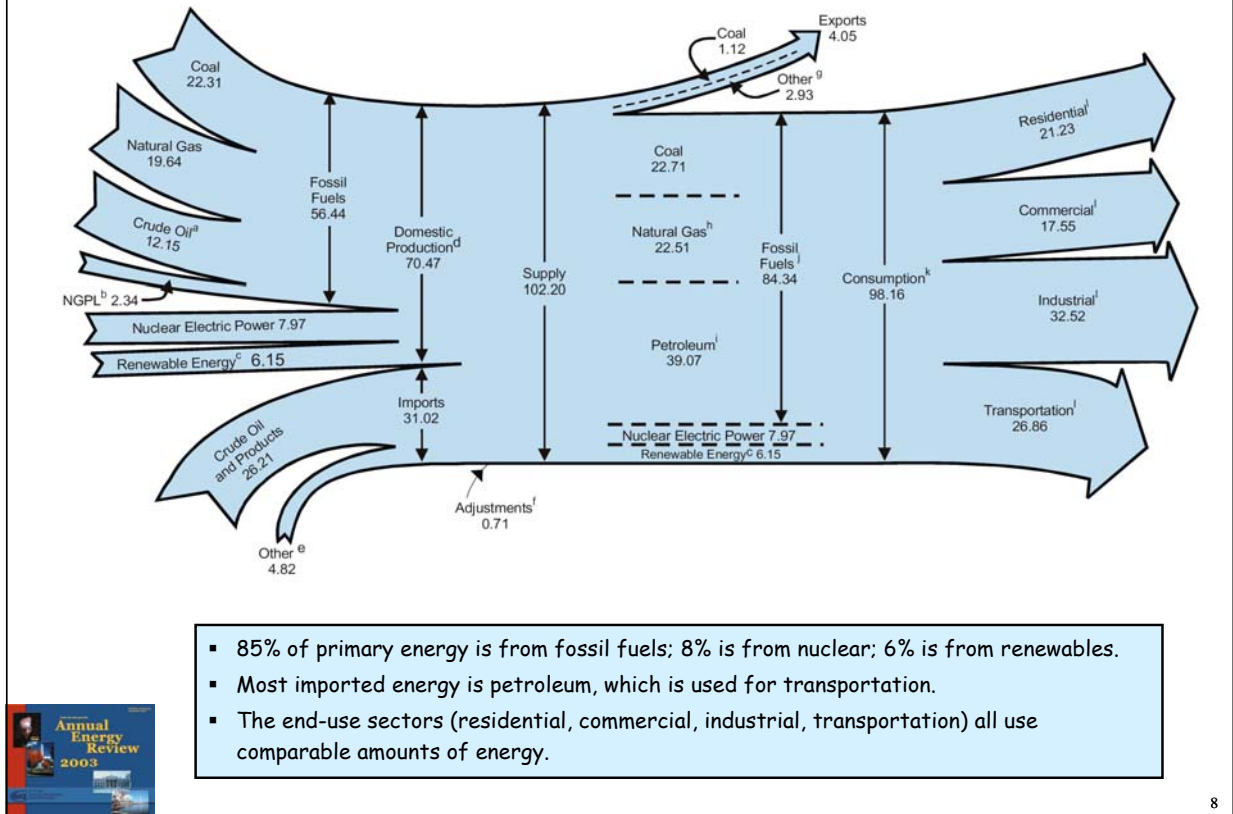
## Projected U.S. Energy Consumption in the Coming Century



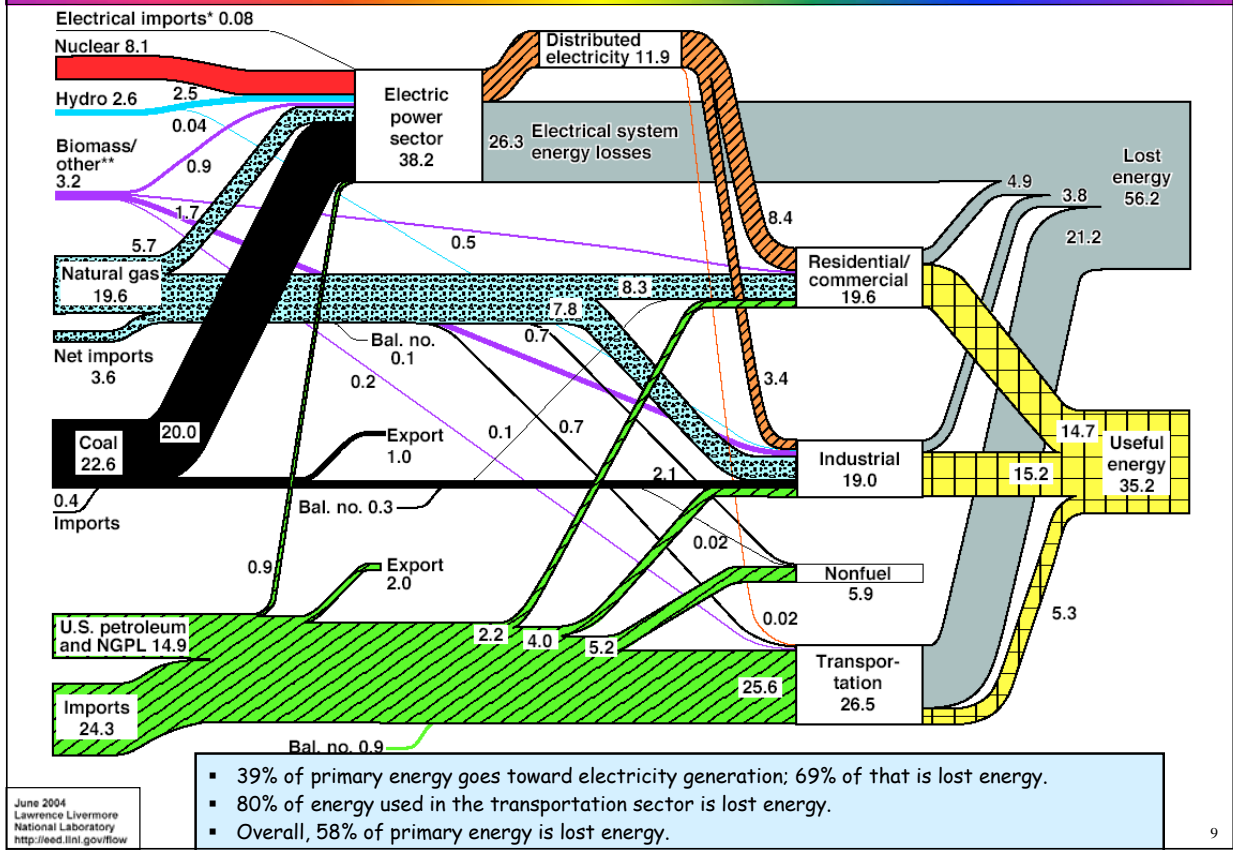
## U.S. Energy Flow, 2003 (Quads)



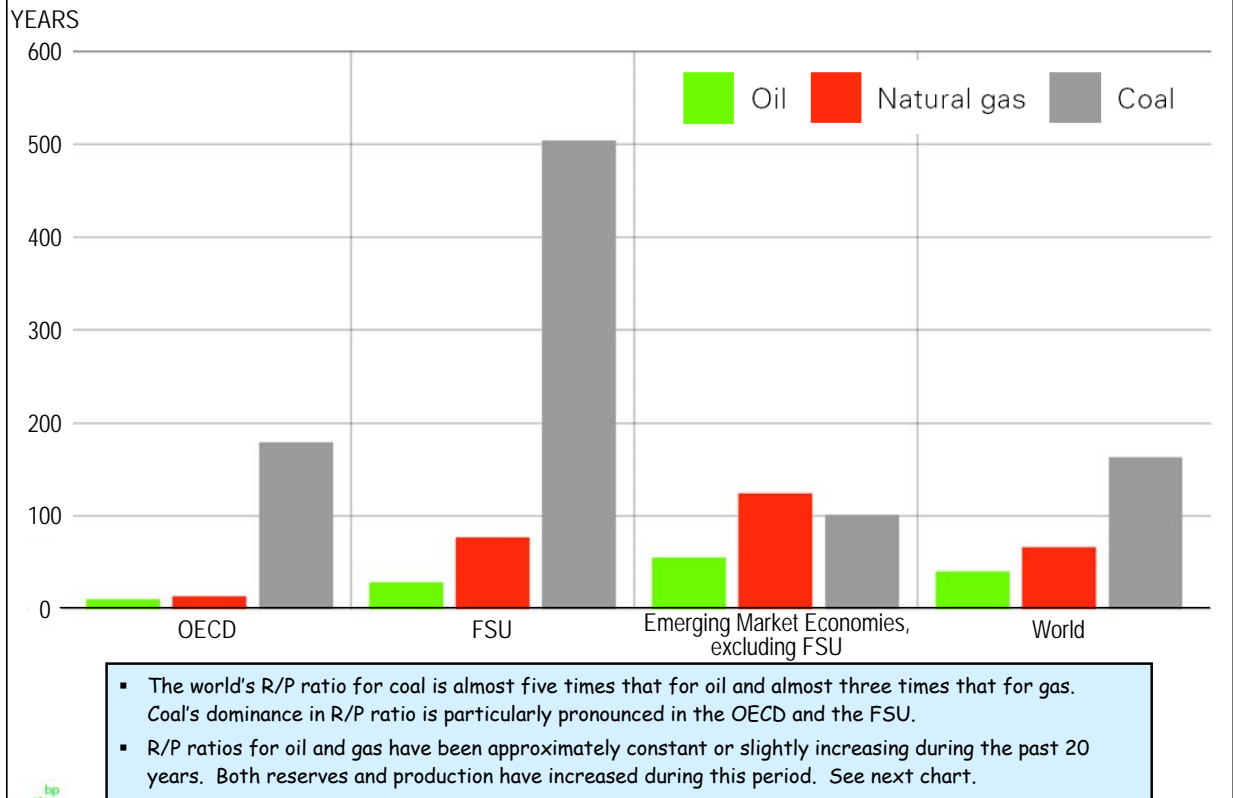
## U.S. Energy Flow, 2003 (Quads)



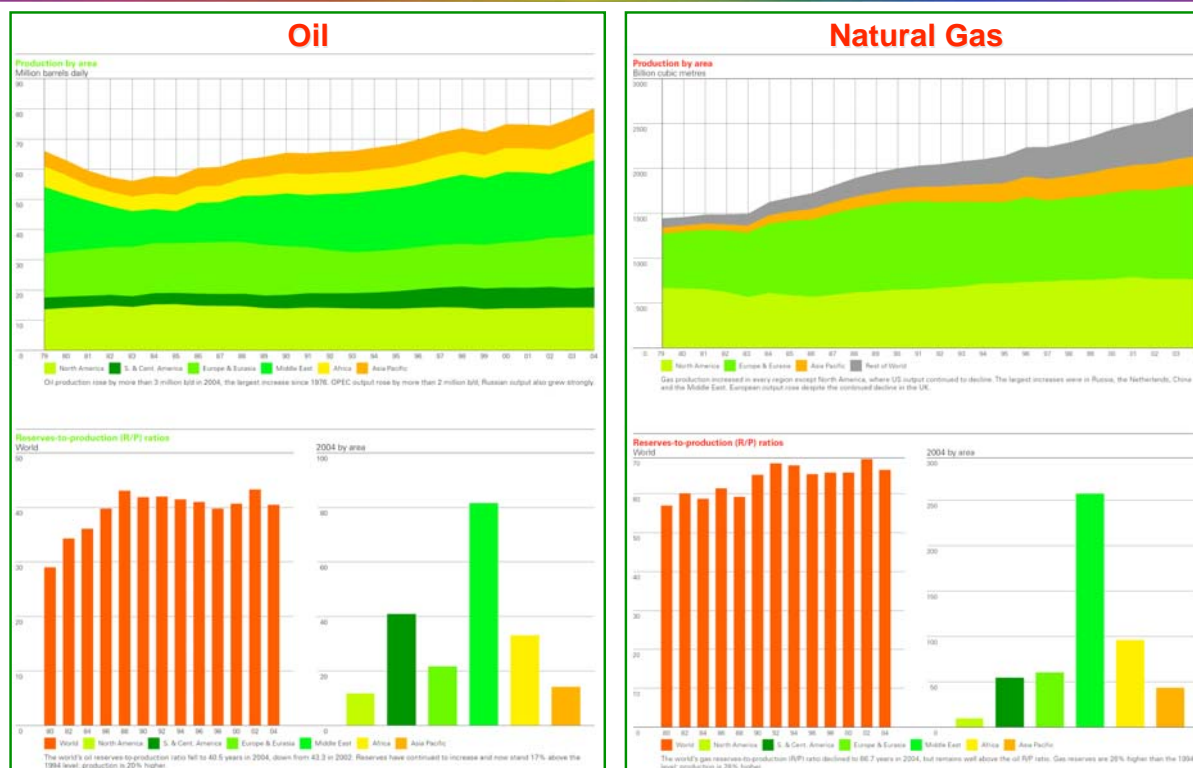
## U.S. Energy Flow, 2002 (Quads)



## Fossil Fuel Reserves-to-Production (R/P) Ratios at End 2004



## Reserves-to-Production (R/P) Ratios at End 2004



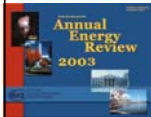
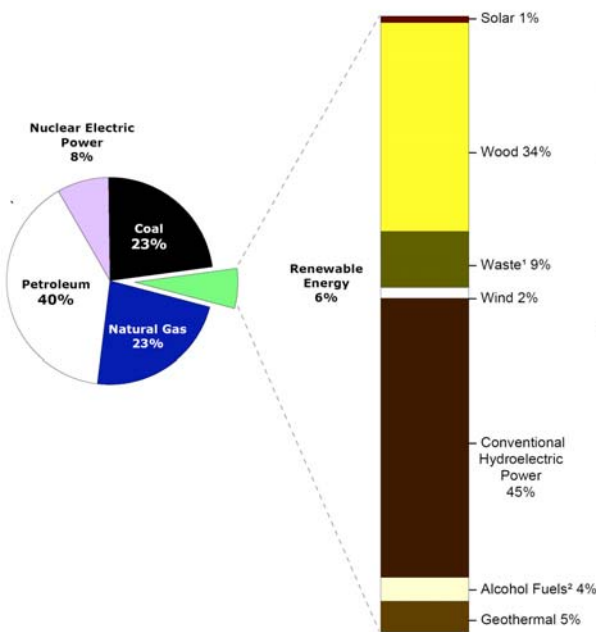
## 36 Estimates of the Time of the Peak of World Oil Production (There are More)

Published	By	Peak Year/Range	Published	By	Peak Year/Range
1972	ESSO	About 2000	1999	Parker	2040
1972	UN	By 2000	2000	Bartlett	2004 or 2019
1974	Hubbert	1991-2000	2000	Duncan	2006
1976	UKDOE	About 2000	2000	EIA	2021-2167; 2037 most likely
1977	Hubbert	1996	2000	IEA (WEO)	Beyond 2020
1977	Ehrlich, et al.	2000	2001	Deffeyes	2003-2008
1979	Shell	Plateau by 2004	2001	Goodstein	2007
1981	World Bank	Plateau around 2000	2002	Smith	2010-2016
1985	Bookout	2020	2002	Campbell	2010
1989	Campbell	1989	2002	Cavallo	2025-2028
1994	Ivanhoe	OPEC Plateau 2000-2050	2003	Greene, et al.	2020-2050
1995	Petroconsultants	2005	2003	Laherrère	2010-2020
1997	Ivanhoe	2010	2003	Lynch	No visible peak
1997	Edwards	2020	2003	Shell	After 2025
1998	IEA (WEO)	2014	2003	Simmons	2007-2009
1998	Campbell/Laherrère	2004	2004	Bakhitari	2006-2007
1999	Campbell	2010	2004	CERA	After 2020
1999	Odell	2060	2004	PFC Energy	2015-2020

EIA's short answer to "When will oil production peak?" is "Not soon, but within the present century." The most probable scenarios put the peak at about mid century.

## Renewable Energy Consumption by Major Sources

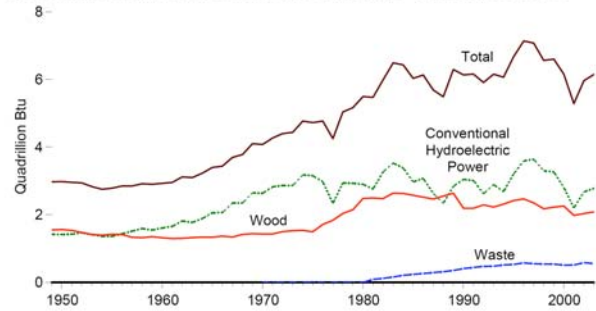
Renewable Energy as Share of Total Energy, 2003



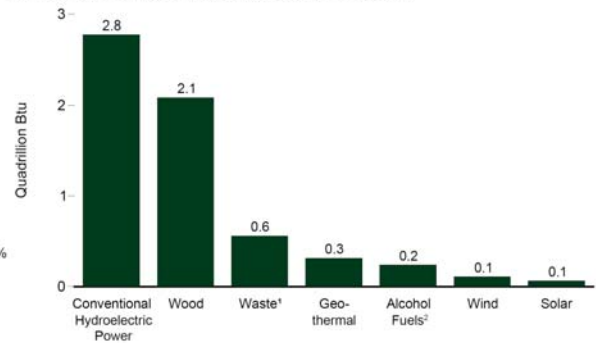
<sup>1</sup> Municipal solid waste, landfill gas, sludge waste, tires, agricultural byproducts, and other biomass.

<sup>2</sup> Ethanol blended into motor gasoline.

