U.S. DEPARTMENT OF ENERGY | Office of Science

Basic Energy Sciences

Accelerators and Detector R&D Principal Investigators Meeting

August 22, 2011

Harriet Kung
Director, Office of Basic Energy Sciences
Office of Science, 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

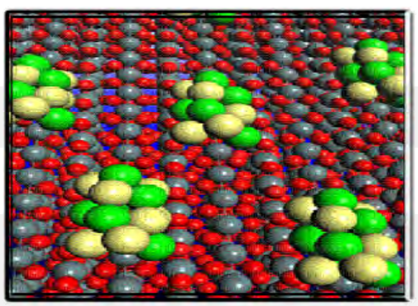
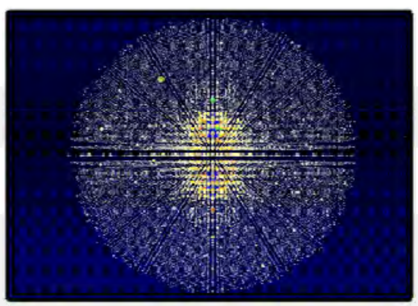
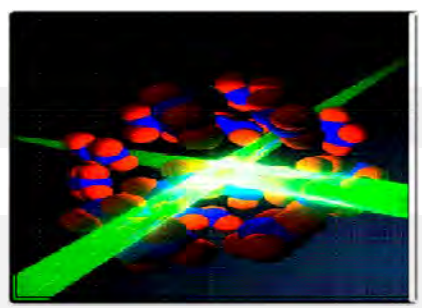
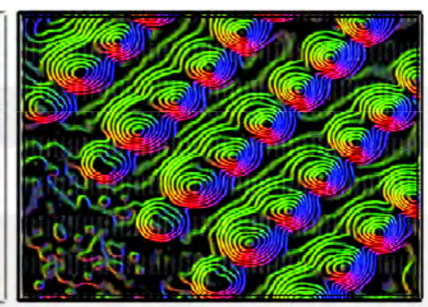
Chemical sciences, geosciences, and energy biosciences—exploring the fundamental aspects of chemical reactivity and energy transduction over wide ranges of scale and complexity and their applications to energy technologies

