A person in a purple shirt stands on the peak of a rocky mountain, arms raised in a gesture of triumph or challenge. The background shows a vast, hazy mountain range under a cloudy sky.

Directing Matter and Energy: Five Challenges for Science and the Imagination

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ADVISORY COMMITTEE**

FEBRUARY 21, 2008

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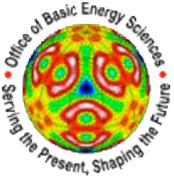
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* BESAC Chair

** BESAC Member



Why Grand Challenges Now?

Necessity

Opportunity



Why Grand Challenges Now?

19th Century

Average Behavior of
Continuous Systems

Thermodynamics

20th Century

Discrete and
Fluctuating Systems
Quantum Mechanics

21st Century

Control of Matter & Energy

“During the 20th Century, scientists developed increasingly sophisticated technologies and instrumentation for the study of quantum effects. Our understanding of these phenomena has reached the point where we are ready to move beyond simple observation and take the steps that will enable us to direct and control matter and energy at the quantum level.”

--Grand Challenges report, Chapter 1

Humanity's Top Problems for next 50 years

ENERGY
WATER
FOOD
ENVIRONMENT
POVERTY
TERRORISM & WAR
DISEASE
EDUCATION
POPULATION



2003	6.3	Billion People
2050	8-10	Billion People

The US Department of Energy

Energy

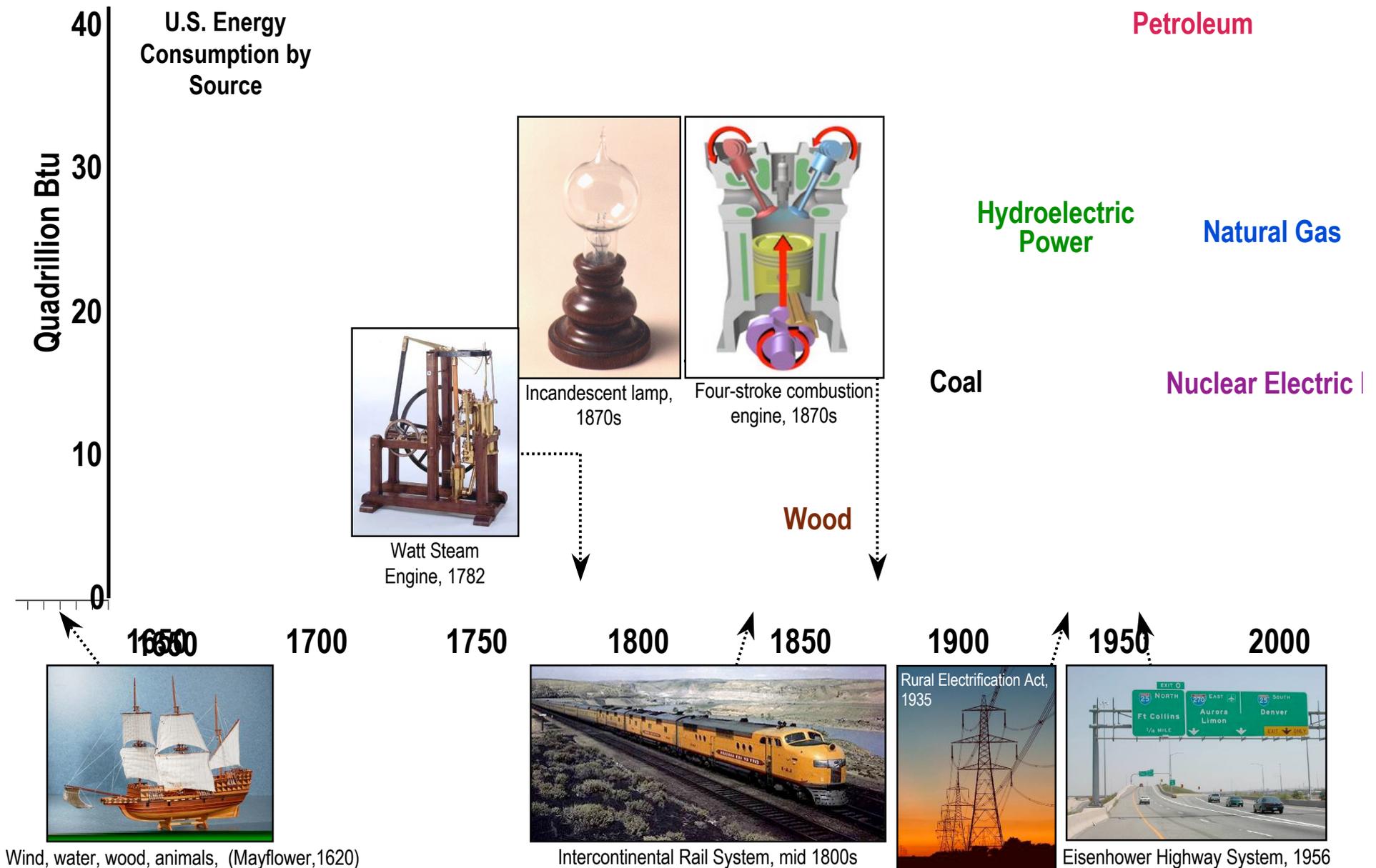
The Environment

and

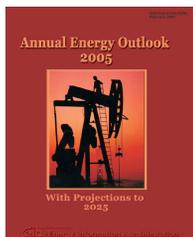
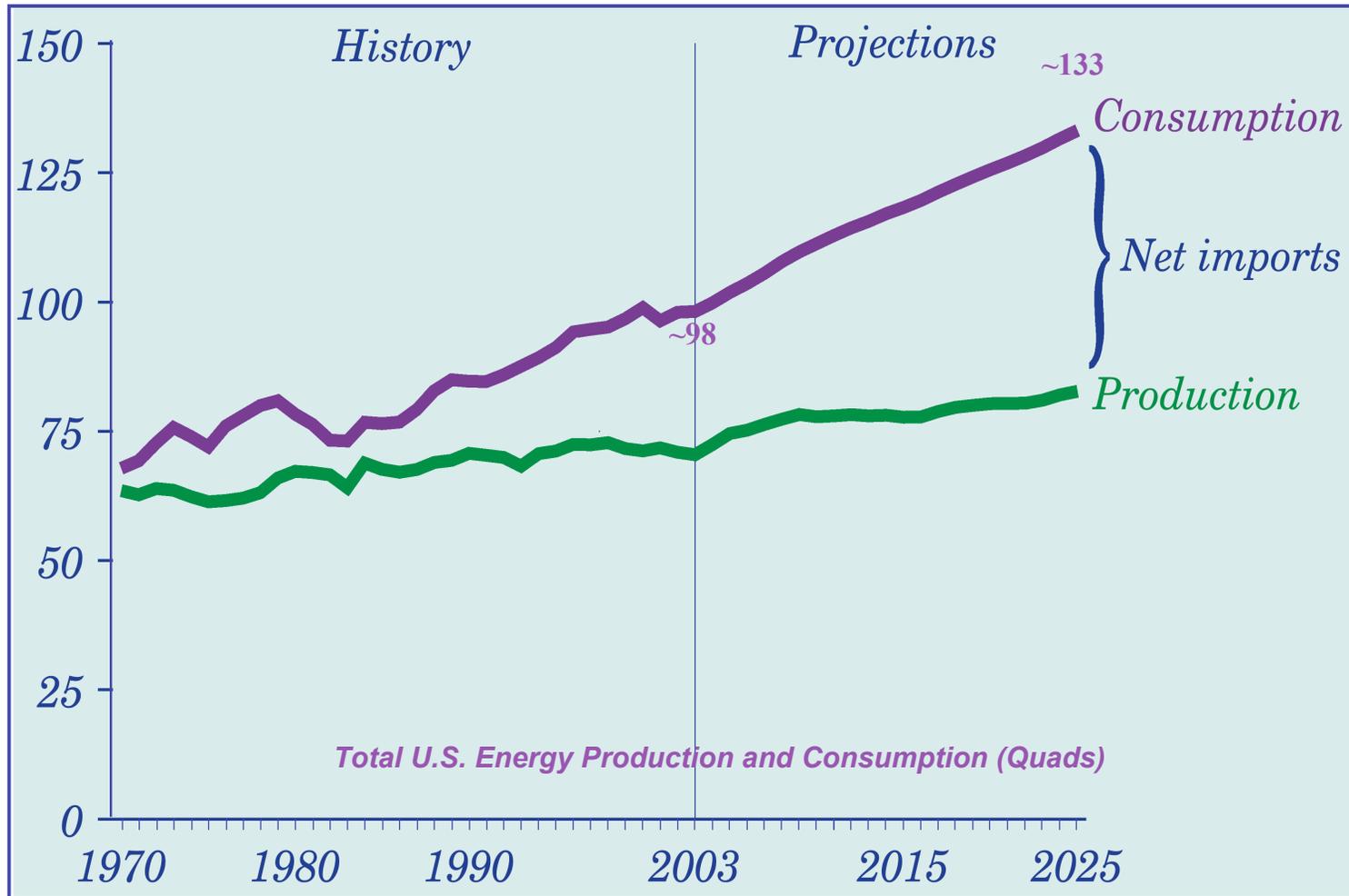
Global Change

Technology, Energy, and Society are Inextricably Intertwined

Today's Energy Technologies and Infrastructures are Firmly Rooted in the 20th Century