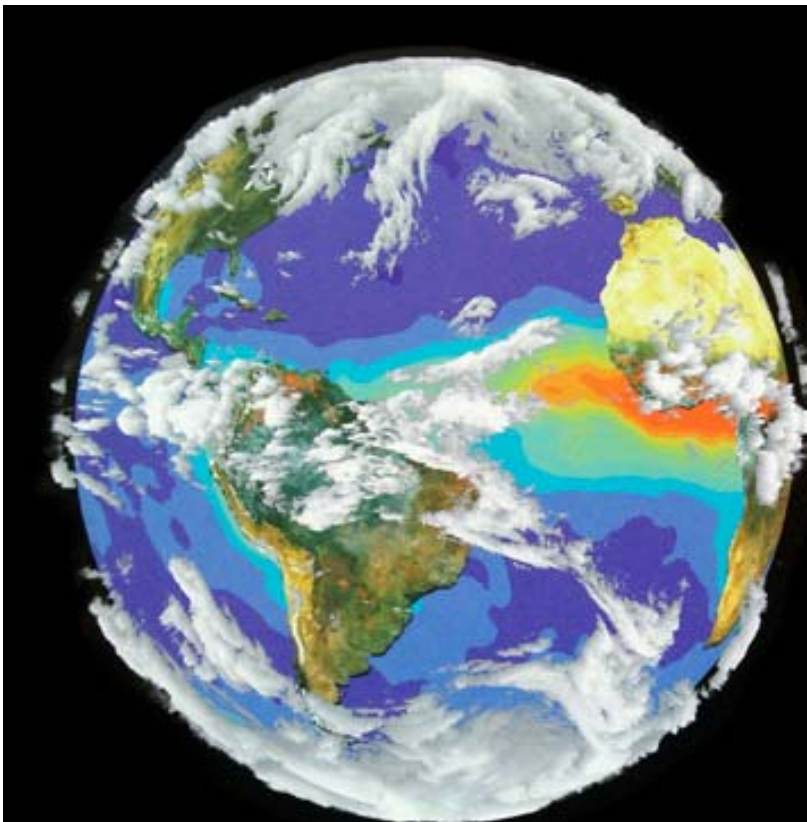
Renewable Energy Total Consumption and Major Sources, 1949-2003



Renewable Energy Consumption by Source, 2003



Note: Because vertical scales differ, graphs should not be compared. Sources: Tables 1.3 and 10.1.



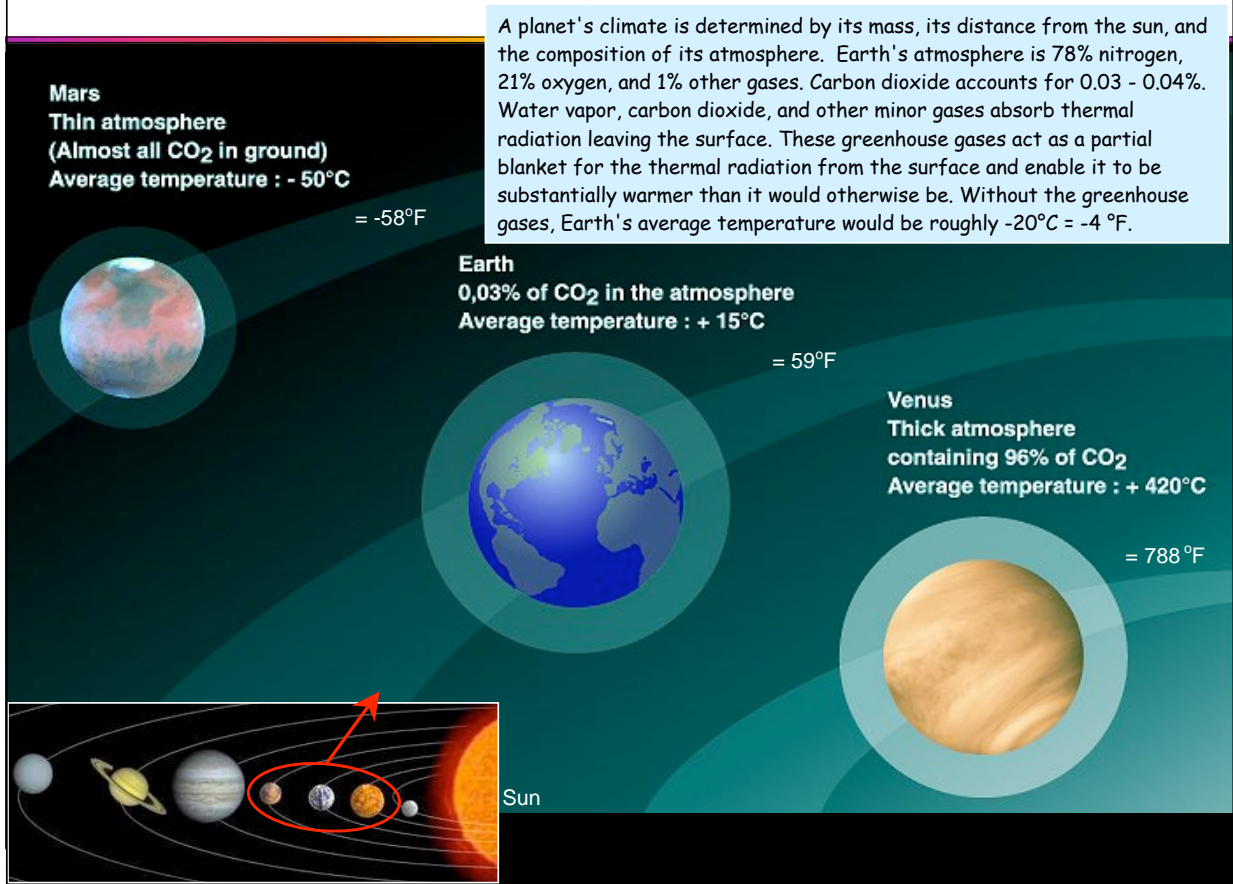
*How do the Earth's land, water, air, and life interact to affect the environment?*

This Earth image is a compilation of data from several different satellites that remotely sense vegetation, clouds, fires, and aerosols.

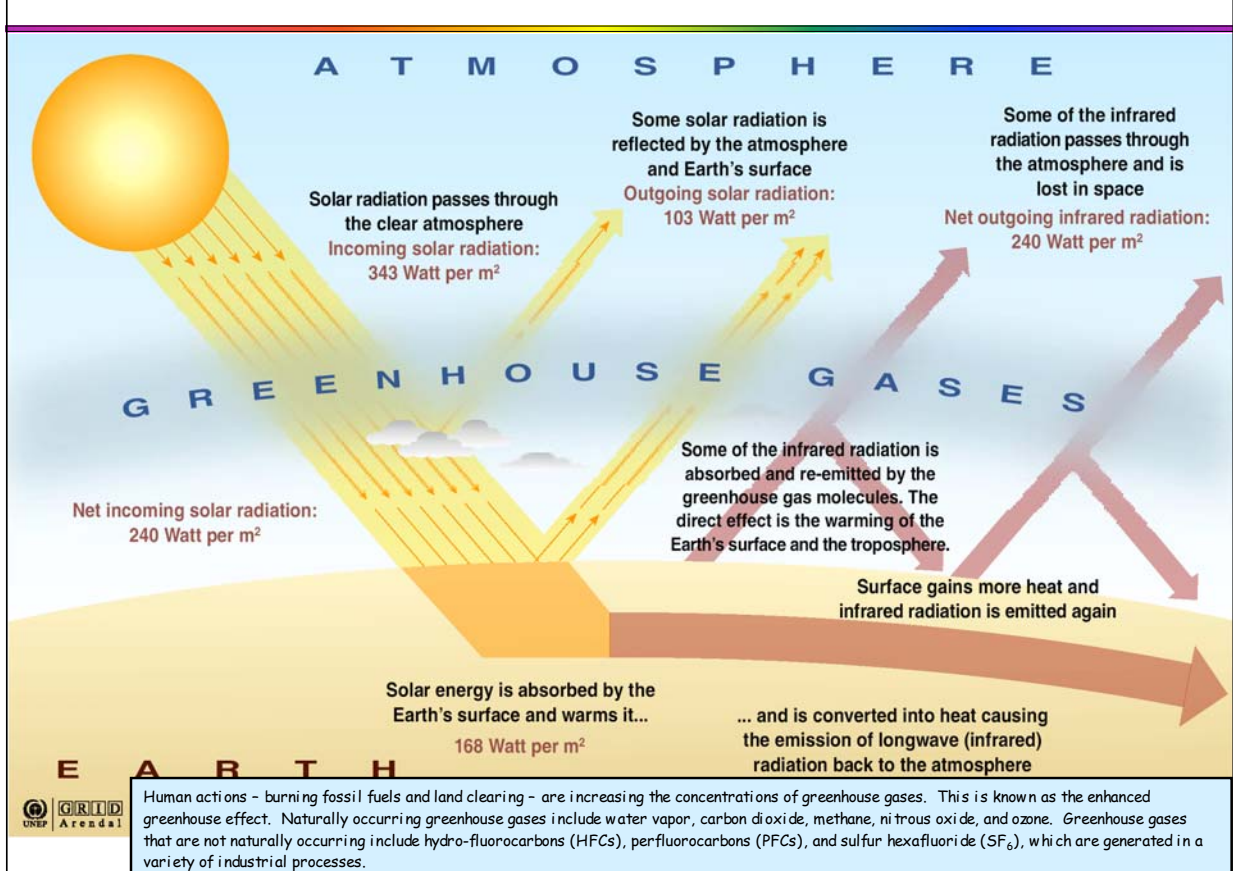
Image Source: NASA, Earth Science Enterprise, *Understanding Our Changing Planet*  
 URL: <http://departments.weber.edu/sciencecenter/nasa/lithographs/126.jpg>



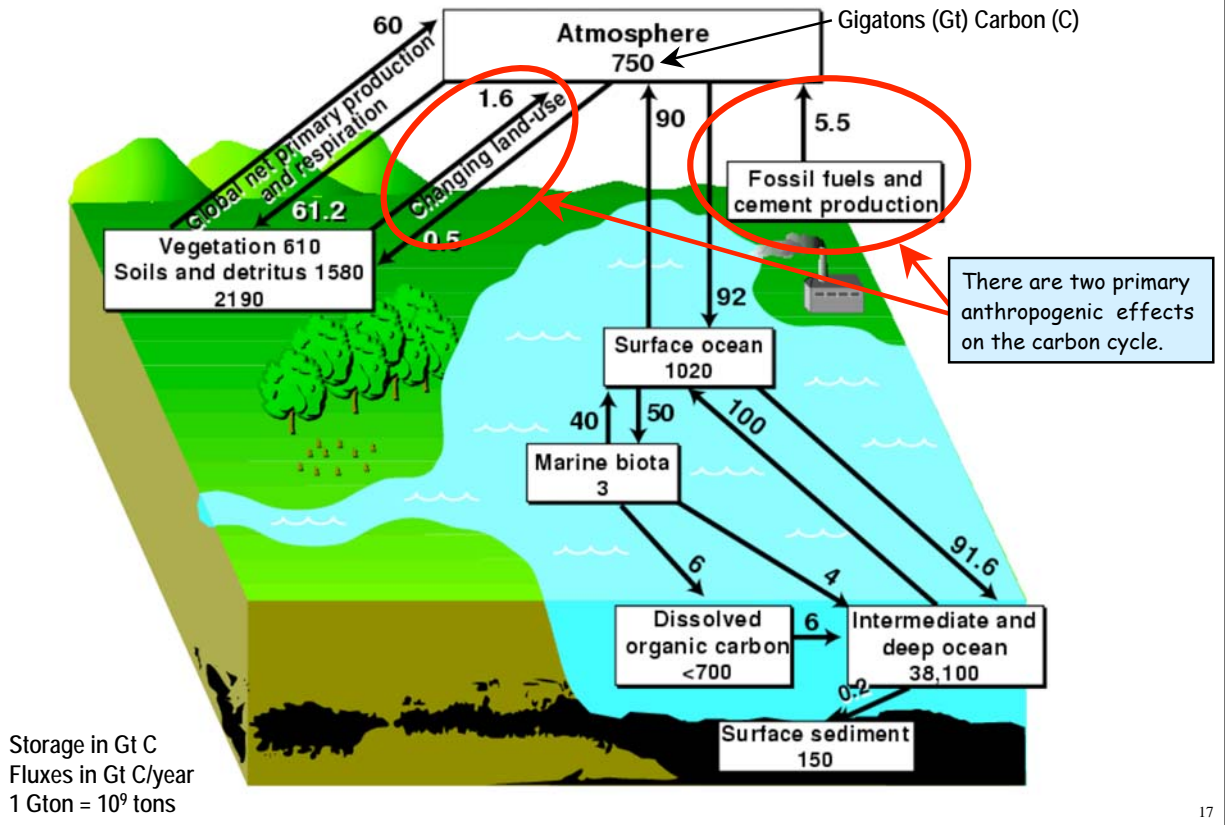
## Planets, Atmospheres, and Climate



## The Greenhouse Effect

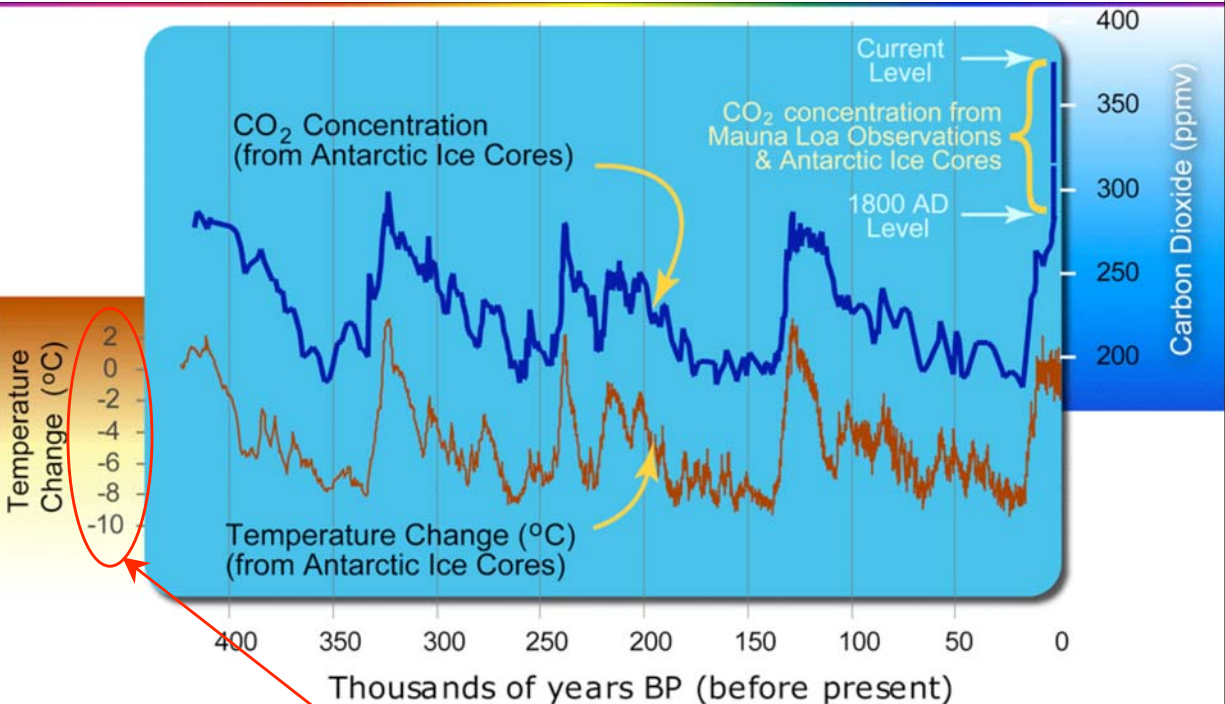


## The Earth's Carbon Cycle



17

## CO<sub>2</sub> Concentrations and Temperature Change



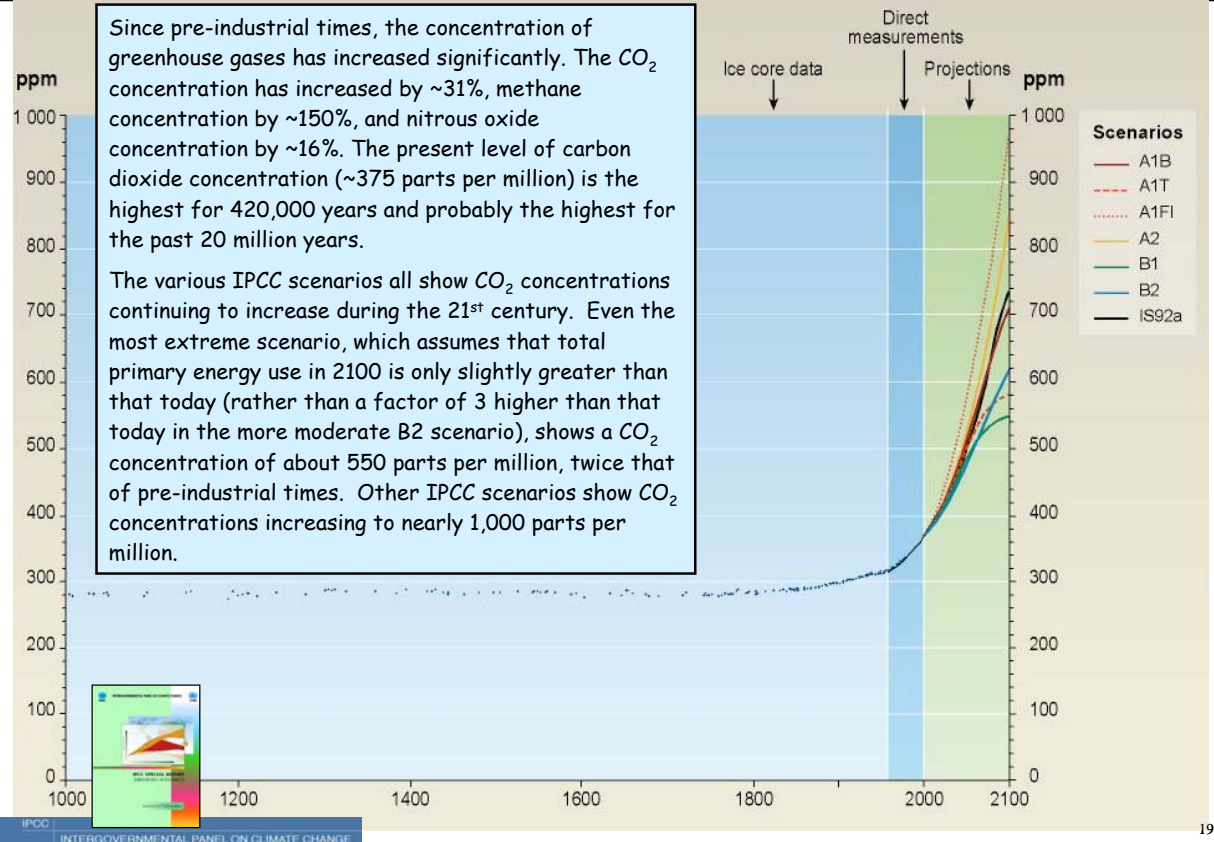
Data Source CO<sub>2</sub>: <ftp://cdiac.ornl.gov/pub/trends/co2/vostok.icecore.co2>  
Data Source Temp: <http://cdiac.esd.ornl.gov/ftp/trends/temp/vostok/vostok.1999.temp.dat>

Note that total temperature change across several ice ages was only about 12°C or about 22°F.

