U.S. DEPARTMENT OF ENERGY | Office of Science

Office of Science Overview

University Research Associates, Inc.
Council of Presidents

Dr. William F. Brinkman
Director, Office of Science
U.S. Department of Energy

January 27, 2010

U.S. DEPARTMENT OF
ENERGY

- **Office of the Secretary**
  Dr. Steven Chu
  Daniel B. Poneman, Deputy Secretary
  - **Office of the Under Secretary**
    Kristina Johnson
    - Asst. Secretary for Energy Efficiency & Renewable Energy – Cathy Zoi
    - Asst. Secretary for Fossil Energy – James Markowski
    - Asst. Secretary for Nuclear Energy – Pete Miller
    - Asst. Secretary for Energy Delivery – Pat Hoffman (A)
  - **Office of the Under Secretary for Science**
    Steven E. Koonin
    - **Office of Science**
      William Brinkman
      - Basic Energy Sciences – Harriet Kung
      - High Energy Physics – Dennis Kovar
      - Advanced Scientific Computing Research – Michael Strayer
      - Nuclear Physics – Tim Hallman
      - Biological & Environmental Research – Anna Palmisano
      - Fusion Energy Sciences – Ed Synakowski
      - Workforce Development for Teachers & Scientists – Bill Valdez
  - **Advanced Research Projects Agency – Energy**
    Arun Majumdar

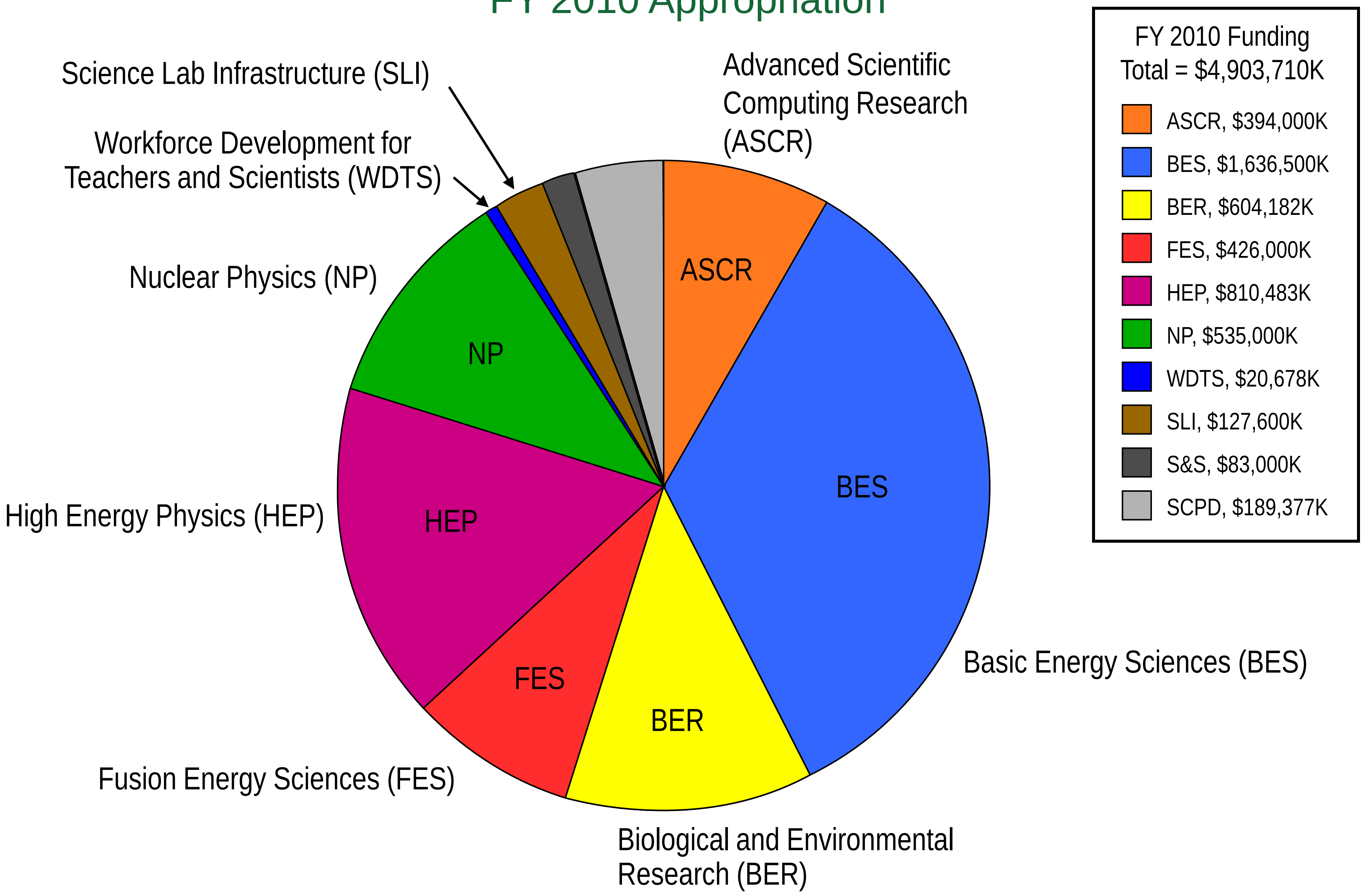
DOE's Office of Science

<u>Three themes</u> describe the work supported by the Office of Science:

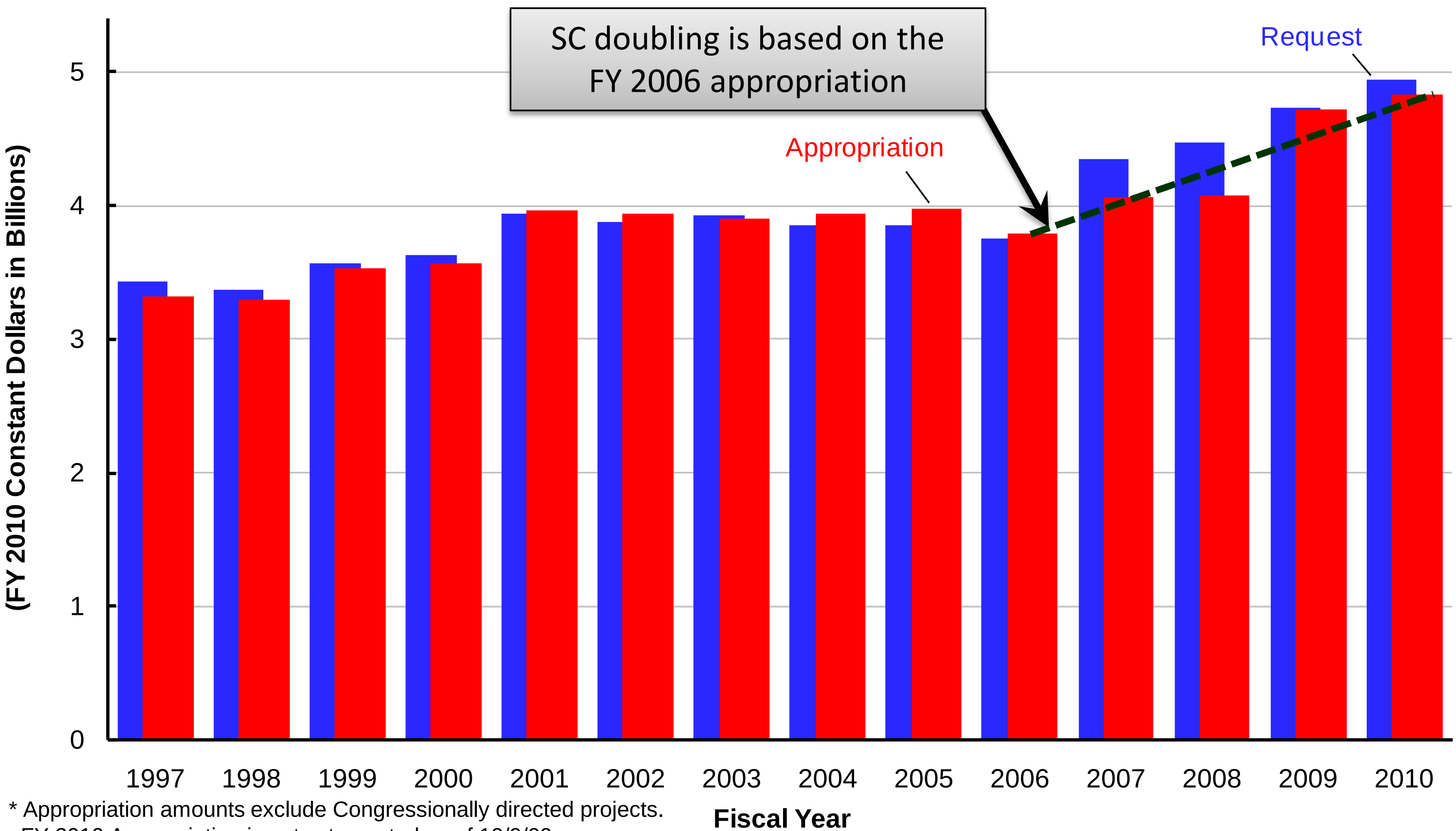
- **Science for discovery**
  - Unraveling Nature's deepest mysteries—from the study of subatomic particles; to atoms and molecules that make up the materials of our everyday world; to DNA, proteins, cells, and entire natural ecosystems
- **Science for national need**
  - Advancing a clean energy agenda through basic research on energy production, storage, transmission, and use
  - Advancing our understanding of the Earth's climate through basic research in atmospheric and environmental sciences and in climate modeling
  - Supporting DOE's missions in national security
- **National user facilities, the 21st century tools for science, engineering, and technology**
  - Providing the Nation's researchers with the most advanced tools of modern science including accelerators, colliders, supercomputers, light sources and neutron sources, and facilities for studying the nanoworld, the environment, and the atmosphere

Office of Science Programs

FY 2010 Appropriation



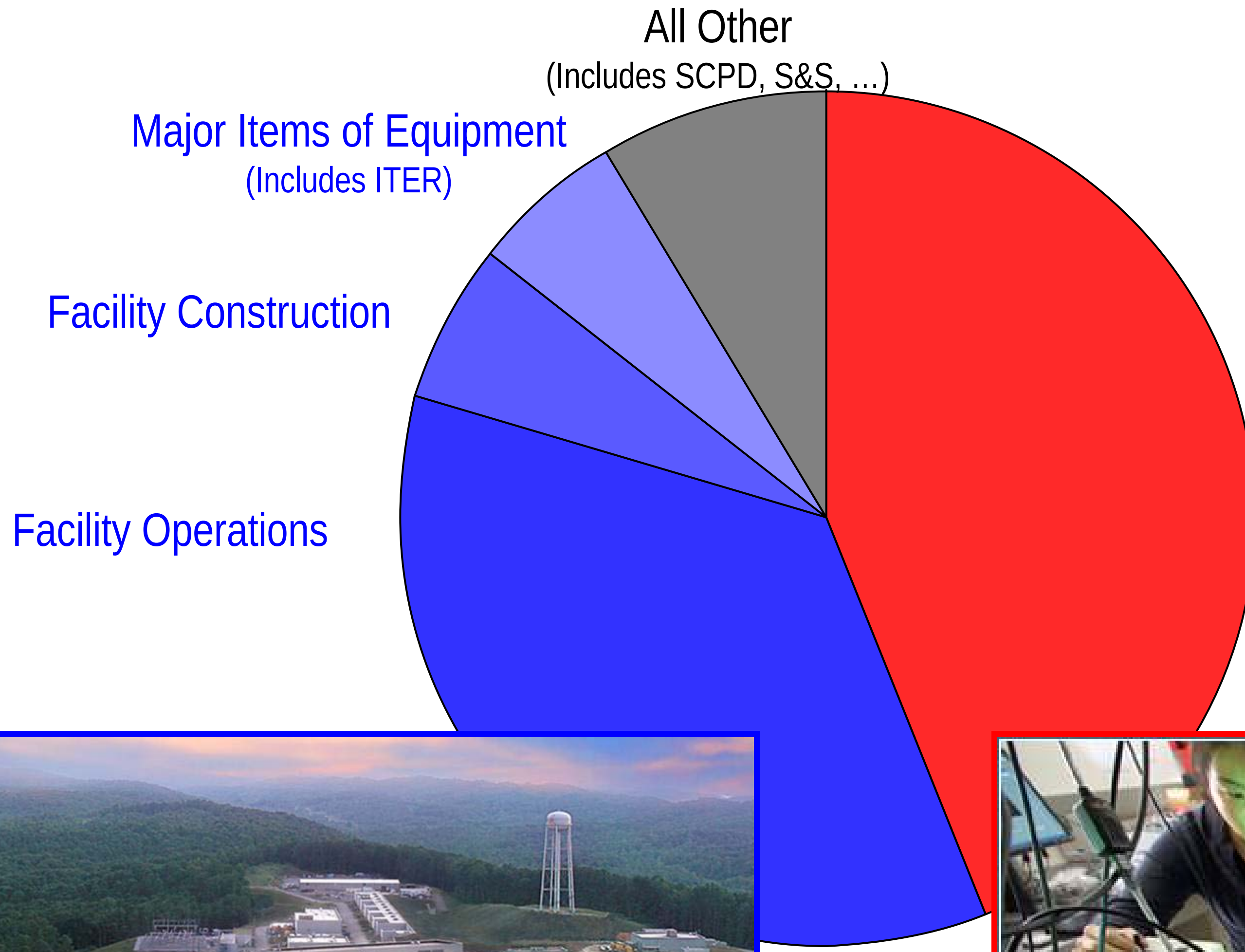
SC Request vs. Appropriation (FY 2010 Constant $s)

