U.S. DEPARTMENT OF ENERGY | Office of Science

Basic Energy Sciences

BERAC Meeting

February 16, 2012

Harriet Kung

Associate Director of Science
for Basic Energy Sciences
U.S. Department of Energy

Basic Energy Sciences

The Program:

Materials sciences & engineering—exploring macroscopic and microscopic material behaviors and their connections to various energy technologies

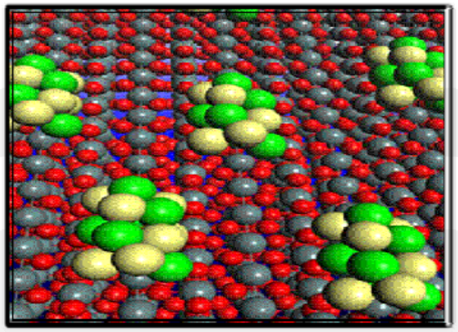
Chemical sciences, geosciences, and energy biosciences—exploring the fundamental aspects of chemical reactivity and energy transduction over wide ranges of scale and complexity and their applications to energy technologies

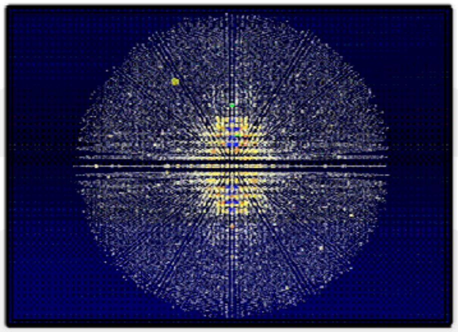
Scientific User Facilities—supporting the largest collection of facilities for electron, x-ray, and neutron scattering in the world

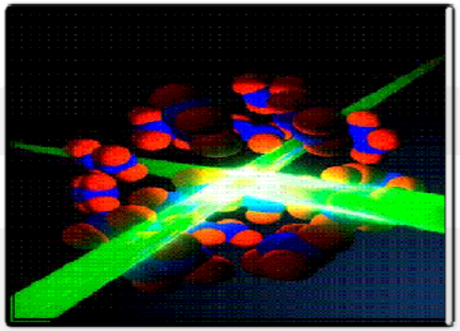
The Scientific Challenges:

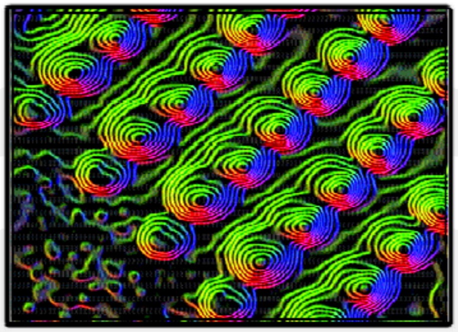
- Synthesize, atom by atom, new forms of matter with tailored properties, including nano-scale objects with capabilities rivaling those of living things
- Direct and control matter and energy flow in materials and chemical assemblies over multiple length and time scales
- Explore materials & chemical functionalities and their connections to atomic, molecular, and electronic structures
- Explore basic research to achieve transformational discoveries for energy technologies

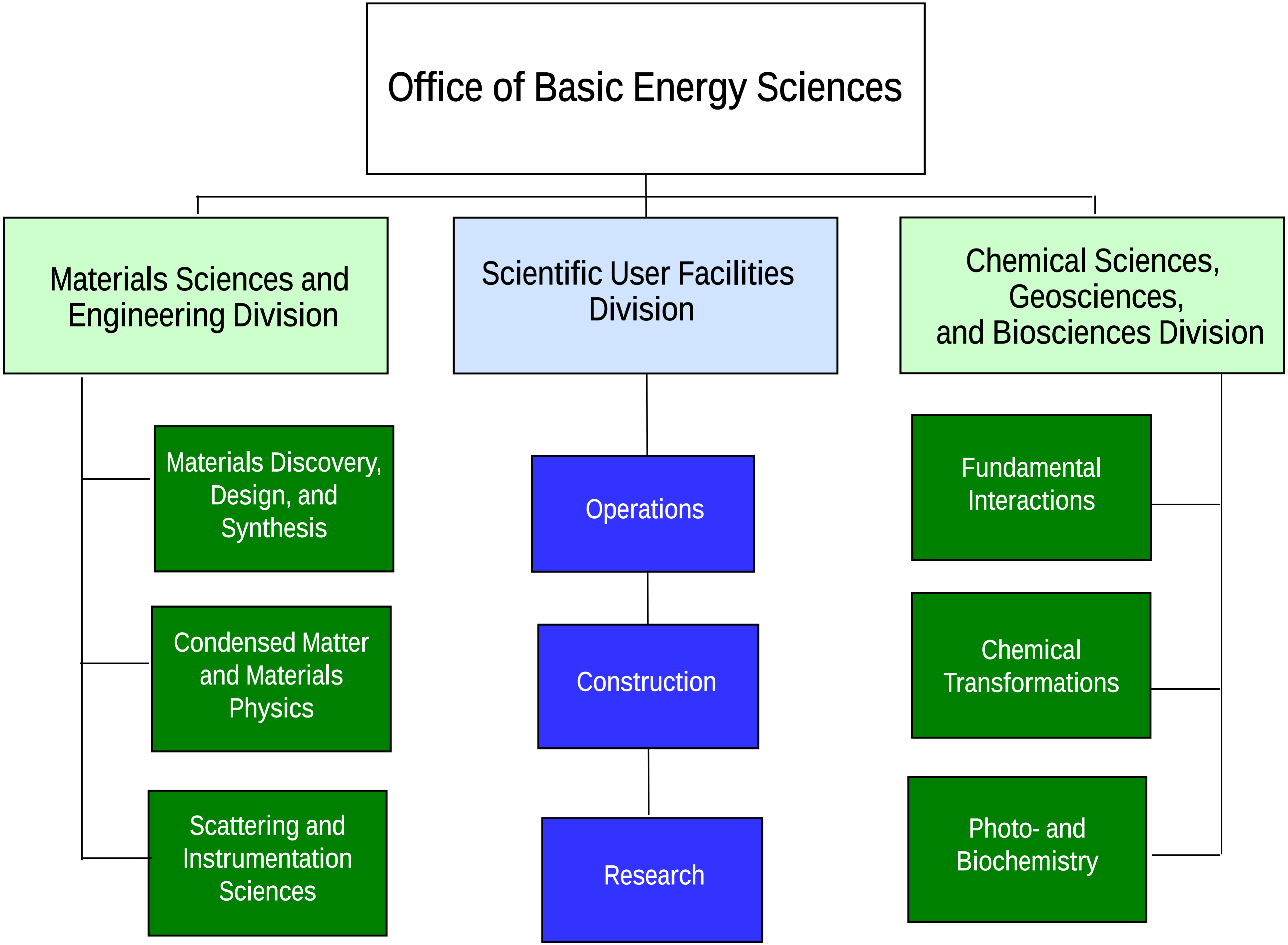
Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels





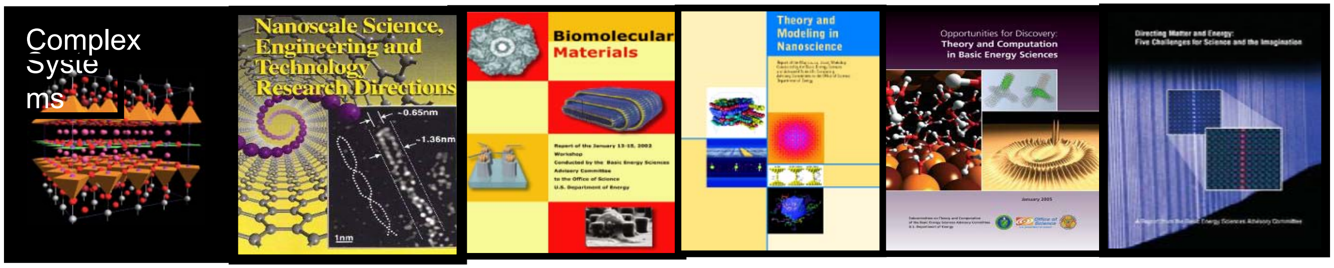





Office of Basic Energy Sciences
Materials Sciences and Engineering Division
Scientific User Facilities Division
Chemical Sciences, Geosciences, and Biosciences Division
Materials Discovery, Design, and Synthesis
Condensed Matter and Materials Physics
Scattering and Instrumentation Sciences
Operations
Construction
Research
Fundamental Interactions
Chemical Transformations
Photo- and Biochemistry

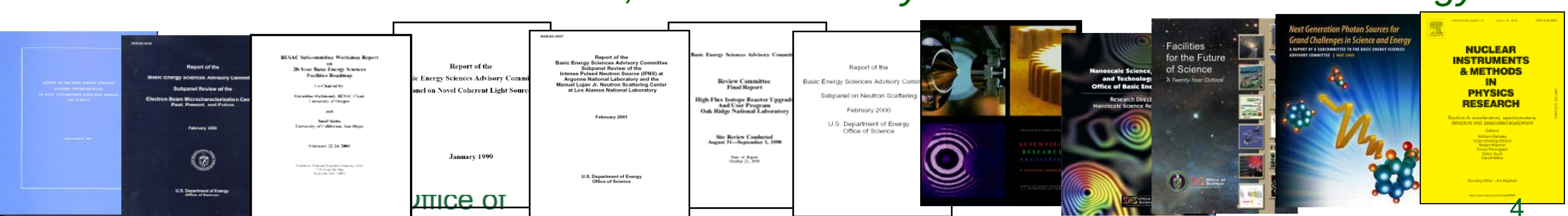
BES Strategic Planning Activities

- *Science for Discovery*



- *Science for National Needs*

- *National Scientific User Facilities, the 21st century Tools of Science & Technology*