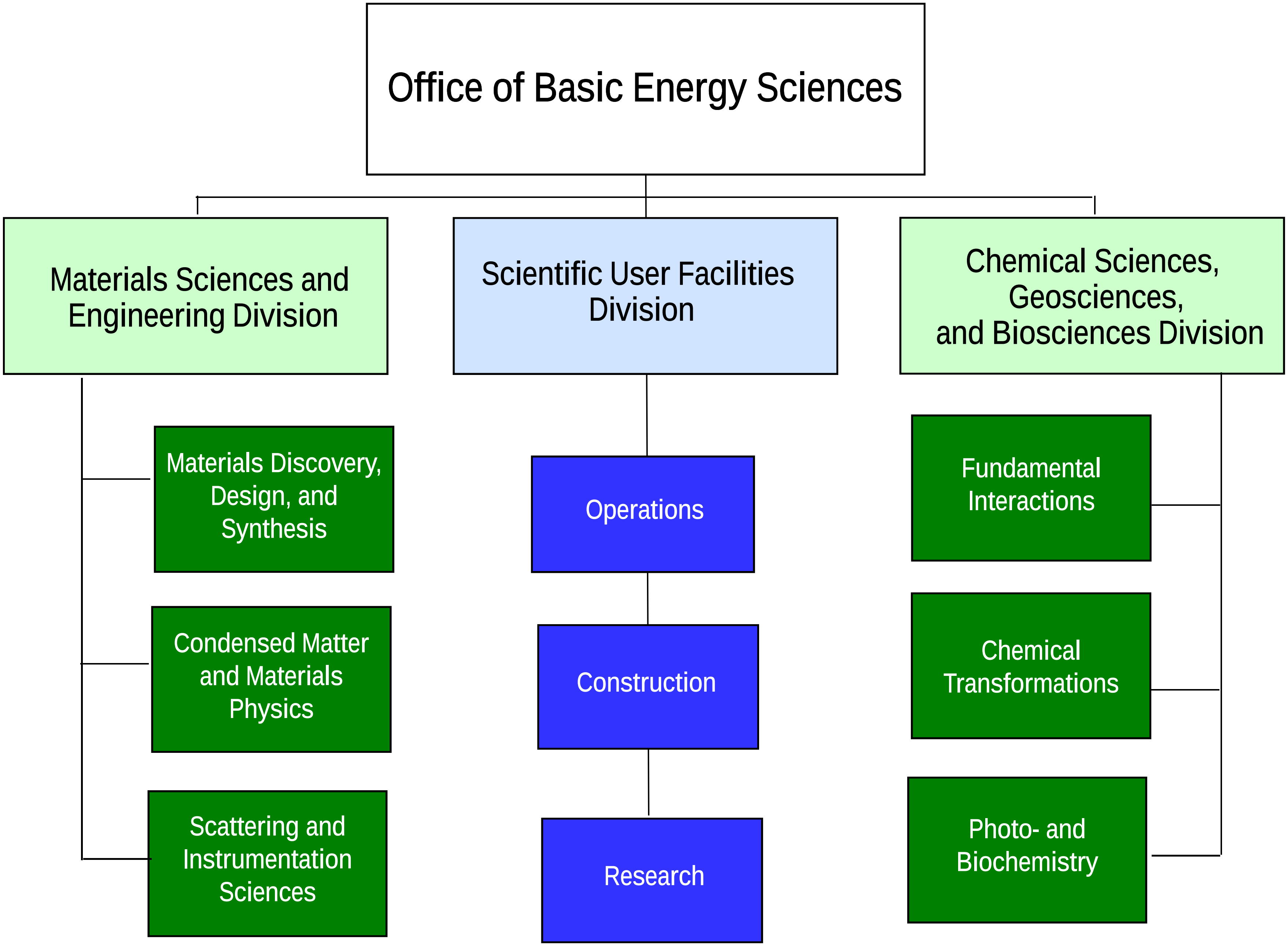
Scientific User Facilities—supporting the largest collection of facilities for electron, x-ray, and neutron scattering in the world

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

Office of Basic Energy Sciences

Harriet Kung, Director
Wanda Smith, Administrative Specialist

BES Budget and Planning
- Bob Astheimer, Senior Technical Advisor
- Margie Davis, Financial Management

BES Operations
- Kerry Gorey, Program Support Specialist
- Robin Hayes, AAAS Fellow
- Katie Perine, Program Analyst / BESAC
- Ken Rivera, Laboratory Infrastructure / ES&H
- Vacant, DOE and Stakeholder Interactions
- Vacant, DOE Technical Office Coordination

Materials Sciences and Engineering Division

Linda Horton, Director
Teresa Crockett, Program Analyst
Vacant

- **Materials Discovery, Design, and Synthesis** — Arvind Kini; Jorge Mariani, P.A.
  - Materials Chemistry: Arvind Kini; Vacant; ● John Schlueter, ANL; ● Darryl Sasaki, SNL
  - Biomolecular Materials: Mike Markowitz
  - Synthesis and Processing: Bonnie Gersten
  - Tech. Coordination Program Management: John Vetrano; Vacant
- **Condensed Matter and Materials Physics** — Jim Horwitz; Marsophia Agnant, P.A.
  - Exp. Cond. Mat. Phys.: Andy Schwartz; ● Doug Finnemore, Ames; Vacant
  - Theo. Cond. Mat. Phys.: Jim Davenport; ■ Kim Ferris, PNNL
  - Physical Behavior of Materials: Refik Kortan
  - Mechanical Behavior and Radiation Effects: John Vetrano; ● Richard Wright, INL
- **Scattering and Instrumentation Sciences** — Helen Kerch; Cheryl Howard, P.A.
  - X-ray Scattering: Lane Wilson
  - Neutron Scattering: Thiyaga P. Thiyagarajan
  - Electron and Scanning Probe Microscopies: Jane Zhu
  - DOE EPSCoR*: Tim Fitzsimmons; ● Helen Farrell, INL; ● John Schlueter, ANL