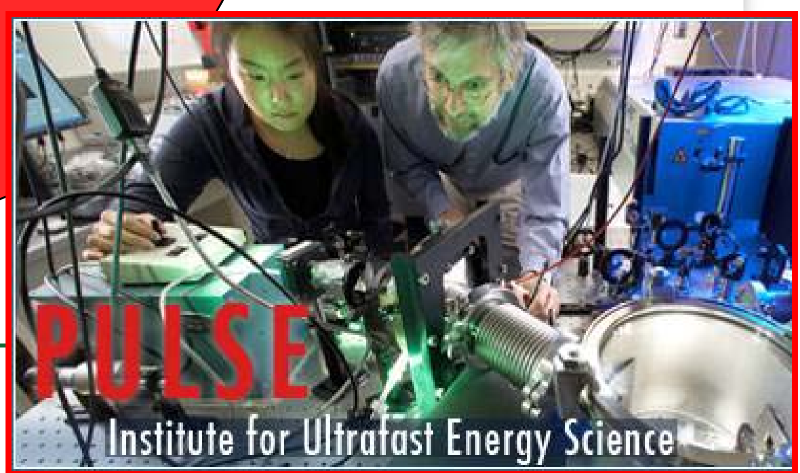


* Appropriation amounts exclude Congressionally directed projects.
FY 2010 Appropriation is not yet enacted as of 10/9/09.

Office of Science Functional Support

FY 2010 Funding
Total = $4,903,710K

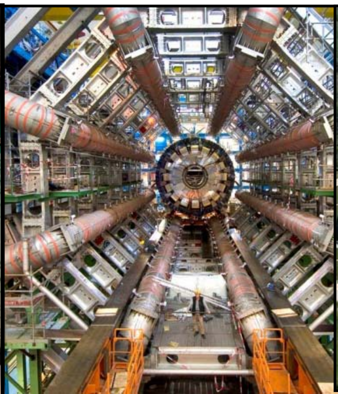




User Facilities

- Advanced **computational resources** – terascale to petascale computing and networks for open science
- Four **synchrotron light sources**, and two next-generation light sources in construction
- Three **neutron sources** for scattering
- **Particle accelerators/colliders/detectors** for high energy and nuclear physics
- **Fusion/plasma facilities**, including **ITER** which seeks to demonstrate a burning plasma
- Five **Nanoscale Science Research Centers** – capabilities for fabrication and characterization of materials at the nanoscale
- **Joint Genome Institute** for rapid whole genome sequencing
- **Environmental Molecular Science Laboratory** – experimental and computational resources for environmental molecular sciences
- **Atmospheric and Environmental Facilities** – capabilities for cloud and aerosol measurement and for carbon cycling measurements





Distribution of Users by Facility

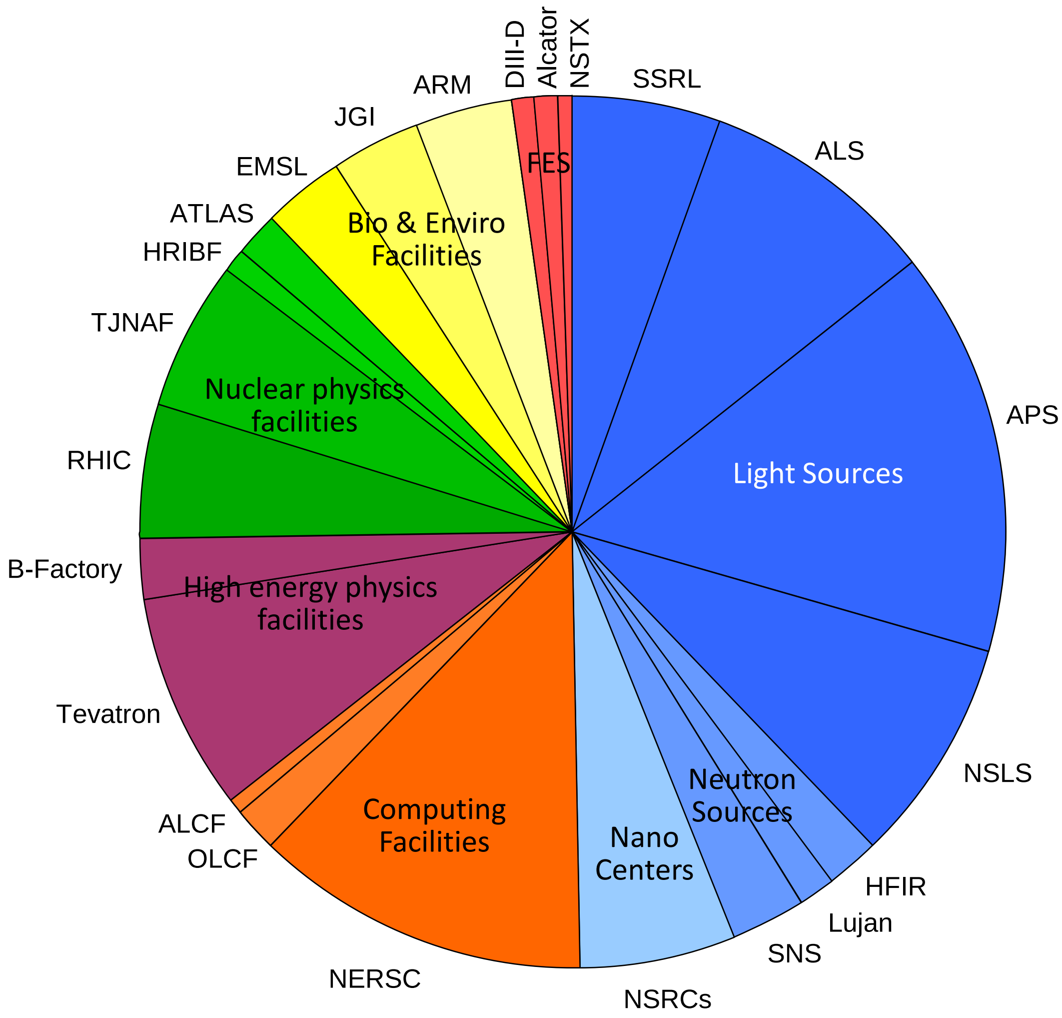
Breakdown by facility of ~25,000 users in FY 2010

~25,000 users at the facilities in FY 2010:

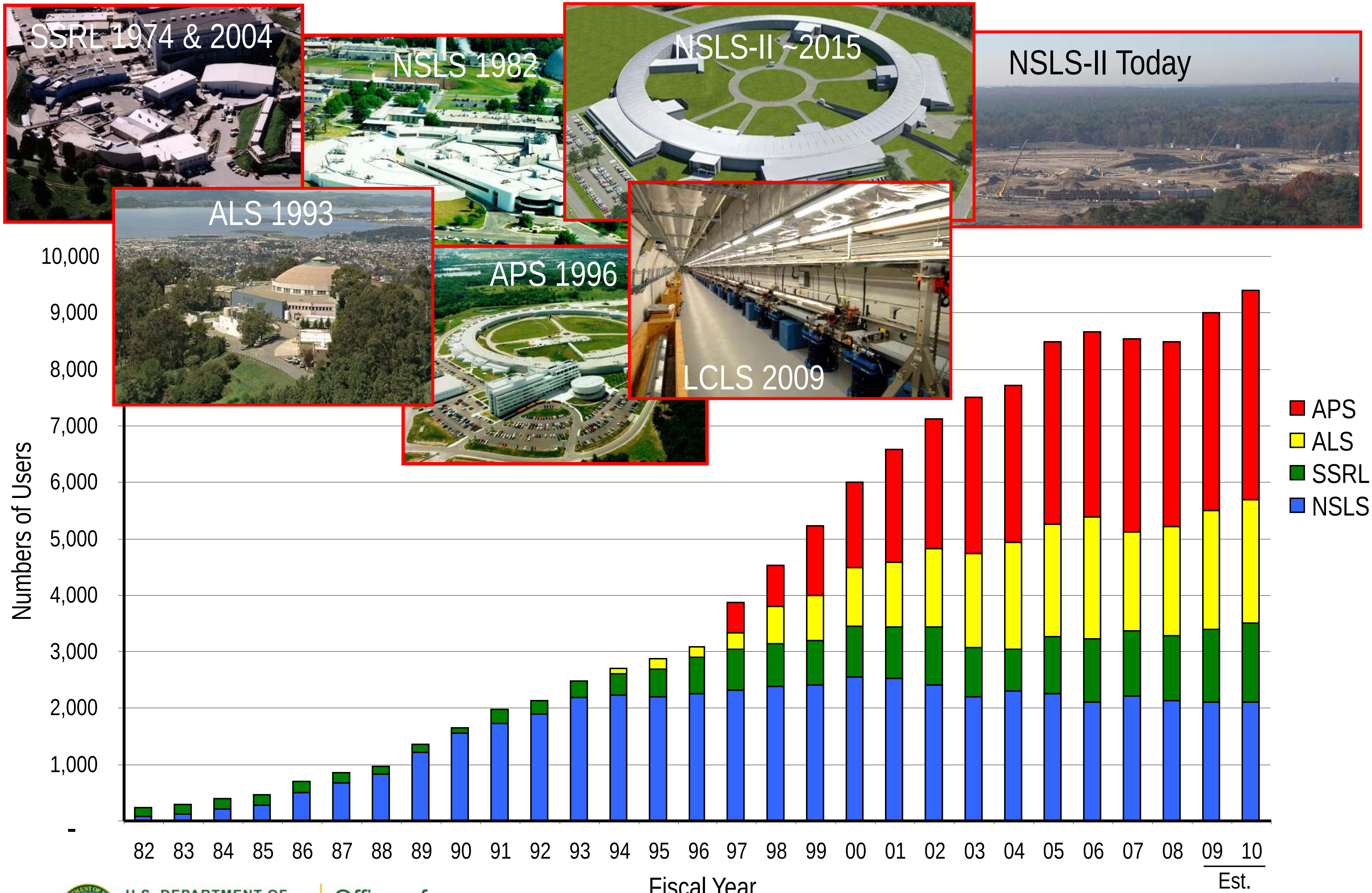
~1/2 from universities;

~1/3 from national labs;

and the remainder from industry, other agencies, and international entities.