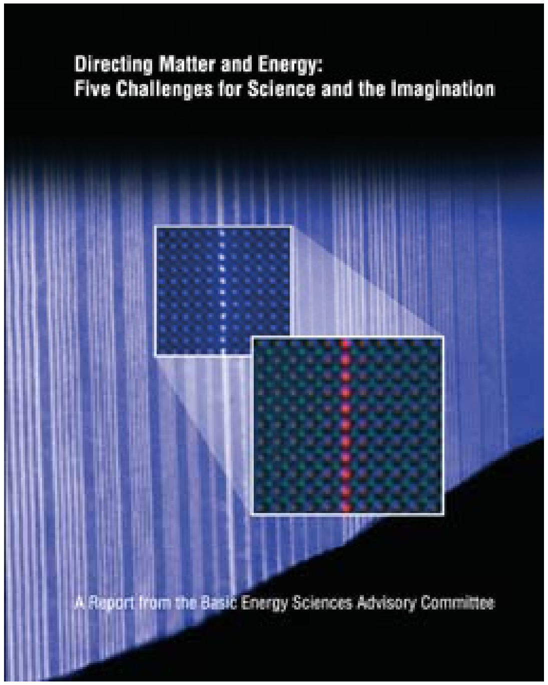


Office of Science

ENERGY

BESAC Grand Challenges Report

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



BESAC Grand Challenges Report 2007

- Control the quantum behavior of electrons in materials
- Synthesize, atom by atom, new forms of matter with tailored properties
- Control emergent properties that arise from the complex correlations of atomic and electronic constituents
- Synthesize man-made nanoscale objects with capabilities rivaling those of living things
- Control matter very far away from equilibrium

"Basic Research Needs" Reports

Sustainable Energy = High Tech Materials and Chemistry

Energy Sustainability and Materials

Traditional Energy Materials	*Sustainable Energy Materials*
Fuels: coal, oil, gas $CH_{0.8}$, CH_2, CH_4	Diverse Functions PV, Superconductors, Photocatalysts Battery Electrodes Electrolytic Membranes
Passive Function: Combustion	Active Function: Converting Energy
Value: Commodities High Energy Content	Value: Functionality 30 year Lifetime

Greater Sustainability = Greater Complexity,
higher functional materials

Transforming the Discovery Process

- Over the past 2 decades, the U.S. has developed and deployed the world's most powerful collection of research facilities for materials and chemical sciences
  - World-leading x-ray and neutron sources
  - Nanoscale science centers
  - High-performance computers
- For the first time in history, we are able to synthesize, characterize, and model materials and chemical behavior at the length scale where this behavior is controlled
- This transformational leap conveys a significant competitive advantage and forms the framework of BES programs.

BES Research — Science for Discovery & National Needs

Three Major Types of Funding Modality

increasing progression of scientific scope and level of effort

- **Core Research**

  Support single investigator and small group projects to pursue their specific research interests.

  - Enable seminal advances in the core disciplines of the basic energy sciences—materials sciences and engineering, chemistry, and aspects of geosciences and biosciences. Scientific discoveries at the frontiers of these disciplines establish the knowledge foundation to spur future innovations and inventions.

- **Energy Frontier Research Centers**

  $2-5 million-per-year research centers, established in 2009, focused on fundamental research related to energy

  - Multi-investigator and multi-disciplinary centers to harness the most basic and advanced discovery research in a concerted effort to accelerate the scientific breakthroughs needed to create advanced energy technologies. Bring together critical masses of researchers to conduct fundamental energy research in a new era of grand challenge science and use-inspired energy research.

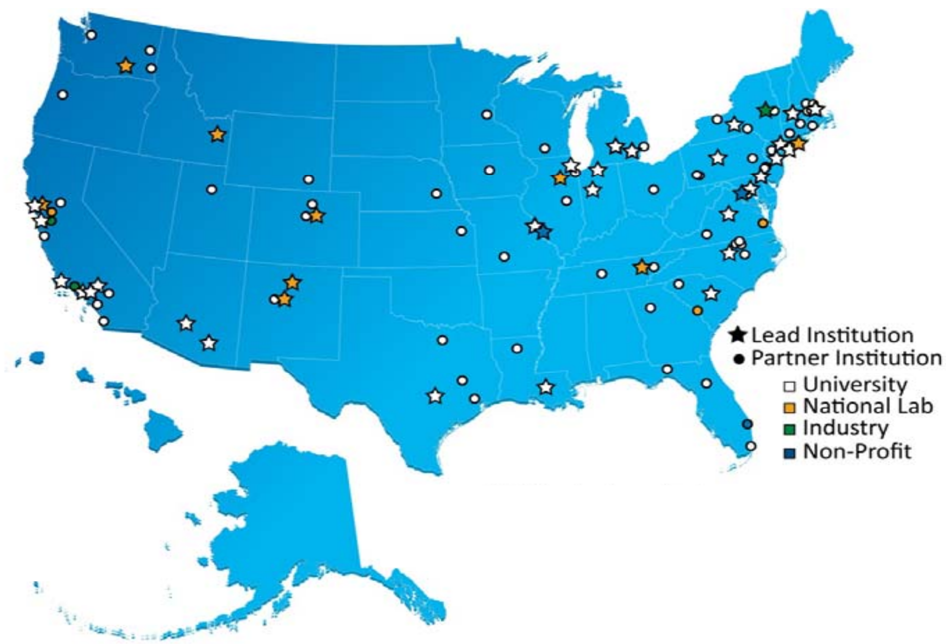
- **Energy Innovation Hubs**

  $25 million-per-year research centers will focus on co-locating and integrating multi-components, multi-disciplinary research with technology development to enable transformational energy applications

Energy Frontier Research Centers

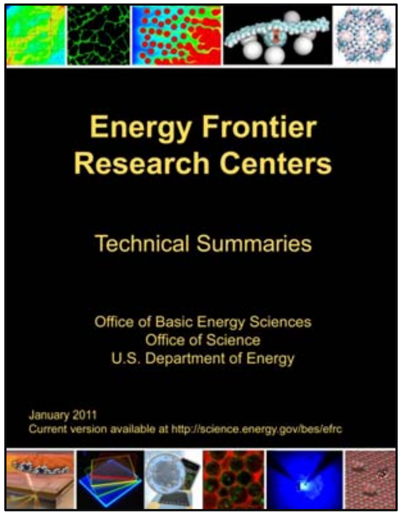
46 EFRCs in 35 States were launched in Fall 2009

- ~860 senior investigators and ~2,000 students, postdoctoral fellows, and technical staff at ~115 institutions
- > 250 scientific advisory board members from 12 countries and > 35 companies



Impact to date:

- >1,000 peer-reviewed papers including more than 30 publications in *Science* and *Nature*.
- > 40 patents applications and nearly 50 additional patent/invention disclosures by 28 of the EFRCs.
- at least 3 start-up companies with EFRC contributions



Assessment of progress:

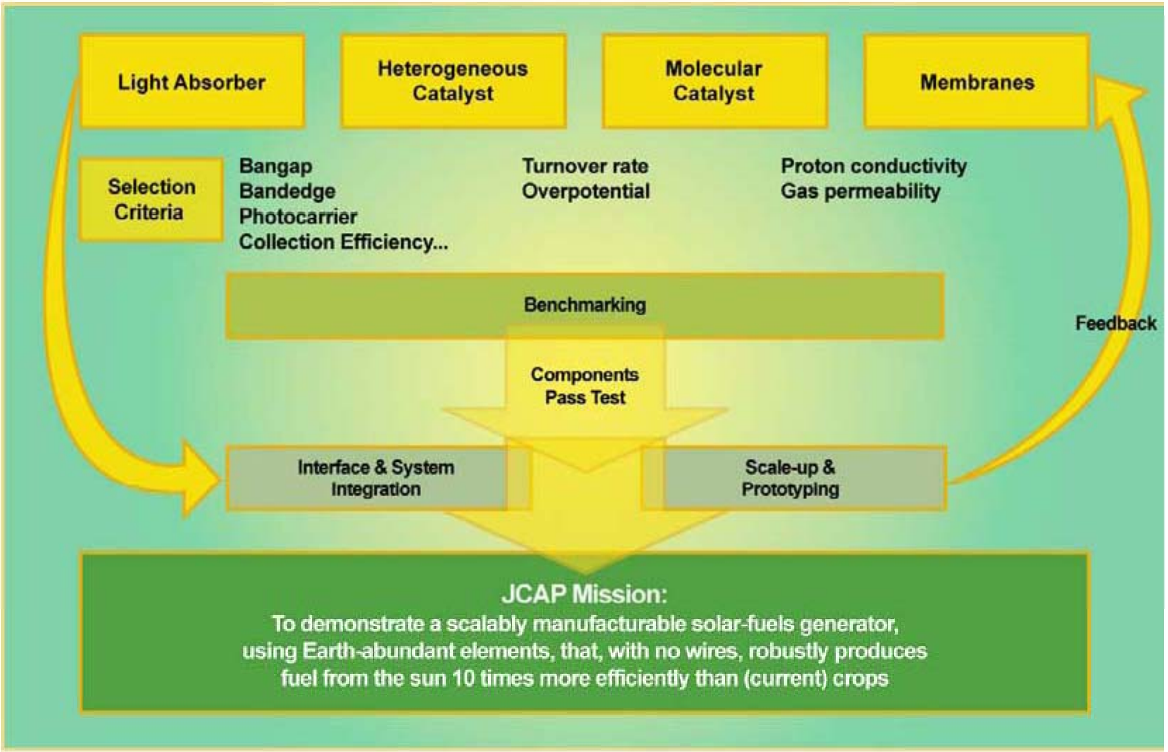
- All EFRCs are undergoing mid-term peer review to assess progress towards goals and plans for the next 2 years of R&D.