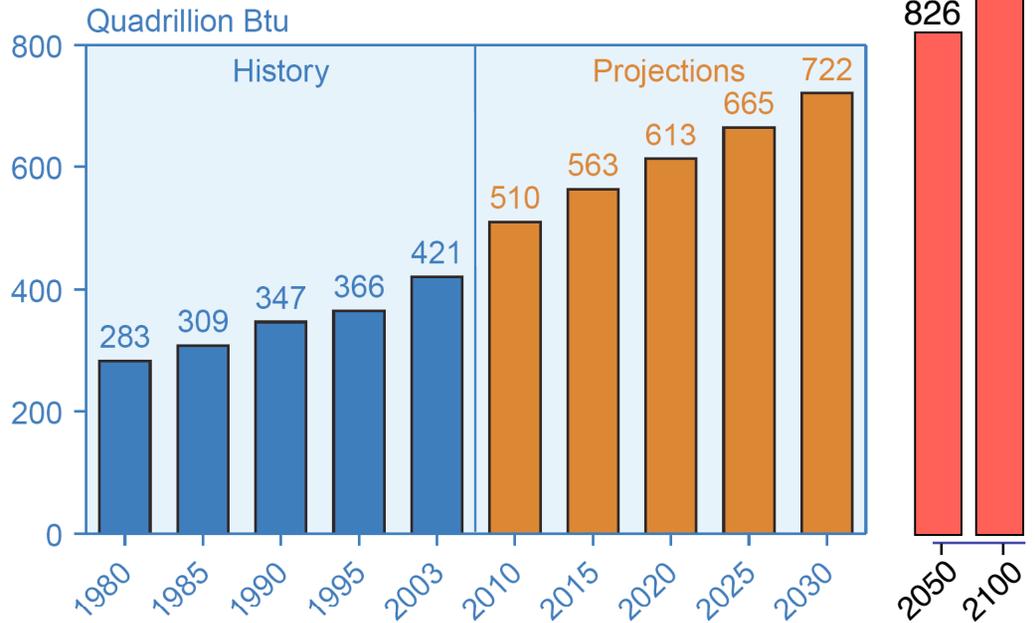


U.S. Overall Energy Needs Continue to Grow and Outpace Domestic Supply



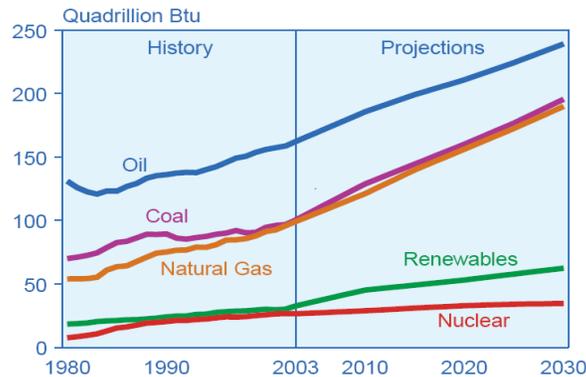
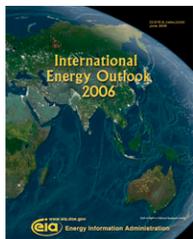
World Energy Needs will Grow Significantly in the 21st Century

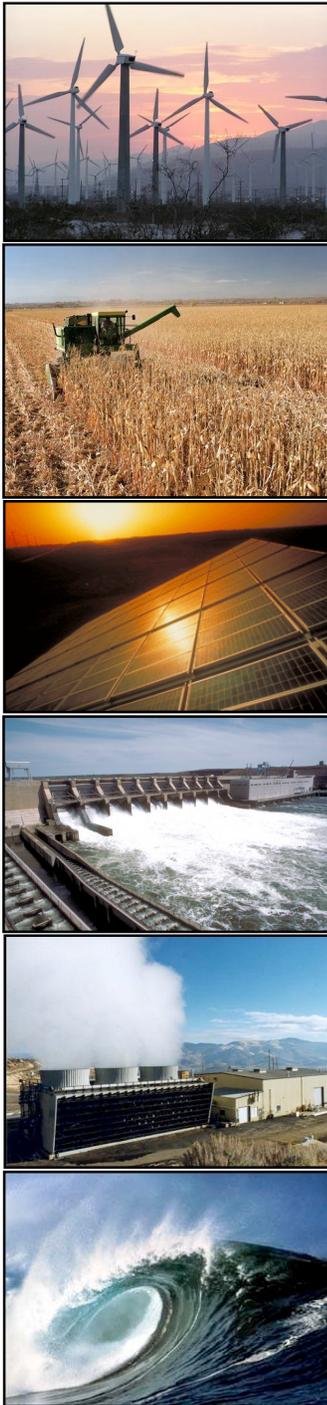
World Primary Energy Consumption (Quads)



Projections to 2030 are from the Energy Information Administration, International Energy Outlook, 2006.

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

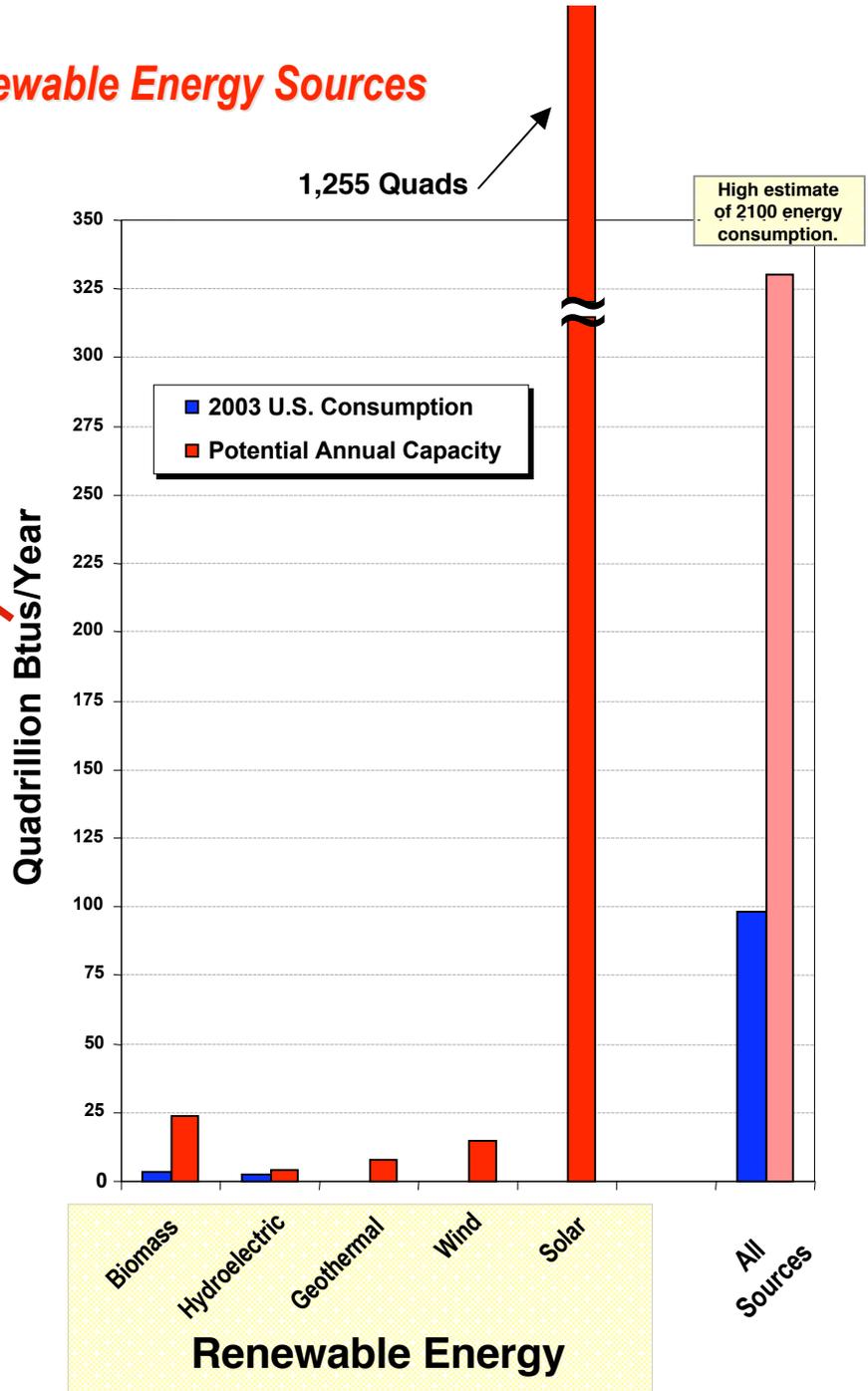




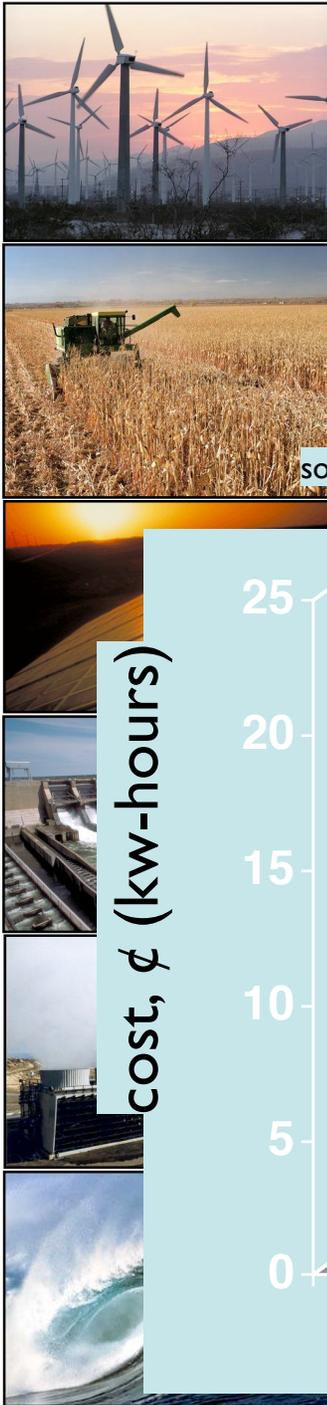
Potentials of U.S. Renewable Energy Sources

United States Renewable Energy (Quads/Year)	
Wind	
<u>2003 Consumption</u>	<u>Potential Capacity</u>
0.11	15
Biomass	
<u>2003 Consumption</u>	<u>Potential Capacity</u>
2.88	24
Solar	
<u>2003 Consumption</u>	<u>Potential Capacity</u>
0.06	1,255
Hydroelectric	
<u>2003 Consumption</u>	<u>Potential Capacity</u>
2.78	4
Geothermal	
<u>2003 Consumption</u>	<u>Potential Capacity</u>
0.31	8