35 Years of Light Sources



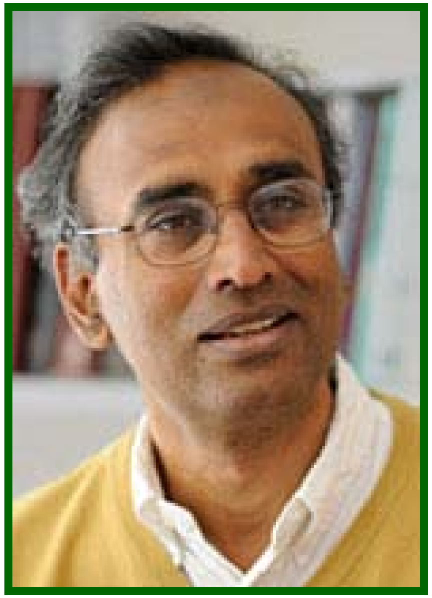
U.S. DEPARTMENT OF ENERGY | Office of Science

X ray Light Sources are Revolutionizing Biology

- The Protein Data Bank archive contains the structures of proteins, nucleic acids, and complex assemblies. Synchrotrons account for 70.6% of all structures (1995-2009 to date).
- These structures are used by researchers world wide to understand the functions of biologically important proteins with applications as diverse as developing new pharmaceuticals for combating disease to creating new enzymes to produce bioenergy.

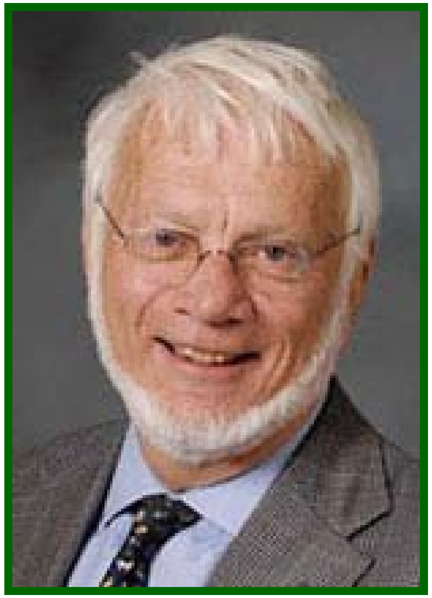
Advanced Photon Source	7,227
National Synchrotron Light Source	4,391
Advanced Light Source	2,729
Stanford Synchrotron Radiation Laboratory	2,621
European Synchrotron Radiation Facility (France)	5,868
EMBL/DESY (Germany)	2,080
Swiss Light Source	1,170
SPring-8 (Japan)	2,444
Photon Factory (Japan)	1,449

2009 Nobel Prize in Chemistry based on X-ray Crystallography



Venkatraman Ramakrishnan

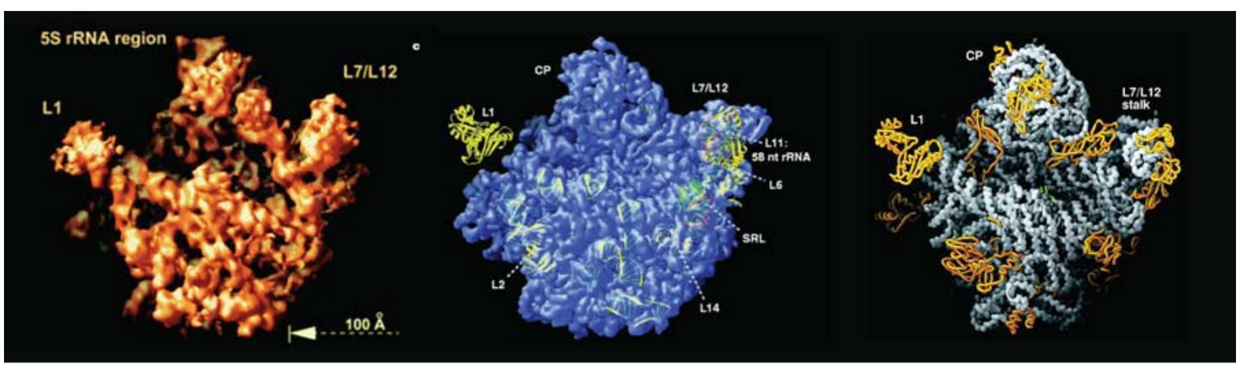
Ada Yonath



Thomas Steitz

- Three molecular biologists who mapped the structure and inner workings of the ribosome — the cell's machinery for churning out proteins from the genetic code — have won the Nobel Prize in Chemistry in 2009.
- Venkatraman Ramakrishnan, who works at the Medical Research Council's Laboratory of Molecular Biology in Cambridge, UK; Ada Yonath of the Weizmann Institute of Science in Rehovot, Israel, and Thomas Steitz at Yale University in New Haven, Connecticut, share the prize equally.

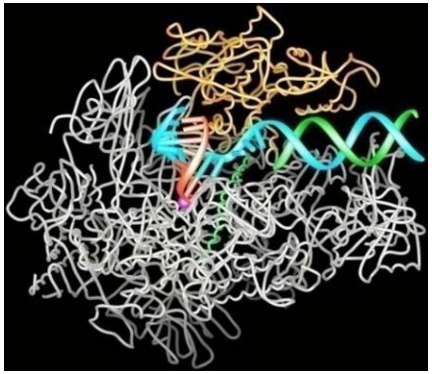
- Ribosome translates the genetic instructions encoded by DNA into chains of amino acids that make up proteins. The ribosome is composed of two subunits: 30S, which reads the code; and 50S, which links up the amino acids. The structures of 30S and 50S have been crucial to understanding everything from how the ribosome achieves its amazing precision to how different antibiotics bind to the ribosome, knowledge that could help researchers come to grips with the problem of multiresistant bacteria.



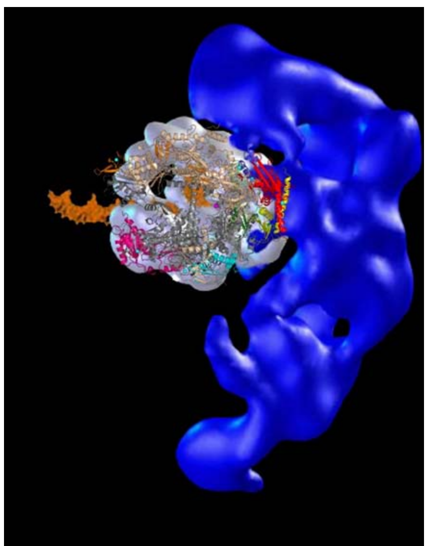
The 50S subunit structure at 9Å resolution (left, 1998), 5Å resolution (middle, 1999), and 2.4Å resolution (right, 2000) (From Ban et al., 1998; 1999; 2000).

Reading the Genetic Code –
How Does DNA Transcription Occur - How Is It Regulated?

The SSRL Structural Molecular Program is funded by DOE-BER, NIH-NCRR and NIH-NIGMS

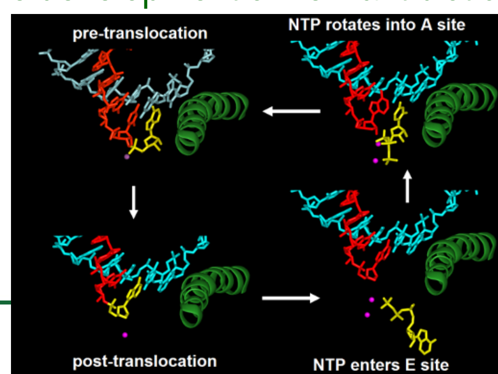


- Transcription is the process by which DNA is “read” and converted into a message that directs protein synthesis with extremely high fidelity. Protein synthesis is carried out by the ribosome.
- Three main stages are initiation, elongation and termination, which are carried by an exceedingly complex molecular machine and associated proteins (RNA Polymerase-II)
- Synchrotron-enabled studies have provided molecular-level insight into the function of this molecular machine
- Most of the synchrotron work was performed at SSRL and strongly enabled by beam line automation and robotics

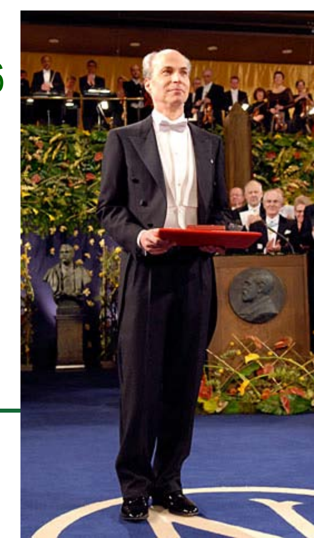


Structure of Pol II (white) and full mediator complex (blue) determined from EM. The high resolution crystallographic structure of Pol II has been fitted into the lower resolution structure from EM.

This structural information now serves to guide the development of new antibiotics

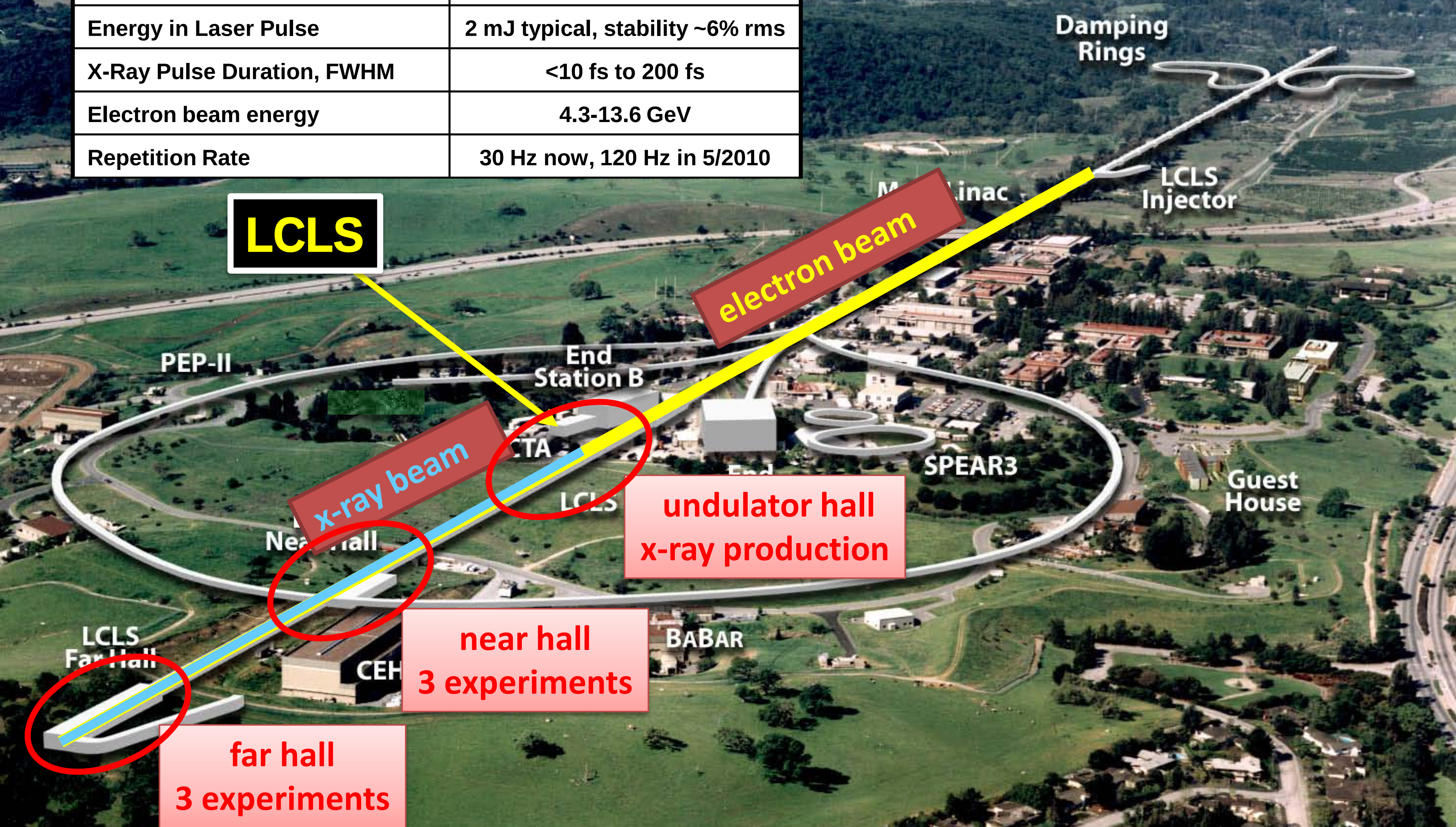


Roger Kornberg receiving the 2006 Nobel Prize in Chemistry for his research on RNA Polymerase II



Linac Coherent Light Source at SLAC

LCLS Present Performance	
Operating wavelength range (eV)	0.15-1.5 nm (8,000-800 eV)
Energy in Laser Pulse	2 mJ typical, stability ~6% rms
X-Ray Pulse Duration, FWHM	<10 fs to 200 fs
Electron beam energy	4.3-13.6 GeV
Repetition Rate	30 Hz now, 120 Hz in 5/2010



LCLS: 132 meters of FEL Undulators

LCLS Instruments

AMO - Atomic, Molecular & Optical Science

Will enable the study of the interaction of LCLS X-ray pulses and the basic constituents of matter.