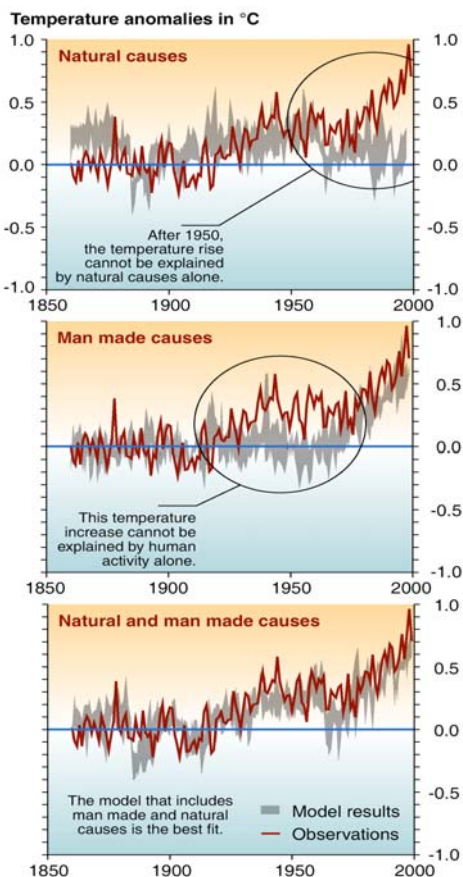


18

## Past and Future CO<sub>2</sub> Atmospheric Concentrations for Various IPCC Scenarios



19



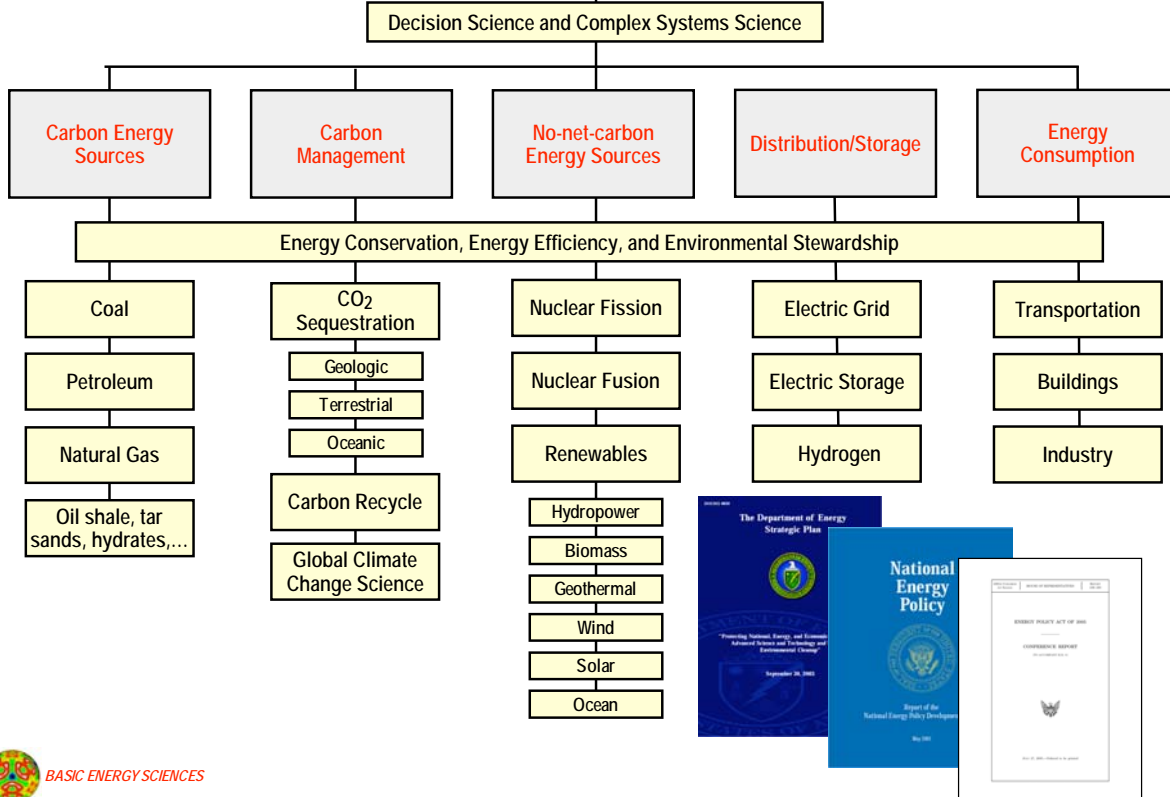
### Climate Models, CO<sub>2</sub> Concentrations, and Temperature Change for Past Data

- Recorded global temperature change can be compared with computer models that predict temperature change under different "forcing" scenarios, (with "forcings" signifying external influences on the solar radiative budget of the planet - greenhouse gases, aerosols, increased solar radiation, and other agents). The charts compare observed temperature anomalies from the historic mean (red line) with the results of computer models that attempt to predict temperature based on the interactions of other environmental influences (gray line).
- The top two charts illustrate that models using natural and anthropogenic influences alone [Natural causes & Man-made causes] fail to match the observed record of temperature anomalies since 1866. But the combination of natural and anthropogenic models [Natural and man-made causes] produces a close match to the measured data. This is seen as a clear "thumbprint" of human impacts on climate change.
- Based on results such as these, the Intergovernmental Panel on Climate Change (IPCC) 2001 report stated that "concentrations of atmospheric greenhouse gases and their radiative forcing have continued to increase as a result of human activities."

20

# Research for a Secure Energy Future

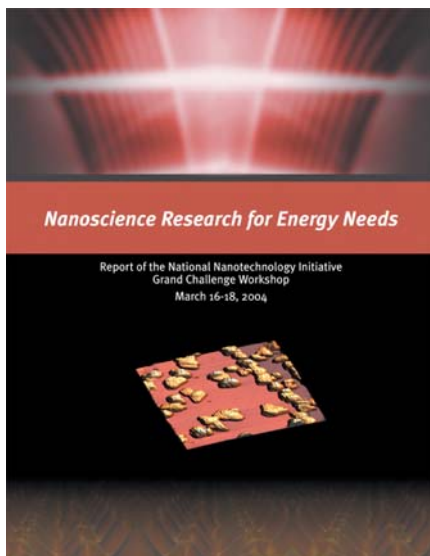
## Supply, Distribution, Consumption, and Carbon Management,



21

## Nanoscience Research for Energy Needs

"All the elementary steps of energy conversion (charge transfer, molecular rearrangement, chemical reactions, etc.) take place on the nanoscale. Thus, the development of new nanoscale materials, as well as the methods to characterize, manipulate and assemble them, creates an entirely new paradigm for developing new and revolutionary energy technologies."



- The workshop identified nine key areas of energy technology in which nanoscience is expected to have a substantial impact:
  - Scalable methods to split water with sunlight for hydrogen production
  - Reversible hydrogen storage materials operating at ambient temperatures
  - Harvesting of solar energy with 20 percent power efficiency and 100 times lower cost
  - Solid-state lighting at 50 percent of the present power consumption
  - Highly selective catalysts for clean and energy-efficient manufacturing
  - Super-strong light-weight materials to improve efficiency of cars, airplanes, etc.
  - Power transmission lines capable of 1 gigawatt transmission
  - Low-cost fuel cells, batteries, thermoelectrics, and ultra-capacitors built from nanostructured materials
  - Materials synthesis and energy harvesting based on the efficient and selective mechanisms of biology
- The strategy for achieving these targets lies in growing R&D efforts in six areas:
  - Catalysis by nanoscale materials
  - Using interfaces to manipulate energy carriers
  - Linking structure and function at the nanoscale
  - Assembly and architecture of nanoscale structures
  - Theory, modeling, and simulation for energy nanoscience
  - Scalable synthesis methods

22

## *A Series of Workshops to Understand Basic Research Needs for Energy*



### **Basic Research Needs to Assure a Secure Energy Future**

**Basic Energy Sciences Advisory Committee Workshop**

**October 21-25, 2002**

*The foundation workshop that set the model for the focused workshops that follow.*

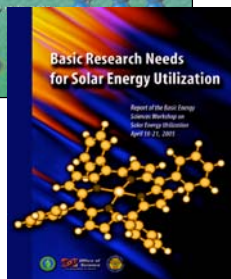


### **Basic Research Needs for the Hydrogen Economy**

**Basic Energy Sciences Workshop**

**May 13-15, 2003**

*Led to BES solicitation in FY 2005 that awarded \$21M in new funding as part of the President's Hydrogen Fuel Initiative.*



### **Basic Research Needs for Solar Energy Utilization**

**Basic Energy Sciences Workshop**

**April 18-21, 2005**

*Heavily attended workshop (>200) with very enthusiastic participation in breakout sessions. Report published in July 2005.*

- Each focused workshop seeks to define the basic research needed to overcome both short-term technology showstoppers and long-term scientific grand challenges.
- Future workshops will examine basic research needs for advanced nuclear reactors including advanced fuel cycles, solid-state lighting, superconductivity, and more.

23

## **ADDITIONAL REFERENCE MATERIALS**

24

## Prefixes and Names for Large and Small Numbers

Metric Prefix	Metric Symbol	Common Name (American and modern British "short scale")	Decimal Equivalent	Exponential
		google <sup>1</sup>		10 <sup>100</sup>
yotta	Y	septillion	1,000,000,000,000,000,000,000,000,000	10 <sup>24</sup>
zetta	Z	sextillion	1,000,000,000,000,000,000,000,000	10 <sup>21</sup>
exa	E	quintillion	1,000,000,000,000,000,000,000	10 <sup>18</sup>
peta	P	quadrillion	1,000,000,000,000,000,000	10 <sup>15</sup>
tera	T	trillion	1,000,000,000,000	10 <sup>12</sup>
giga	G	billion	1,000,000,000	10 <sup>9</sup>
mega	M	million	1,000,000	10 <sup>6</sup>
kilo	k	thousand	1,000	10 <sup>3</sup>
hecto	h	hundred	100	10 <sup>2</sup>
deca	da	ten	10	10 <sup>1</sup>
no prefix		one	1	10 <sup>0</sup>
deci	d	tenth	0.1	10 <sup>-1</sup>
centi	c	hundredth	0.01	10 <sup>-2</sup>
milli	m	thousandth	0.001	10 <sup>-3</sup>
micro	μ	millionth	0.000001	10 <sup>-6</sup>
nano	n	billionth	0.000000001	10 <sup>-9</sup>
pico	p	trillionth	0.000000000001	10 <sup>-12</sup>
femto	f	quadrillionth	0.000000000000001	10 <sup>-15</sup>
atto	a	quintillionth	0.00000000000000001	10 <sup>-18</sup>
zepto	z	sextillionth	0.0000000000000000001	10 <sup>-21</sup>
yocto	y	septillionth	0.000000000000000000001	10 <sup>-24</sup>

<sup>1</sup> Invented more for fun than for use, the googol lies outside the regular naming systems.

25

## Some Useful Conversion Factors

### Approximate conversion factors

#### Crude oil\*

From	To tonnes (metric)	kilolitres	barrels	US gallons	tonnes/year
	<b>Multiply by</b>				
Tonnes (metric)	1	1.165	7.33	307.86	–
Kilolitres	0.8581	1	6.2898	264.17	–
Barrels	0.1364	0.159	1	42	–
US gallons	0.00325	0.0038	0.0238	1	–
Barrels/day	–	–	–	–	49.8

\*Based on worldwide average gravity.

#### Products

From	To convert barrels to tonnes	tonnes to barrels	kilolitres to tonnes	tonnes to kilolitres
	<b>Multiply by</b>			
LPG	0.086	11.6	0.542	1.844
Gasoline	0.118	8.5	0.740	1.351
Kerosene	0.128	7.8	0.806	1.240
Gas oil/diesel	0.133	7.5	0.839	1.192
Fuel oil	0.149	6.7	0.939	1.065

#### Natural gas and LNG

From	To billion cubic metres NG	billion cubic feet NG	million tonnes oil equivalent	million tonnes LNG	trillion British thermal units	million barrels oil equivalent
	<b>Multiply by</b>					
1 billion cubic metres NG	1	35.3	0.90	0.73	36	6.29
1 billion cubic feet NG	0.028	1	0.026	0.021	1.03	0.18
1 million tonnes oil equivalent	1.111	39.2	1	0.805	40.4	7.33
1 million tonnes LNG	1.38	48.7	1.23	1	52.0	8.68
1 trillion British thermal units	0.028	0.98	0.025	0.02	1	0.17
1 million barrels oil equivalent	0.16	5.61	0.14	0.12	5.8	1

#### Units

1 metric tonne = 2204.62 lb  
= 1.1023 short tons  
1 kilolitre = 6.2898 barrels  
1 kilolitre = 1 cubic metre  
1 kilocalorie (kcal) = 4.187 kJ = 3.968 Btu  
1 kilojoule (kJ) = 0.239 kcal = 0.948 Btu  
1 British thermal unit (Btu) = 0.252 kcal  
= 1.055 kJ  
1 quadrillion British thermal units (Btus)  
= 1 Quad = 1.055 exa Joules (EJ)  
= 0.03346 terawatt-year (TW-year)

1 kilowatt-hour (kWh) = 860 kcal  
= 3600 kJ = 3412 Btu

#### Caloric equivalents

One tonne of oil equivalent equals approximately:

Heat units	10 million kilocalories 42 gigajoules 40 million Btu
Solid fuels	1.5 tonnes of hard coal 3 tonnes of lignite
Gaseous fuels	see natural gas and LNG table
Electricity	12 megawatt-hours

One million tonnes of oil produces about 4500 gigawatt-hours (= 4.5 terawatt-hours) of electricity in a modern power station.



## Projected World Energy Consumption in the Coming Century

### How much energy will the world need in the coming century?

The most widely used scenarios for future world energy consumption have been those developed by technical experts brought together by the Intergovernmental Panel on Climate Change (IPCC), an organization jointly established by the World Meteorological Organization (WMO) and the United Nations Environment Programme (UNEP). A scenario from their most recent set is illustrated in Table 1. Though this scenario should not be thought of as any more probable than the others in the set, it is based on "moderate" assumptions on population and economic growth, and hence can be viewed as neither overly conservative nor overly aggressive. The quantities listed and defined in Table 1 are fundamental factors, such as population (N), per capita GDPs (GDP/N), and energy consumption intensities (energy consumed per unit of GDP,  $\dot{E}/\text{GDP}$ ), underlying the energy consumption rate ( $\dot{E}$ ):

$$\dot{E} = N \cdot (\text{GDP}/N) \cdot (\dot{E}/\text{GDP}).$$

One can see from this Table that as population and per capita gross domestic product increase, even as energy consumption intensity decreases (due to improved energy-usage-efficiency), the energy consumption rate is projected to double and then triple, from 12.9 TW in 2000 to 27.6 TW in 2050 and 43.0 TW in 2100.

Quantity	Definition	Units	2000	2050	2100
N	Population	Billion persons	6.1	9.4	10.4
GDP	Gross Domestic Product	TS/yr	28	110	235
GDP/N	per capita Gross Domestic Product	\$(/person-yr)	4,640	11,650	22,590
$\dot{E}/\text{GDP}$	Energy Consumption Intensity	W/(\$/yr)	0.46	0.25	0.18
$\dot{E}$	Energy Consumption Rate	TW	12.9 <sup>2</sup>	27.6	43.0
C/E	Carbon Emission Intensity	kgC/(W·yr)	0.62	0.40	0.31
$\dot{C}$	Carbon Emission Rate	GtC/yr	8.0	11.0	13.3
$\dot{C}$	Equivalent CO <sub>2</sub> Emission Rate	GtCO <sub>2</sub> /yr	29.3	40.3	48.8

Table 1: Energy Statistics and Projections.<sup>3</sup>

<sup>2</sup> This quantity is slightly lower than that estimated in *International Energy Outlook 2004* (U.S. Department of Energy Energy Information Administration, 2004) ([http://www.eia.doe.gov/oiat/ieo/pdf/0484\(2004\).pdf](http://www.eia.doe.gov/oiat/ieo/pdf/0484(2004).pdf)):  $\dot{E} = (398.9 \text{ Quads/yr}) \cdot (33.4 \text{ GWyr/Quad}) \cdot (10^{-3} \text{ TW/GW}) = 13.3 \text{ TW}$ .

<sup>3</sup> After scenario B2, as discussed in Nebojsa Nakicenovic and Rob Swart, Eds., *Special Report on Emissions Scenarios* (Intergovernmental Panel on Climate Change, 2000) (<http://www.grida.no/climate/ipcc/emission/index.htm>).

27

## IPCC Socioeconomic Scenarios for Climate Modeling

**The A1 scenario** describes a future world of very rapid economic growth, a global population that peaks in mid-century and declines thereafter, and the rapid introduction of new and more efficient technologies. Specific regional patterns tend to disappear as a result of increased cultural and social interaction. The gap between regions, regarding per capita income, reduces substantially. This scenario develops into three groups that describe alternative in the development of energy supply: fossil intensive (A1FI), non-fossil energy sources (A1T), or a balance (A1B) across all sources.