DRAFT

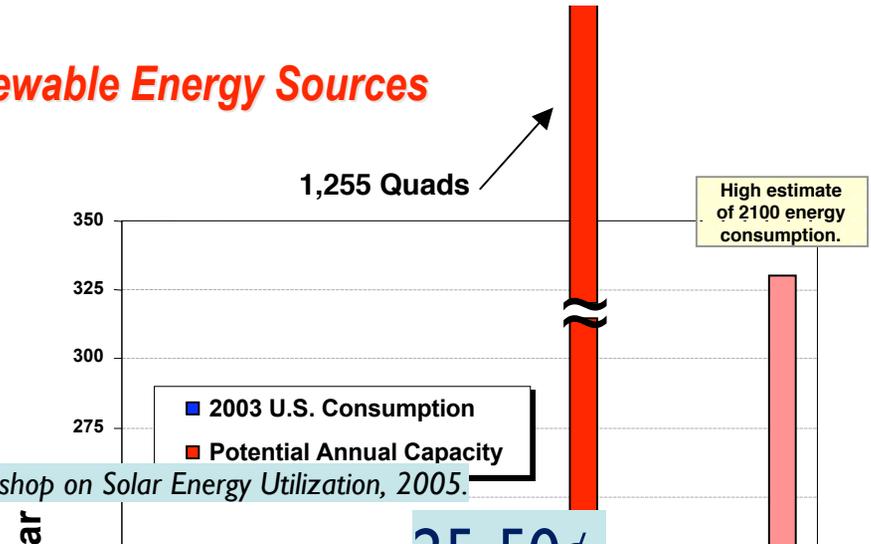


Potentials of U.S. Renewable Energy Sources

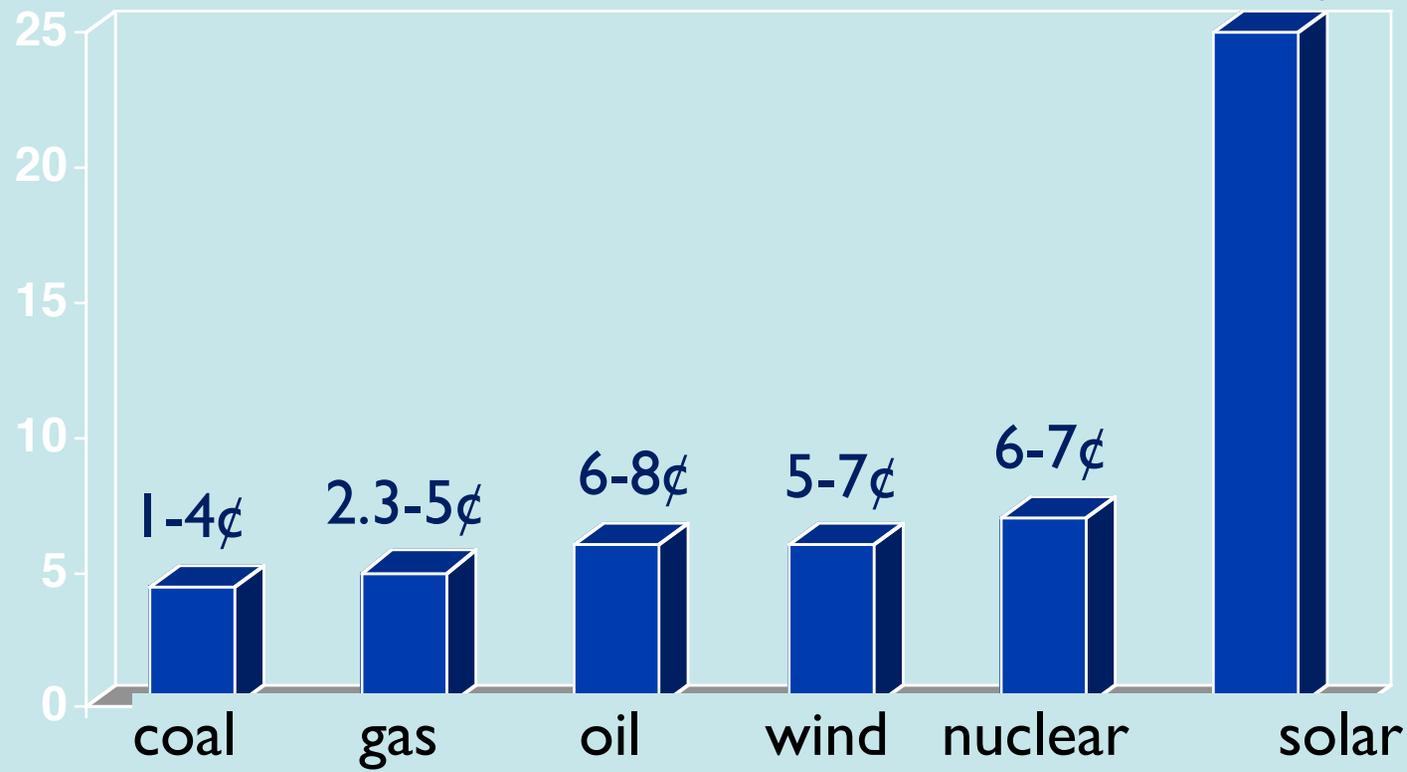


United States Renewable Energy (Quads/Year)	
2003 Consumption	Potential Capacity
11	125

source: DOE Report of the Basic Energy Sciences Workshop on Solar Energy Utilization, 2005.



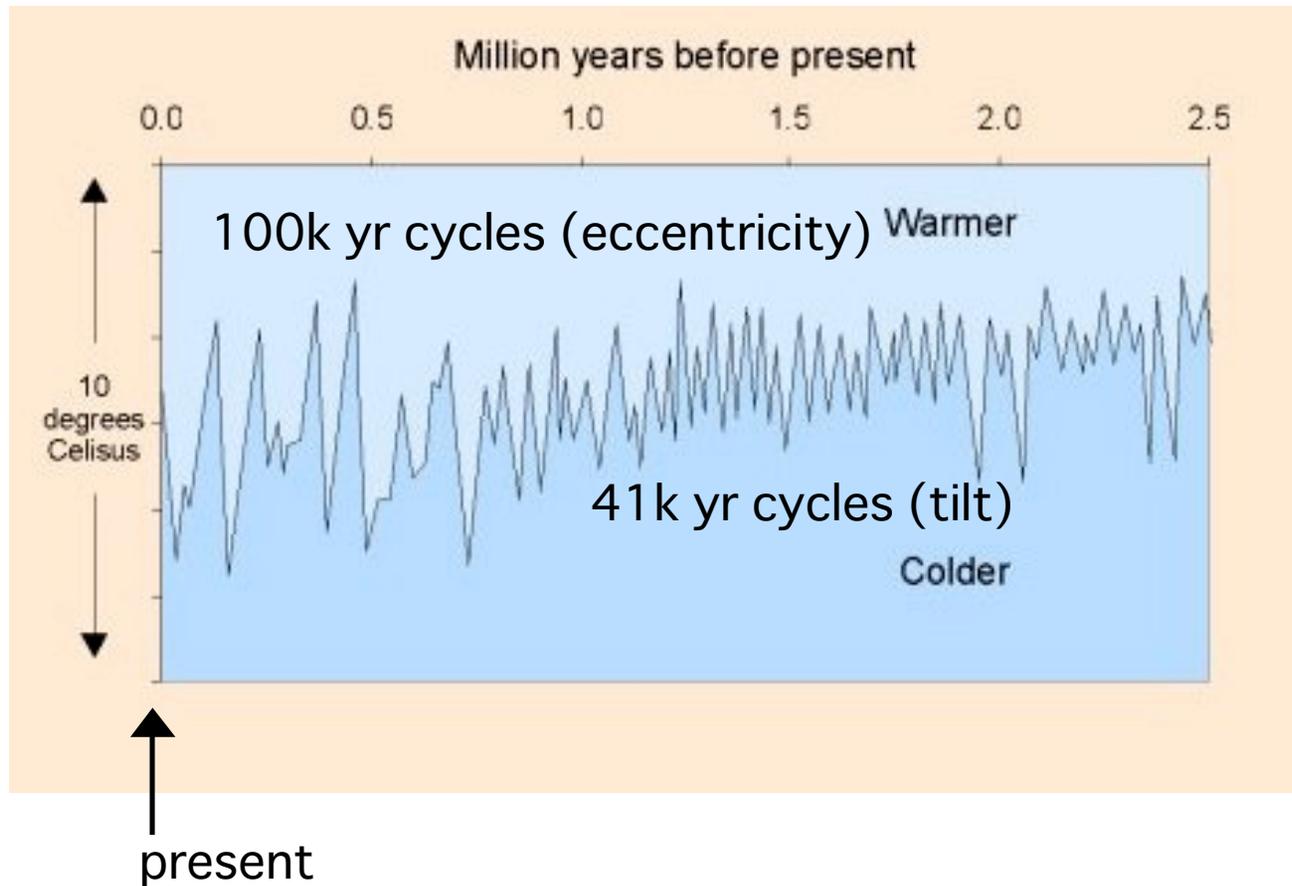
cost, ¢ (kw-hours)