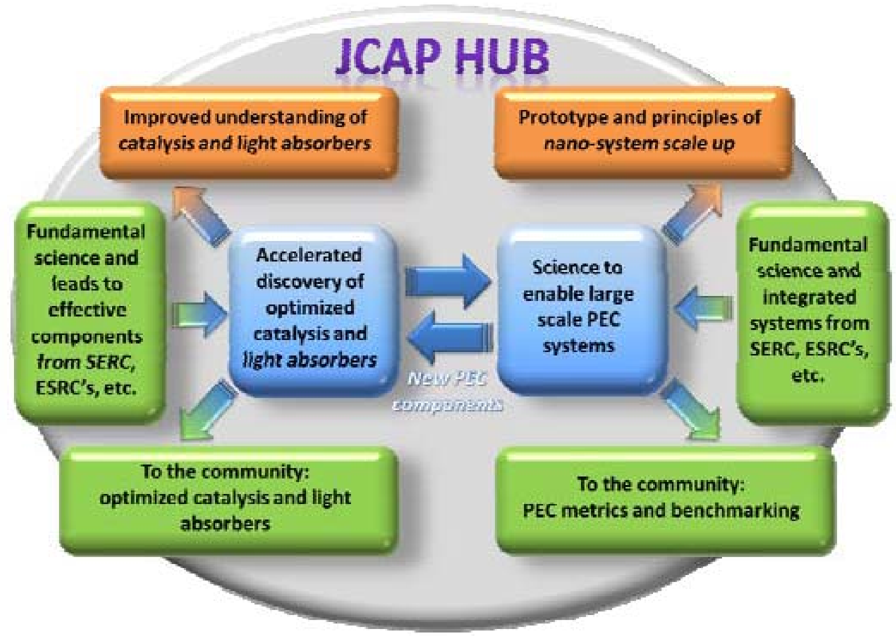
FY 2013 plans:

- Enhanced integration with DOE Technology programs to ensure implementation of scientific advances

http://science.energy.gov/bes/efrc/

JCAP as an Integrative Hub





JCAP R&D will focus on:

- ➢ Robustness of components
- ➢ Accelerating the rate of catalyst discovery for solar fuel reactions
- ➢ Discovering earth-abundant, robust, inorganic light absorbers with optimal band gap
- ➢ System integration, benchmarking, and scale-up

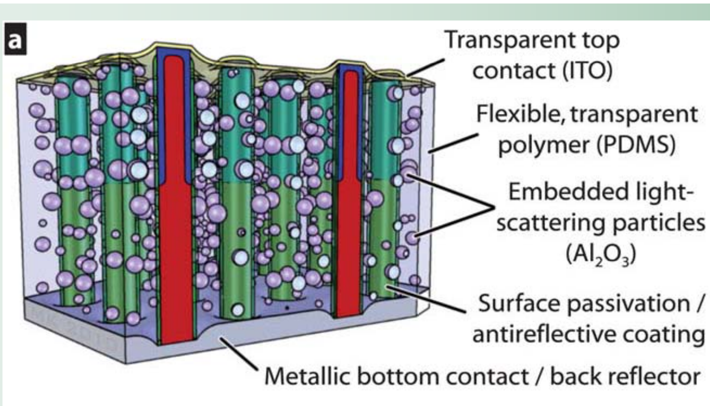
JCAP's role as a solar fuels Hub:

- ➢ Incorporating the latest discoveries from the community (EFRCs, single-PI or small-group research)
- ➢ Providing metrics and benchmarking to the community

Inexpensive Solar Cell Absorbs Nearly All Available Light

From Fundamental Research to Rooftop Applications

Basic Science
Energy Frontier Research Center



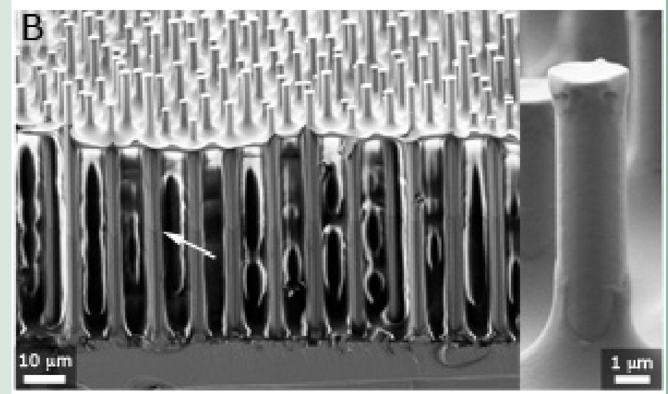
Light absorbing nanowires surrounded by polymer that contains Al_2O_3 scattering particles

Sunlight can be efficiently collected and redirected: Materials that occupy as little as 2% of the solar cell volume absorb up to 85% of the available sunlight

Manufacturing/ Commercialization

Caelux, a start-up company funded by the DOE PV Solar Incubator Program, develops solar cell designs and flexible manufacturing process that minimize the use of semiconducting material.

This invention has the potential to significantly improve device efficiency while dramatically reducing production costs.



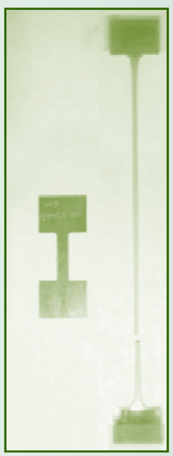
Breakthrough Award from *Popular Mechanics* 2010

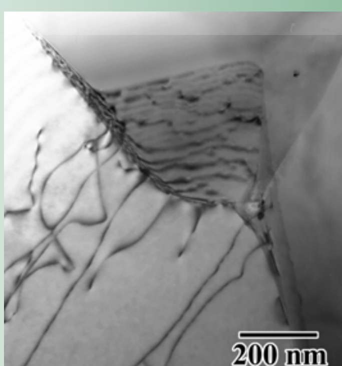
Superplastic Forming

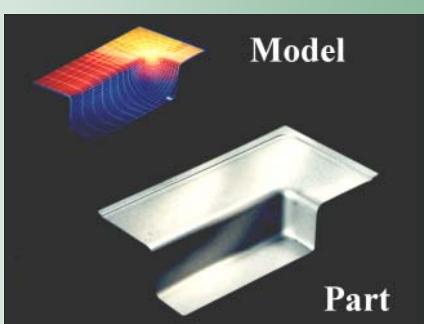
Basic Science Reduces Vehicle Weight, Improves Fuel Economy, Reduces Emissions

Basic Science

Fundamental research provided mechanistic understanding of the aluminum alloy microstructure and the superplastic deformation.







Applied R&D

Refined superplastic forming and optimized alloys to produce high quality, affordable, mass-produced aluminum parts.

PNNL worked with Kaiser Aluminum to develop new alloys based on the basic understanding of grain boundary sliding and recrystallization

Transportation Technology, Lab Technology Research Program (DOE), and NASA funded this applied research. Partnership with MARC Analysis to advance finite element modeling.

Manufacturing/ Commercialization

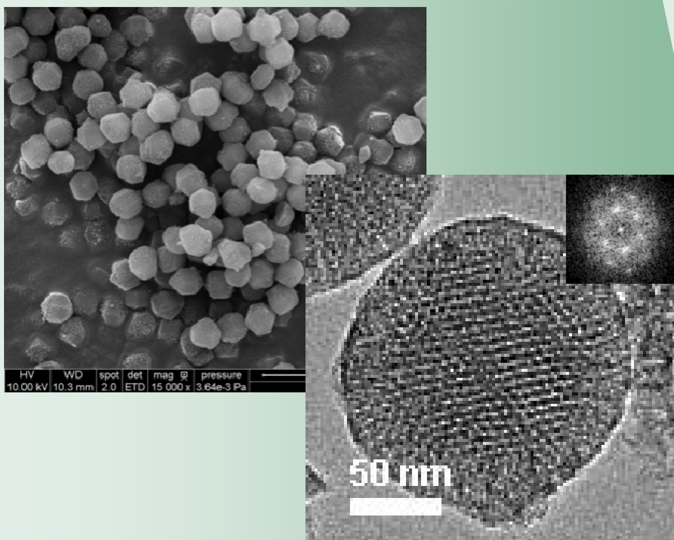
General Motors further developed the technology and reduced the cycle time. Used in Cadillac STS, Oldsmobile Aurora, and Chevy Malibu Maxx.

MARC Analysis – refined material simulation

Kaiser Aluminum -- new aluminum alloy.

Rational Catalyst Design for Cost Effective Biodiesel Production

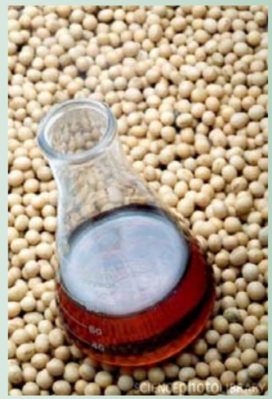
Basic Science

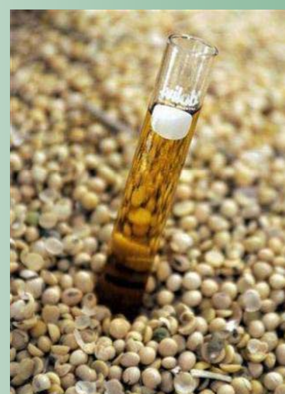


Discovery that co-locating catalysts and substrates in confined spaces greatly increases reaction rates leads to a new series of bi-functional mixed metal oxide materials for cooperative catalysis. One was identified as having both basic and acidic sites making it ideal for biodiesel production.

Applied R&D

Biodiesel is produced from vegetable and algal oils via transesterification, which is commercially catalyzed by a strong base.