CXI - Coherent X-ray Imaging

Will allow imaging of non-periodic nanoscale objects, including single or small clusters of biomolecules at or near atomic resolution.

MEC - Matter in Extreme Conditions

Will observe matter at temperatures exceeding 10,000 Kelvin and at pressures 10 million times the earth's atmospheric pressure at sea-level.

SXR - Soft X-ray Materials Science

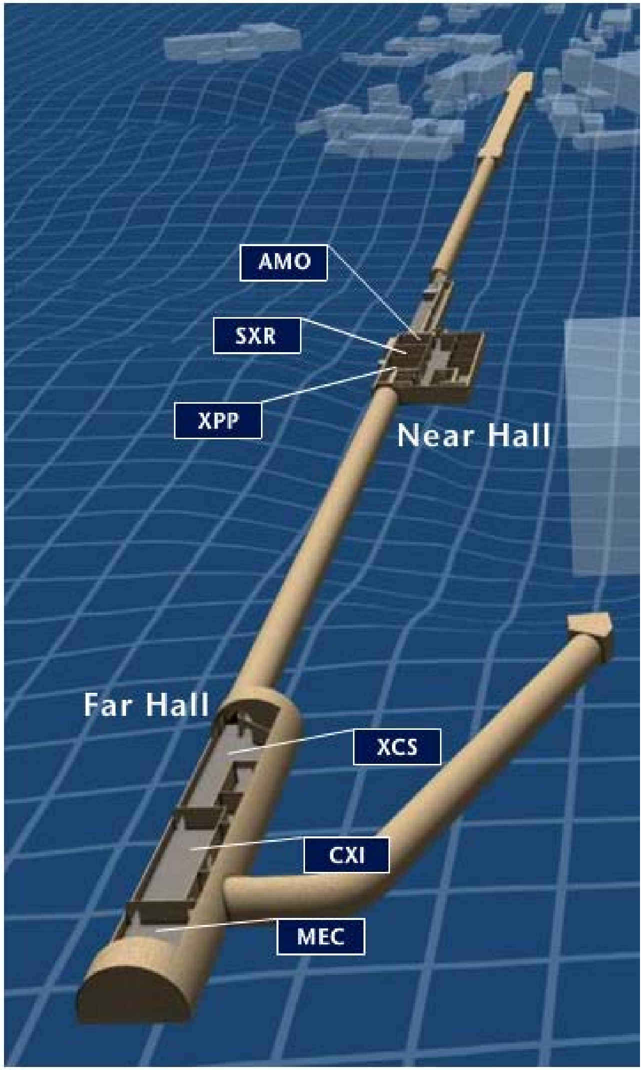
Will enable the LCLS to be applied to scattering and imaging experiments that require the use of soft X-rays.

XCS - X-ray Correlation Spectroscopy

Will enable observation of dynamical changes of large groups of atoms in condensed matter systems over a wide range of time scales.

XPP - X-ray Pump Probe

Will enable use of a fast optical laser to generate transient states of matter for probing by the LCLS.



ORNL's Jaguar Supercomputer is World's Fastest

- The upgrade of ORNL's Cray XT5 "Jaguar" to 37,376 six-core AMD Istanbul processors has increased performance 70 percent over that of its quad-core predecessor.
- Achieved #1 ranking on the Top500 with a speed of 1.759 petaflops/s on the benchmark High-Performance Linpack.
- Enabled by $19.9M in Recovery Act funds.
- Scientists in industry, academia, and government have requested more than 2 billion processor hours on Jaguar for 2010. The six-core upgrade on Jaguar will enable Oak Ridge to allocate 1 billion processor hours, up from 470 million in 2009.

Science Applications are Running on the Upgraded Jaguar

Two major science applications are already running at close to the full capability of the machine:

Name of code: DCA++

- **Largest # cores used thus far: 213,120**
- **Performance: 1.892 Petaflop/s**
- **Description: Study role of nano-scale inhomogeneities in high temperature superconductors**

Name of code: WL-LSMS

- **Largest # cores used thus far: 223,232**
- **Performance: 1.837 Petaflop/s**
- **Description: Ab initio calculations of free energies in nanomagnets**

SC Leadership Goals and Challenges

- Maintain excellence and world leadership in
  - Our scientific programs
  - Planning, construction, and operations of our scientific user facilities
  - Management of our 10 DOE laboratories
  - Our federal and contractor workforces
- Develop new approaches to integrate basic and applied research to address the challenges of energy technologies
  - Establish Energy Innovation Hub using lessons learned from 3 Bioenergy Research Centers
  - Establish 46 Energy Frontier Research Centers
  - Work with the technology offices and the new ARPA-E office to advance energy technology in innovative ways

Energy Frontier Research Centers

Tackling Our Energy Challenges in a New Era of Science

- To engage the talents of the nation's researchers for the broad energy sciences
- To accelerate the scientific breakthroughs needed to create advanced energy technologies for the 21st century
- To pursue the fundamental understanding necessary to meet the global need for abundant, clean, and economical energy

46 centers awarded ($777M over 5 years), representing 102 participating institutions in 36 states and D.C.

Pursue *collaborative* basic research that addresses both energy challenges and science grand challenges in areas such as:

- Solar Energy Utilization
- Combustion
- Bio-Fuels
- Catalysis
- Energy Storage
- Solid State Lighting
- Geosciences for Energy Applications
- Superconductivity
- Advanced Nuclear Energy Systems
- Materials Under Extreme Environments
- Hydrogen

DOE Energy Innovation Hubs

Hubs appropriated in FY 2010:

- **Fuels from Sunlight (SC lead)**
- **Energy Efficient Building Systems Design (EERE)**
- **Modeling and Simulation for Nuclear Fuel Cycles and Systems (NE)**

Each Hub will comprise a world-class, multi-disciplinary, and highly collaborative research and development team.

Strong scientific leadership *must* be located at the primary location of the Hub. Each must have a clear organization and management plan that "infuses" a culture of empowered central research management throughout the Hub.

The Department hopes to add additional Hubs in FY 2011.

Office of Science Early Career Research Program

The Department of Energy is now reviewing proposals for the DOE Office of Science Early Career Research Program to support the research of outstanding scientists early in their careers.

Purpose: To support the development of individual research programs of outstanding scientists early in their careers and to stimulate research careers in the disciplines supported by the Office of Science.

- **July 2, 2009:** Funding announcements released
- **August 3, 2009:** ~2,200 letters of intent received
- **September 1, 2009:** ~1,800 proposals received
- **Now through January 1, 2010:** Proposals under peer review
- **January 15, 2009:** Selections and award/decline notifications
- **March or April, 2010:** Awards issued

Office of Science Graduate Fellowship program

The Office of Science established the DOE Office of Science Graduate Fellowship program to support outstanding students pursuing graduate training in basic research in areas of physics, biology, chemistry, mathematics, engineering, computational sciences, and environmental sciences relevant to the Office of Science.

- The fellowship award provides partial tuition support ($10.5K/year), an annual stipend for living expenses ($35K) , and a research stipend ($5K) for full-time graduate study and thesis/dissertation research at a U.S. academic institution for three years.
- The fellowship is open to students who are currently an undergraduate senior or in their first or second year of graduate school.
- The program was announced and began accepting applications for the FY10-11 academic year on September 30, 2009.
- Recovery Act funds ($12.5M) will fully support approximately 80 fellowships; FY 2010 appropriated funds will support approximately 80 additional fellowships in the program's first year.
- http://www.scied.science.doe.gov/SCGF.html

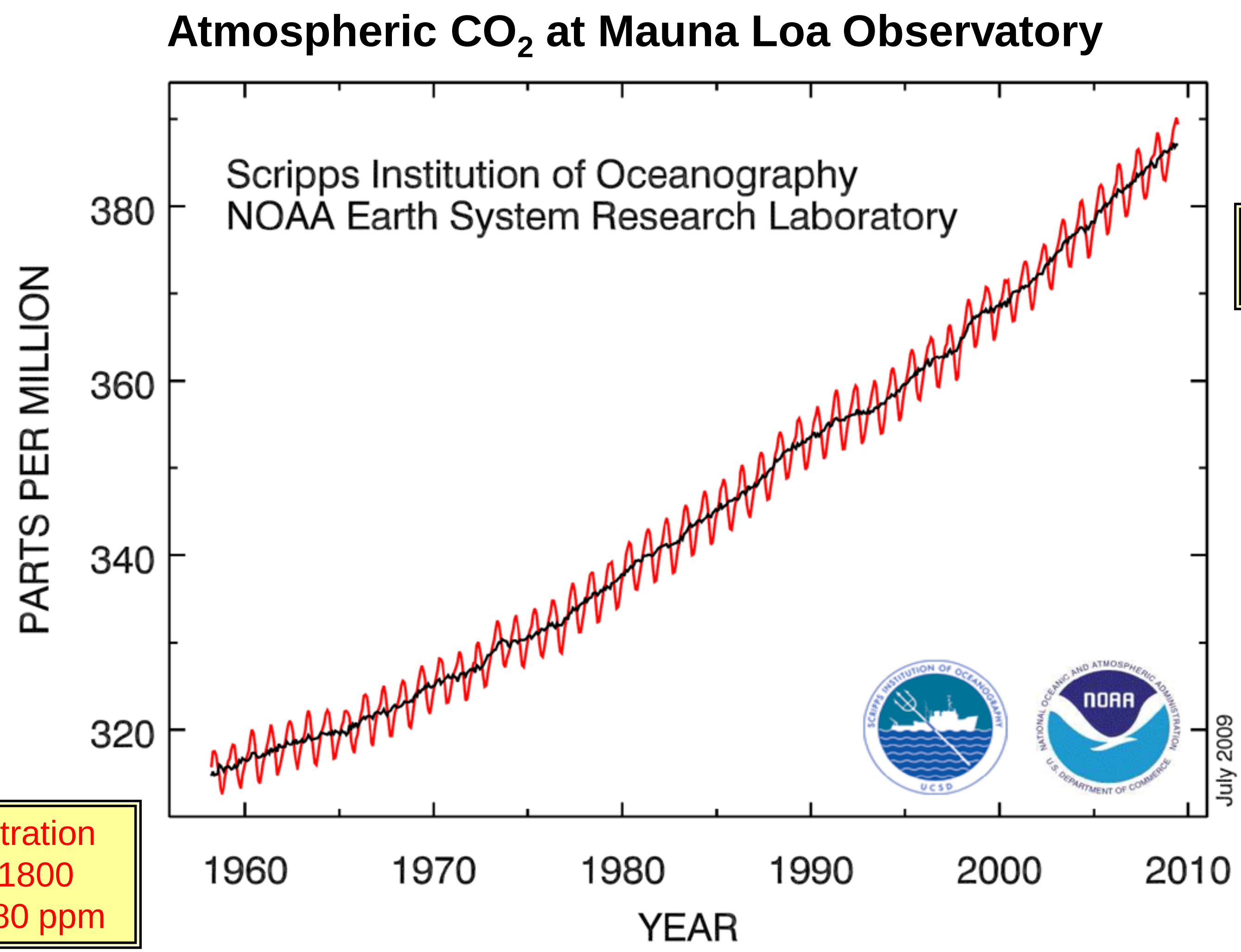
Office of Science Graduate Fellowship program