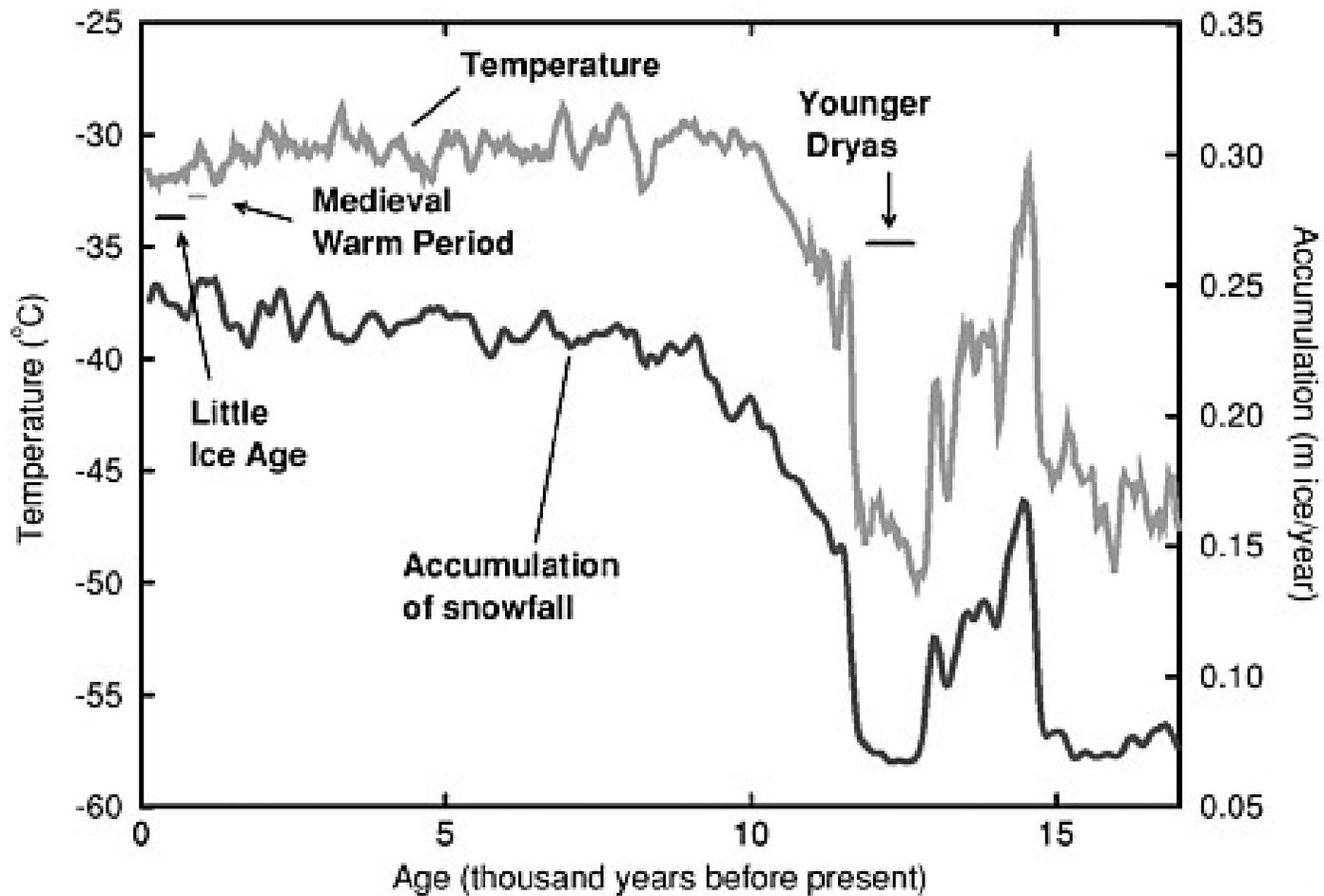
■ Cost

Climate Changes

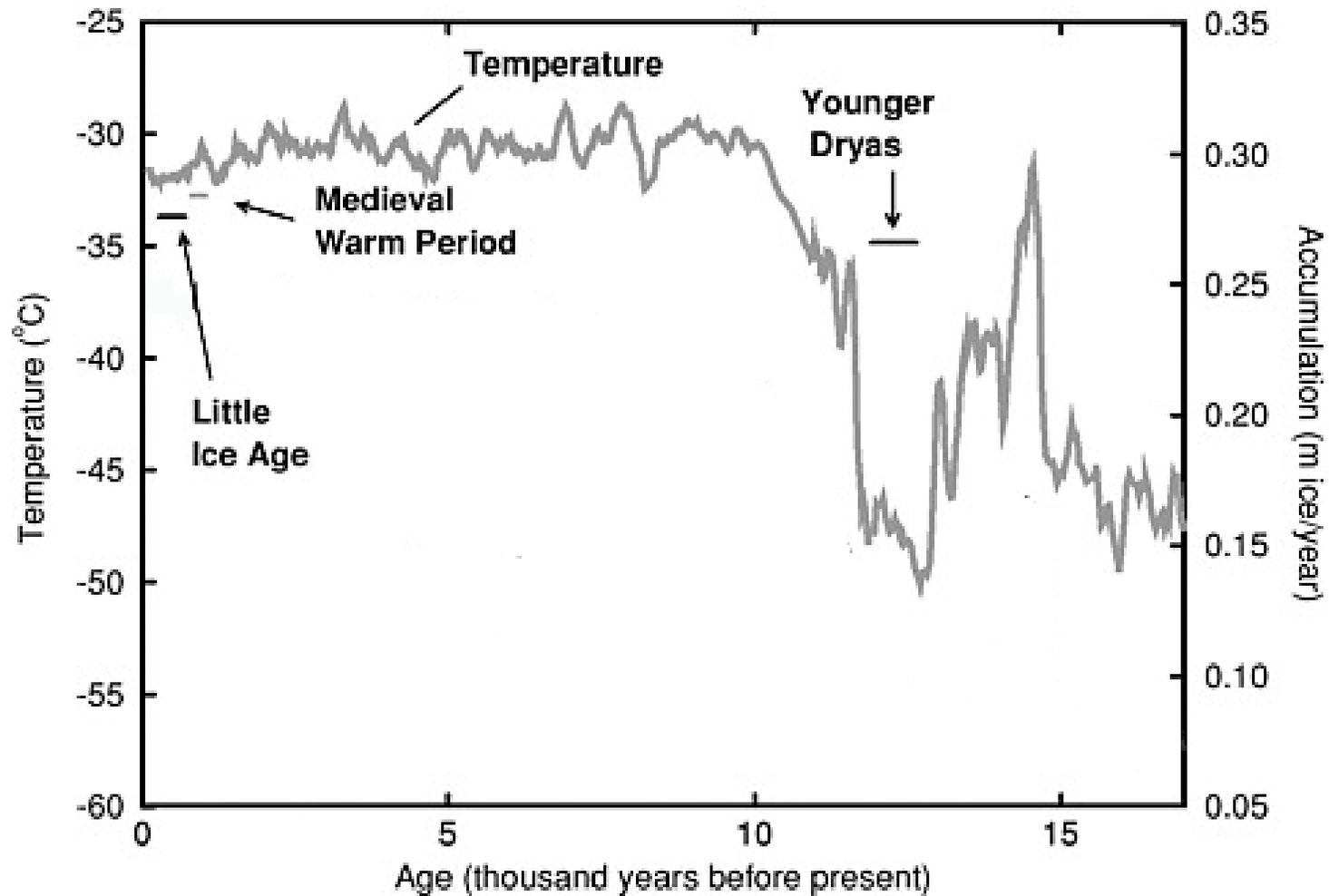
Ice Age Temperature Data



An Example of Abrupt Climate Change: the Younger-Dryas Central Greenland Temperatures



An Example of Abrupt Climate Change: the Younger-Dryas Central Greenland Temperatures



There is an Historic Correlation between CO₂ Concentration and Temperature

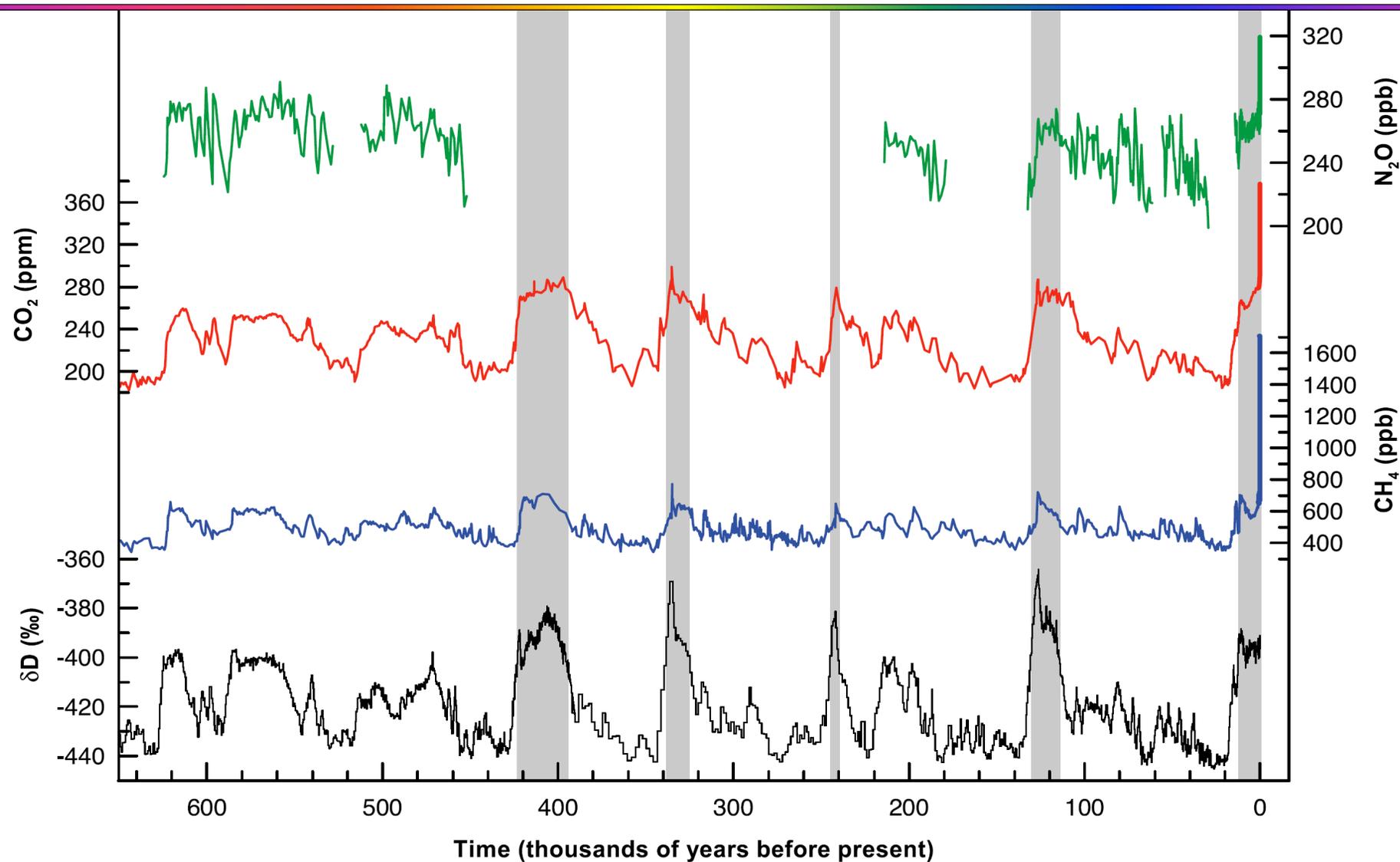
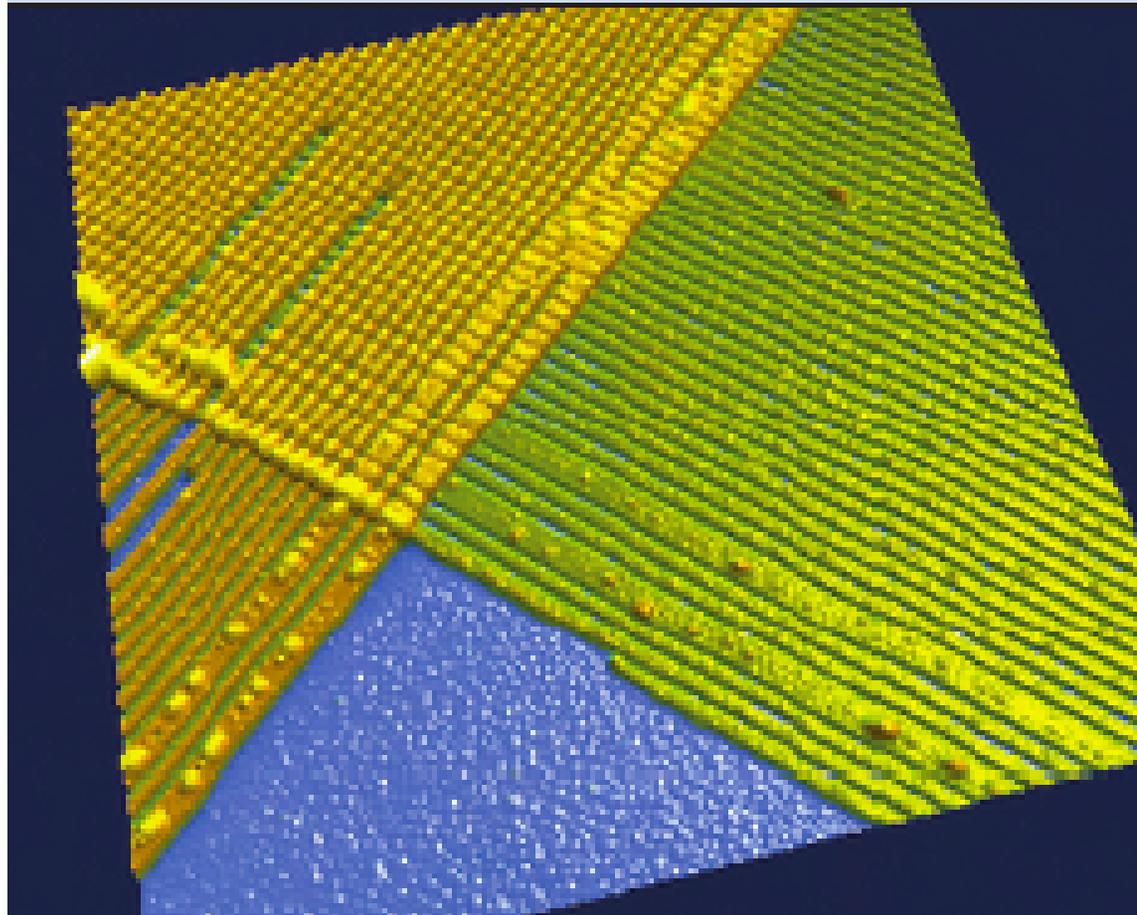