**The B1 scenario** describes a convergent world with a population that peaks in mid-century and declines thereafter (as in the A1 scenario), but with a rapid change in economic structures towards a service and information economy, with reductions in material intensity and the introduction of clean and resource efficient technologies. The emphasis is on global solutions to economic, social and environmental sustainability, including improved equity, but without additional climate initiatives.

MORE  
MARKET-ORIENTED

**The A2 scenario** describes a very heterogeneous world, based on the continued separation and preservation of local identities. Fertility patterns across regions converge very slowly, which results in a continuously increasing population. Economic development is regionally oriented and per capita economic growth and technological change more fragmented and slower than in the A1 scenario.

MORE  
GLOBAL

MORE  
REGIONAL

MORE  
ENVIRONMENTAL

**The B2 scenario** describes a world in which the emphasis is on local solutions to economic, social, and environmental sustainability rather than the global approach in B1. It is a world with a continuously increasing global population, but at a slower rate than other scenarios, intermediate levels of economic development, and slow but diverse technological change. Society is oriented towards environmental protection and social equity, and focuses on the local and regional level.

28

## About the Speaker

### Biography

#### Patricia M. Dehmer

Patricia Dehmer is the Director of the Office of Basic Energy Sciences in the Department of Energy's Office of Science. She holds a B.S. in Chemistry from the University of Illinois and a Ph.D. in Chemical Physics from the University of Chicago. After spending more than 20 years as a research scientist and group leader at Argonne National Laboratory, she joined the Department of Energy in 1995. In her current position, she oversees a budget of more than \$1 billion for research in materials sciences, chemistry, geosciences, and biosciences and for the construction and operation of third- and fourth-generation light sources, high-flux neutron sources, and specialized facilities for microcharacterization, nanoscale materials synthesis, combustion research, and ion beam studies. During the ten years that Dr. Dehmer has led the Office of Basic Energy Sciences, she has initiated more than \$3 billion in construction of scientific user facilities and instrumentation for them, and she has led strategic planning for research related to energy needs and for discovery science and articulation of the grand challenges that link the formerly disparate disciplines of chemistry, condensed matter and materials physics, biology, and computational sciences. Several of the recent studies that her office led (*Basic Research Needs to Assure a Secure Energy Future*, *Basic Research Needs for the Hydrogen Economy*, *Basic Research Needs for Solar Energy Utilization*, and a number of studies on nanoscale science) serve as the basis for today's OSTP briefing.

Dr. Dehmer has held many elected positions in the American Physical Society (APS), the American Association for the Advancement of Science, and the Gordon Research Conferences. She has served as the Chair of the APS Nominating Committee, a member of the APS Council and its Executive Committee, and as Chair of the APS Divisions of Atomic, Molecular, and Optical Physics and Laser Science. She has published 125 papers and given hundreds of scientific and science policy talks.



## Nanoscience and technology in six easy pieces

- The missing length scale
- One at a time
- It takes care of itself –defect tolerance
- High performance at large scales
- The energy connection
- Inspiration from nature- the hybrid system

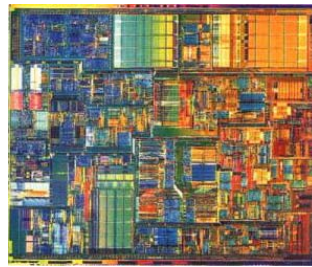
Paul Alivisatos

Assoc. Director for Physical Sciences, Lawrence Berkeley National Lab  
Professor of Chemistry and Materials Science, University of California, Berkeley  
alivis@berkeley.edu

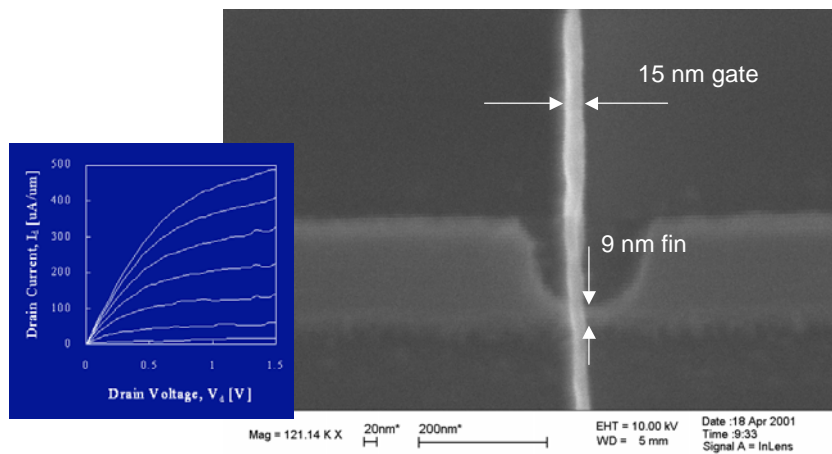
## From Democritus to Gordon Moore



Democritus  
(400 BC)



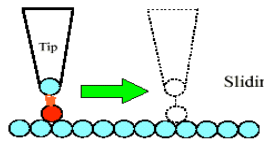
Gordon Moore



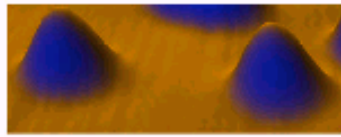
Bokor, King, Hu  
UCB Device Group

*Nano-silicon FinFET with 15 nm gate and 9 nm fin. This is a fully functional MOS transistor with excellent electrical performance.*

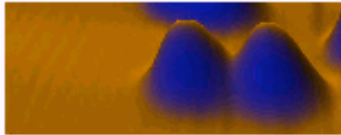
## Atom Manipulation: then and now



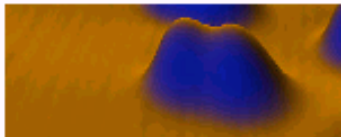
### Building a Ni Dimer on Au(111)



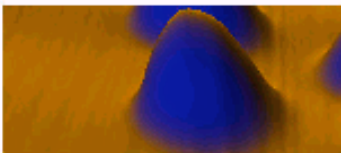
$r \sim 25 \text{ \AA}$



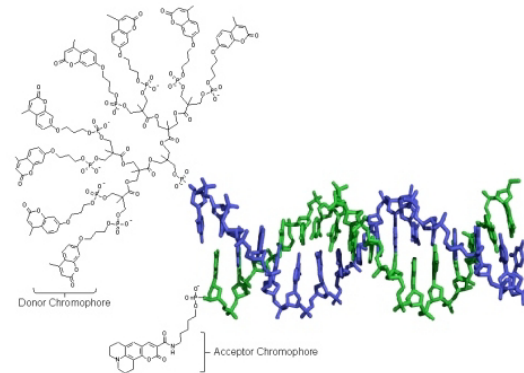
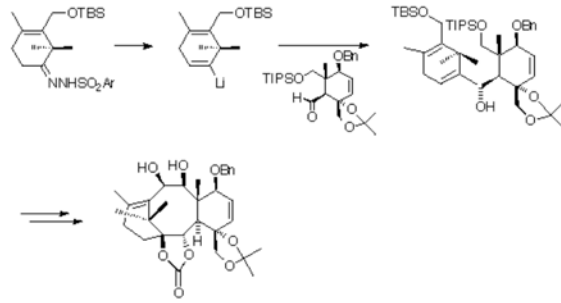
$r \sim 10 \text{ \AA}$



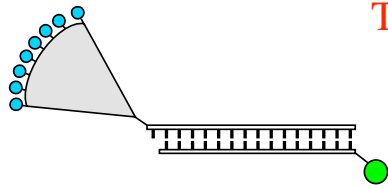
$r \sim 6 \text{ \AA}$



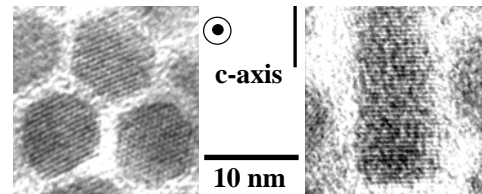
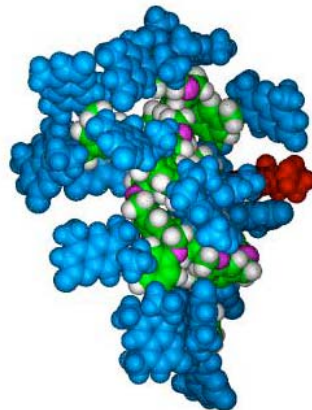
$r \sim 3 \text{ \AA}$



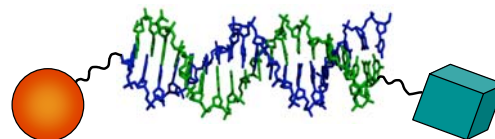
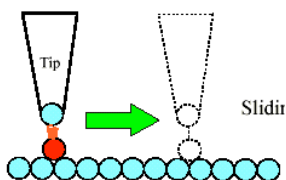
## The Building Blocks



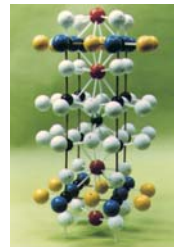
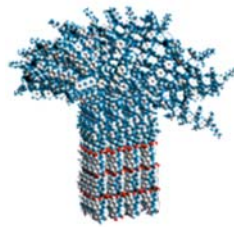
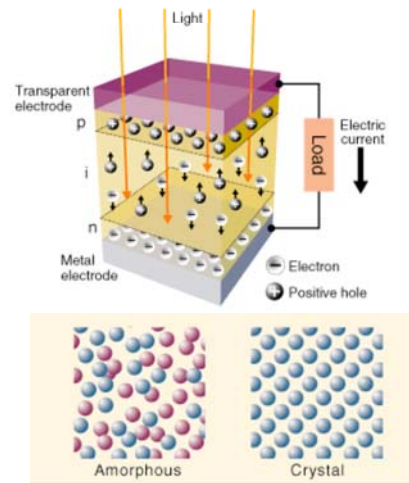
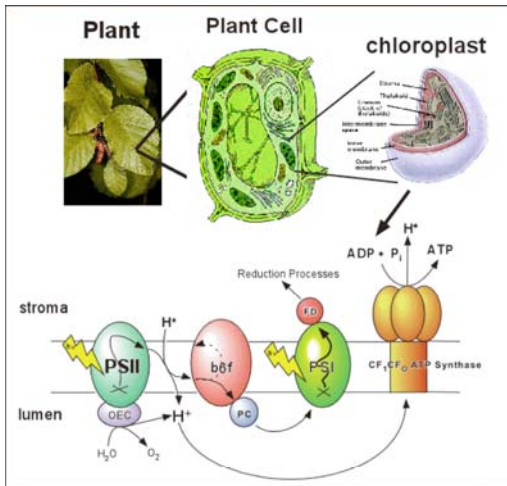
- Dendrimer
- Nanocrystal
- Nanorods
- Scanning Probe Tip.



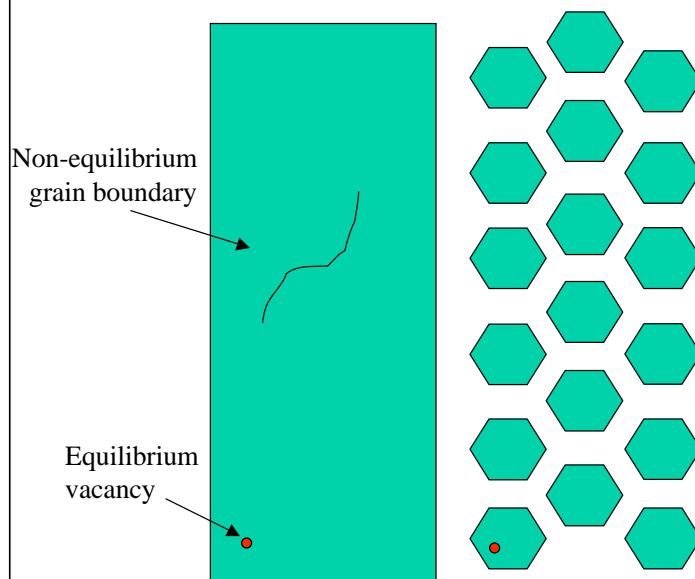
- Patterned Surface
- Cell Membrane
- DNA
- ...



# Heirarchical assembly of a complete system



## A comparison of defects in extended solids and nanocrystals

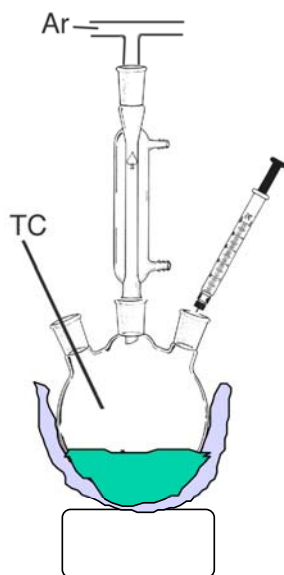


- 1 defect can affect an entire bulk solid
- On average, nanocrystals contain no equilibrium defects
- Easier to anneal out non-equilibrium defects in nanocrystals

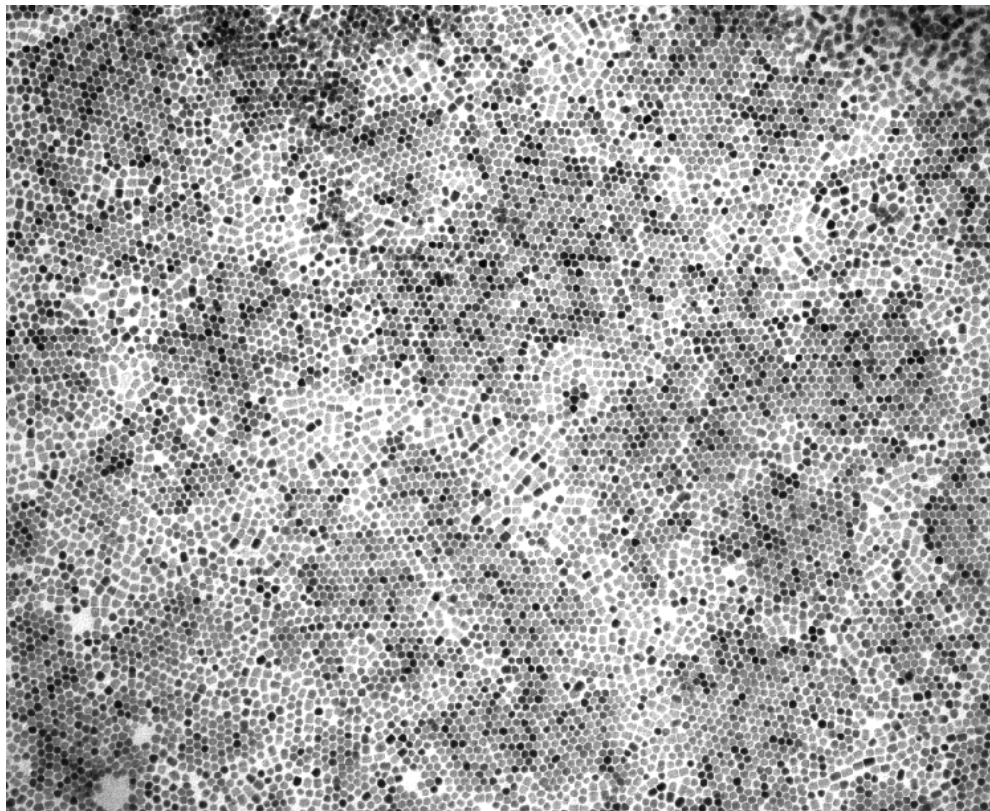


## Fabrication methods are key

### Molecular Beam Epitaxy of Quantum Structures



### A wide field view of 7nm diameter surfactant capped CdSe nanocrystals



## Some SCALING LAWS for nanoscale properties

Energy level spacing (band gap)  $E_g \sim A/r^2$

Density of states, oscillator strength ( $\sim V$ )

Charging energy ( $\sim 1/r$ )

Melting temperature ( $\sim 1/r$ )

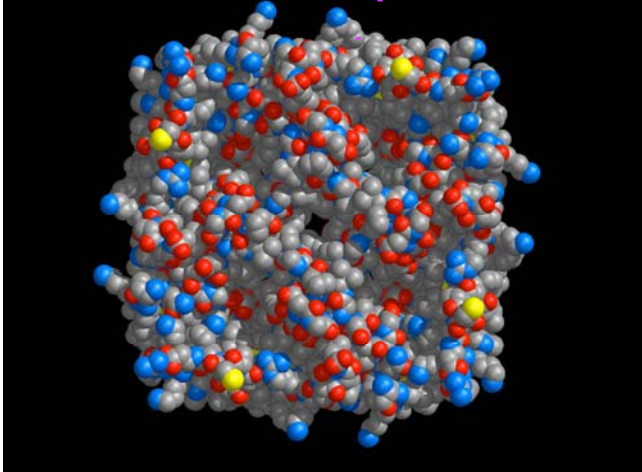
Magnetic relaxation time ( $\sim N$ )

Timescale for structural metastability ( $\sim N$ )

Control of size and shape will be an important variable  
in the design of new materials