* Experimental Program to Stimulate Competitive Research

Scientific User Facilities Division

Harriet Kung, Acting Director
~~Linda Cerrone, Program Support Specialist~~ Vacant

- **Operations**
  - X-ray and Neutron Scattering Facilities: Peter Lee; David Price
  - NSRCs and EBMCs**: Mihal Gross; ☆ Tof Carim
  - Accelerator and Detector R&D: Eliane Lessner
  - Facility Coordination; Metrics; Assessment: Van Nguyen
- **Construction**
  - NSLS-II ***: Phil Kraushaar; Vacant
  - Facilities Upgrades: Phil Kraushaar; ◆ Carl Piechowski; Vacant
  - Instrument MIEs****: Phil Kraushaar; ◆ Carl Piechowski; ■ John Tapia, LANL

** Nanoscale Science Research Centers and Electron-beam Microcharacterization Centers
*** National Synchrotron Light Source II
**** Major Item of Equipment projects

Chemical Sciences, Geosciences, and Biosciences Division

Eric Rohlfing, Director
Diane Marceau, Program Analyst
Michaelene Kyler-King, Program Assistant

- **Fundamental Interactions** — Michael Casassa; Robin Felder, P.A.
  - Atomic, Molecular, and Optical Sciences: Jeff Krause
  - Gas-Phase Chemical Physics: Wade Sisk
  - Condensed-Phase and Interfacial Mol. Science: Gregory Fiechtner
  - Computational and Theoretical Chemistry: Mark Pederson
- **Photochemistry and Biochemistry** — Rich Greene; Sharron Watson, P.A.
  - Solar Photochemistry: Mark Spitler; ◆ Margaret Ryan, PNNL
  - Photosynthetic Systems: Gail McLean
  - Physical Biosciences: Robert Stack
  - Fuels from Sunlight Energy Innovation Hub: Carol Bessel
- **Chemical Transformations** — John Miller; Vacant, P.A.
  - Catalysis Science: Paul Maupin; Raul Miranda; ◆ Jan Hrbek, BNL
  - Separations and Analysis: Larry Rahn
  - Heavy Element Chemis[try]: Philip Wilk; ● Norm Edelstein, LB[NL]
  - Geosciences: Nick Woodward; ● Jennifer Blank, LBNL
  - Technology Office Coordination: Marvin Singer

LEGEND
- ◆ Detailee (from DOE laboratories)
- ☆ On Detail to OSTP
- ◆ On Detail from HS-71
- ■ Detailee, ½ time, not at HQ
- ● Detailee, ¼ time, not at HQ
- P.A. Program Assistant

(oval) Vacancy

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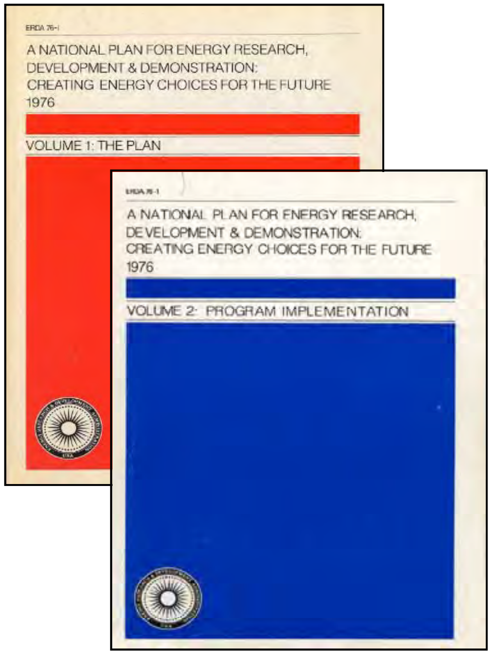
History of Basic Energy Sciences



ERDA's 1976 R&D plan, *A National Plan for Energy Research, Development, and Demonstration: Creating Energy Choices for the Future (April 15, 1976)*.