- **September 30, 2009:** Program announced and applications opened
- **October 15, 2009:** More than 1,700 potential applicants have registered
- **November 30, 2009:** Applications due to DOE
- **November 2009 through February 2010:** Applications subjected to peer review
- **March 2010:** Selections and award/decline notifications
- **September 1, 2010:** Fellowship terms begin

Climate change

Modern CO_2 Concentrations are Increasing

The current concentration is the highest in 800,000 years, as determined by ice core data



Concentration now ~388 ppm

Concentration prior to 1800 was ~280 ppm

U.S. DEPARTMENT OF ENERGY | Office of Science

Greenland Ice Mass Loss – 2002 to 2009

Increasing rates of ice mass loss from the Greenland and Antarctic ice sheets revealed by GRACE (Gravity Recovery and Climate Experiment) satellite:

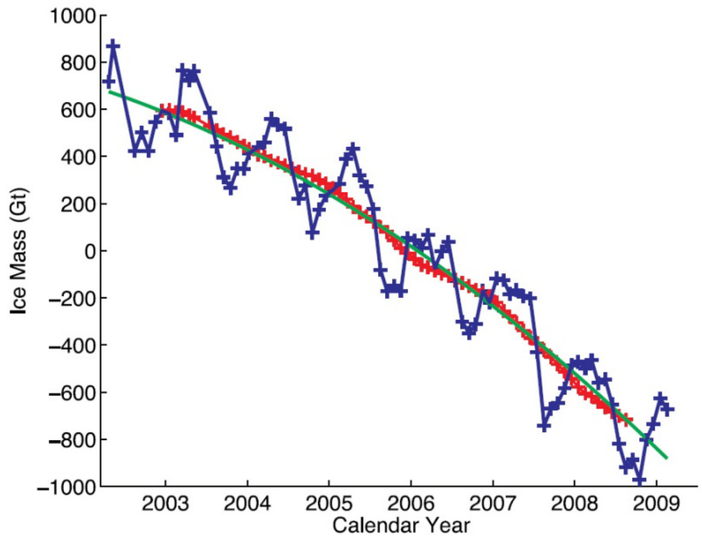
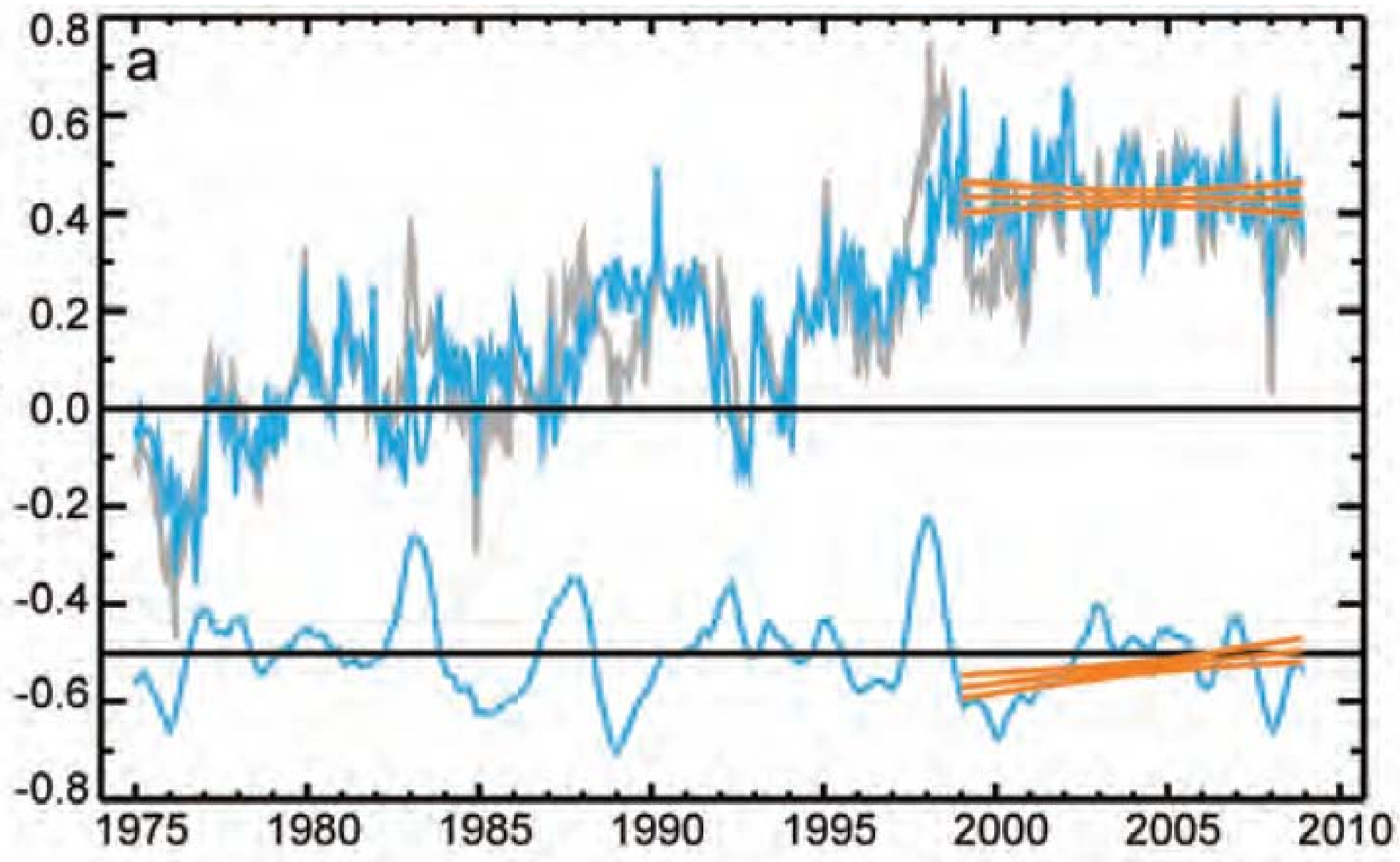
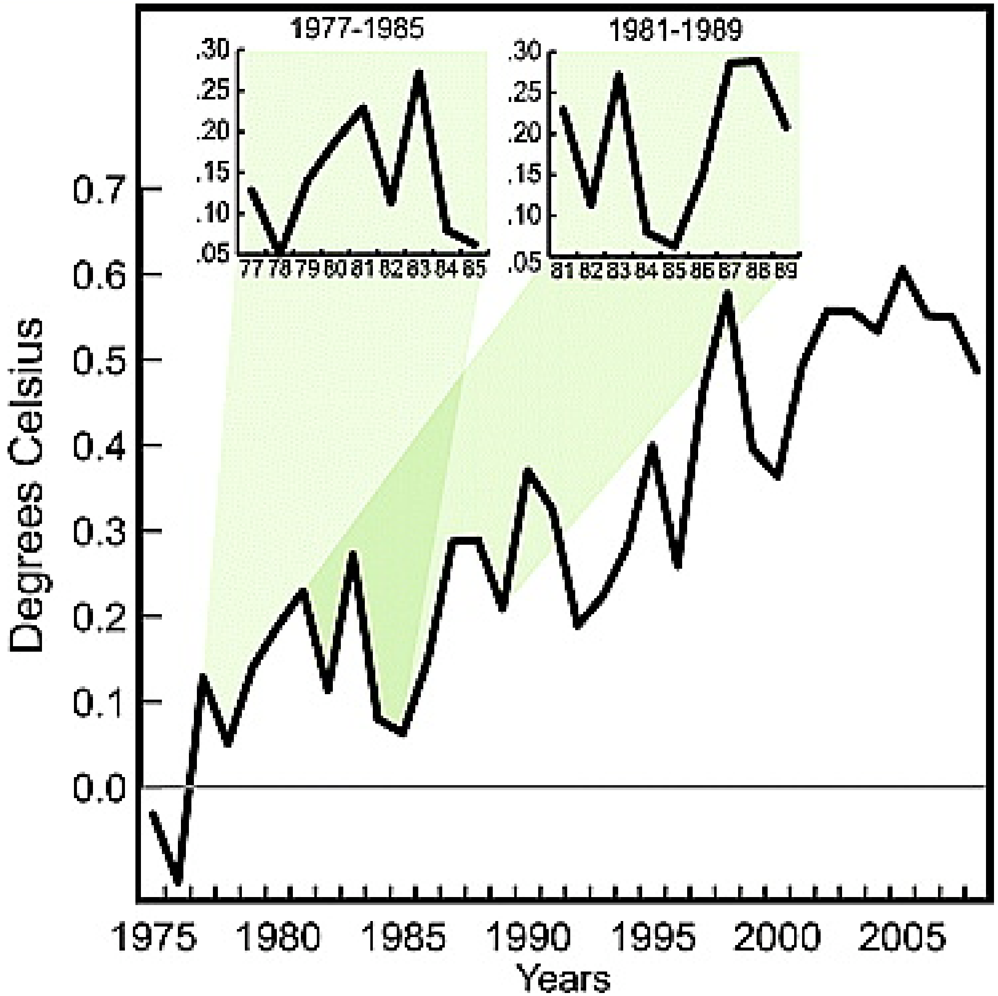


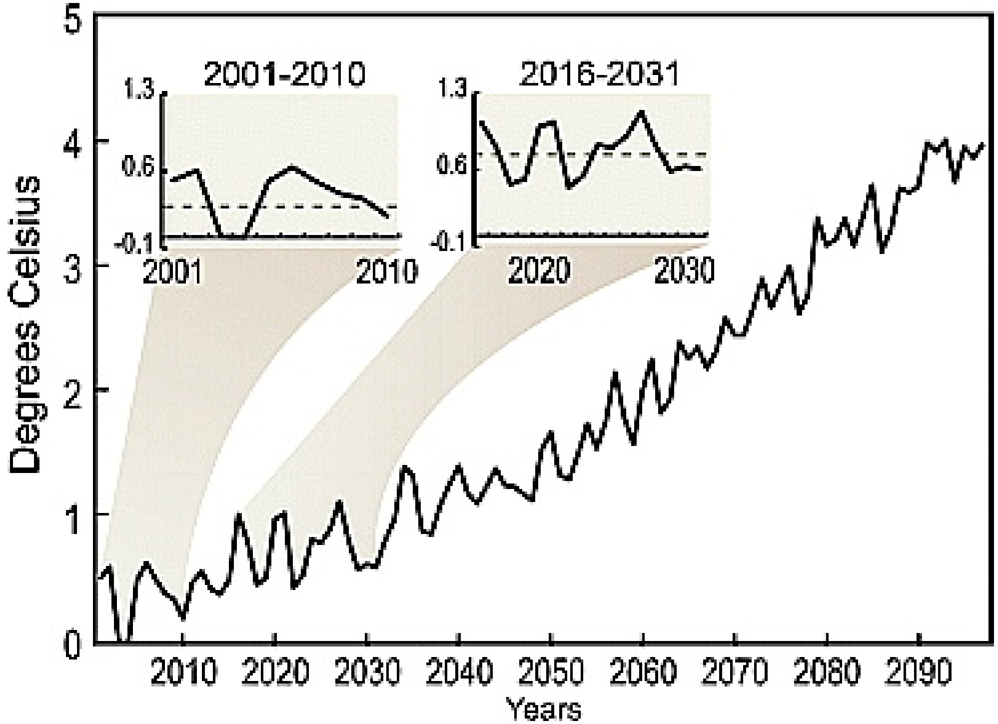
Figure 1. Time series of ice mass changes for the Greenland ice sheet estimated from GRACE monthly mass solutions for the period from April 2002 to February 2009. Unfiltered data are blue crosses. Data filtered for the seasonal dependence using a 13-month window are shown as red crosses. The best-fitting quadratic trend is shown (green line). The GRACE data have been corrected for leakage and GIA.