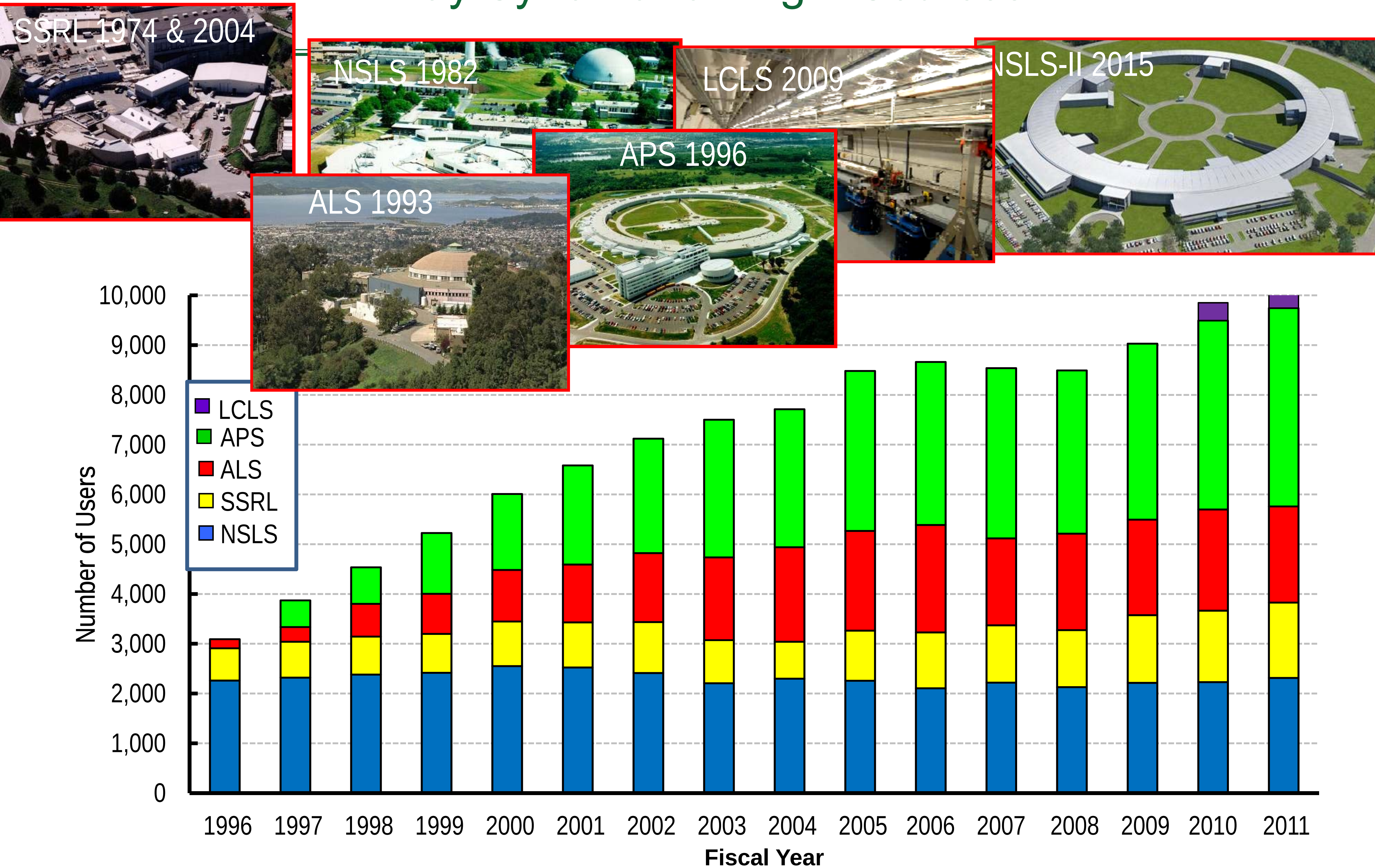
Current catalysts require pure feedstocks, and high temperature and pressure, making them unsuitable. EERE-supported work demonstrated that the new catalyst can make biodiesel from broader spectrum feedstocks and works even in the presence of impurities, such as acids and metals.

Manufacturing/ Commercialization

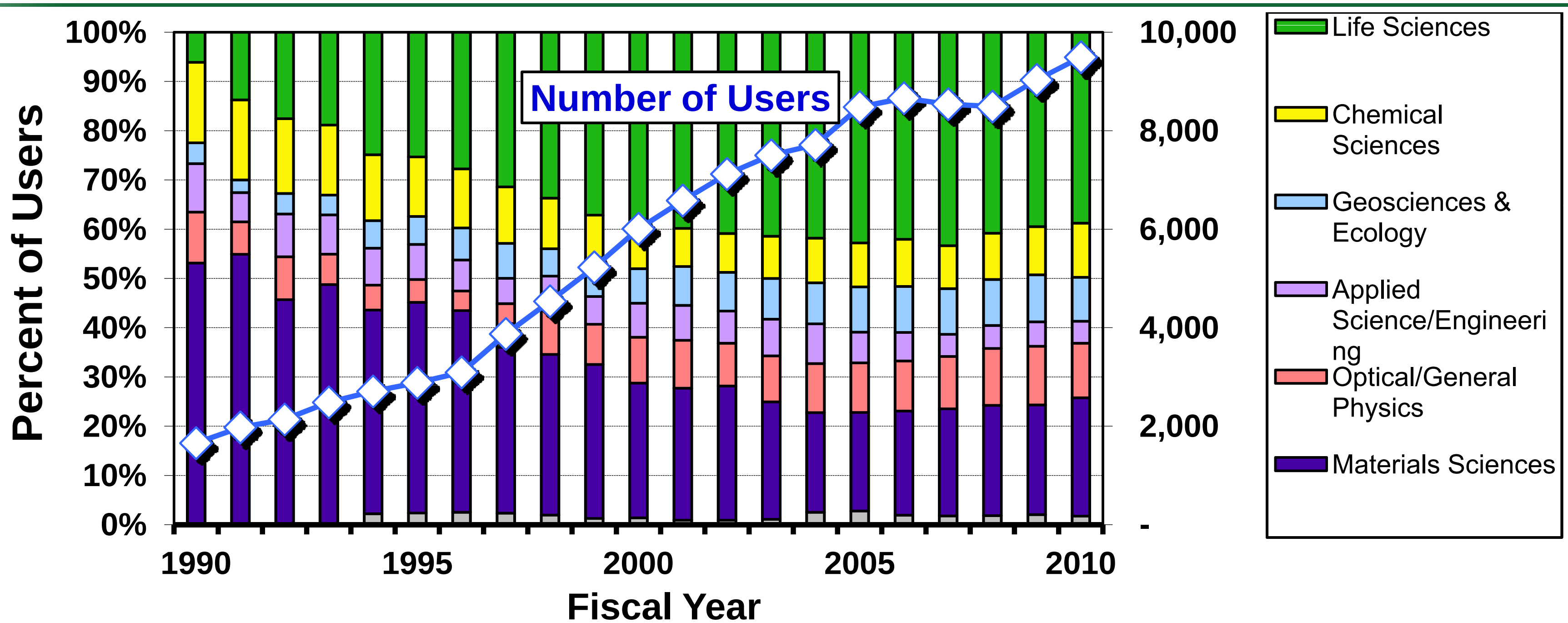
In 2007 the technology's commercial value attracted investor capital and Catilin, Inc. was born. Scale-up synthesis and pilot-plant demonstration was funded by EERE. In May 2011, Albemarle Corp. acquired Catilin, making the catalyst available as GoBio™ T300.