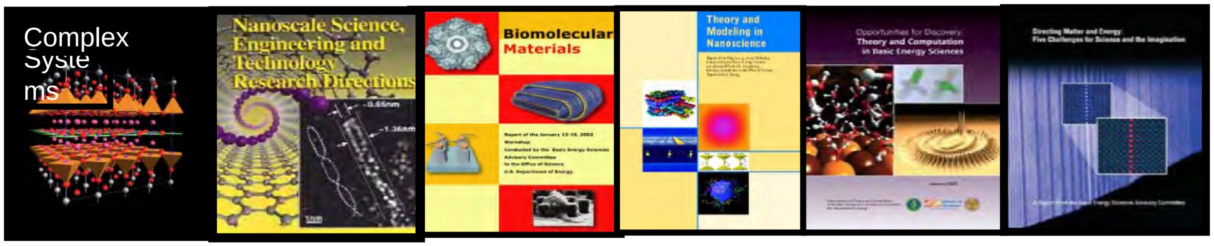
- **The formation of BES was part of the *Department of Energy Organization Act of 1977* to provide for basic energy research in non-nuclear areas.**
- **Basic research activities within the *Energy Research and Development Administration* (ERDA) were first grouped as the BES program in the FY 1977 Budget Request (released February 1976). The BES organization was formed in June 1977 in preparation for the creation of DOE in October 1977.**
- **While BES has gone through many changes in structure and program emphases, the mission of BES has not changed. As stated in 1976, "The primary purpose of the BES program is to increase knowledge of the physical phenomena relevant to the goal of meeting our nation's energy needs."**

The research activities and subprograms of BES have undergone substantial changes over the past three decades. For a detailed evolution of the BES program, see: http://science.energy.gov/bes/about/bes-organizational-history/

The origins of the federal research programs that became BES are rooted in the nation's research efforts to win World War II. The goals of the early U.S. science programs that evolved into BES were to explore fundamental phenomena, create scientific knowledge, and provide unique user facilities. In this sense, the BES program predates the establishment of the *Atomic Energy Commission* in 1946, which became part of ERDA on October 11, 1974, as a result of the *Energy Reorganization Act of 1974*.

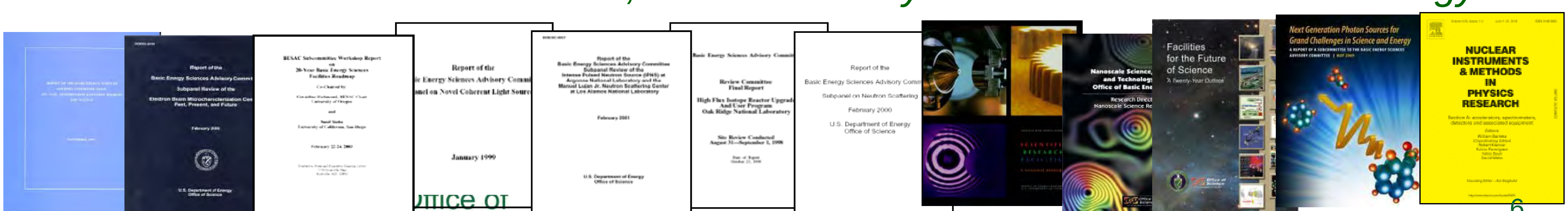
BES Strategic Planning Activities

- *Science for Discovery*



- *Science for National Needs*

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



Science for Discovery - Directing and Controlling Matter and Energy

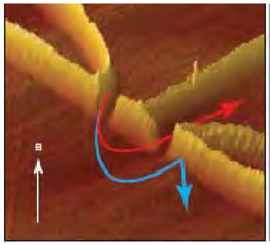
- **Control the quantum behavior of electrons in materials**
  Direct manipulation of the charge, spin, and dynamics of electrons to control and imitate the behavior of physical, chemical and biological systems, such as digital memory and logic using a single electron spin, the pathways of chemical reactions and the strength of chemical bonds, and efficient conversion of the Sun's energy into fuel through artificial photosynthesis.