- In Greenland, the mass loss increased from 137 Gt/yr in 2002–2003 to 286 Gt/yr in 2007–2009
- In Antarctica, the mass loss increased from 104 Gt/yr in 2002–2006 to 246 Gt/yr in 2006–2009

I. Velicogna, GEOPHYSICAL RESEARCH LETTERS, VOL. 36, L19503, doi:10.1029/2009GL040222, 2009


a
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
1975
1980
1985
1990
1995
2000
2005
2010


1977-1985
.30
.25
.20
.15
.10
.05
77 78 79 80 81 82 83 84 85
1981-1989
.30
.25
.20
.15
.10
.05
81 82 83 84 85 86 87 88 89
Degrees Celsius
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
1975 1980 1985 1990 1995 2000 2005
Years


Degrees Celsius
5
4
3
2
1
0
2001-2010
1.3
0.6
-0.1
2001
2010
2016-2031
1.3
0.6
-0.1
2020
2030
2010
2020
2030
2040
2050
2060
2070
2080
2090
Years

Tackling Energy Challenges

- Fusion Energy
- Carbon Capture and Sequestration
- Biofuels
- Catalysis for Energy Applications

Fusion Energy Sciences Grand Challenges

There are at least three major scientific needs for establishing credibility for fusion energy:

(1) We must generate, study, optimize, and learn to predict the properties of the burning plasma state

(2) We must develop the scientific basis for robust control strategies for the burning plasma state: in MFE, this includes developing the scientific understanding to enable long plasma pulses.

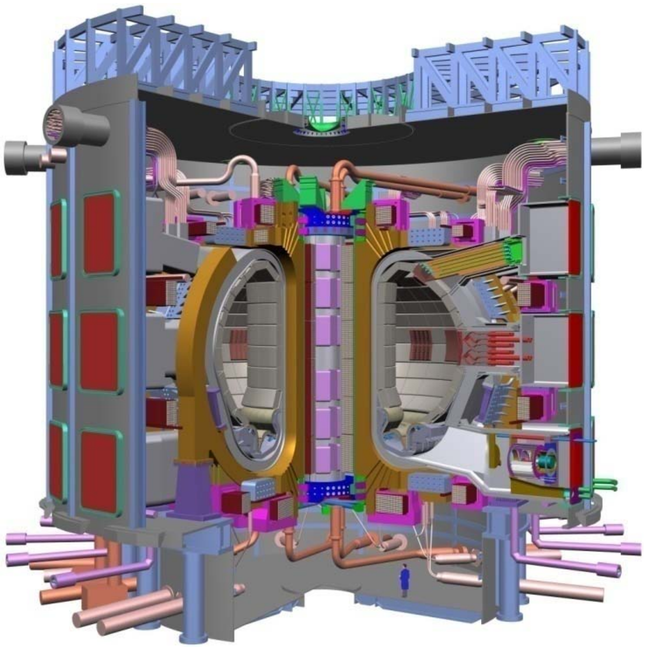
(3) We must develop the understanding of the material/plasma interface, and the fusion nuclear science needed to endure the fusion environment and to harness fusion power

A grand challenge for fusion: Controlling the burning plasma state

- <u>Burning plasmas</u>: energy released by fusion exceeds the energy required to heat and control it. The basis of any future fusion reactor

- <u>Science critical to fusion energy</u>: the nonlinear physics of a self-heated plasma. Developing a robust and predictable approach to controlling the dynamics of this plasma state

- <u>Leading research tools</u>: ITER, an international project being built in Cadarache, France, will create the world's first sustained burning plasma in the 2020's. U.S magnetic fusion science program supports burning plasma research: scaled ITER simulation experiments, ITER design, fundamental understanding of underlying plasma state



A grand challenge for fusion: Materials science and harnessing fusion power

- Plasma-wall interactions: managing heat fluxes of many MW/m^2 in a fusion reactor for long times (weeks and longer). Fuel retention in materials; sputtering; surviving explusions of plasma heat from instabilities

- Neutron fluences: materials have to be able to withstand ~ 100 atomic displacements due to neutron bombardment before replacement

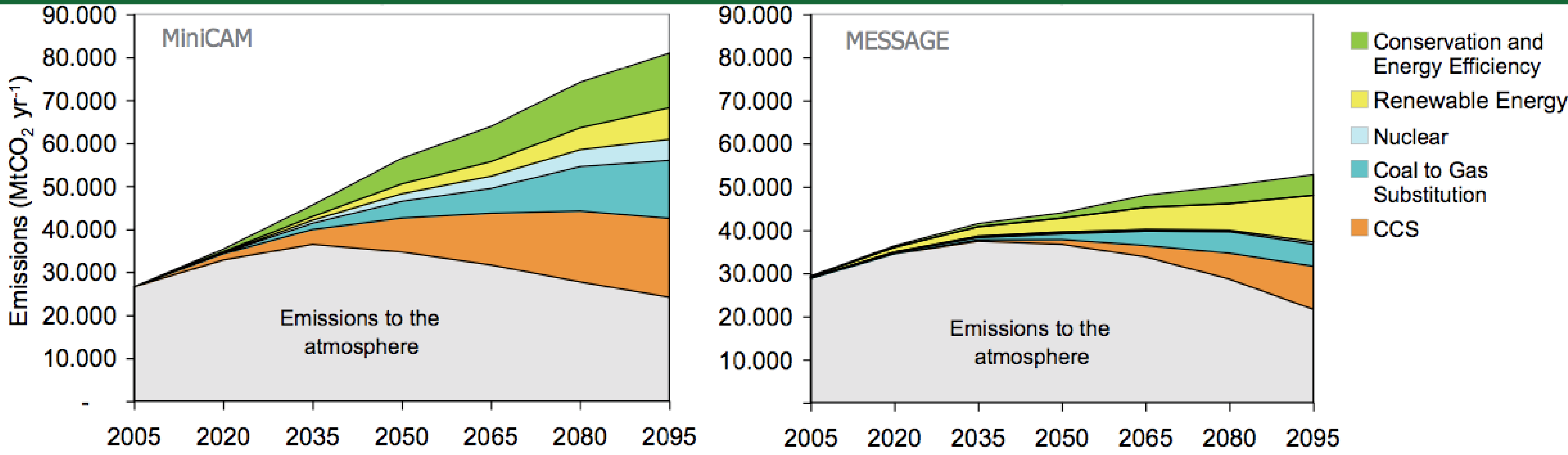
- Technology challenge of extracting heat from a fusion plasma, creating fuel in the process

- U.S. opportunity for world leadership: fusion nuclear science and materials science. Develop partnerships across DOE. Test stands, computation, design of a volume neutron source to benefit both magnetic and inertial fusion

Tackling Energy Challenges

- Carbon Capture and Sequestration

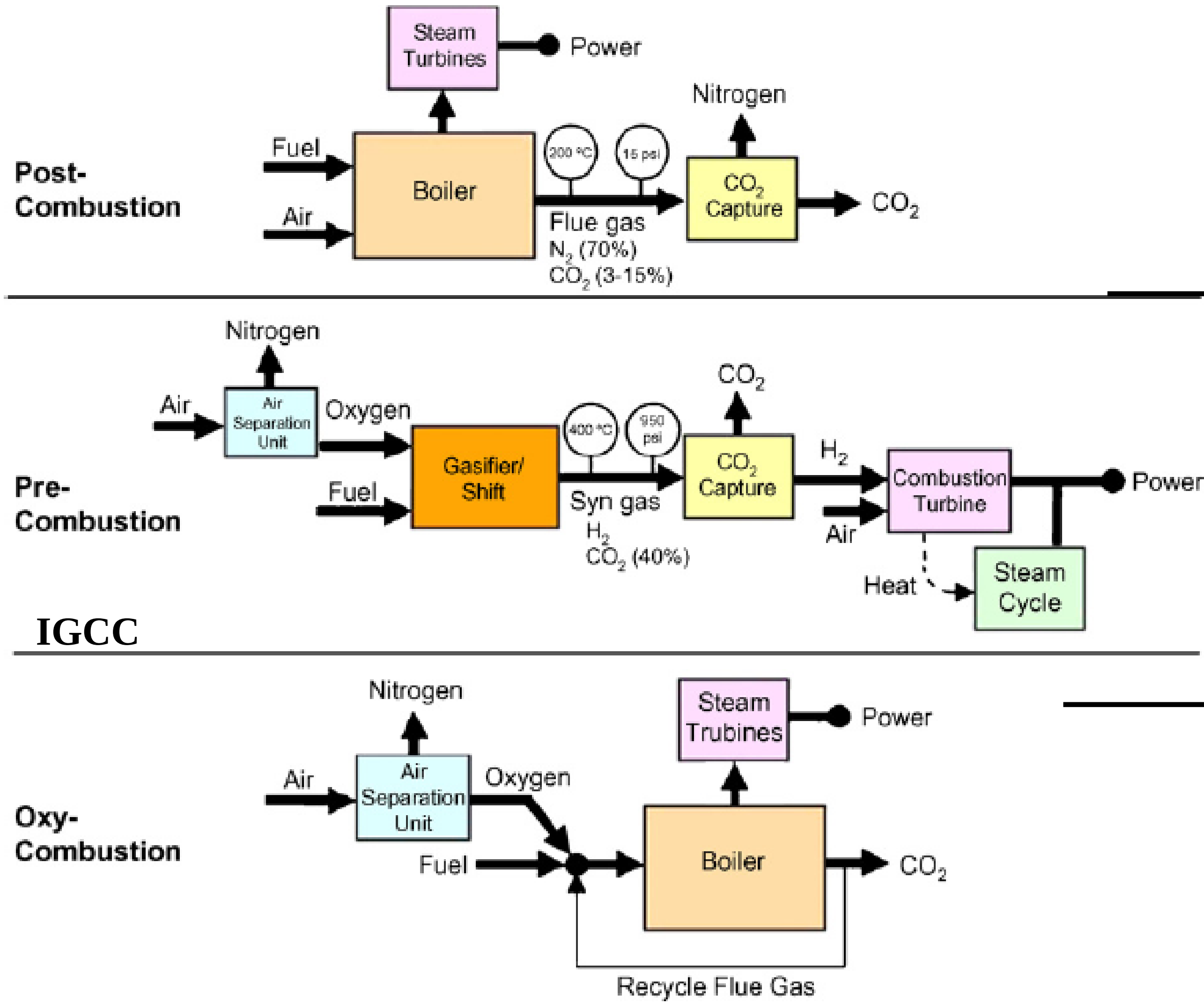
Carbon Capture and Sequestration



Two scenarios for reducing carbon dioxide emissions to keep atmospheric concentrations at 450-750 ppmv. Left: high-emission scenario, where nuclear plays an important role. Right low-emission scenario. In both cases, carbon capture and storage (CCS) – the orange wedge - plays a critical role. (IPCC report, 2007)

- Continued use of fossil fuel while capping the atmospheric concentration of carbon dioxide to about double the pre-industrial level requires the sequestration of ~10 GT of CO_2 per year.
- Current technologies for the post-combustion capture of CO_2 are too expensive.
- "Underground" as a long-term storage container
  - Advantages: Enormous volume; distance from subsurface environment; pre-made container
  - Disadvantages: Designed by nature, only approximately fits the design criteria for containment; complex materials and processes; difficult to see and monitor; uncertainty about long-term performance

Today's Carbon Capture Options



Challenges

- Low CO_2 Concentration
- High Energy for regeneration

- Mostly new plants
- Oxygen production – Air Separation Units (ASUs) have high electricity cost (chemical looping, ITMs)

- ASUs consume considerable energy
- Expense - corrosion resistant materials

Science challenges for post-combustion capture

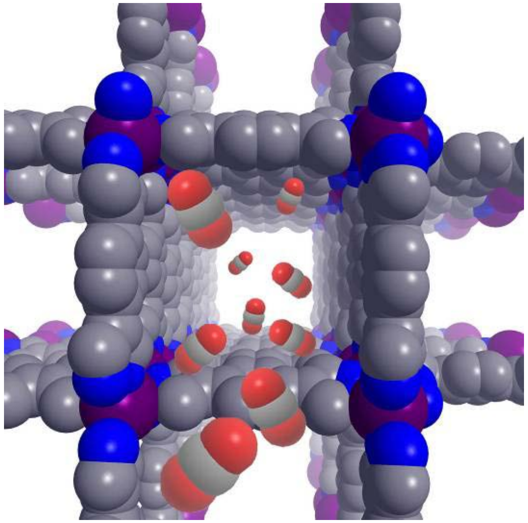
- CO_2 sorbent that can be stripped with minimal energy
    - Look to Nature for ideas on triggers but unlikely to be a biological solution
    - Electrical, electrochemical, pressure, light, pH, phase change (liquid crystal)*
    - Nanoscale approaches

- Build the knowledge base to facilitate a rationale design of sorbents from first principles
    - – Advanced computational modeling and theory - First-principles methods for capture and release of nonpolar molecules
    - – Advanced characterization tools, including those supported by BES, to
        - Identify structure of binding sites
        - Understand kinetics and thermodynamics of sorption/desorption in realistic conditions
    - – New chemistries for advanced sorbents
        - New sorbents
        - Synthesis

*Source: *Advanced Post-Combustion CO_2 Capture*, prepared for Clean Air Task Force, Howard Herzog, Jerry Meldon and Alan Hatton

EFRC: Center for Gas Separations Relevant to Clean Energy Technologies -- Berend Smit (UC Berkeley)

This EFRC will develop new strategies and materials that allow for energy efficient selective capture or separation of CO_2 from gas mixtures based on molecule-specific chemical interactions.