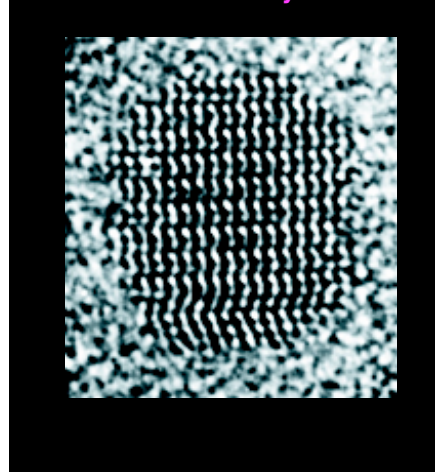
## Conjunction of Soft and Hard Matter

Glpf Cytoplasmic surface - Glycerol in the channels



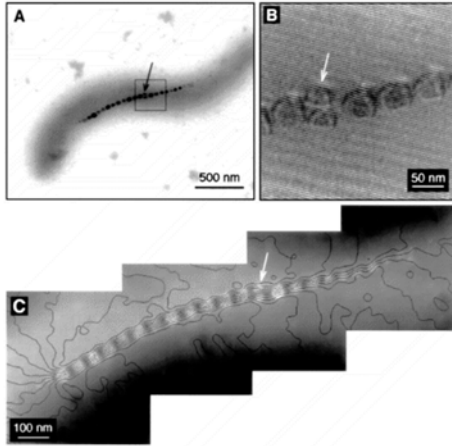
5nm

CdSe Nanocrystal



5nm

## Nanocrystals in Magnetotactic Bacteria

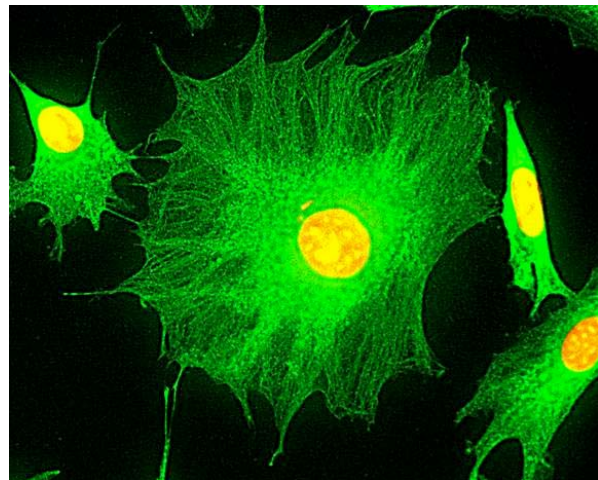
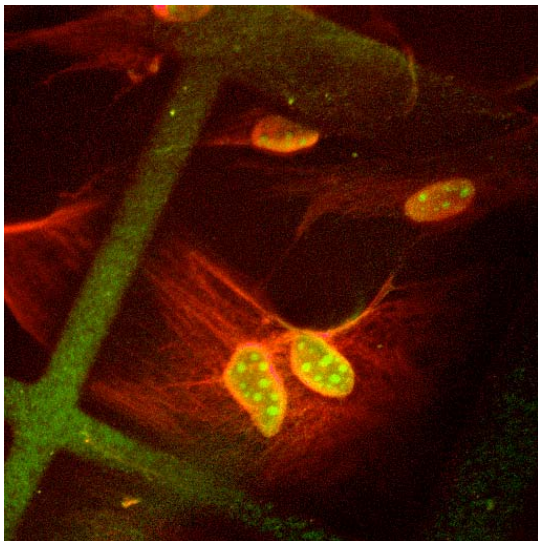


*Magnetospirillum magnetotacticum*

TEM images from Frankel, R.  
B., Bazylinski, D. A., et. al.  
*Science* **1998**, 282, 1868-1870

- Exploitation of a fundamental scaling law
- Maximum size for a magnet to be a “single domain,” with no defects (tens of nm)
- Least amount of material to achieve the greatest degree of magnetization.

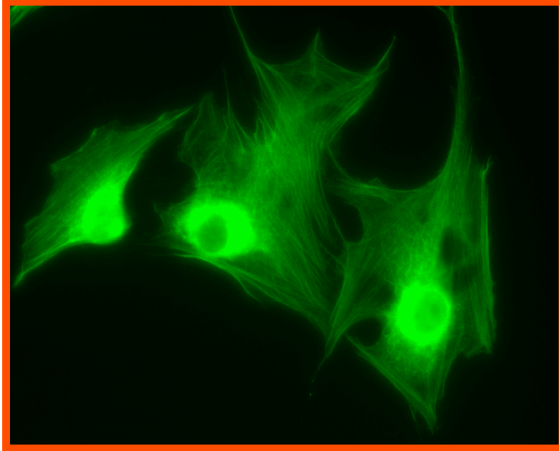
## Quantum Dot Cell Labeling



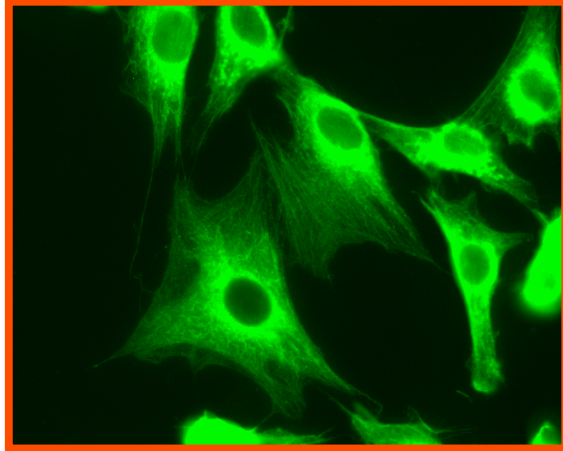
Bruchez, M.; Moronne, M.; Gin, P.; Weiss, S.; Alivisatos, A. P., *Science* **1998**, 281, 2013-2016.

## Photostability Comparison (Video)

### Alexa 488



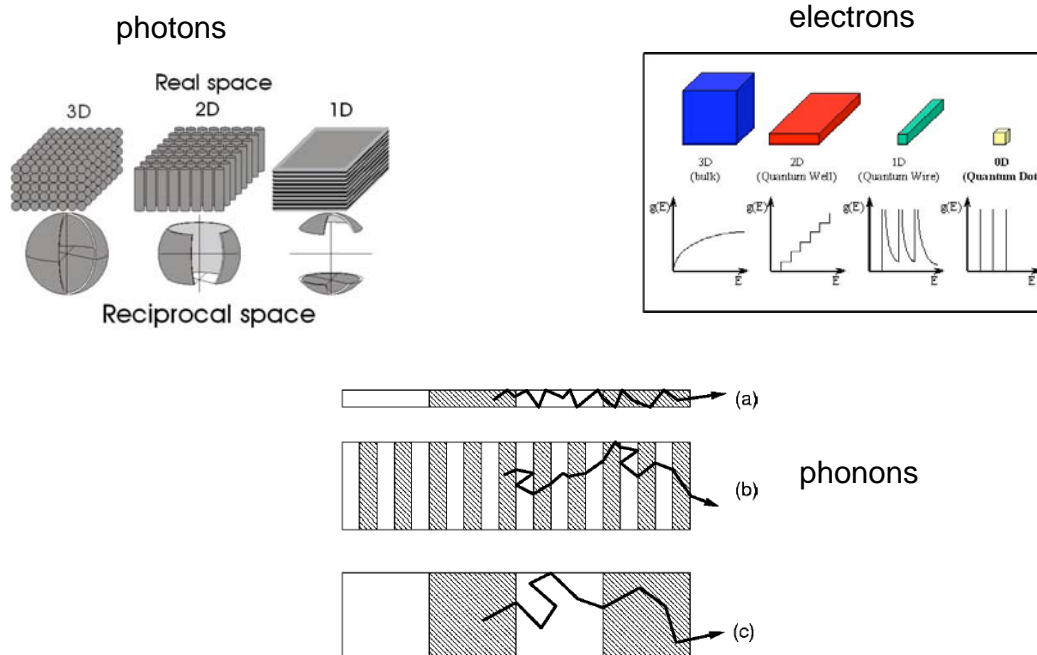
### Green QDs



Courtesy Quantum Dot Corporation

Streptavidin coated QDs are now available for purchase from [www.qdots.com](http://www.qdots.com)

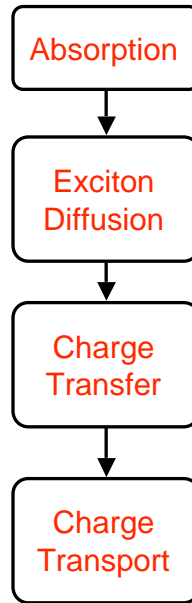
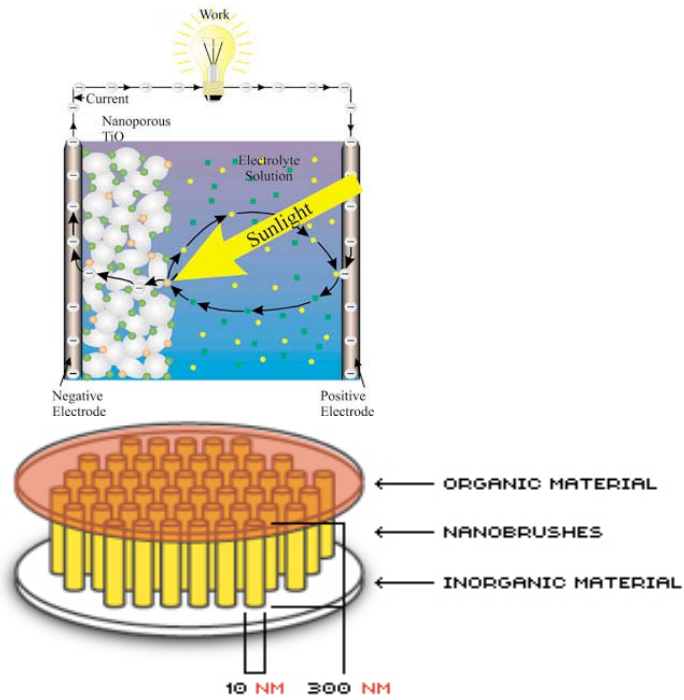
## dimensionality to control light, electricity, and heat...



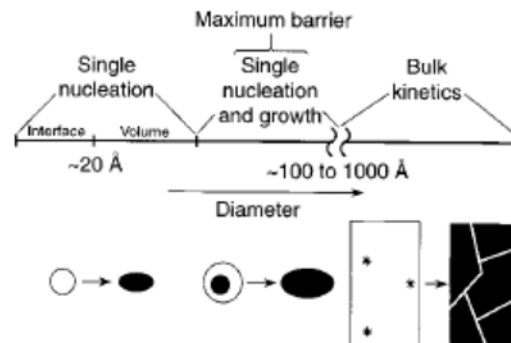
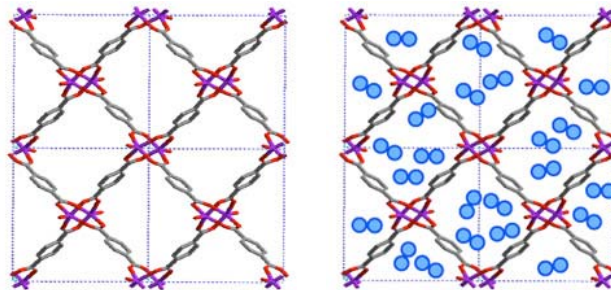
Measurement of scaling laws, synthetic control...

# Nanotechnology solar cells

Grätzel cell

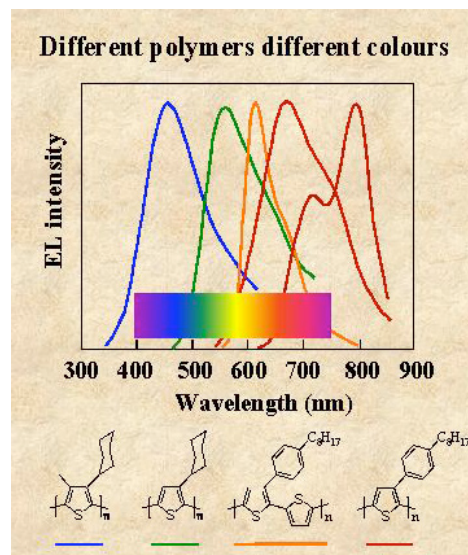
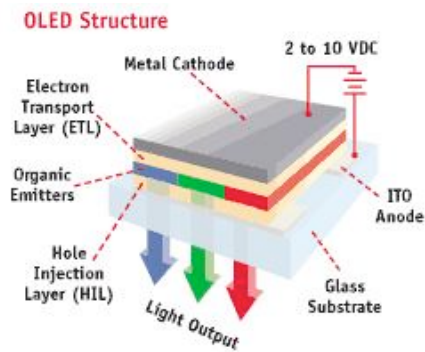


# Nanotechnology and Hydrogen Storage

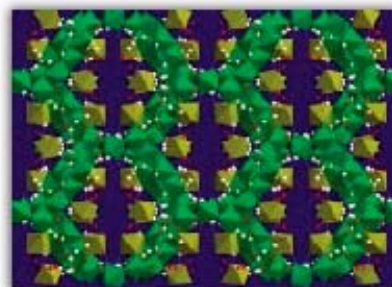
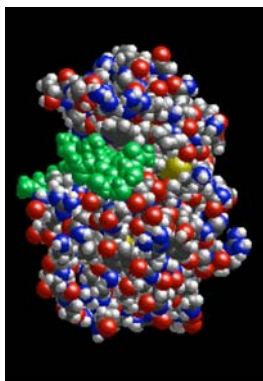




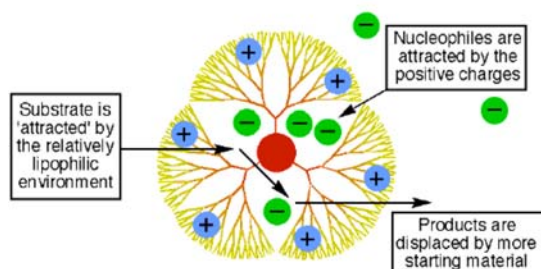
## Nanotechnology and Solid State Lighting



## Nanotechnology and selective chemical transformation



### *A Dendritic Catalyst for Reactions of Anionic Nucleophiles in Water*



## Issues of production



## Nanoscience and technology in six easy pieces

- The missing length scale
- One at a time
- It takes care of itself –defect tolerance
- High performance at large scales
- The energy connection
- Inspiration from nature- the hybrid system

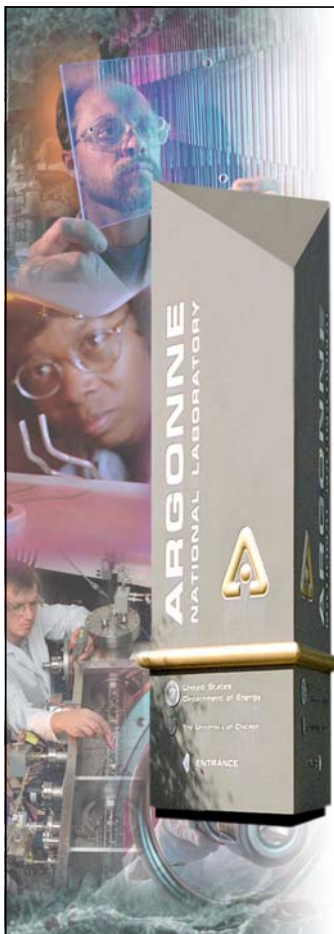
Paul Alivisatos

Assoc. Director for Physical Sciences, Lawrence Berkeley National Lab  
Professor of Chemistry and Materials Science, University of California, Berkeley  
alivis@berkeley.edu

## About the Speaker

### Paul Alivisatos

Paul Alivisatos is Professor of Chemistry and Materials Science at the University of California, Berkeley, and Assoc. Director for Physical Sciences at the Lawrence Berkeley National Lab. His research concerns the structural, optical, electrical, and thermodynamic properties of nanocrystals. He is a member of the National Academy of Science, the founding editor of Nano Letters, and the scientific founder of Quantum Dot corporation and Nanosys, Inc.



# Nanotechnology for the Hydrogen Economy

George Crabtree  
Senior Scientist and Director  
Materials Science Division

with  
Millie Dresselhaus MIT  
Michelle Buchanan ORNL

OSTP Hot Topics in Science and Technology  
Nanotechnology: Energizing our Future  
August 10, 2005

**Argonne National Laboratory**



A U.S. Department of Energy  
Office of Science Laboratory  
Operated by The University of Chicago



## Preview

### Hydrogen: a solution to world energy challenges

- supply, security, local/regional pollution, climate change

### Basic research challenges and nanoscience solutions

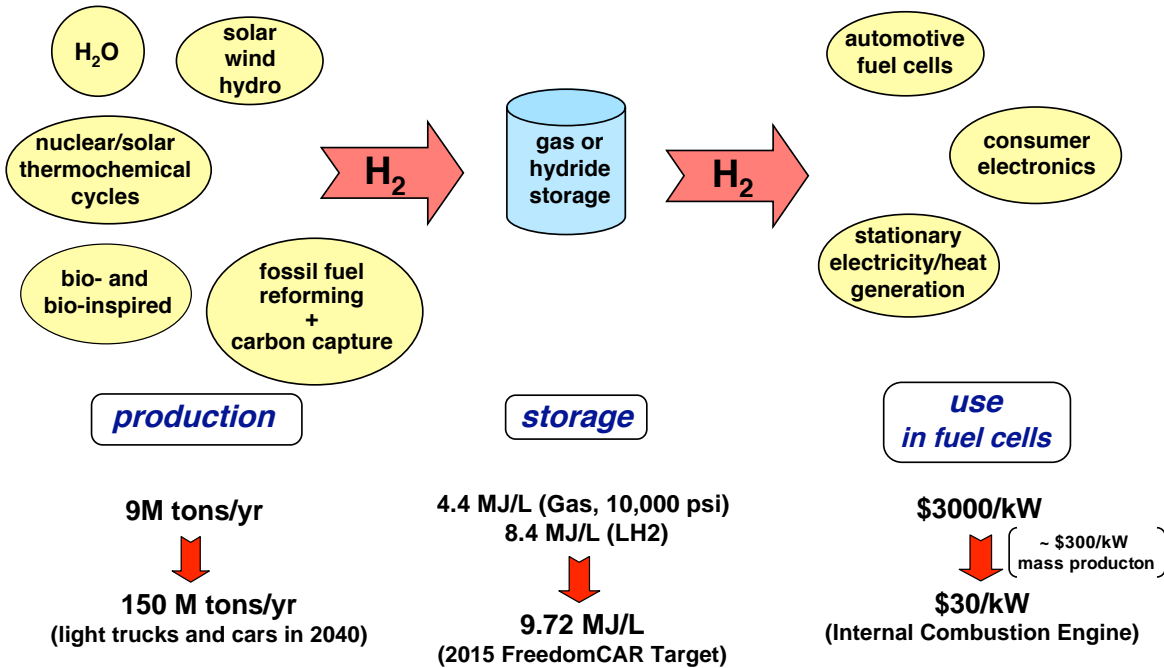
- production
- storage
- use in fuel cells