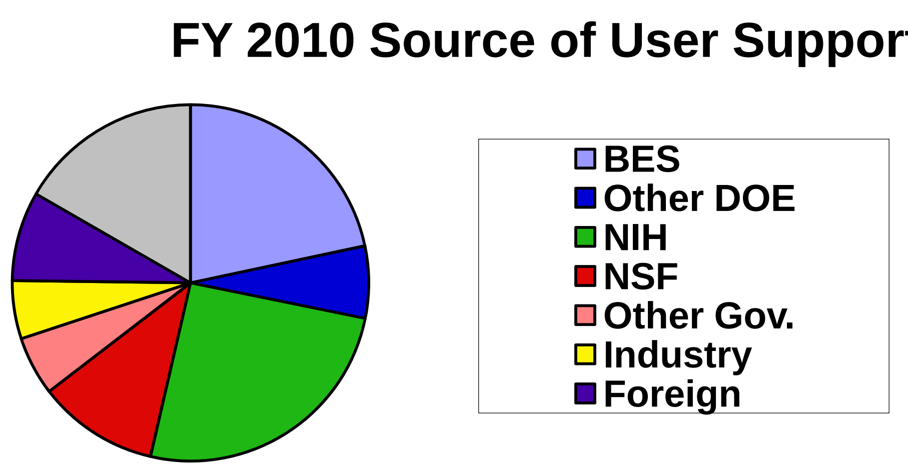
ALBEMARLE CATILIN

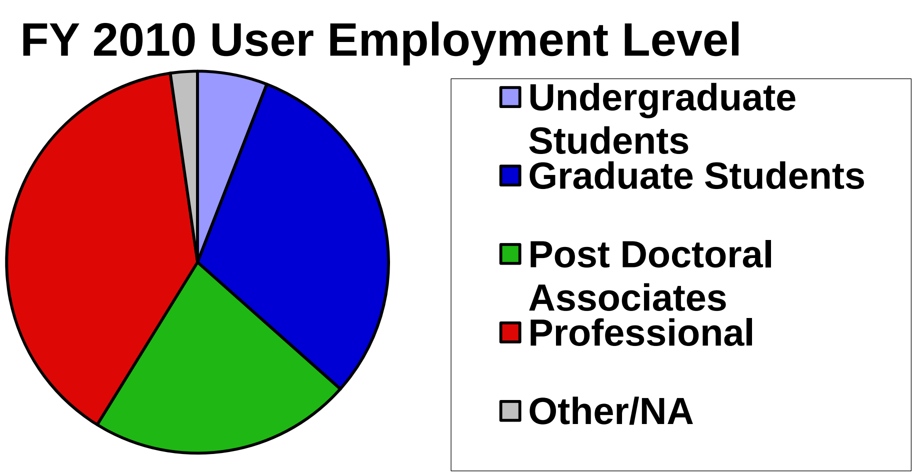
X-ray Synchrotron Light Sources



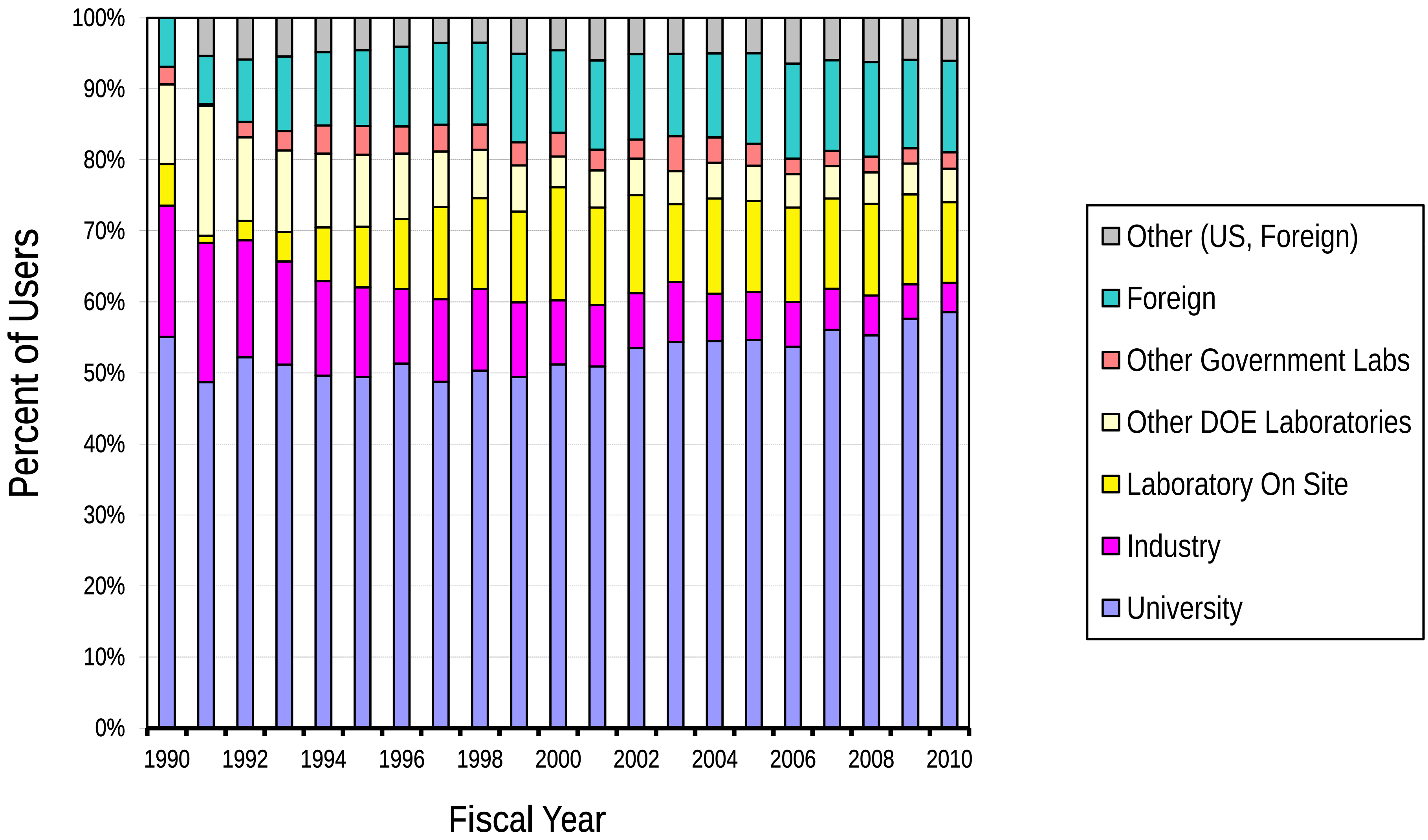
Characteristics of Users at the Synchrotron Light Sources







User Profile by Employer at the Synchrotron Radiation Light Sources

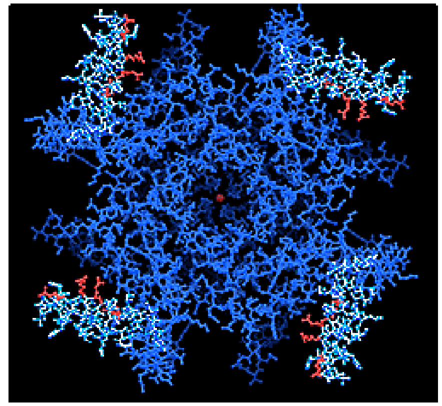


3 Nobel Prizes in 6 Years Using X-ray Crystallography

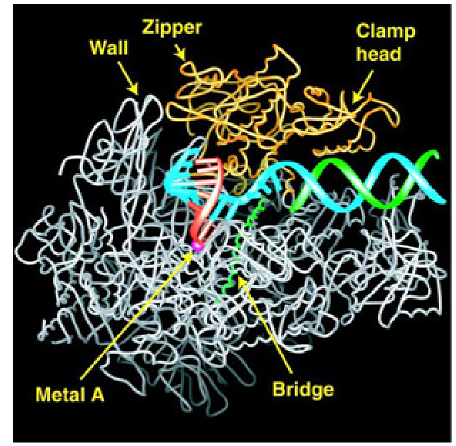
2003: Roderick MacKinnon (Chemistry) for “structural and mechanistic studies of ion channels.”
Used NSLS beamlines X25 and X29.

2006: Roger Kornberg (Chemistry) "for his studies of the molecular basis of eukaryotic transcription.”
Used SSRL macromolecular crystallography beamlines.

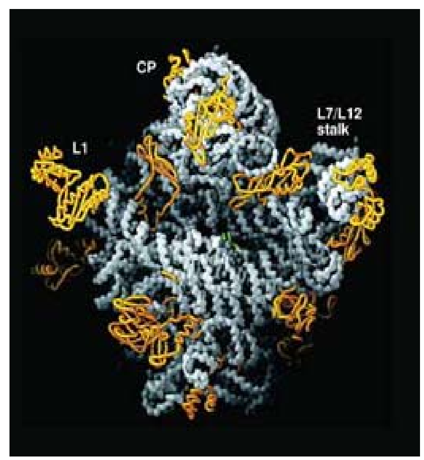
2009: Venkatraman Ramakrishnan, Thomas A. Steitz, and Ada E. Yonath (Chemistry) "for studies of the structure and function of the ribosome.”
Used all 4 DOE light sources.



An overhead view of a voltage-dependent potassium ion channel shows four red-tipped "paddles" that open and close in response to positive and negative charges. This structure, discovered by Rockefeller scientists, shows for the first time the molecular mechanism by which potassium ions are allowed in and out of living cells during a nerve or muscle impulse.



The transcription process visualized by Roger Kornberg and his colleagues. The protein chain shown in grey is RNA polymerase, with the portion that clamps on the DNA shaded in yellow. The DNA helix being unwound and transcribed by RNA polymerase is shown in green and blue, and the growing RNA stand is shown in red.



The 50S subunit structure at 2.4Å resolution.

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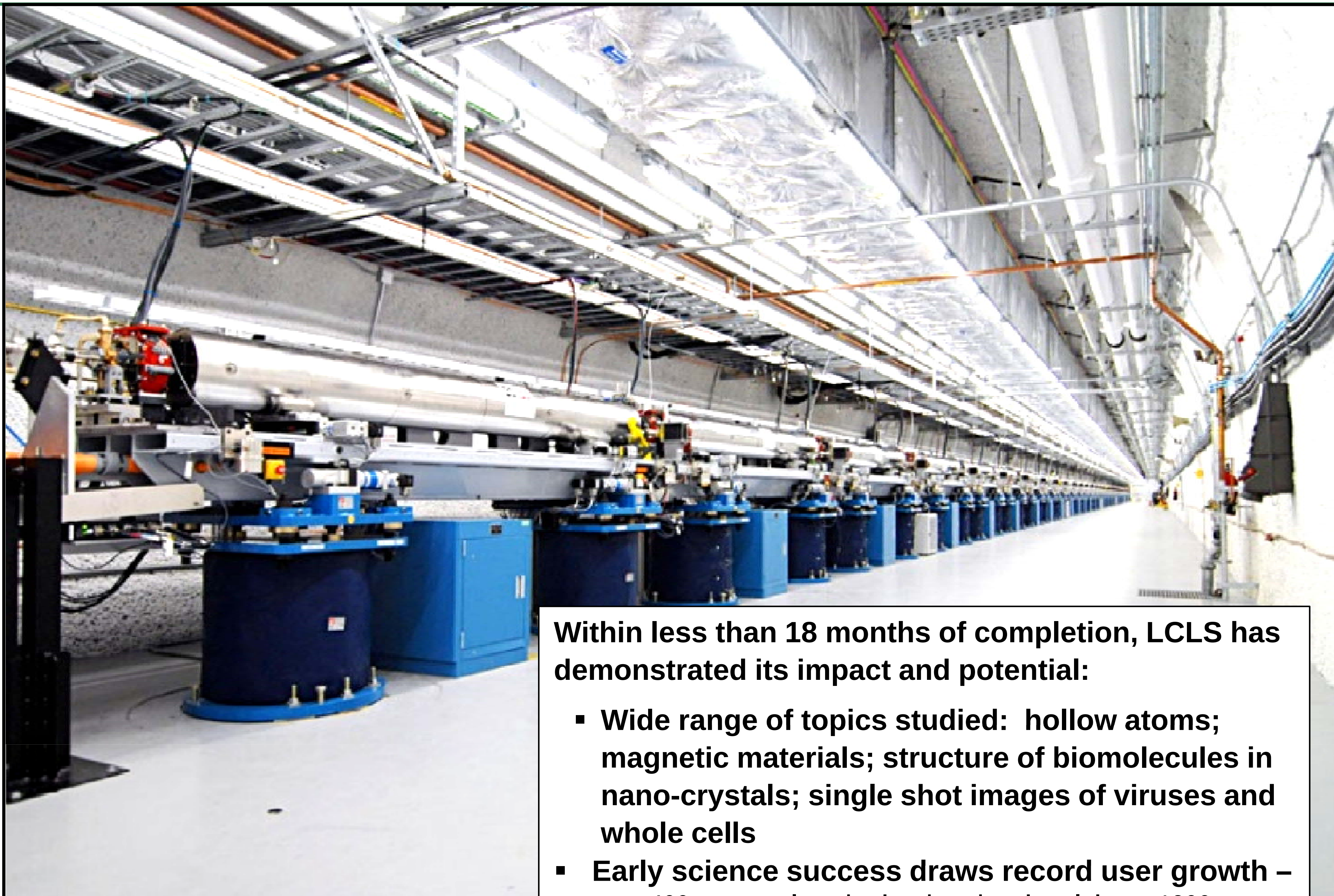
Expect the unexpected from new tools

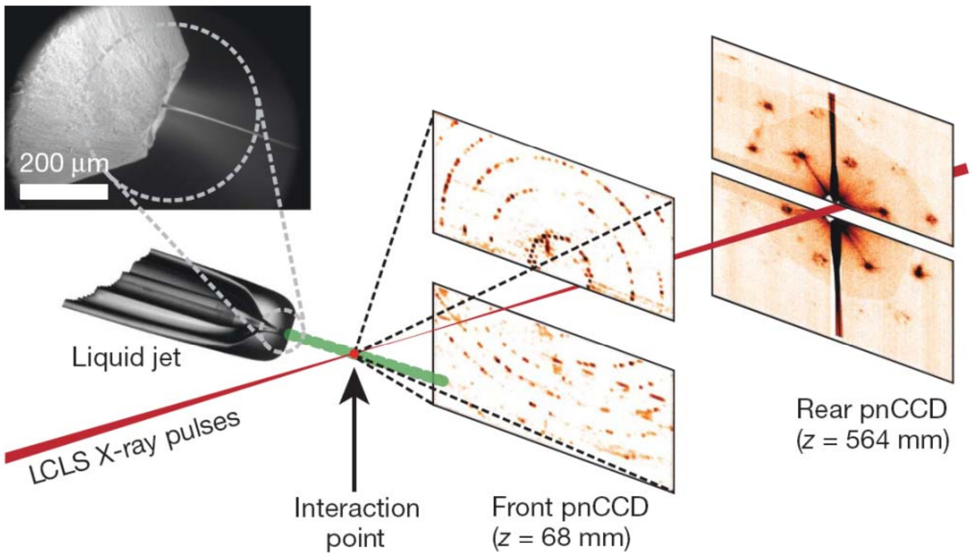
The World's First Hard X-ray Laser



Within less than 18 months of completion, LCLS has demonstrated its impact and potential:

- **Wide range of topics studied: hollow atoms; magnetic materials; structure of biomolecules in nano-crystals; single shot images of viruses and whole cells**
- **Early science success draws record user growth –** over 400 proposals submitted to date involving ~1300 unique scientists

LCLS @ SLAC: Femtosec Crystallography

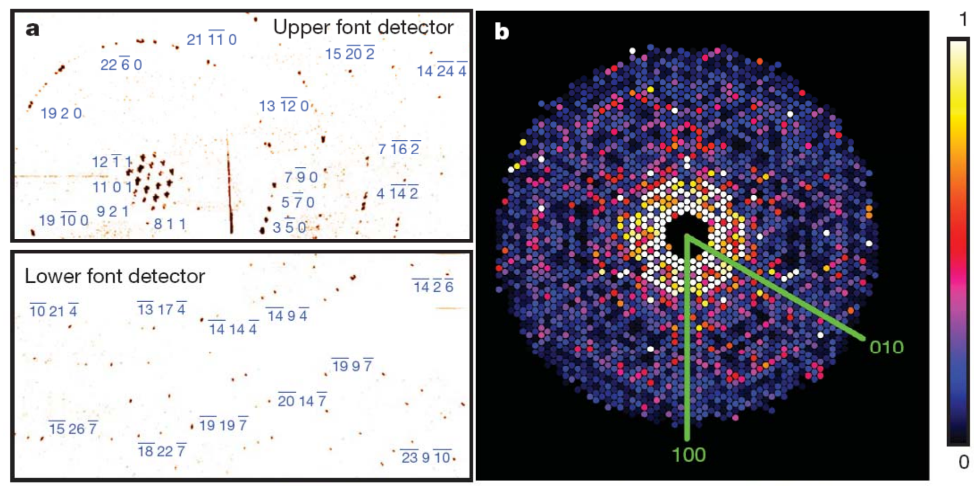


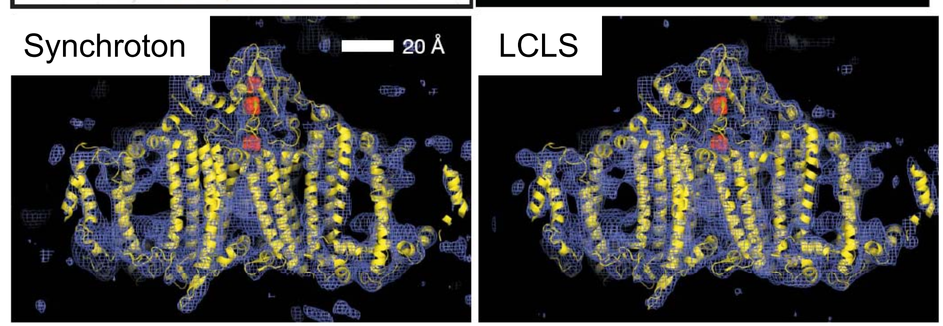
LETTER

doi:10.1038/nature09750

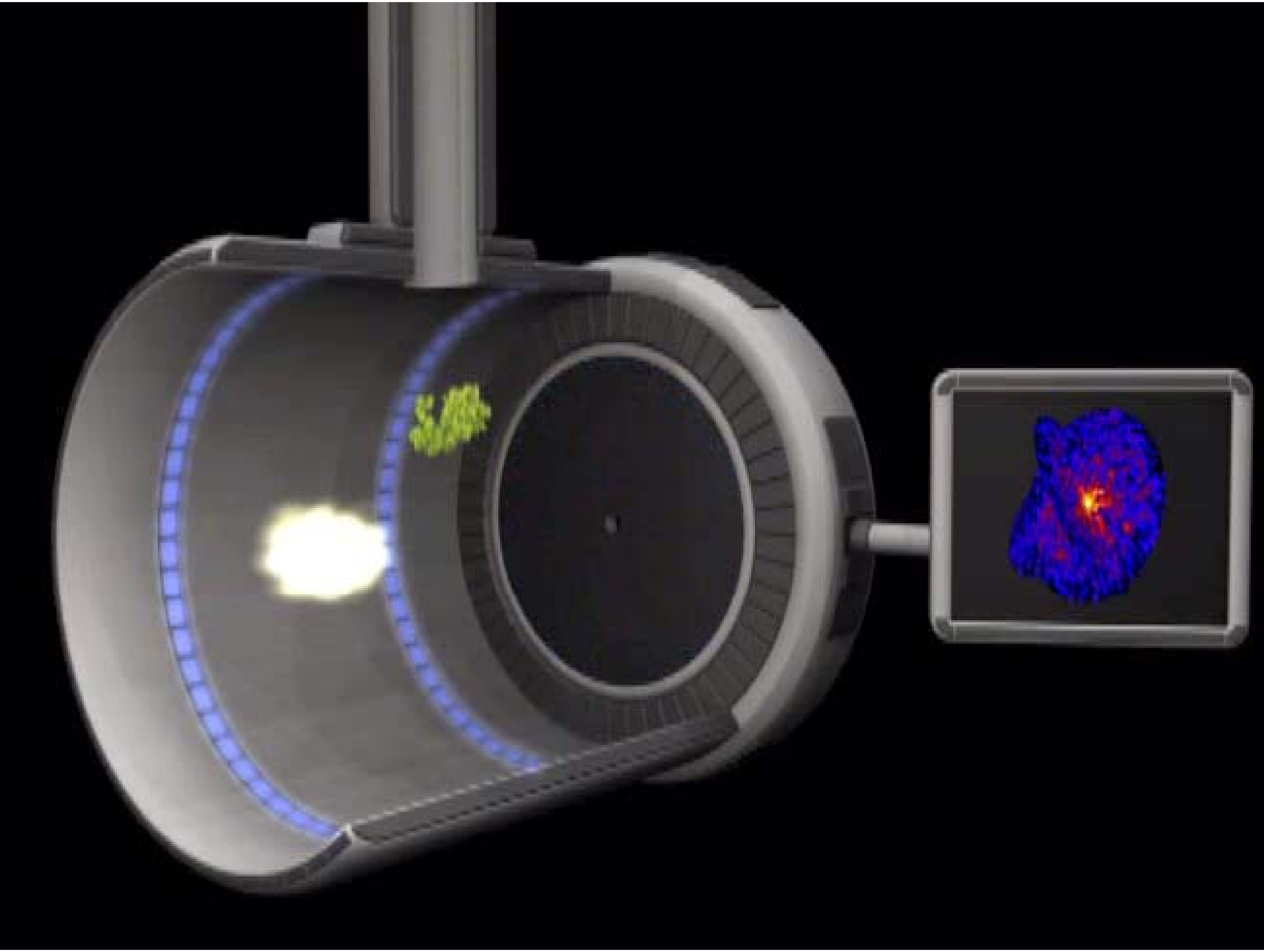
Femtosecond X-ray protein nanocrystallography

Henry N. Chapman[1,2], Petra Fromme[3], Anton Barty[1], Thomas A. White[1], Richard A. Kirian[4], Andrew Aquila[1], Mark S. Hunter[3], Joachim Schulz[1], Daniel P. DePonte[1], Uwe Weierstall[4], R. Bruce Doak[4], Filipe R. N. C. Maia[5], Andrew V. Martin[1], Ilme Schlichting[6,7], Lukas Lomb[7], Nicola Coppola[1]†, Robert L. Shoeman[7], Sascha W. Epp[6,8], Robert Hartmann[9], Daniel Rolles[6,7], Artem Rudenko[6,8], Lutz Foucar[6,7], Nils Kimmel[10], Georg Weidenspointner[11,10], Peter Holl[9], Mengning Liang[1], Miriam Barthelmess[12], Carl Caleman[1], Sébastien Boutet[13], Michael J. Bogan[14], Jacek Krzywinski[13], Christoph Bostedt[13], Saša Bajt[12], Lars Gumprecht[1], Benedikt Rudek[6,8], Benjamin Erk[6,8], Carlo Schmidt[6,8], André Hömke[6,8], Christian Reich[9], Daniel Pietschner[10], Lothar Strüder[6,10], Günter Hauser[10], Hubert Gorke[15], Joachim Ullrich[6,8], Sven Herrmann[10], Gerhard Schaller[10], Florian Schopper[10], Heike Soltau[9], Kai-Uwe Kühnel[8], Marc Messerschmidt[13], John D. Bozek[13], Stefan P. Hau-Riege[16], Matthias Frank[16], Christina Y. Hampton[14], Raymond G. Sierra[14], Dmitri Starodub[14], Garth J. Williams[13], Janos Hajdu[5], Nicusor Timneanu[5], M. Marvin Seibert[5]†, Jakob Andreasson[5], Andrea Rocker[5], Olof Jönsson[5], Martin Svenda[5], Stephan Stern[1], Karol Nass[2], Robert Andritschke[10], Claus-Dieter Schröter[8], Faton Krasniqi[6,7], Mario Bott[7], Kevin E. Schmidt[4], Xiaoyu Wang[4], Ingo Grotjohann[3], James M. Holton[17], Thomas R. M. Barends[7], Richard Neutze[18], Stefano Marchesini[17], Raimund Fromme[3], Sebastian Schorb[19], Daniela Rupp[19], Marcus Adolph[19], Tais Gorkhover[19], Inger Andersson[20], Helmut Hirsemann[12], Guillaume Potdevin[12], Heinz Graafsma[12], Björn Nilsson[12] & John C. H. Spence[4]