Figure TS.1. Variations of deuterium (δD) in antarctic ice, which is a proxy for local temperature, and the atmospheric concentrations of the greenhouse gases carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O) in air trapped within the ice cores and from recent atmospheric measurements. Data cover 650,000 years and the shaded bands indicate current and previous interglacial warm periods. {Adapted from Figure 6.3}

Defectology



An AFM topograph of a crossbar circuit fabricated by imprint lithography at a feature size (half-pitch) of 17nm.

Directing Matter and Energy: Five Challenges for Science and the Imagination, Chapter 5(pg 79) Sidebar on “Defectology and the End of Moore’s Law”, Figure Courtesy of Greg S. Snider and R. Stanley Williams (Hewlett-Packard)).

There are Four Broad Energy Goals in the DOE Strategic Plan

PRIORITIES

SCIENTIFIC AND TECHNOLOGICAL INNOVATION

NUCLEAR SECURITY

- Nation's nuclear deterrent and infrastructure transformation
- Nuclear WMD/radiological threat prevention
- Naval Reactors

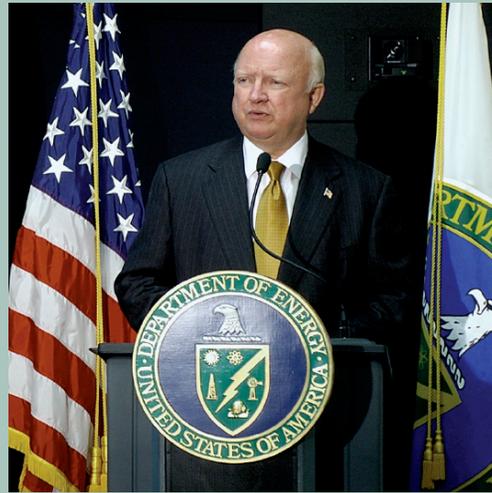
ENERGY SECURITY

- Nuclear power development
- Solar and biomass advancement
- Clean coal
- Hydrogen

ENVIRONMENTAL STEWARDSHIP

OPERATING PRINCIPLES

- Ensure safe, secure, and environmentally responsible operations
- Act with a sense of urgency
- Work together
- Treat people with dignity and respect
- Make the tough choices
- Keep our commitments
- Embrace innovation
- Always tell the truth
- Do the right thing



VISION

RESULTS IN OUR LIFETIME TO ENSURE . . .

- Energy Security
- National Security
- Science-Driven Technology Revolutions
- One Department of Energy - Keeping our Commitments

STRATEGIC THEMES

- Promoting America's energy security through reliable, clean, and affordable energy
- Ensuring America's nuclear security
- Strengthening U.S. scientific discovery, economic competitiveness, and improving quality of life through innovations in science and technology
- Protecting the environment by providing a responsible resolution to the environmental legacy of nuclear weapons production
- Enabling the mission through sound management

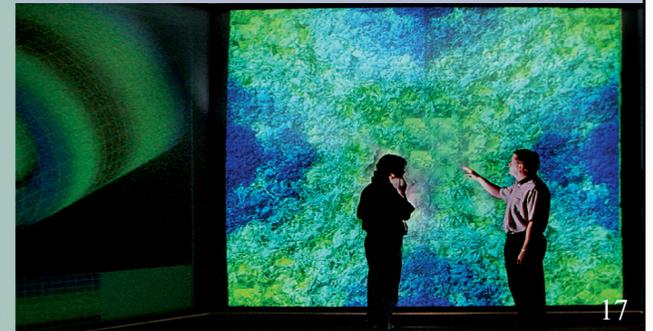
www.ENERGY.gov

DOE/CF-0011



2006 STRATEGIC PLAN THE DEPARTMENT OF ENERGY

MISSION:
Discovering the solutions to power
and secure America's future



There are Four Broad Energy Goals in the DOE Strategic Plan

Energy Diversity

Increase our energy options and reduce dependence on oil, thereby reducing vulnerability to disruptions and increasing the flexibility of the market to meet U.S. needs.

Environmental Impacts of Energy

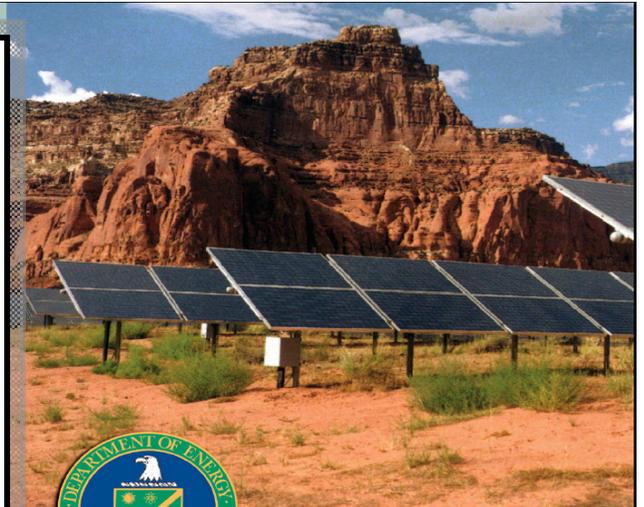
Improve the quality of the environment by reducing greenhouse gas emissions and environmental impacts to land, water, and air from energy production and use.

Energy Infrastructure

Create a more flexible, more reliable, and higher capacity U.S. energy infrastructure.

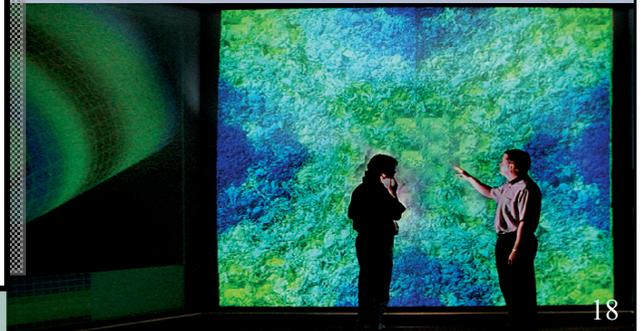
Energy Productivity

Cost-effectively improve the energy efficiency of the U.S. economy.