- **Synthesize, atom by atom, new forms of matter with tailored properties**
  Create and manipulate natural and synthetic systems that will enable catalysts that are specific and produce no unwanted byproducts, or materials that operate at the theoretical limits of strength and fracture resistance, or that respond to their environment and repair themselves like those in living systems

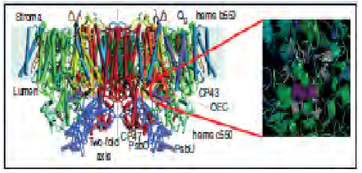
- **Control emergent properties that arise from the complex correlations of atomic and electronic constituents**
  Orchestrate the behavior of billions of electrons and atoms to create new phenomena, like superconductivity at room temperature, or new states of matter, like quantum spin liquids, or new functionality combining contradictory properties like super-strong yet highly flexible polymers, or optically transparent yet highly electrically conducting glasses, or membranes that separate CO_2 from atmospheric gases yet maintain high throughput.

- **Synthesize man-made nanoscale objects with capabilities rivaling those of living things**
  Master energy and information on the nanoscale, leading to the development of new metabolic and self-replicating pathways in living and non-living systems, self-repairing artificial photosynthetic machinery, precision measurement tools as in molecular rulers, and defect-tolerant electronic circuits

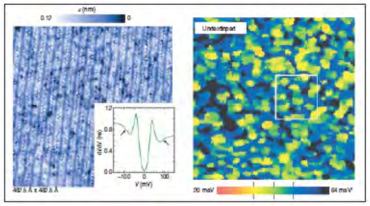
- **Control matter very far away from equilibrium**
  Discover the general principles describing and controlling systems far from equilibrium, enabling efficient and robust biologically-inspired molecular machines, long-term storage of spent nuclear fuel through adaptive earth chemistry, and achieving environmental sustainability by understanding and utilizing the chemistry and fluid dynamics of the atmosphere.



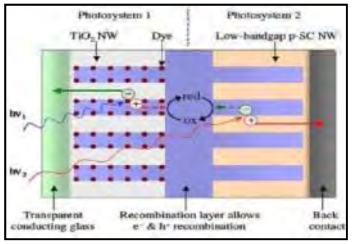
Atomic force micrograph of a device used to separate electrons according to their spin



Structure of nature's photosynthetic membrane. The inset shows the manganese-based biological machine.



(Left) Atomic-resolution scanning tunneling microscope image at 4.2K of BiSrCaCuO, (Right) A map of the superconducting gap.



Tandem photovoltaics combine two systems for photon capture and charge separation, analogous to natural photosynthesis.

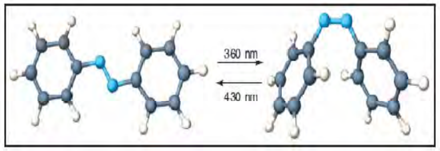


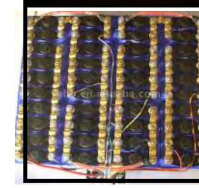
Photo-interconversion of two isomers of the azobenzene molecule. The direction of the interconversion depends on the wavelength of the light.

"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

Basic and Applied R&D Coordination

How Nature Works ··· to ··· Design and Control ··· to ··· Technologies for the 21st Century

Grand Challenges
How nature works

- Controlling materials processes at the level of quantum behavior of electrons
- Atom- and energy-efficient syntheses of new forms of matter with tailored properties
- Emergent properties from complex correlations of atomic and electronic constituents
- Man-made nanoscale objects with capabilities rivaling those of living things
- Controlling matter very far away from equilibrium

Discovery and Use-Inspired Basic Research
Materials properties and chemical functionalities by design

- Basic research for fundamental new understanding on materials or systems that may revolutionize or transform today's energy technologies
- Development of new tools, techniques, and facilities, including those for the scattering sciences and for advanced modeling and computation
- Basic research, often with the goal of addressing showstoppers on real-world applications in the energy technologies

Applied Research

- Research with the goal of meeting *technical milestones*, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes
- Proof of technology concepts

Technology Maturation & Deployment

- Scale-up research
- At-scale demonstration
- Cost reduction
- Prototyping
- Manufacturing R&D
- Deployment support

BESAC & BES Basic Research Needs Workshops

BESAC Grand Challenges Panel

DOE Technology Office/Industry Roadmaps

U.S. DEPARTMENT OF ENERGY | Office of Science

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.