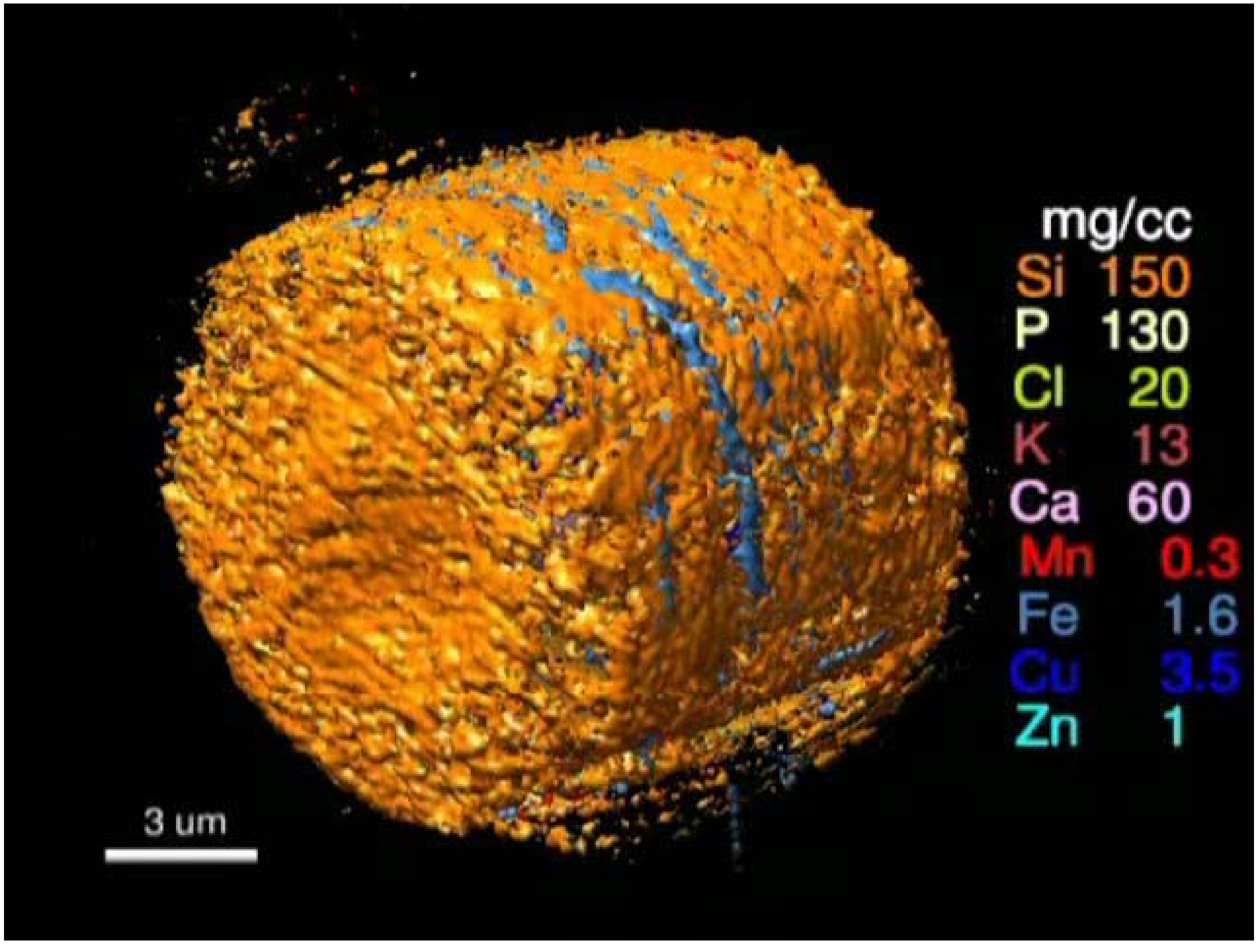




- **Low resolution structure of Photosystem I determined from ~15,000 nanocrystals**
- **Each crystal was illuminated sequentially and destroyed by the LCLS beam**
- **Dose >30 times larger than classical damage limit**
- **Recent experiment**
  ~ 18 Terabytes collected in 8 hours!



3-D Elemental Mapping within a Single Cell



Martin D. de Jonge et. al., Proc Nat Acad Sci. USA 107, 15676 (2010)

Trace elements in the freshwater diatom *Cyclotella meneghiniana*

Surprisingly, Mn is concentrated at the end caps of the frustule, and Fe incorporated into the siliceous shell, at the girdle bands.

Cell likely caught in early stages of cell division;

APS-U provides the higher resolution needed to see internal structures of cell organelles.

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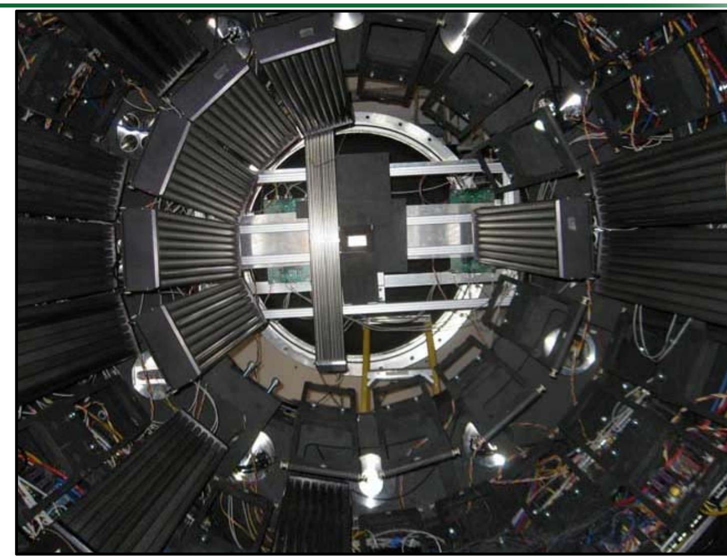
Neutron Scattering Facilities

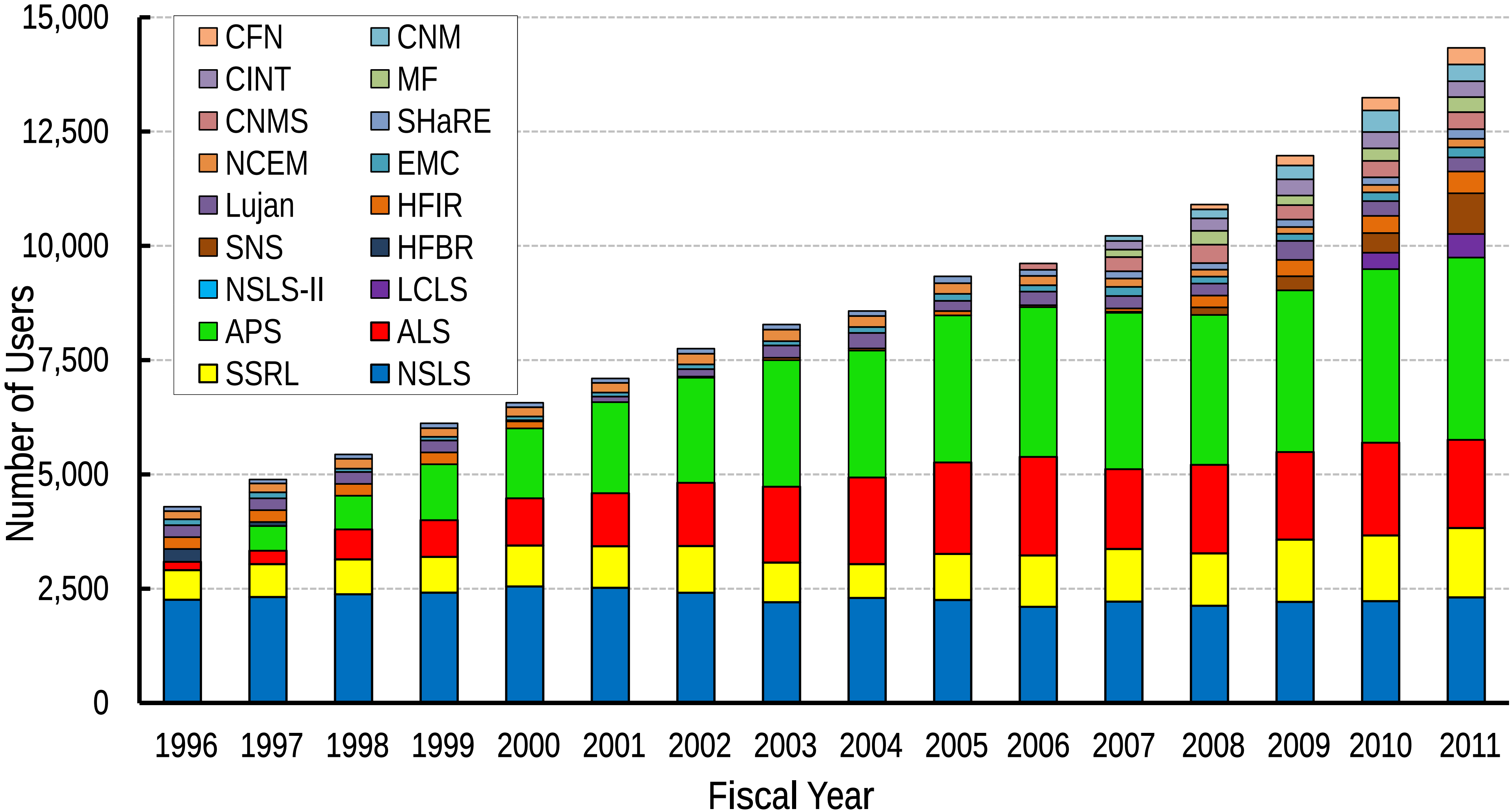
- The Spallation Neutron Source (SNS), the world's most intense neutron source, continues to expand the experimental capabilities for neutron scattering, with significant improvement in operation and user support.
    - 14 instruments in user program
    - 890 users in FY11
- The High Flux Isotope Reactor (HFIR) is upgrading existing instruments and developing new capabilities for neutron scattering; it continues reliable operations for nuclear materials research and isotope production:
    - New detector for GS-SANS
    - New neutron imaging station
    - 470 users in FY11
- The Lujan Center, a pulsed spallation source operating at about 100 kW, supports a target hall constructed by SC and instruments fabricated by SC and NNSA that address the needs of both the basic research community and the NNSA mission of science-based stockpile stewardship.
    - 308 users in FY11