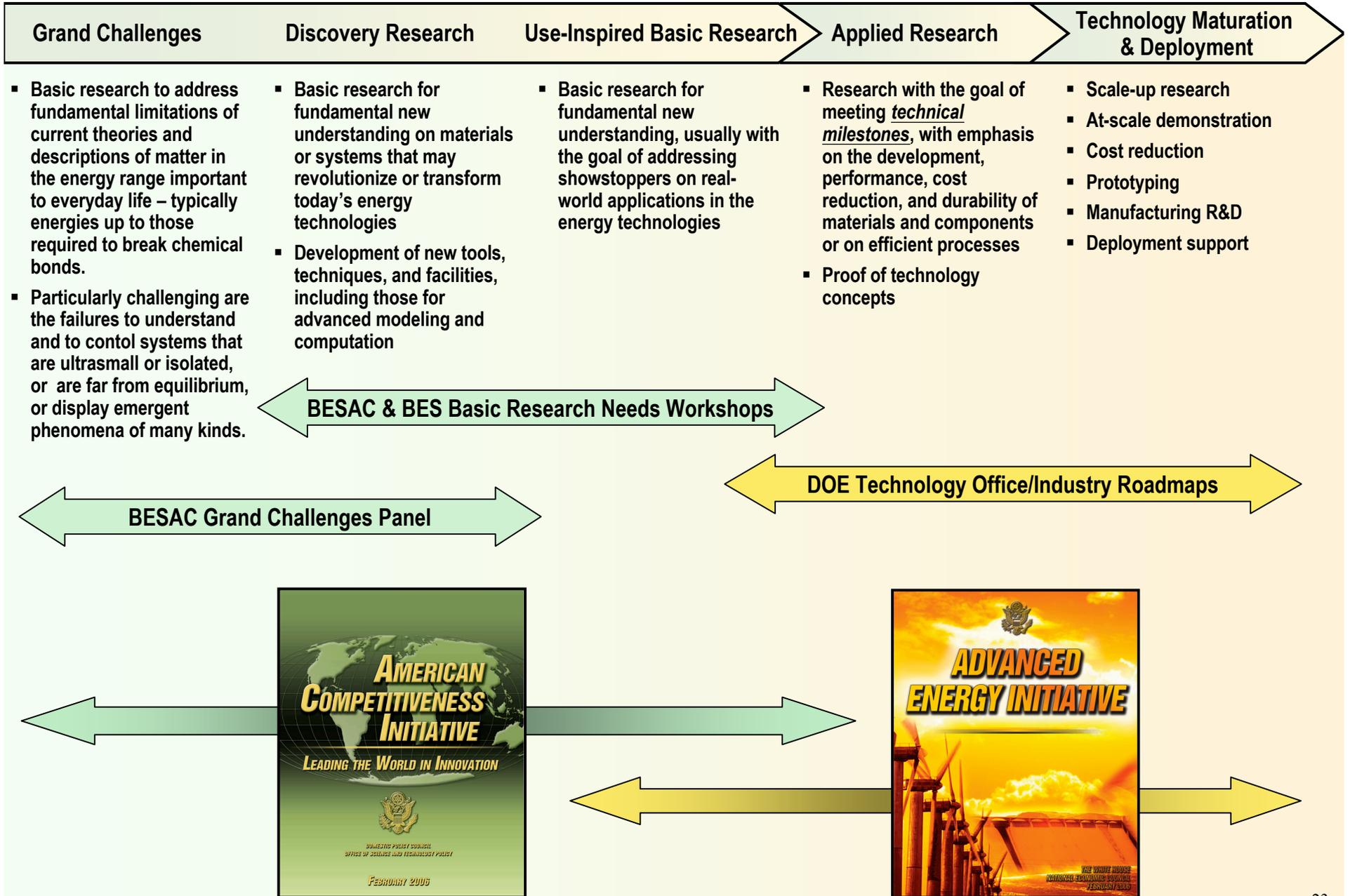


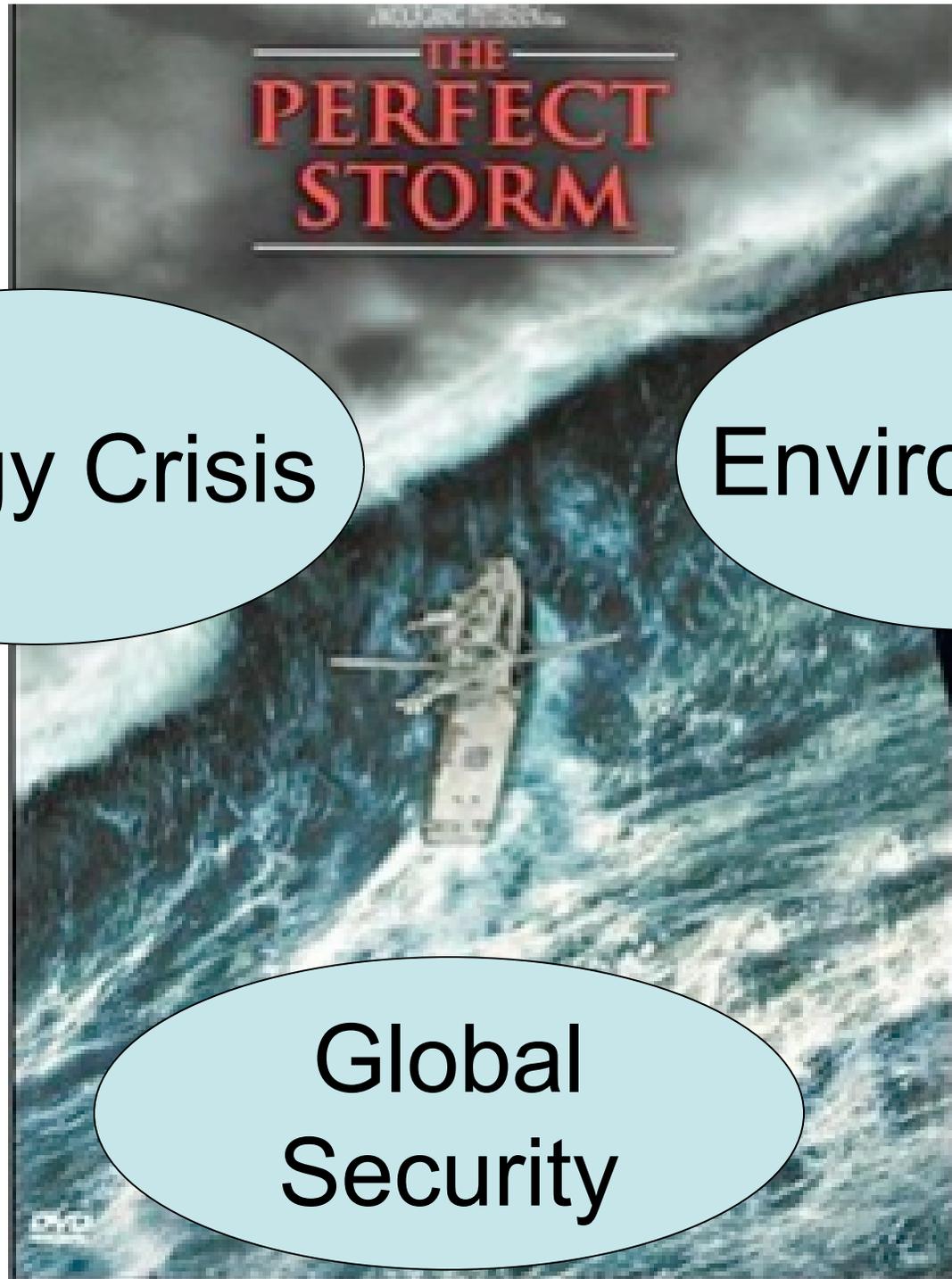
2006 STRATEGIC PLAN THE DEPARTMENT OF ENERGY

MISSION:
Discovering the solutions to power
and secure America's future



Overview of Relationships between BES Activities and the ACI & AEI





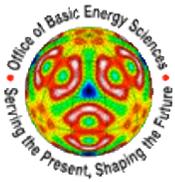
Energy Crisis

Environment

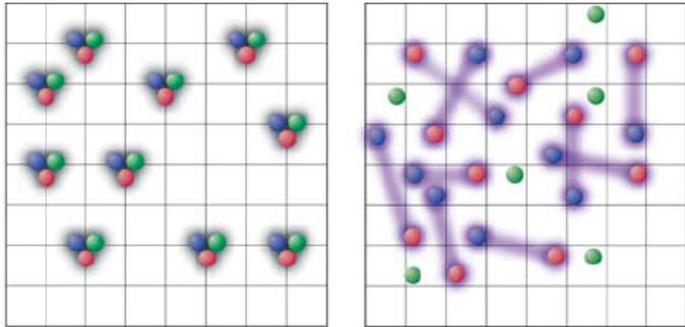
Global Security

Five Grand Challenges for

- *How do we control materials and processes at the level of electrons?*
- *How do we design and perfect atom- and energy-efficient synthesis of new forms of matter with tailored properties?*
- *How do remarkable properties of matter emerge from complex correlations of atomic and electronic constituents and how can we control these properties?*
- *Can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living systems?*
- *How do we characterize and control matter away—especially very far away—from*

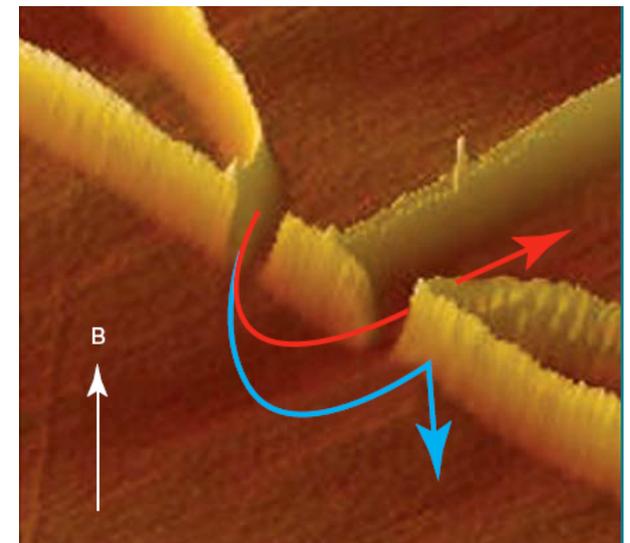
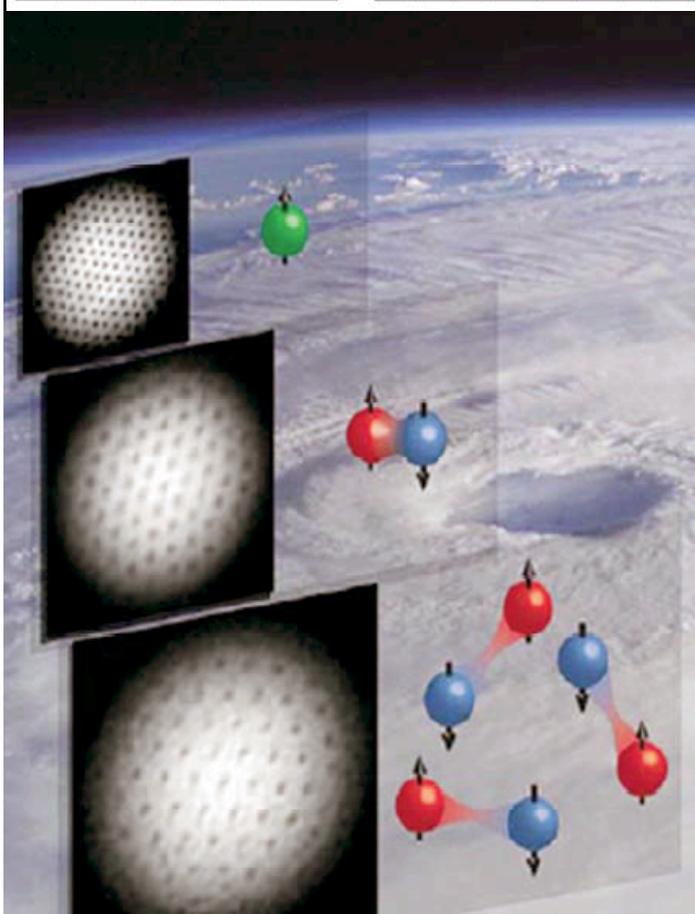


Grand Challenge: *How do we control materials and processes at the level of electrons?*