### The two hydrogen economies

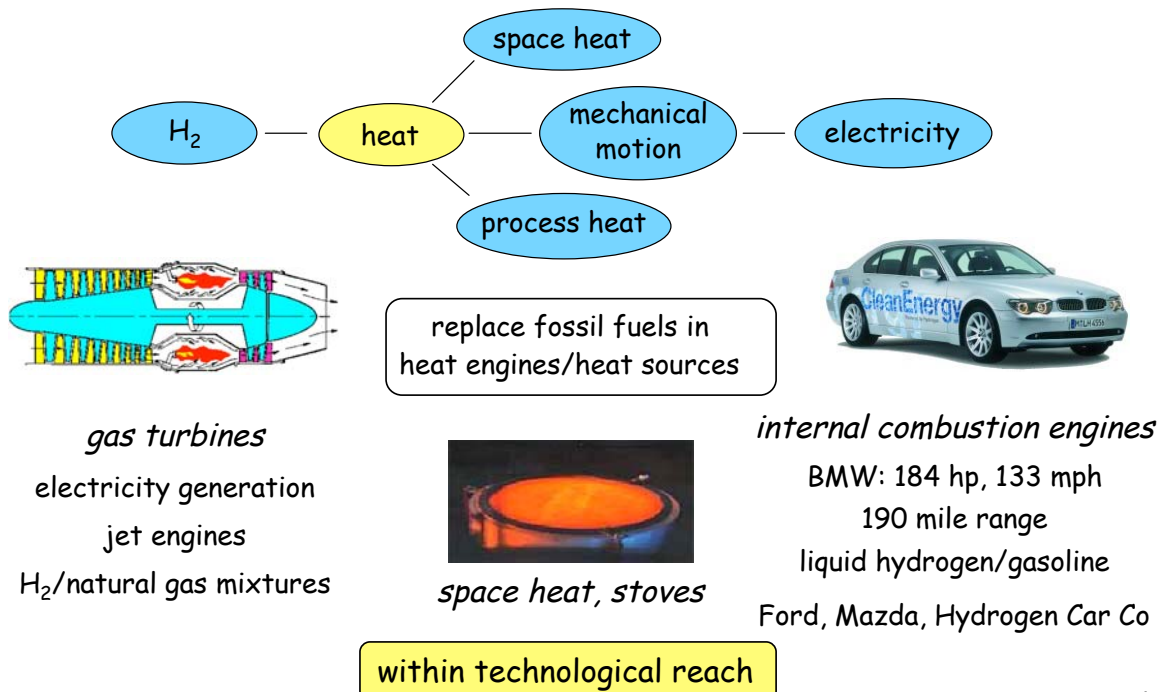
- incremental: where we are now
- mature: where we need to be
- nanotechnology bridges the gap



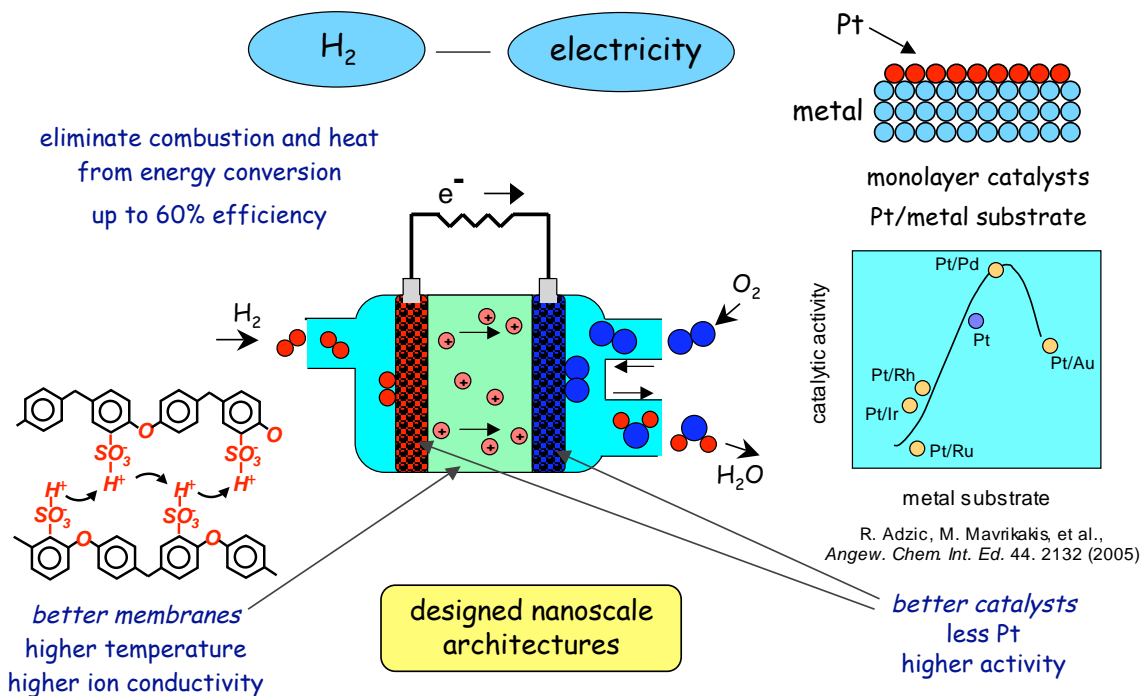
# The Hydrogen Economy



# Hydrogen Use Today: Combustion



# Hydrogen Use Tomorrow: Fuel Cells



# Hydrogen Storage Today: Gas and Liquid



*gaseous storage*

5000 psi = 350 bar  
10000 psi = 700 bar  
fiber reinforced composite containers



*liquid storage*

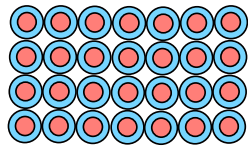
standard in stationary applications  
portable cryogenics for auto  
30-40% energy lost to liquifaction

**within technological reach**

# Hydrogen Storage Tomorrow: Solid State

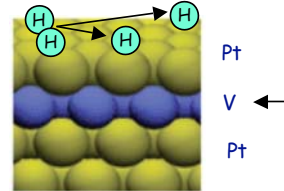
300 mile driving range  $\Rightarrow$  storage density higher than liquid  $H_2$   
 short refill time, good acceleration  $\Rightarrow$  fast charge, release rates

grand challenge for hydrogen economy:  
 viable hydrogen compounds



core-shell architecture  
 nanoparticle medium  
 high surface area

composite nanostructured media



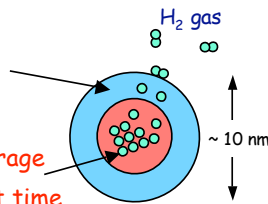
near-surface alloys

sub-surface atom controls surface behavior

- low  $H_2$  surface binding energy
- high  $H_2$  surface dissociation rate

shell: dissociation  
 $H_2 \rightleftharpoons 2H$

core: high density storage  
 nanoscale  $\Rightarrow$  fast transit time

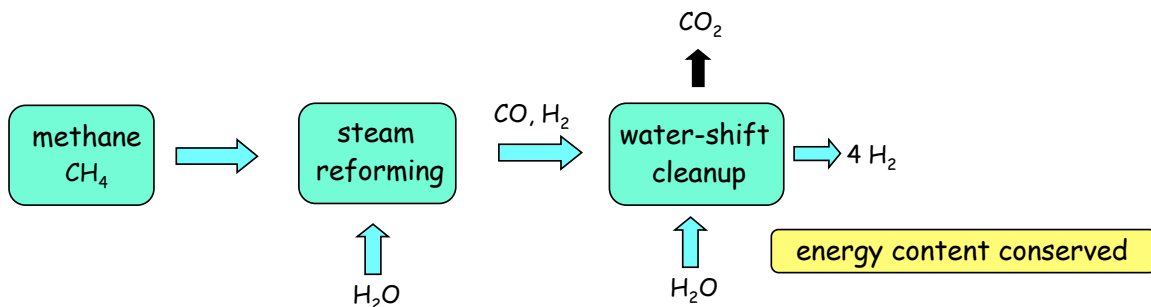


design by computer modeling  
 multi-node clusters, density functional theory  
 target promising nanoscale architectures

M. Mavrikakis et al., *Nature Materials* 3, 810 (2004)



# Hydrogen Production Today: Reform Fossil Fuels



need 10 - 15 times today's production  
 for light trucks and cars in 2040

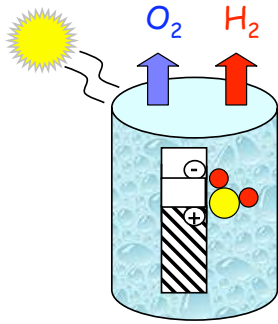
technology in place  
 incremental effect on energy

**Energy Impact**

- depletion of fossil resource
- dependence on foreign supply
- fossil pollution unchanged
- greenhouse emissions unchanged



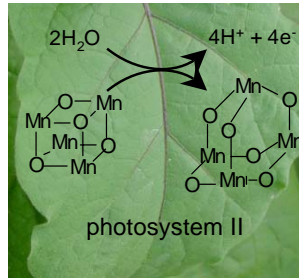
# Hydrogen Production Tomorrow: Splitting H<sub>2</sub>O



*solar electrolysis*

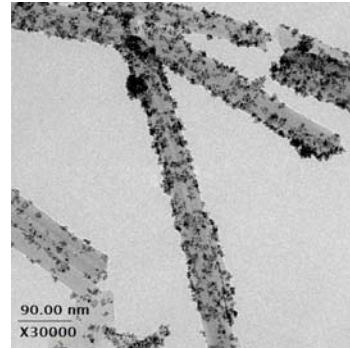
functional integration  
at the nanoscale  
molecular transfer of  
energy and charge  
6-18% efficiency in laboratory

*abundant resource  
no geopolitical constraints  
environmentally benign*



*bio-inspired nanoscale  
assemblies*

inexpensive Mn catalyst  
room temperature  
"one molecule at a time"



*porphyrin nanotube hybrids*

porphyrin: harvests light  
Pt, Au: catalyst & electrodes  
assembly splits water  
in sunlight

J A Shelnutt., et al.,  
*J. Am. Chem. Soc.* 126, 635 (2004)

nanoscale hydrogen production



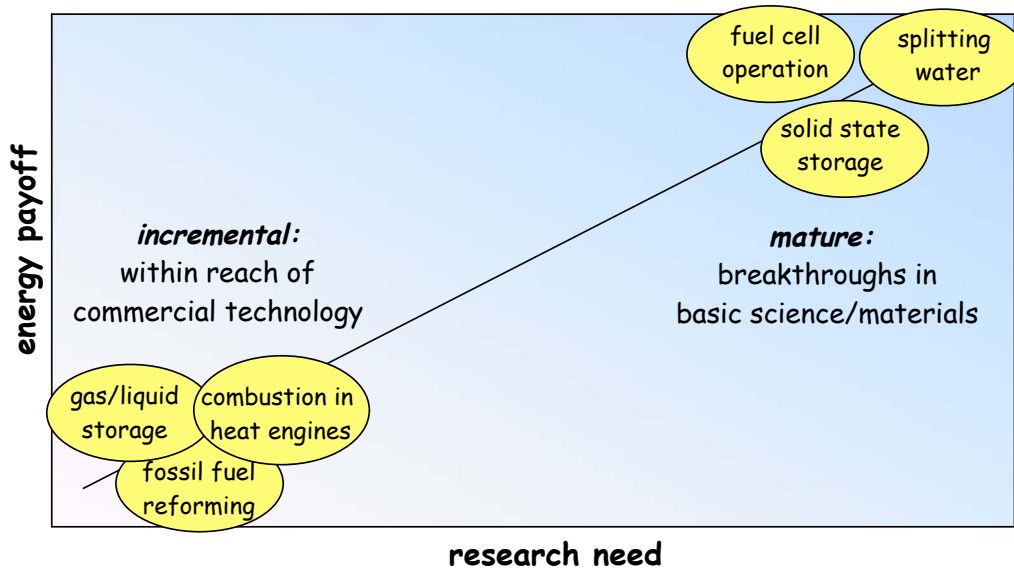
Pioneering  
Science and  
Technology

Office of Science  
U.S. Department  
of Energy



9

# The Two Hydrogen Economies



nanoscience bridges the gap



Pioneering  
Science and  
Technology

Office of Science  
U.S. Department  
of Energy



10



## About the Speaker

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### George W. Crabtree

George Crabtree is a Senior Scientist at Argonne National Laboratory and Director of its Materials Science Division. He holds a B.S. in Engineering from Northwestern University and Ph.D. in Condensed Matter Physics from the University of Illinois at Chicago, specializing in the electronic properties of metals. He has won numerous awards, most recently the Kammerlingh Onnes Prize for his work on the properties of vortices in high temperature superconductors. This prestigious prize is awarded only once every three years; Dr. Crabtree is its second recipient. He has won the University of Chicago Award for Distinguished Performance at Argonne twice, and the U.S. Department of Energy's Award for Outstanding Scientific Accomplishment in Solid State Physics four times, a notable accomplishment. He has an R&D 100 Award for his pioneering development of Magnetic Flux Imaging Systems, is a Fellow of the American Physical Society, and is a charter member of ISI's compilation of Highly Cited Researchers in Physics.

Dr. Crabtree has served as Chairman of the Division of Condensed Matter of the American Physical Society, as a Founding Editor of the scientific journal *Physica C*, as a Divisional Associate Editor of *Physical Review Letters*, as Chair of the Advisory Committee for the National Magnet Laboratory in Tallahassee, Florida, and as Editor of several review issues of *Physica C* devoted to superconductivity. He has published more than 400 papers in leading scientific journals, and given approximately 100 invited talks at national and international scientific conferences. His research interests include materials science, nanoscale superconductors and magnets, vortex matter in superconductors, and highly correlated electrons in metals. Most recently he served as Associate Chair of the Basic Energy Sciences Workshop on Solar Energy Utilization, the subject of his presentation to the San Diego Regional Energy Office Conference on Solar Energy.

11

# Solar Energy and Nanotechnology

Based on:

## Basic Research Needs for Solar Energy Utilization:

Report of the Basic Energy Sciences Workshop on Solar Energy Utilization

Nathan S. Lewis

George L. Argyros Professor of Chemistry

California Institute of Technology

with

George Crabtree, Argonne NL

Arthur Nozik, NREL

Mike Wasielewski, Northwestern

Paul Alivisatos, UC-Berkeley



## Solar Energy Utilization

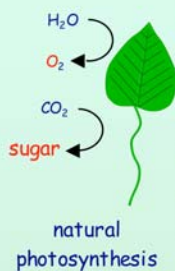


Solar Electric

.001 TW PV  
\$0.30/kWh w/o storage



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



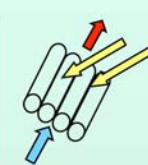
Solar Fuel

1.4 TW solar fuel (biomass)



11 TW fossil fuel  
(present use)

~ 14 TW additional energy by 2050



50 - 200 °C  
space, water  
heating



500 - 3000 °C  
heat engines  
electricity generation  
process heat

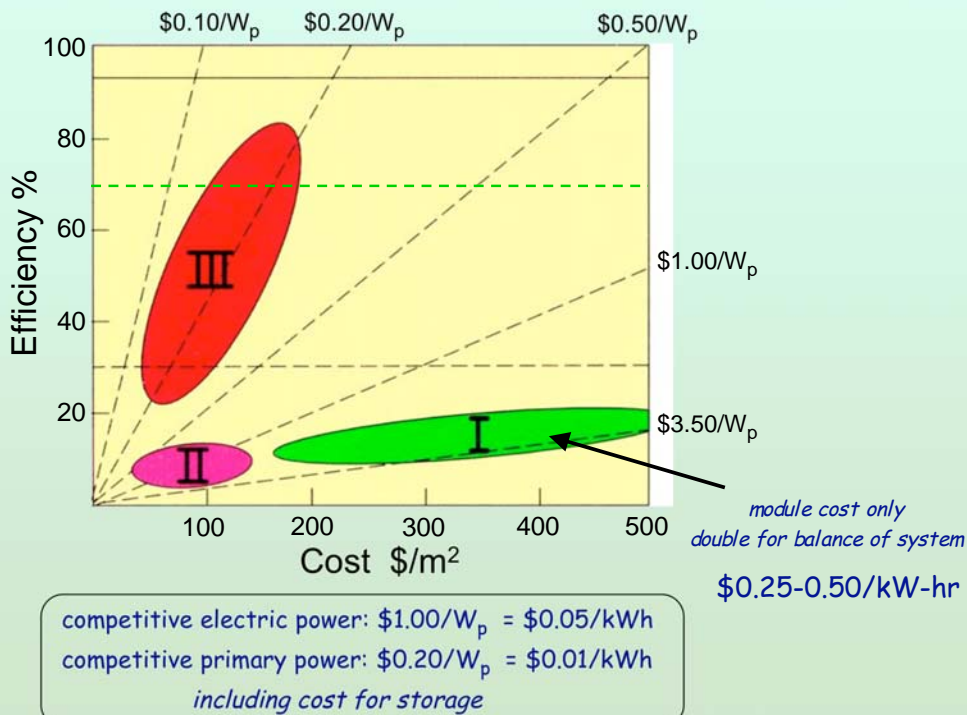
Solar Thermal

0.002 TW

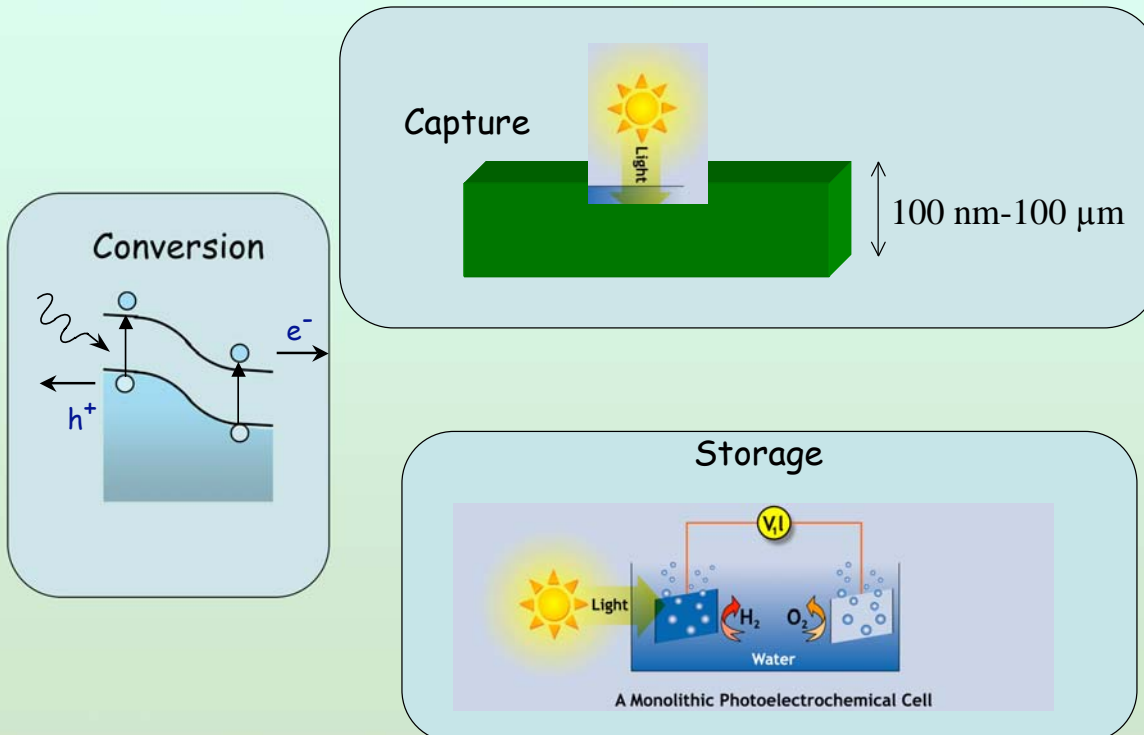


2 TW  
space and water  
heating

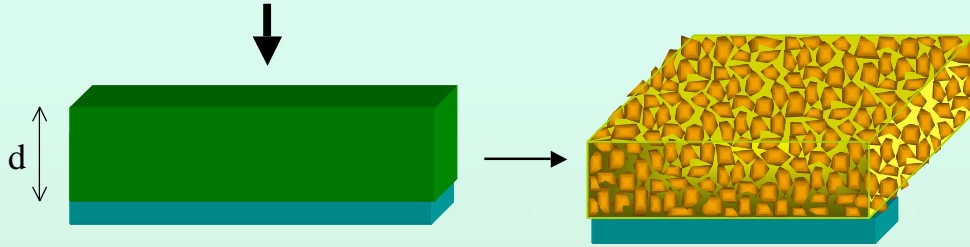
# Solar Energy Costs



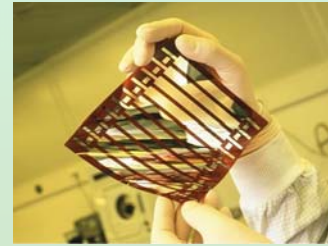
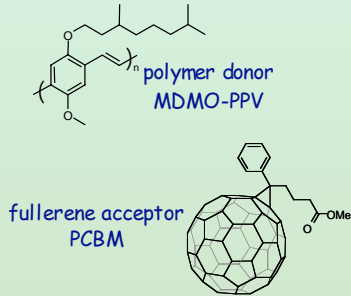
# Solar Energy Conversion



# "Solar Paint"

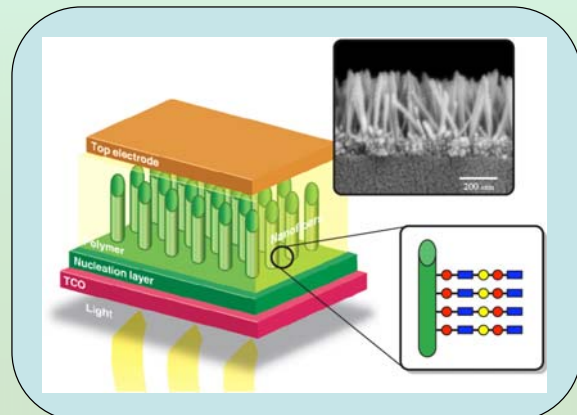
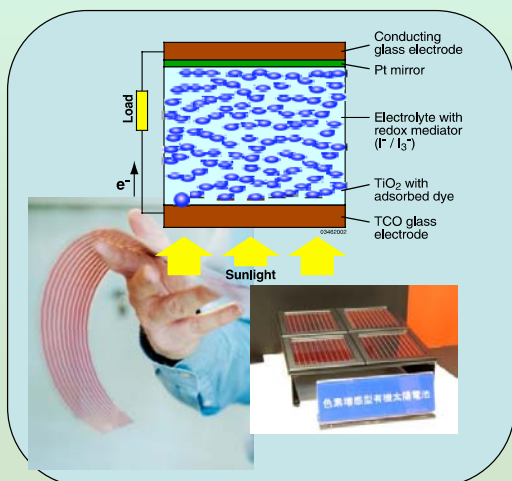
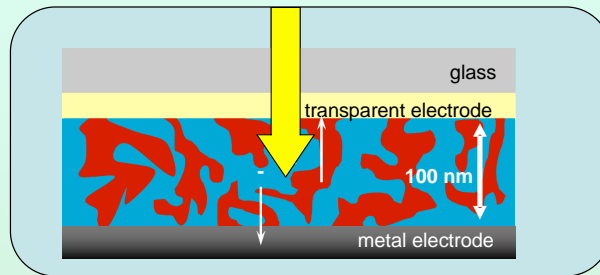


"Fooling" inexpensive particles into behaving as single crystals

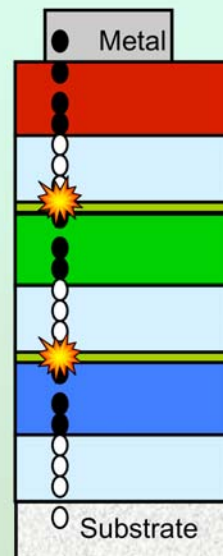
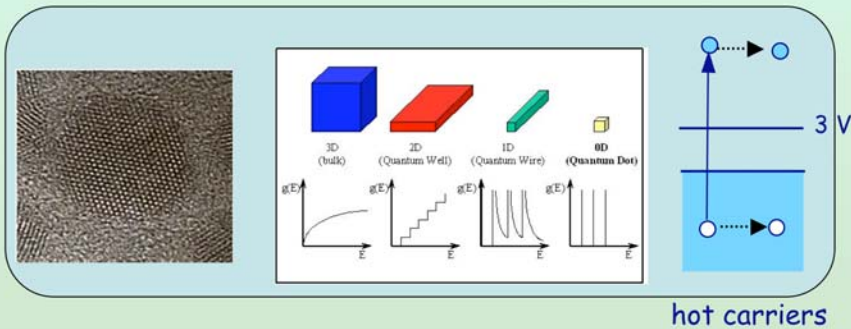


inexpensive processing, conformal layers

# Interpenetrating Nanostructured Networks



# Ultra-high Efficiency Solar Cells

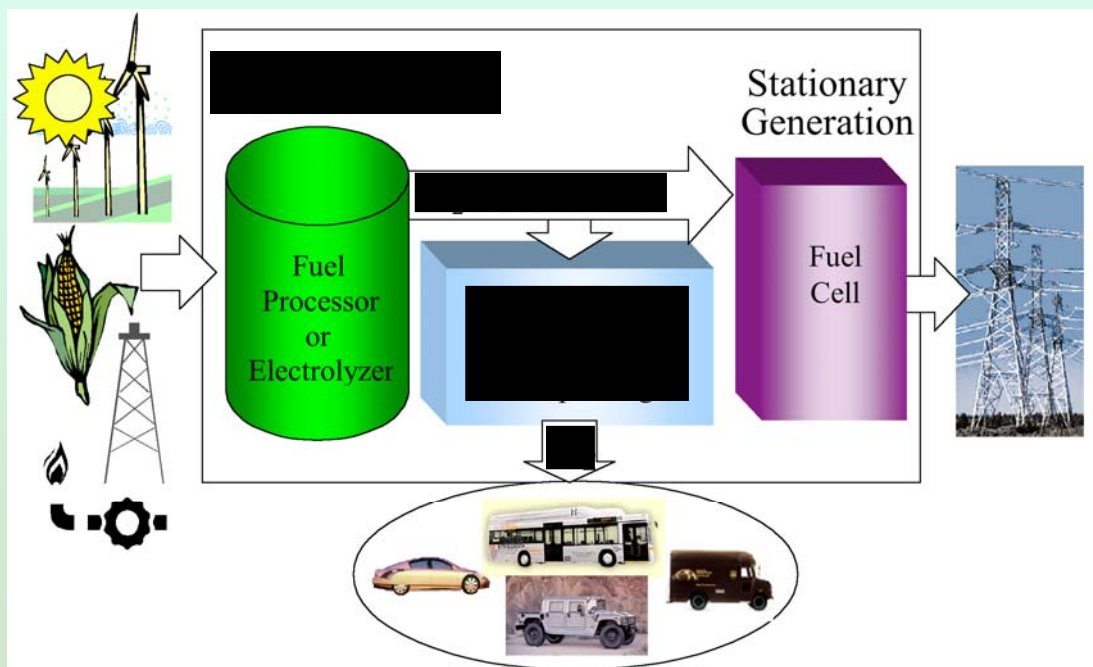


rich variety of new physical phenomena understand and implement

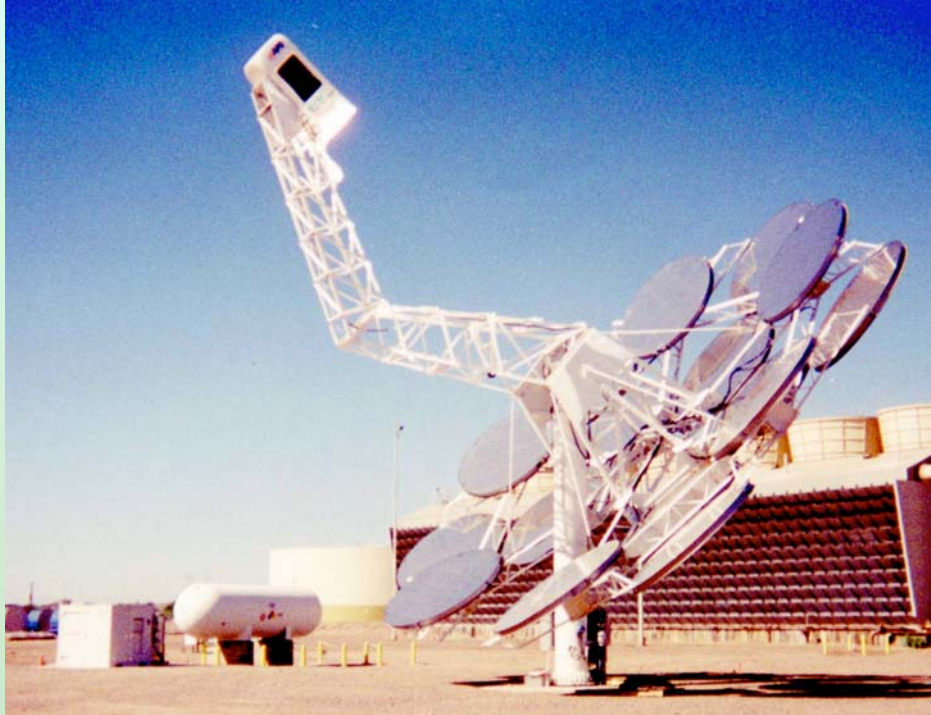
multiple junctions

# Storage: The Need to Produce Fuel

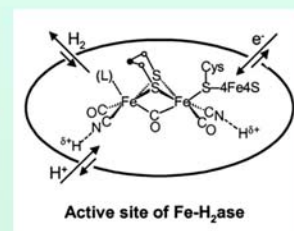
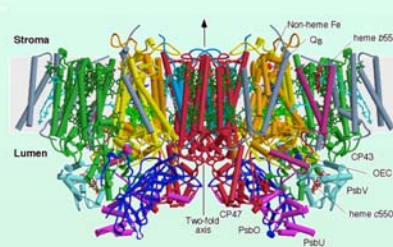
"Power Park Concept"



# Solar Thermal + Electrolyzer System

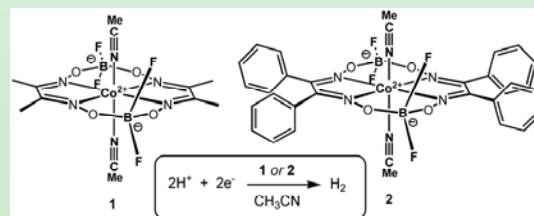
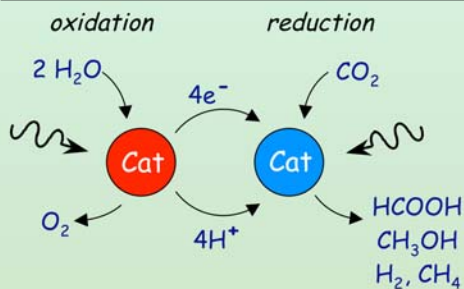


# Solar-Powered Catalysts for Fuel Formation



photosystem II

hydrogenase  
 $2\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{H}_2$

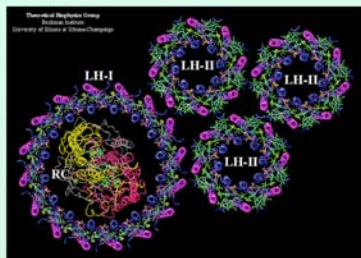


# Solar Land Area Requirements

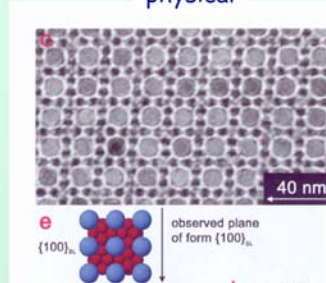


# Control of Materials Properties Through Nanoscience

biological



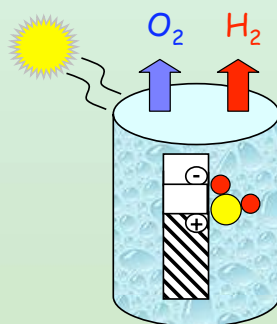
physical



mechanical



Self-assembly of complex structures



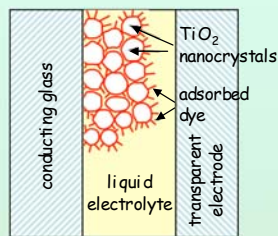
Hydrogen from water and sunlight



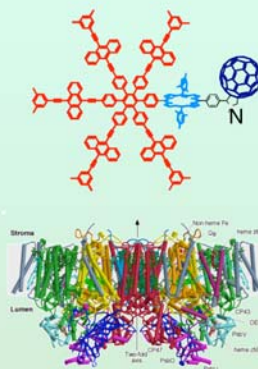
demonstrated efficiencies 10-18% in laboratory

# Nanoscience and Solar Energy

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 is interdisciplinary nanoscience

## 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 the earth uses 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>



## About the Speaker

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### Nathan S. Lewis

Nathan S. Lewis is the George L. Argyros Professor of Chemistry at the California Institute of Technology. He holds a B.S. and M.S. degree in 1977 Chemistry from Caltech, and a Ph.D. in 1981 from MIT. From 1981-1986, he was an Assistant Professor at Stanford University, from 1986-1988 he was an Associate Professor at Caltech, and from 1988-present he is a full professor at Caltech. Lewis' research interests involve artificial photosynthesis to enable solar energy conversion to directly form chemical fuels, and chemical microsensors for widely disseminated early warning systems for chemical terrorist events in homeland security.

Lewis is an author or co-author of over 200 papers, and has received numerous awards including a Presidential Young Investigator Award, the American Chemical Society Award in Pure Chemistry, and the Princeton Environmental Award. He has served on the editorial boards of the *Journal of the Electrochemical Society* and *Accounts of Chemical Research*, and is currently on the board of *Chemical Reviews*. He has attended the World Economic Forum in 2000 and 2001, and consults for government, industry, and academia on energy technology and energy policy. He is a member of the Technology Advisory Council of BP, and has been a founding participant in several successful start-up high technology companies. He also consults for government on a broad array of national security-related topics, and has been the chair of the visiting committee for the Department of Applied Science at Brookhaven National Laboratory. Along with George Crabtree, Lewis was the co-chair of the recent workshop sponsored by the DOE Office of Basic Energy Sciences on *Basic Research Needs for Solar Energy Utilization*, which is the basis for today's OSTP briefing.