Nanosale Ordered Materials Diffractometer (NOMAD) Detectors Tank at SNS

Triple-Axis Spectrometer at HFIR

BES User Facilities Hosted Over 14,000 Users in FY 2011



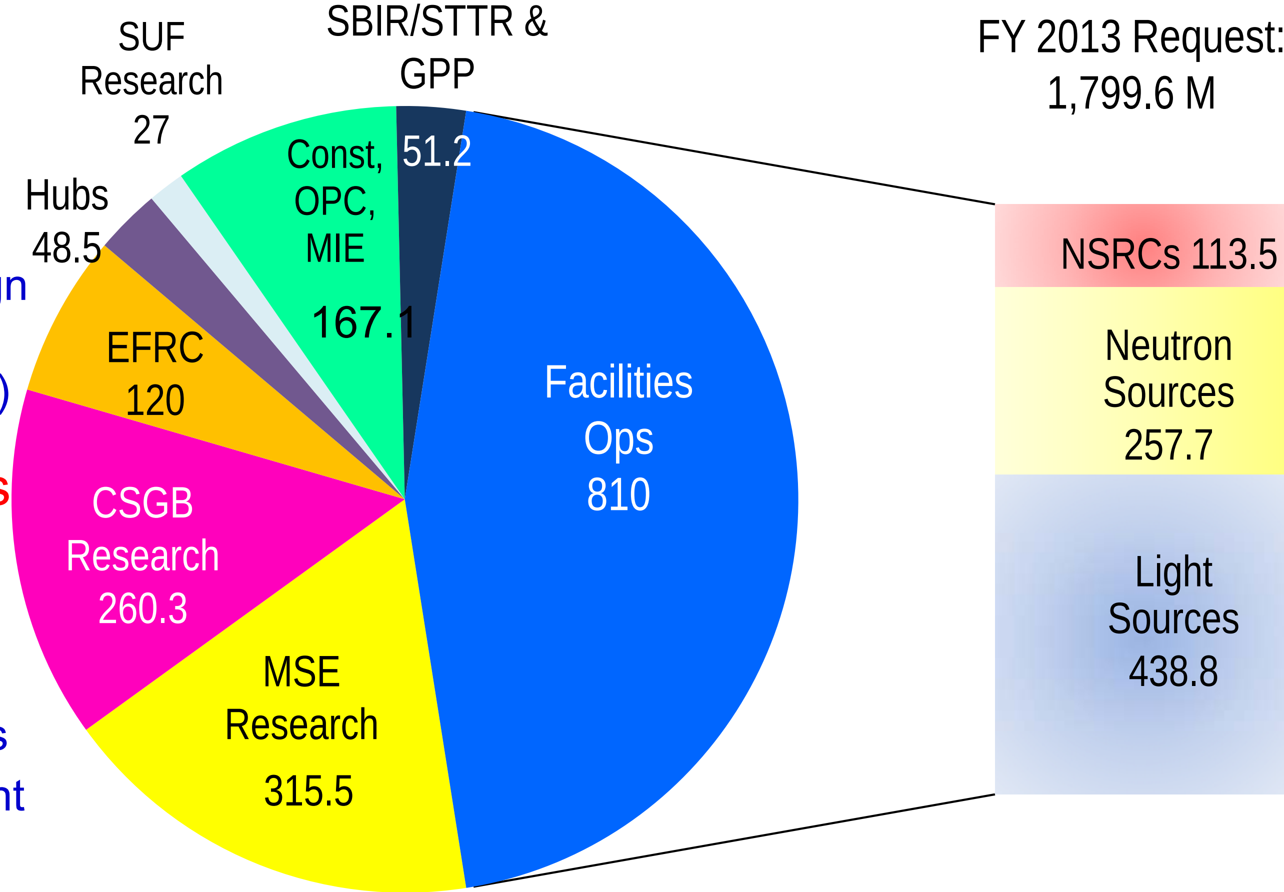
More than 300 companies from various sectors of the manufacturing, chemical, and pharmaceutical industries conducted research at BES scientific user facilities. Over 30 companies were Fortune 500 companies.

Fortune 500 Users of BES Scientific Facilities

BOEING
United Technologies
GE
MONSANTO
NORTHROP GRUMMAN
HALLIBURTON
SAIC
P&G
DOW
DUPONT
Honeywell
Chevron
ExxonMobil
Rockwell Collins
Building trust every day
3M
Sun Data Center Efficiency Resource Kit
SOFTWARE. HARDWARE. COMPLETE.
Sun
ORACLE
Ford
GM
JOHN DEERE
CAT
WD Western Digital
Kodak
MOTOROLA
intel
Boston Scientific
Defining tomorrow, today.
MERCK
ITT
TEXAS INSTRUMENTS
Abbott
A Promise for Life
Medtronic
Pfizer
IBM
hp
Bristol-Myers Squibb
Johnson & Johnson
AMGEN
Lilly

FY 2013 BES Budget Request

- **Research programs**
  - Energy Innovation Hubs
  - Energy Frontier Research Centers
    - Joint EERE R&D ($+20M)
  - Core Research
    - Materials and Chemistry by Design ($+20M)
    - Science for Clean Energy ($+42M)



- **Scientific user facilities operations**

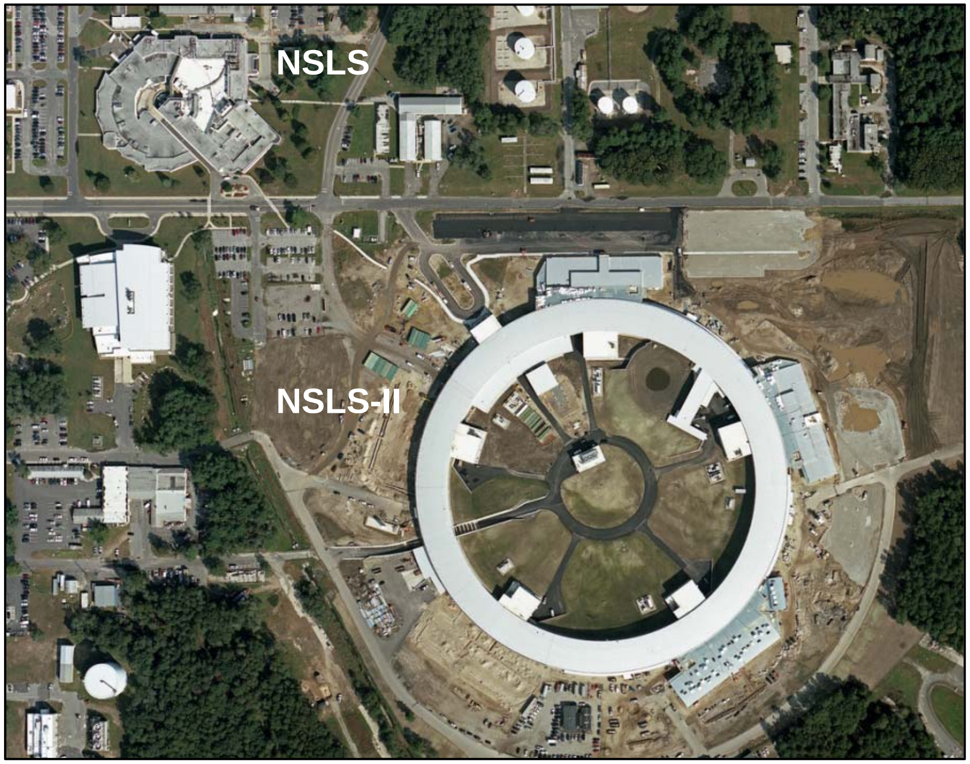
Near optimum operations of all facilities
  - Synchrotron light sources
  - Neutron scattering facilities
  - Nanoscale Science Research Centers
  - Instrumentation for clean energy – joint with EERE ($+15M)

- **Construction and instrumentation**
  - National Synchrotron Light Source-II ($71.6M)
  - NSLS-II instrumentation (NEXT) ($12M)
  - Advanced Photon Source upgrade ($20M)
  - Linac Coherent Light Source-II ($63.5M)

Maintaining World Leadership in Light Sources
National Synchrotron Light Source-II, 67% Complete

Highly optimized x-ray synchrotron:
- exceptional brightness and beam stability
- suite of advanced instruments, optics, and detectors that capitalize on these capabilities

Capabilities:
- ~ 1 nm spatial resolution
- ~ 0.1 meV energy resolution
- single atom sensitivity



Aug 2005	CD-0, Approve Mission Need	(Complete)
Jul 2007	CD-1, Approve Alternative Selection and Cost Range	(Complete)
Jan 2008	CD-2, Approve Performance Baseline	(Complete)
Jan 2009	CD-3, Approve Start of Construction	(Complete)
Feb 2009	Contract Award for Ring Building	(Complete)
Aug 2009	Contract Award for Storage Ring Magnets	(Complete)
May 2010	Contract Award for Booster System	(Complete)
Mar 2011	1st Pentant Bldg Beneficial Occ; Start Accel Installation	(Complete)
Feb 2012	Beneficial Occupancy of Experimental Floor	
Apr 2012	Start LINAC Commissioning	
Oct 2012	Start Booster Commissioning	
May 2013	Start Storage Ring Commissioning	
Jun 2015	CD-4, Approve Start of Operations	

Maintaining World Leadership in Light Sources
Upgrades and Instrumentation

Linac Coherent Light Source-II (LCLS-II)
- LCLS-II will provide a second, independently controlled FEL to the facility
- Expanded x-ray energy range (250eV – 13keV), x-ray polarization control, control pulse length down to ~1 femtosecond
- New experimental hall with 4 experimental stations
- Cost Range: $350M - $500M (Line Item Construction)
- FY 2012 $30M, FY 2013 Request $64M for R&D, design, and construction

Advanced Photon Source Upgrade (APS-U)
- Temporal resolution to 1 picosecond, spatial resolution to <1 nm above 25keV
- Accelerator and x-ray source upgrades, new and upgraded beamlines, enabling technical capabilities
- Cost Range: $310M - $450M (Major Item of Equipment)
- FY 2012 $20M, FY 2013 Request $20M for R&D, design, and long lead procurement

NSLS-II Experiment Tools (NEXT)
- Enhance NSLS-II with 4 to 6 best-in-class beamlines chosen from peer reviewed proposals
- Beamlines will support 300-400 users per year
- CD-1 Cost Range: $83M - $90M (Major Item of Equipment)
- FY 2012 $12M, FY 2013 Request $12M for R&D, design, long lead procurement, and construction