Making quantum systems work for us

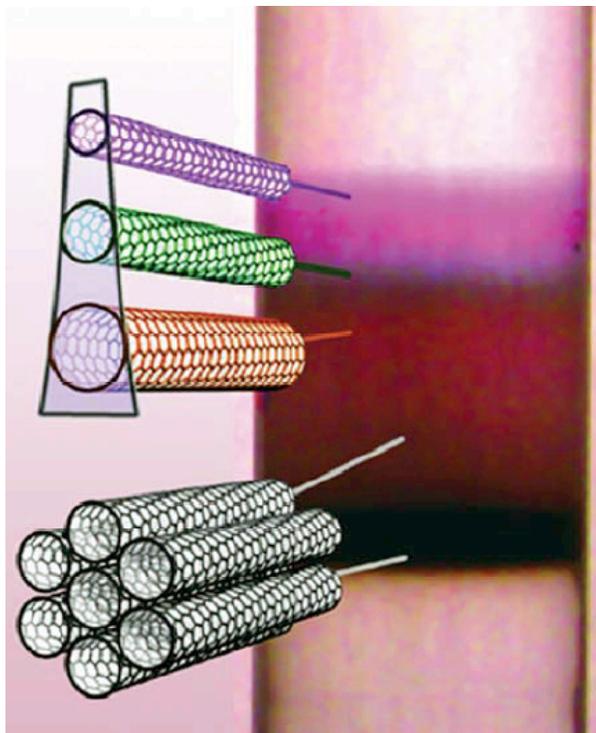
- ◆ Attosecond optical pulses, high intensity excitation
 - Failure of Born-Oppenheimer Approx.
 - Conical intersections
- ◆ Control of spins (spintronics)
- ◆ Quantum computing and the use of coherence in devices.
- ◆ Quantum simulators



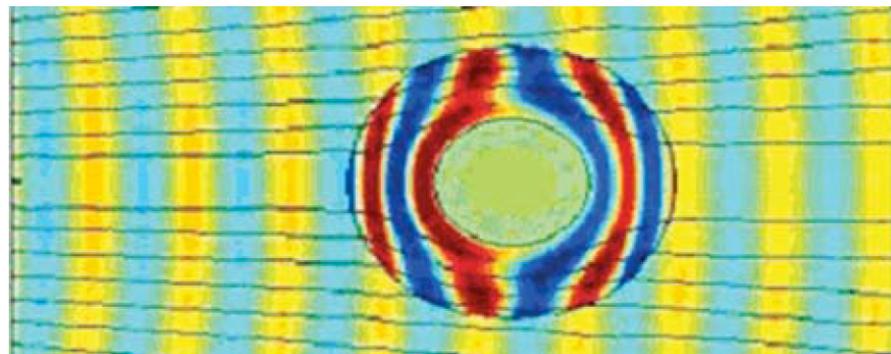
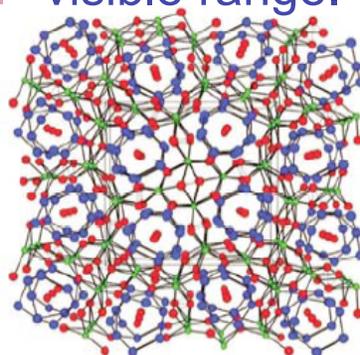
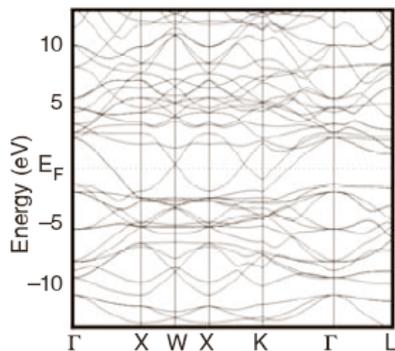


Grand Challenge: How do we design and perfect atom- and energy-efficient synthesis of new forms of matter with tailored properties?

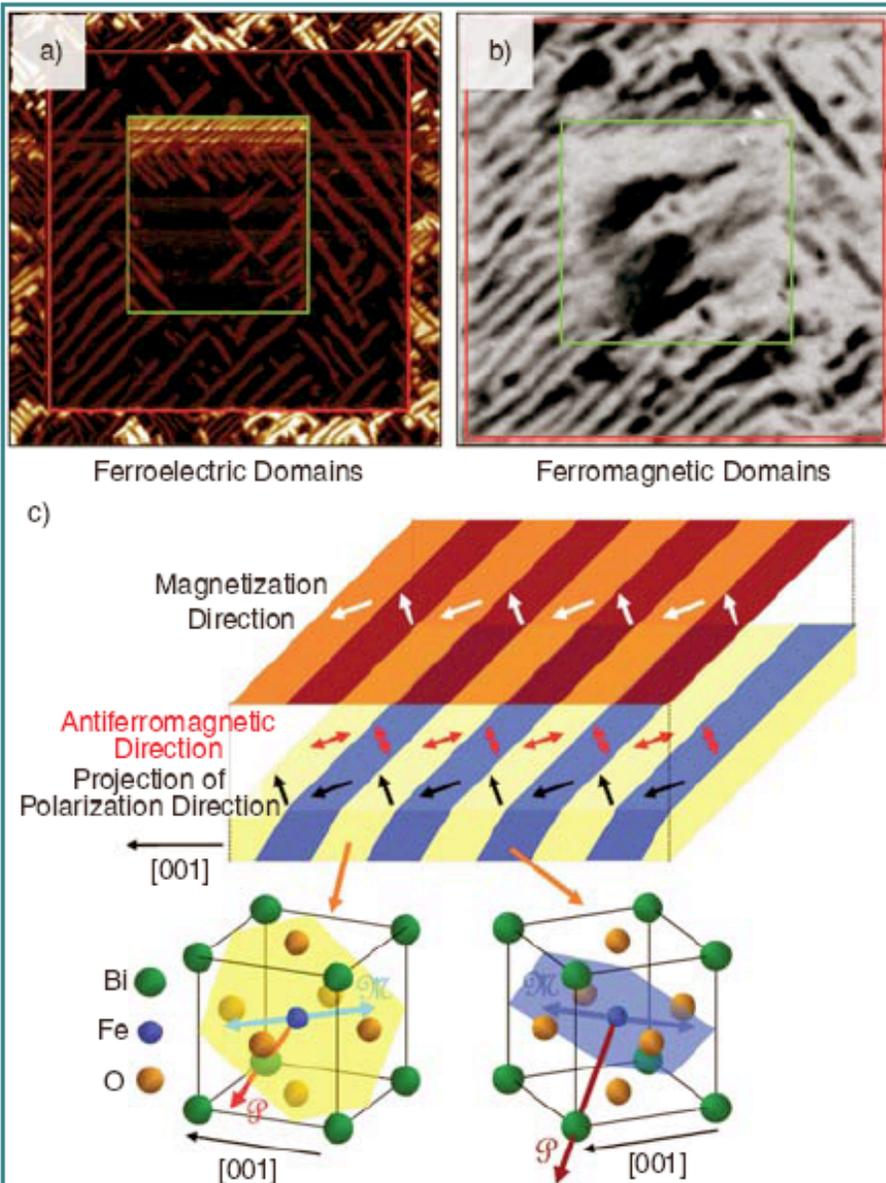
Directing the “un-glueing” and “re-glueing” of electrons



- ◆ Design for a particular electronic structure by finding the optimum combination of crystal structure & elements that yields (e.g. a specified band structure).
- ◆ Design for self regulation and even self repair of catalysts
- ◆ Low cost efficient solar cells
- ◆ Designing molecular logic
- ◆ Contra indicated properties (e.g. transparent conductors).
- ◆ Meta materials: perfect lenses, invisibility cloaks in the visible range.

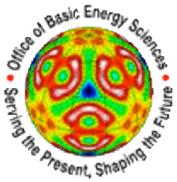


Grand Challenge: How do remarkable properties of matter emerge from complex correlations of atomic and electronic constituents and how can we control these properties?



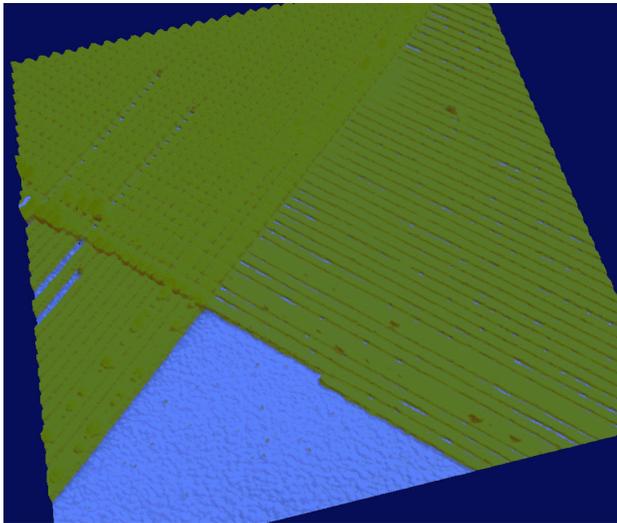
Uncovering the fundamental rules of correlations and emergence & learning to control them

- ◆ Create successor to current semiconductors from strongly correlated materials (e.g. multiferroics combine and couple electric & magnetic action—electrical control of magnetism)
- ◆ Quantum correlated liquids
 - Quantum spin liquids: artificial photons, fractional quasi particle (error free quantum computing)
- ◆ Strongly correlated atoms
 - quantum emulators & simulators (e.g. tests of the Hubbard Model for cuprates)
- ◆ Soft matter
- ◆ Biology

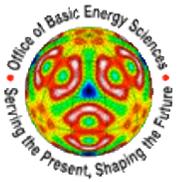


Grand Challenge: *Can we master energy and information on the nanoscale?*

Creating new technologies with capabilities rivaling those of living systems

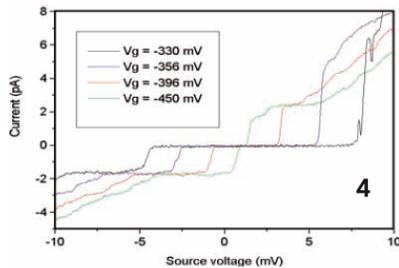
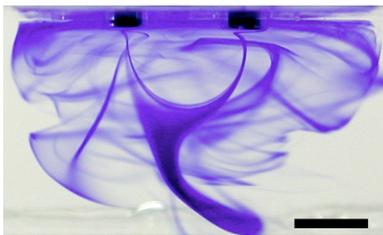
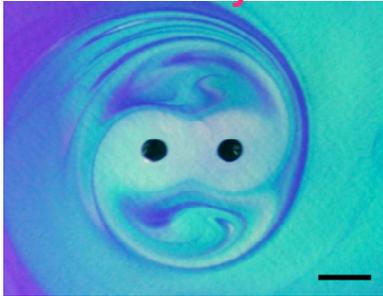


- ◆ Tap the existing world of biological nanotechnology by constructing interfaces between living cells and synthetic technology
- ◆ Fabricate devices with functionalities approaching those of living systems, but with different hardware implementation.
- ◆ Nano-macro junctions: covering the gap from a few tenths to a few hundred nanometers (photonic, electrical & magnetic, mechanical)
- ◆ Defects and the end of Moore's law
 - adaptive probabilistic computing
- ◆ Energy transduction at the nanoscale
 - stochastic processes, signals & noise)
- ◆ Ad hoc networking among nanoscale devices

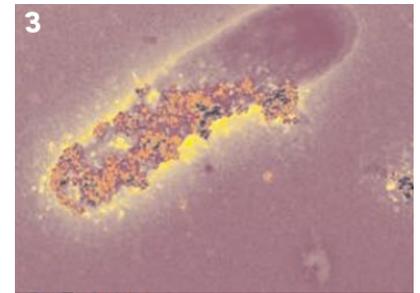


Grand Challenge: How do we characterize and control matter away—especially very far away—from equilibrium?