# OSTP Hot Topics in Science and Technology Series Nanotechnology: Energizing Our Future

## *Nanotechnology for Solid State Lighting*

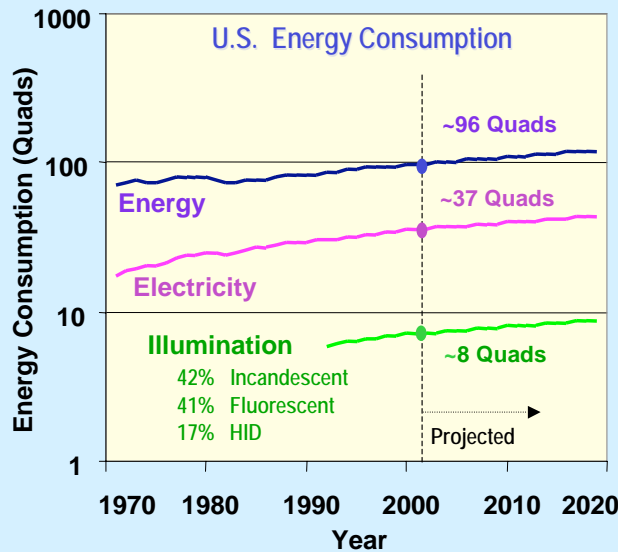
10 August 2005

Harriet Kung

Director, Materials Sciences and Engineering Division  
Office of Basic Energy Science  
Office of Science, DOE

harriet.kung@science.doe.gov  
(301) 903-1330

## *Lighting is a Large Fraction of Energy Consumption*



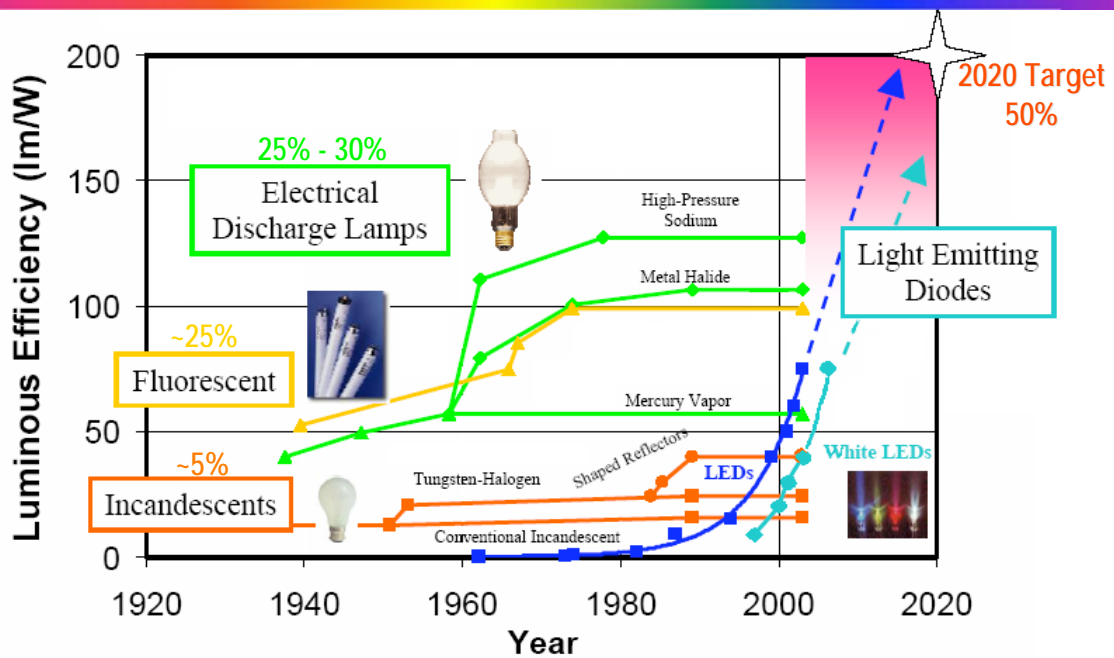
### Efficiencies of Energy Technologies in Buildings

Heating:	70-80%
Electrical Motors:	85-95%
Incandescent Lighting:	~5%
Fluorescent Lighting:	~25%
Metal Halide Lighting:	~30%

*Lighting consumes ~20% of U.S electricity and yet has very low efficiency*



## Solid State Lighting Offers Great Potential for Energy Savings



50% conversion efficiency (200 lm/W) in SSL in 2025 could lead to:

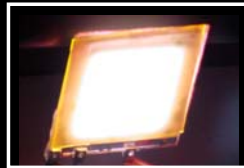
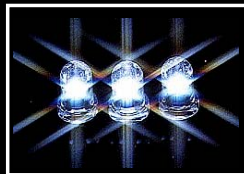
- Reduced Electricity Consumption (525 TW-hr/Yr) and Cost (\$35 B/Yr)
- Decreases in New Power Plant Needs (75 GW) and CO<sub>2</sub> Emission (87 Mtons)

Ref: J.Y. Tsao, Laser Focus World, May 2003 and references therein

## Solid State Lighting: Semiconductor-Based Lighting Technology

### Inorganic Light Emitting Diodes (LEDs)

- III-V semiconductors-based device
- High brightness point sources
- Potential high efficiency & long lifetime

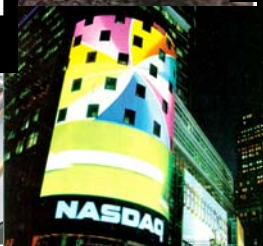
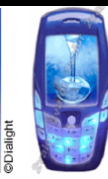


### Organic Light Emitting Diodes (OLEDs)

- Organic semiconductors-based device
- Large area diffuse sources
- Thin and flexible
- Ease of fabrication

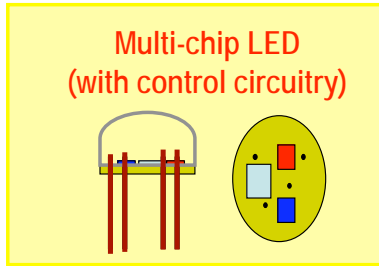


Current LEDs are predominantly in mono-chrome or niche applications.  
High brightness, broad-band white light is needed for general illumination applications.



# White Light Solid State Lighting

## Multi-LED

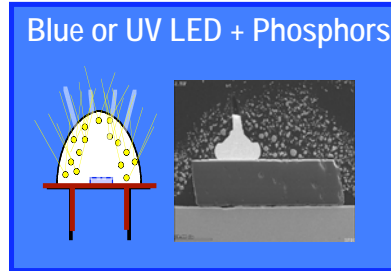


Mix light from multiple LEDs of different color

- ✓ Potential High Efficiency
- ✓ Precise Control of Color and Power Output

Color Likely Sensitive to Temperature  
Higher Materials and Processing Costs

## LED + Phosphors



Use blue or near-UV LED to pump a mixture of phosphors

- ✓ Good Temperature Stability
- ✓ Lower Cost

Limited Control of Color and Power Output  
Lower Energy Conversion Efficiency

## Current Market Status & Technology Gaps

	Efficiency (lm/W)	Price (\$/klm)
Incandescent (75 W)	13	~\$0.60
Fluorescent (T8)	83	~\$0.73
HID (Metal Halide)	100	~\$1.27
SSL (White Light)	~50 → (200*)	~\$150 → (less than \$2*)

\* 2020 Milestones in a SSL Technology Roadmaps developed by SSL Community <http://lighting.sandia.gov>

## LED Research Advancements and Opportunities

### New Materials

New Classes of Light Emitters:

AlInGaP – Red, Yellow    InGaN – Blue, Green

Lattice Matched Substrates

Semiconductor Nanomaterials and Nanostructures

Thin Film and Bulk Crystal Growth, Self-Assembly

UV-Stable Packaging / Encapsulant Materials

### Photon Creation

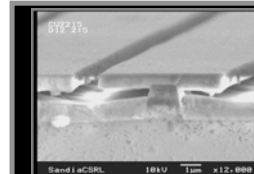
Interplay between Electron-hole Injection and Recombination, Band Structure, Defects, Impurities, and Strain

### Photon Extraction

Manipulation of Optical Modes by use of Optical Microcavities and Photonic Lattices  
3D Nanostructuring, Surface Plasmons

### Photon Wavelength Conversion

New Phosphors – New Material Families and Nanoscience Approaches  
New Approaches to Optical Index Matching and Photon Guiding



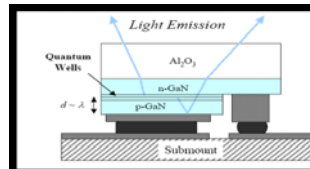
Cantilever epitaxy reduces defect density in GaN  
J. Simmons et al., SNL

### Nanoscale Indium clustering in InGaN

LBNL and Lumileds CRADA, NCEM HRTEM image



2.8 nm  
InGaN  
Quantum Well



Microcavity effects for increased light extraction

Shen et al., *Appl. Phys. Lett.* 82, 2221 (2003).

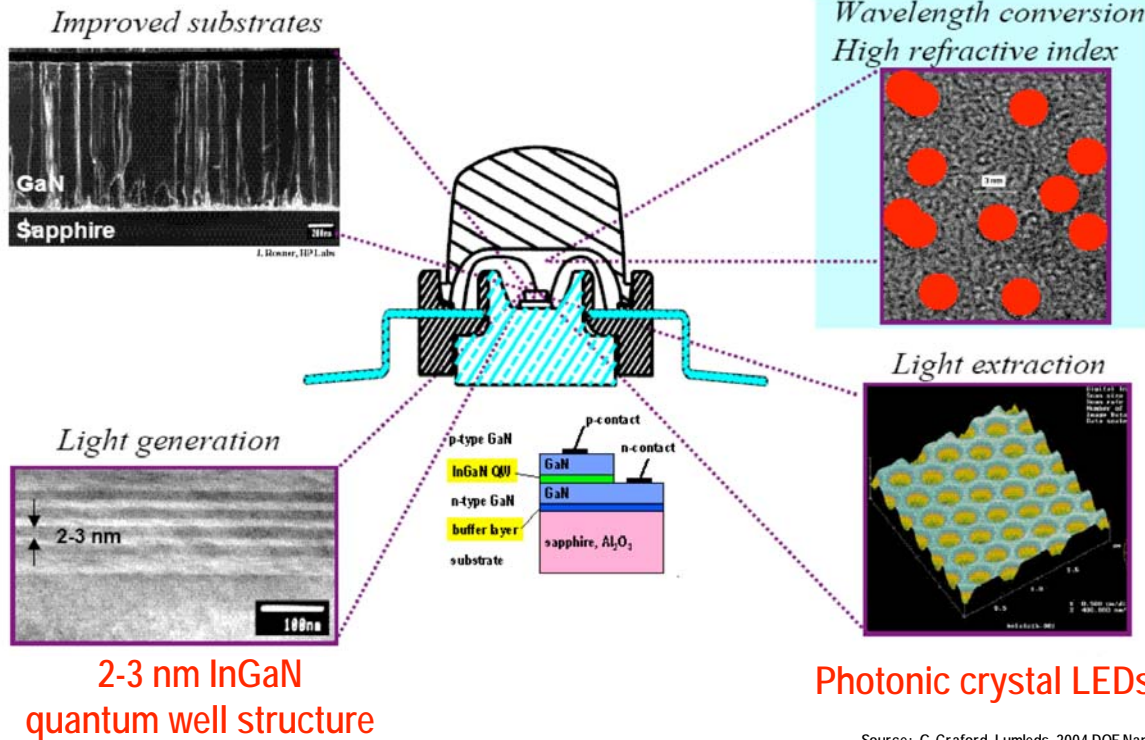


Nano quantum dots provide tunable phosphors

# Nanotechnology-Enabled LED Research Breakthroughs

Nanoscale substrate patterning reduces GaN defects by 100 times

Nano quantum dots as phosphors



Source: G. Craford, Lumileds, 2004 DOE Nanosummit

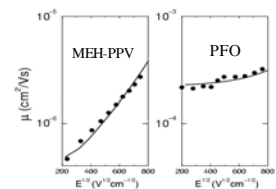
# Nanoscale Research Opportunities in OLEDs

## 1. Organic Semiconductors

Defect Tolerant  
The Wonders of Chemistry-  
Guided by Quantum Chemistry and Intuition  
Widely Tunable Properties



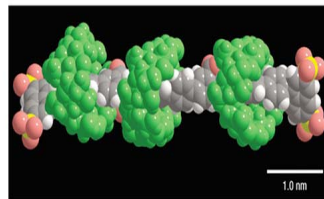
Semiconducting and metallic polymer "inks" A. Heeger, UCSB



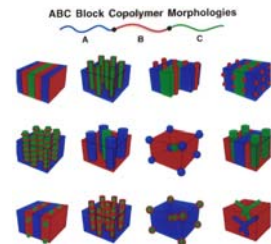
Mobilities Modeling  
D. Smith, LANL

## 2. Synthesis and Processing

Solution and Vacuum Processing  
Self Assembly at the Molecular Level



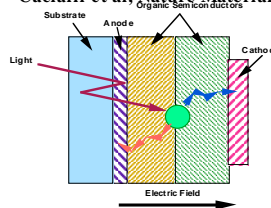
Chemical structures of the polyrotaxanes  
Caciagli et al, Nature Materials



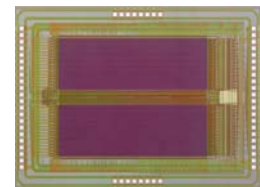
Block Copolymer Morphologies

## 3. Nanoscale Manipulation

Charge Injection  
Tailored Transport & Optical Process  
Will Benefit Other Organic Electronics



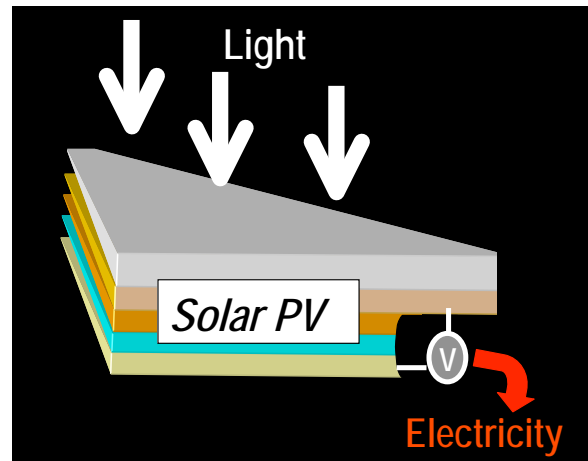
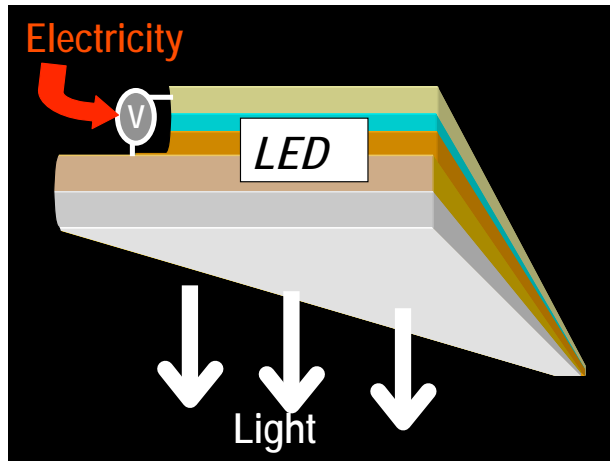
Organic PVs  
Bradley, Imperial College London



1MB prototype chip  
shown by Motorola in June 2002

## Synergy between Solar Photovoltaic & LED

Converting between electricity and light - LED works as a reverse solar PV cell

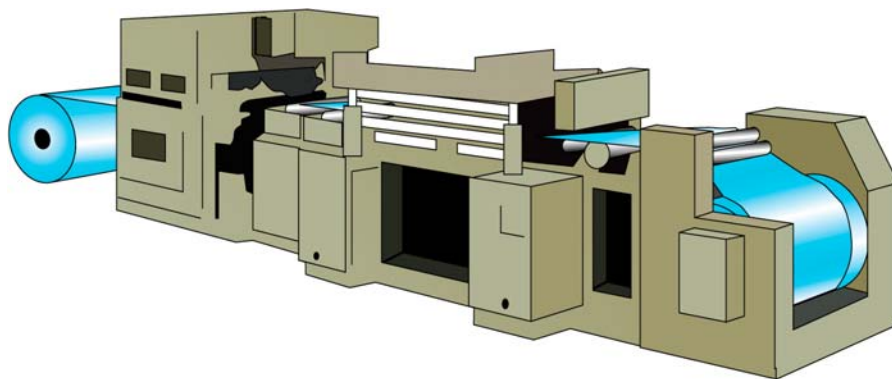


### Common Issues

- Nanomaterials and New Design for High Efficiency Conversion
- Device Reliability and Materials Degradation
- Novel Nanoscale Synthesis & Processing

## OLEDs and Organic Electronics

Semiconductor Processing  $\xrightarrow{?}$  Newspaper Processing



Broad range of applications based on organic electronics:

Organic PV

Organic Sensors

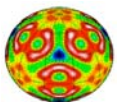
Integrated Circuits

Display and Lighting

**Nanotechnology could assist the paradigm shift.**

## Change a Light, Change the World

- The century old, low conversion efficiency technologies still dominate world lighting application.
- Semiconductor based Light Emitting Diodes offer significant savings in energy consumption.
- Nanoscale basic research presents new opportunities to advance solid-state lighting technologies.



*Basic Energy Sciences*  
*Serving the Present, Shaping the Future*

### Acknowledgments:

DOE-EERE Building Technologies Program: Jim Brodrick  
Univ of Utah: Vally Vardeny; UCSB: Alan Heeger; GE: Anil Duggal  
SNL: Jeff Tsao, Jerry Simmon; LANL: Darryl Smith

## About the Speaker

Dr. Harriet Kung has served as the Director of Materials Sciences and Engineering Division in DOE's Office of Basic Energy Sciences (BES) since June 2004. Her Division supports a broad-based basic research program engaged in fundamental studies of materials sciences and engineering. The research seeks to understand the atomistic basis of materials properties and behavior and how to make materials perform better at acceptable cost through innovative materials design, synthesis, and processing. The program fulfills DOE missions by the development of materials that improve the efficiency, economy, environmental acceptability, and safety in energy generation, conversion, transmission, and utilization.

Before joining DOE in 2002, Dr. Kung was a technical staff member and a project leader in the Materials Science and Technology Division at Los Alamos National Laboratory (LANL). Her main research interest focuses on novel synthesis and characterization of nanostructured materials and their mechanical and physical behavior. In addition, she has conducted research in high temperature superconductivity and devices. She has published ~ 100 refereed papers, and has given more than 50 technical presentations at conferences and universities, including one plenary lecture and 25 invited talks. She has served as a guest editor for several special scientific journal issues, and has been involved in organizing eight international symposia/workshops.

At DOE, she was involved in the planning and execution of three BES-sponsored workshops: *Basic Research Needs to Assure a Secure Energy Future*, *Basic Research Needs for the Hydrogen Economy*, and *Basic Research Needs for Effective Solar Energy Conversion*. She has served as the point of contact for the Office of Science on basic hydrogen research, and has participated in various international hydrogen research coordination activities. She is currently serving as the leader of the Fundamental Research subgroup in an OSTP Hydrogen R&D Task Force to develop interagency coordination plans on basic hydrogen research. She also led a joint BES-EERE workshop on Basic Research Needs for Organic Electronic Materials in support of the solid state lighting technologies.

Dr. Kung received her Ph.D. degree in Materials Science and Engineering with a minor in Applied and Engineering Physics from Cornell University. She is the recipient of numerous awards including the DOE Distinguished Postdoctoral Fellowship award and several performance and leadership service awards at LANL.