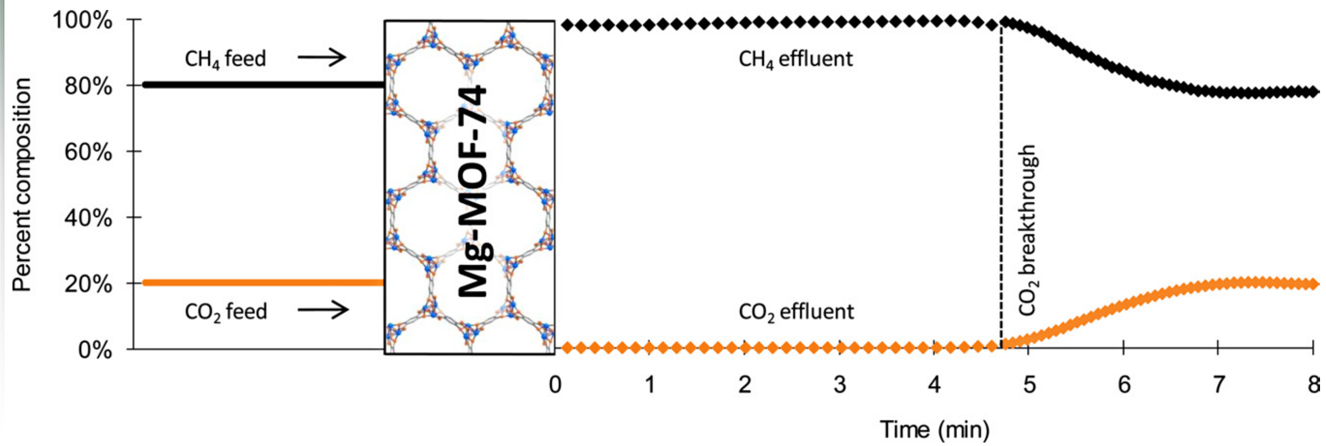
RESEARCH PLAN AND DIRECTIONS

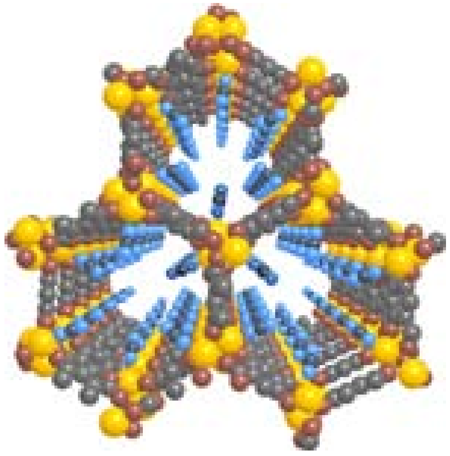
Capture of CO_2 from gas mixtures requires the molecular control offered by nanoscience to tailor-make those materials exhibiting exactly the right adsorption and diffusion selectivity to enable an economic separation process. Characterization methods and computational tools will be developed to guide and support this quest.

New Materials May Aid in Capturing Carbon Dioxide
Omar Yaghi, UCLA

Metal-organic frameworks (MOFs) act as "crystalline sponges" and show promise at reducing the energy penalty for CO_2 capture.

A new magnesium-based MOF is selective in capturing CO_2 in the presence of CH_4 and releases the stored CO_2 at temperatures much lower than current capture media.





Schematic structure of Mg-MOF-74

D. Britt, H. Furukawa, B. Wang, and O. M. Yaghi, PNAS 106, 20637 (2009); also featured in N.Y. Times on Dec. 8, 2009.

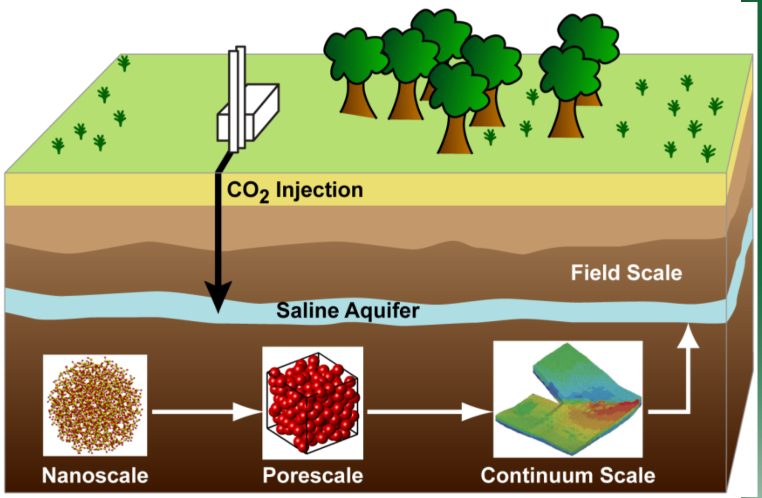
Geological CO_2 Sequestration

Geological Carbon Dioxide Sequestration is the deep well injection of supercritical CO_2 into porous rock formations for permanent disposal. This process initially displaces *in situ* aqueous fluid. Subsequently, the CO_2 buoyantly migrates slowly through the pores, breaking up into immobile bubbles, dissolving within the fluid, or reacting with minerals to form solid phases.

Prediction of CO_2 Sequestration effectiveness depends on understanding:
• Reactive fluid flow properties of multiphase fluids under reservoir conditions in porous and fractured media
• Geochemical stability of mineral phases within deep formations
• Improved geophysical imaging of reservoir-scale properties to track changing reservoir dynamics over long periods of time

EFRC: Center for Frontiers of Subsurface Energy Security
Gary. A. Pope (The University of Texas)

Summary statement: Our goal is scientific understanding of subsurface physical, chemical and biological processes from very small to very large scale so that we can predict the behavior of CO_2 and other byproducts of energy production that may need to be stored in the subsurface.



RESEARCH PLAN AND DIRECTIONS

- Challenges and approaches: Integrate and expand our knowledge of subsurface phenomena across scientific disciplines using both experimental and modeling approaches to better understand and quantify behavior far from equilibrium.
- Unique aspects: The uncertainty and complexity of fluids in geologic media from the molecular scale to the basin scale.
- Outcome: Better understanding of long term behavior of subsurface storage.

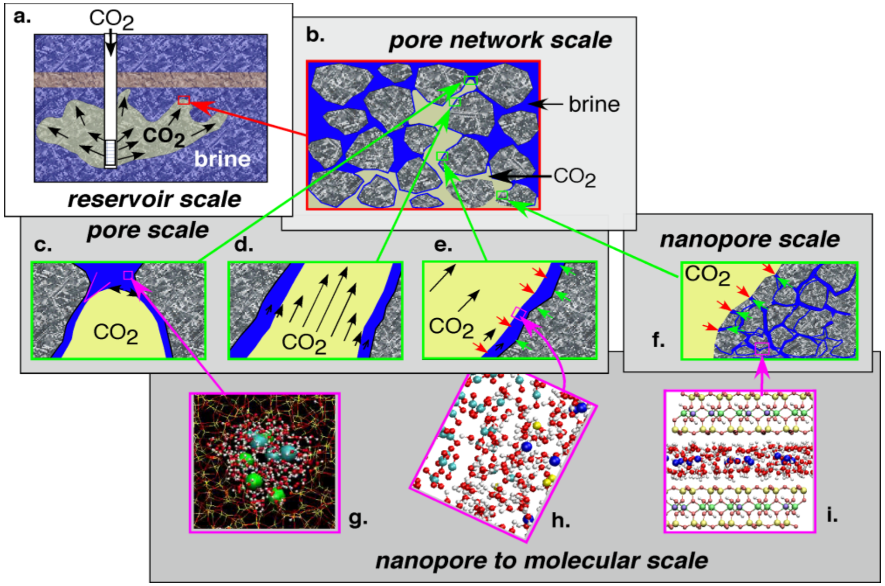
U.S. DEPARTMENT OF ENERGY | Office of Science

TEXAS

Sandia National Laboratories

EFRC: Nanoscale Controls on Geologic CO_2 -- Donald J. DePaolo (LBNL/ESD)

OBJECTIVES are to (1) develop molecular, nano-scale, and pore network scale approaches for controlling flow, dissolution, and precipitation in subsurface rock formations during emplacement of supercritical CO_2; and (2) achieve a new level of prediction of long-term performance



RESEARCH PLAN AND DIRECTIONS

Properties and interactions of complex fluids and minerals must be determined at elevated temperature and pressure, and effects at interfaces and in confined nano-scale pore spaces understood. Novel experimental and computational approaches, and unique DOE experimental facilities (including ALS, SNS, NERSC, Molecular Foundry) will be used.

U.S. DEPARTMENT OF ENERGY | Office of Science | BERKELEY LAB | UCDAVIS PETER A. ROCK Thermochemistry Laboratory | OAK RIDGE NATIONAL LABORATORY Managed by UT-Battelle for the Department of Energy