Magneto-hydrodynamic self-assembly



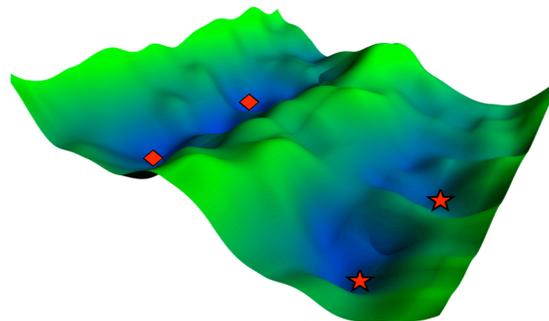
- ◆ Nanoscale thermodynamics
- ◆ Molecular transport junctions
- ◆ Fluctuations; Design, complexity, robustness
 - energy-capture & energy-storage capabilities, mitigate environmental damage
- ◆ Exploring rough landscapes
- ◆ Jamming
- ◆ Science of life



Shewanella



Molecular transport junction

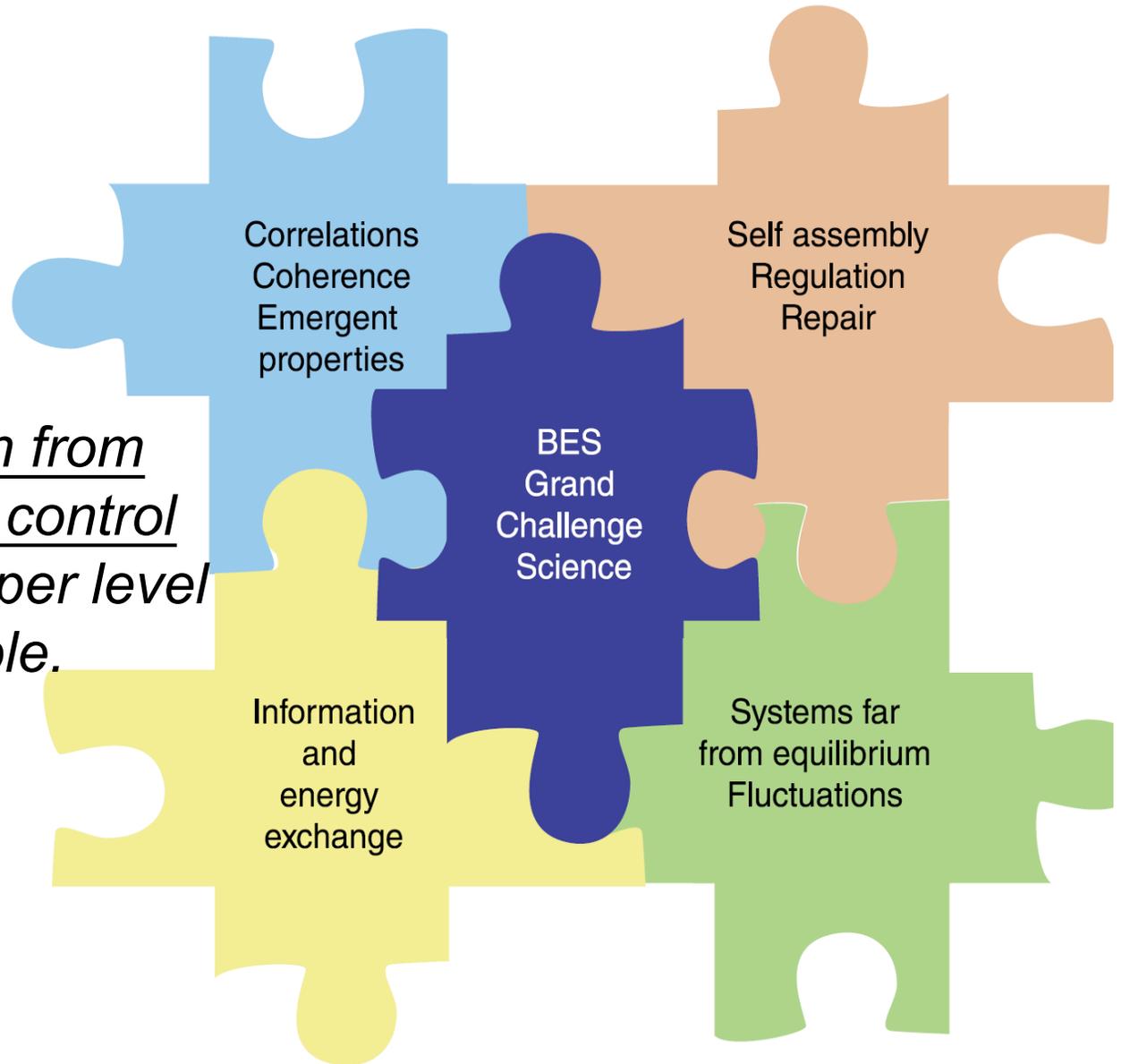


cyclone

Connecting Themes

An underlying set of concepts emerged.

We are on the threshold of a transition from observation science to control science at a much deeper level than is currently possible.

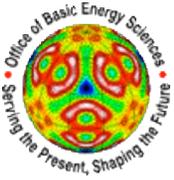


Discovery and Use-Inspired Research

The “Basic Research Needs” Workshops



- **Basic Research Needs to Assure a Secure Energy Future**
BESAC 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**
BES Workshop, May 13-15, 2003
- **Nanoscience Research for Energy Needs**
BES and the National Nanotechnology Initiative, March 16-18, 2004
- **Basic Research Needs for Solar Energy Utilization**
BES Workshop, April 18-21, 2005
- **Advanced Computational Materials Science: Application to Fusion and Generation IV Fission Reactors**
BES, ASCR, FES, and NE Workshop, March 31-April 2, 2004
- **The Path to Sustainable Nuclear Energy: Basic and Applied Research Opportunities for Advanced Fuel Cycles**
BES, NP, and ASCR Workshop, September 2005
- **Basic Research Needs for Superconductivity**
BES Workshop, May 8-10, 2006
- **Basic Research Needs for Solid-state Lighting**
BES Workshop, May 22-24, 2006
- **Basic Research Needs for Advanced Nuclear Energy Systems**
BES Workshop, July 31-August 3, 2006
- **Basic Research Needs for the Clean and Efficient Combustion of 21st Century Transportation Fuels**
BES Workshop, October 30-November 1, 2006
- **Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems**
BES Workshop, February 21-23, 2007
- **Basic Research Needs for Electrical Energy Storage**
BES Workshop, April 2-5, 2007
- **Basic Research Needs for Materials under Extreme Environments**
BES Workshop, June 10-14, 2007
- **Basic Research Needs for Catalysis for Energy**
BES Workshop, August 5-10, 2007



Why Grand Challenges Now?

Necessity

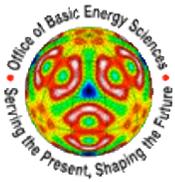
Opportunity



New BESAC Sub-Committee Charge

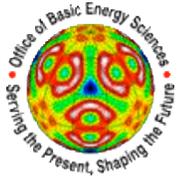
Co-Chairs: George Crabtree, Marc Kastner

Following the completion of the 10 Basic Research Needs (BRNs) workshop reports by BES in the past five years and the recent Grand Challenges study under the auspices of BESAC, BESAC is now embarking on a study to tie together the aforementioned reports. This study has two primary goals: (1) to assimilate the scientific research directions that emerged from these workshop reports into a comprehensive set of science themes; and (2) to identify the new tools required to accomplish the science. Included in this should be the consideration of future light sources with technical characteristics that will address the science questions posed by these BESAC and BES studies.



BESAC Sub-committee Charge (Continued)

1. Summarize the range of scientific research directions that emerged from the 2002 BESAC report *Basic Research Needs for a Secure Energy Future*, the follow-on BES BRNs reports, and the BESAC report “*Directing Matter and Energy: Five Challenges for Science and the Imagination*”. Identify key cross-cutting scientific themes that are common to these reports. In doing so, also make the connections between the themes that resulted from the “use-inspired” BRNs workshops and those that resulted from the consolidation of the fundamental challenges that face our disciplines.
2. Summarize the implementation strategies, and human resources that will be required to accomplish the science described in the aforementioned reports. These strategies may include new experimental and theoretical facilities, instruments and techniques. Consider possible new organizational structures that may be required to implement the strategies and supply the human resources.
3. Identify future light sources needs that will be required to help accomplish the scientific challenges described in these workshops. Specifically, consider the energy range (from vacuum UV to hard X-rays), coherence (both transversal and longitudinal), intensity (photon per pulse and photon per second), brightness (ultrahigh brightness with low electron emittance), and temporal structure (nano to atto seconds) for future light sources.



Grand Challenges

How Do We Control Materials Processes at the Level of Electrons?

How Do We Design and Perfect Atom- and Energy-Efficient Synthesis of Revolutionary New Forms of Matter with Tailored Properties?

How Do Remarkable Properties of Matter Emerge from the Complex Correlations of Atomic or Electronic Constituents and How Can we Control Their Properties?

How Can we Master Energy and Information on the Nanoscale to Create New Technologies with Capabilities Rivaling Those of Living Things?

How Do We Characterize and Control Matter Away—Especially Very Far Away—From Equilibrium?

Implementation Strategies

Grand Challenge Science: The People and the Tools Required

Human Resources:

Attracting and Educating the Next Generation of Students and Young Faculty

Stable Funding for Senior Investigators

Team Science

Theory

New Lab Based Instrumentation

New Facilities