Tackling Energy Challenges

- Biofuels

The DOE Bioenergy Research Centers

Revolutionizing Discovery of Future Energy Solutions

- New paradigm for research—single focus, multi-disciplinary, team-based science
- Transformational science
- Building on DOE's investments in user facilities and fundamental research programs
- Focus on
  - Feedstock characterization & development
  - Feedstock deconstruction
  - Feedstock conversion to liquid fuels

jbei Joint BioEnergy Institute

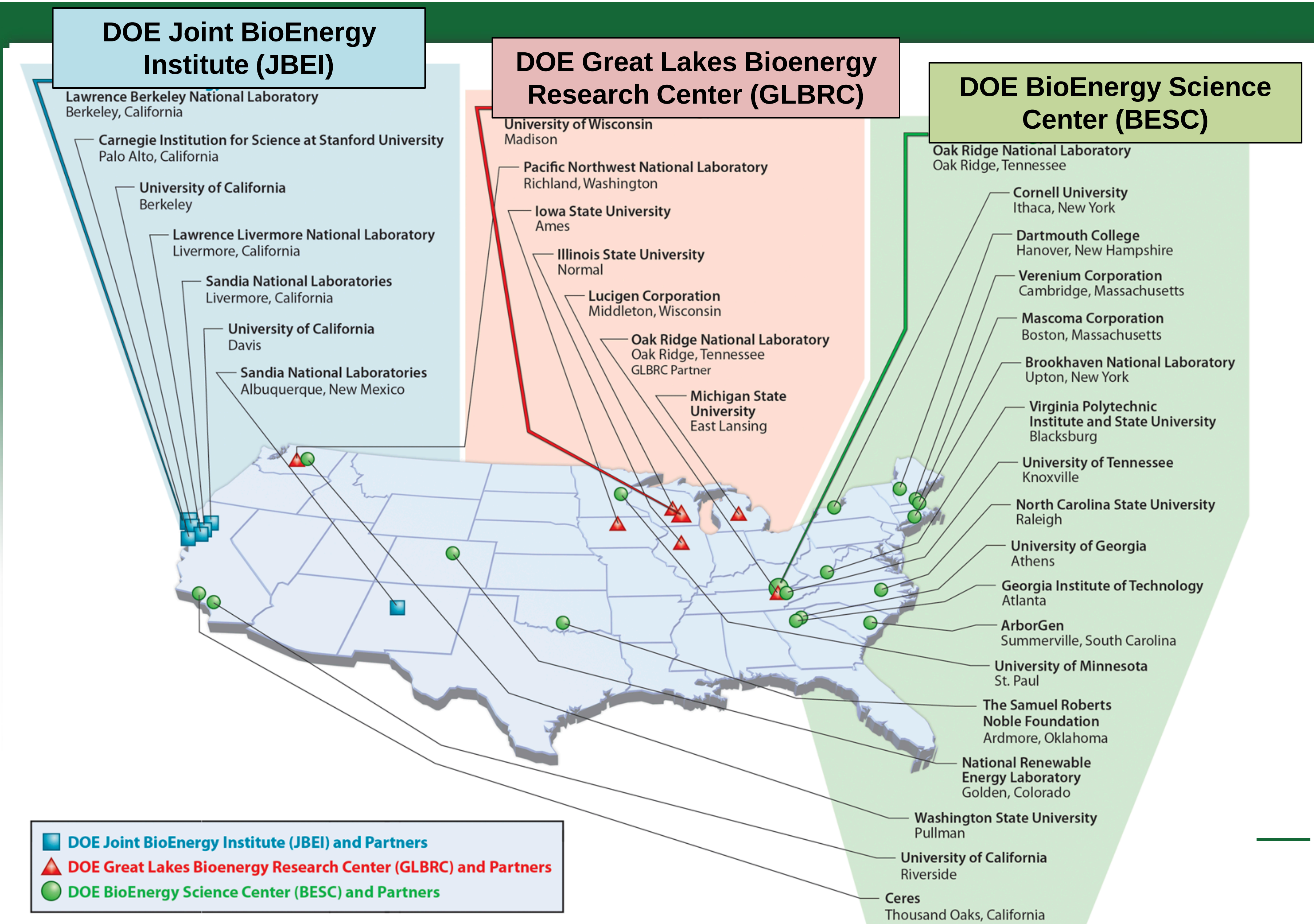
GLBRC Great Lakes Bioenergy Research Center

BESC BioEnergy Science Center

DOE Bioenergy Research Centers

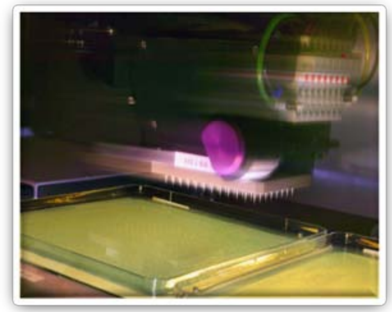
Multi-institutional partnerships

DOE Bioenergy Research Centers



Focus: Model crops (*Arabidopsis* and rice) for rapid advances that can be transferred to bioenergy crops

- **Modifying lignin** to change its monomer composition for easier degradation and access to cellulose
- Using ionic liquids for room-temperature biomass **pretreatments**
- Using **synthetic biology** to look beyond ethanol to green gasoline, diesel, and jet fuels
- Connecting with the **Bay Area Biotech Community** (a hub of bioenergy technology and venture investment)



BioEnergy Science Center (BESC)

Focus: Overcoming "recalcitrance" (resistance of plant fiber, or lignocellulose, to break down into sugars)

- Gene discovery for **recalcitrance** in switchgrass and poplar
- Use of synthetic biology to re-engineer the **cellulosome**
- Long-term **"consolidated bioprocessing"** goal: one microbe or microbial community for processing plants into fuel
- Opportunity to test discoveries in a **demonstration biorefinery** being constructed by the state of Tennessee

Focus: Wide range of plants, including models and potential bioenergy crops (approach leverages the agronomic orientation of the two universities)

- Engineering plants to incorporate **lignin "zippers"** and to produce more starches and oils for biodiesel
- **Developing alternative approaches** to fuels: Microbial biorefineries that use sunlight and biomass to generate hydrogen, electricity, or high-energy chemicals
- **Investigating the sustainability** of biofuel production by studying the environmental and socioeconomic dimensions of a biofuels economy

Tackling Energy Challenges

- Catalysis for Energy Applications

Basic Research Needs: Catalysis for Energy

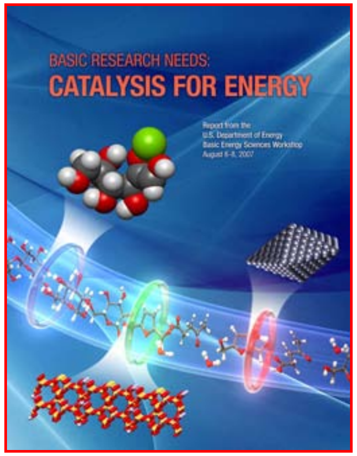
- Grand challenges for catalysis science

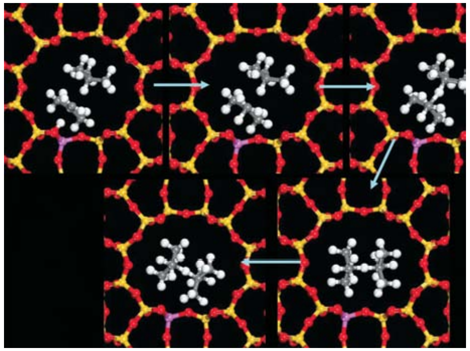
  Understanding the mechanisms and dynamics of catalyzed reactions at the atomic and molecular scale.

  Design and controlled synthesis of catalyst structures.

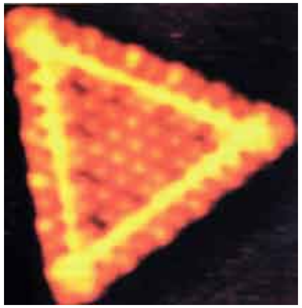
- Advanced catalysts for the conversion of heavy fossil energy feedstocks
  The wide variation in chemical composition demands improved chemical analysis of feedstocks. The dependence of catalyst function on its environment must be elucidated.

- Advanced catalysts for the conversion of biologically derived feedstocks
  Understand the catalytic deconstruction of cellulose and lignin at the molecular level. Design and understand reactions that remove oxygen and increase the hydrogen-carbon ratio.



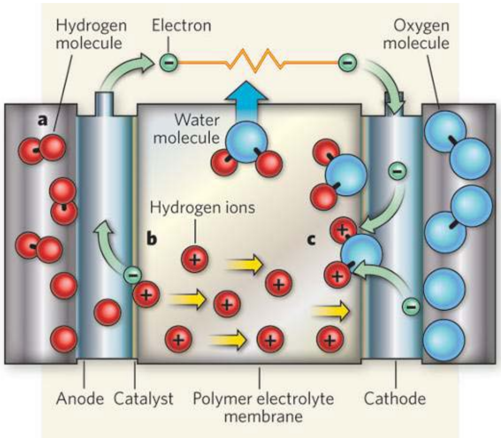


Computed mechanism for the catalytic coupling of two four-carbon molecules to create an eight-carbon, fuel-like molecule



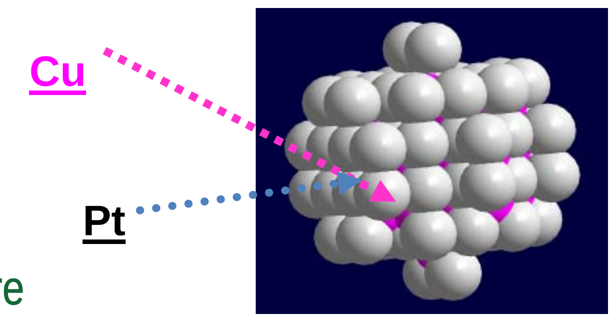
TEM image of a model molbydenum disulfide catalyst showing layers that are only a few atoms across

Pt-Cu Catalysts for Polymer Electrolyte Membrane Fuel Cells



PEMFCs

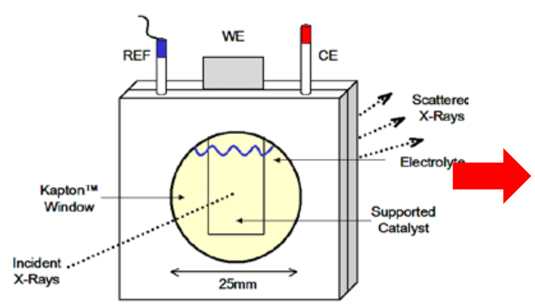
- Pt catalyst in cathode is inefficient & expensive.
- Dealloyed Cu_3Pt nanoparticle catalysts are more active & use less Pt



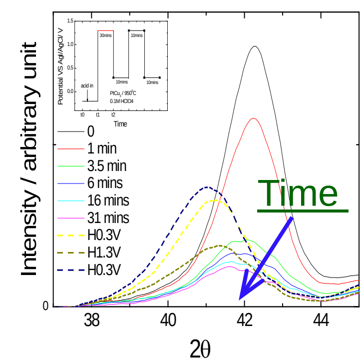
X-ray studies show:

- Dealloyed Cu_3Pt nanoparticle catalyst forms **core-shell** structure with Pt rich shell
- The Pt shell is **compressively strained** & this results in higher catalytic activity
- Dynamics of dealloying and stability studied *in-situ* with X-rays
- Cu_3Pt catalysts are **nearly as stable** as pure Pt

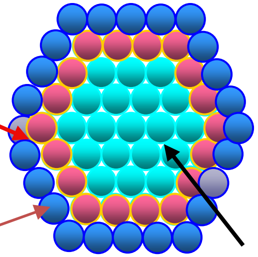
***In-situ* X-ray cell**



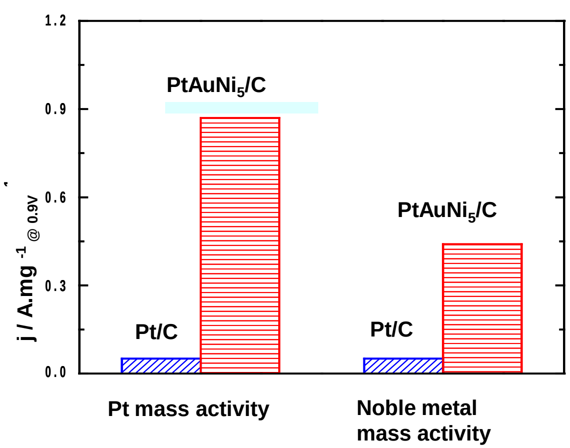
Diffraction: SSRL BL11-3



Tri-Metallic-Decorated Surface Alloys: A New Catalytic Paradigm



Model structure of a trimetallic layered nanoparticle showing a Ni core and noble metal shell.



The activity measurements show trimetallic particles being about 20x more active than monometallic ones (on a Pt-mass basis.)

- A conceptual search for stable electrocatalytic alloys for both anodes (hydrogen oxidation) and cathodes (oxygen reduction) in fuel cells led to the development of novel catalyst nanostructures containing three components: a non-noble metallic core, a palladium or gold shell, and a platinum top monolayer.
- Theoretical electronic structure calculations supported the hypotheses that these new structures would present novel properties, particularly higher activity for both hydrogen and oxygen reactions.
- Recent results successfully confirmed the predictions, providing evidence that the three-layered catalysts can be synthesized and that their activity is 20 times higher than that of regular Pt catalysts.

M.H. Shao, K. Sasaki, R.R. Adzic, *J. Am. Chem. Soc.* 128 (2006) 3526-3527.
M. H. Shao, K. Sasaki, P. Liu, R.R. Adzic, *Z. Phys. Chem.* 221 (2007) 1175-1190.