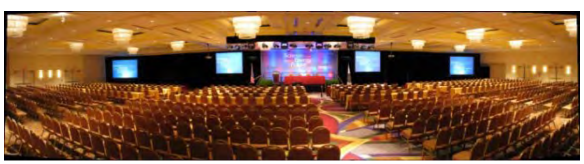
- **Energy Frontier Research Centers**

  $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



Science for Our Nation's Energy Future: EFRC Summit & Forum

May 25-27, 2010 at the Renaissance Penn Quarter Hotel in Washington, D.C.

- Explored the challenges and opportunities in applying America's extraordinary scientific and technical resources to critical energy needs
- Highlighted early successes of the Office of Science Energy Frontier Research Centers
- Promoted collaboration across the national energy enterprise

Participants

- Over 1,060 science and policy leaders from universities, national laboratories, industry and government
- More than 700 EFRC members, including 300 early career scientists
- 195 Institutions, 6 countries, and 36 States + Washington, D.C.

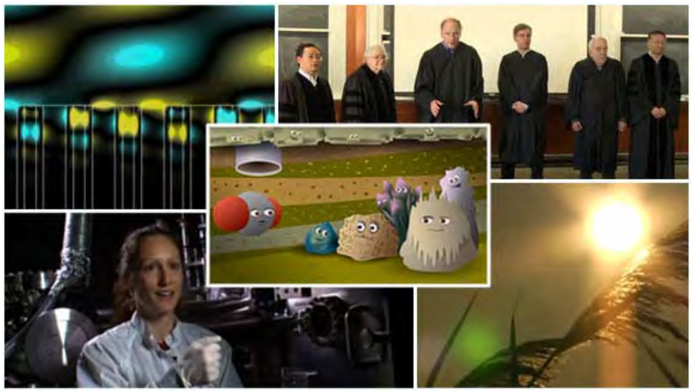
EFRC Summit & Forum Highlights

- Over 35 plenary speakers including Secretary Chu, Senator Jeff Bingaman, Congressman Daniel Lipinski, and Congresswoman Zoe Lofgren
- Screened the winners of the *Life at the Frontiers of Energy Research* video contest
- Summit poster reception featured the 46 Energy Frontier Research Centers
- Nine parallel technical sessions (46 hours of talks), three topical lunch discussions, two poster sessions on EFRC research (300 posters), and one networking poster reception with other DOE offices

Science for our Nation's Energy Future
Energy Frontier Research Centers
Summit & Forum

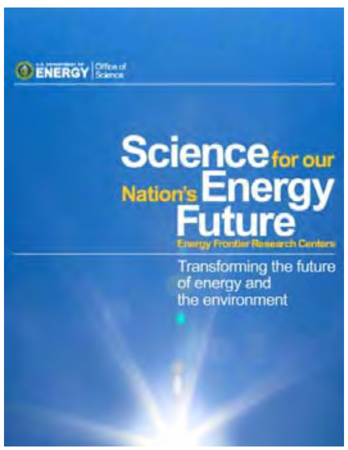
May 25–27, 2011
Washington, D.C.

Renaissance Penn
Quarter Hotel



Life at the Frontiers of Energy Research Video Contest

- Twenty-six EFRCs created short, engaging films that educate, inspire, and entertain an intelligent but not expert audience about the extraordinary science, innovation and people in their centers
- Five winners selected by judges; Over 8,000 votes for the People's Choice Award
- Contest highlighted on the Office of Science news, C&E newscript blog, DOE Facebook, and DOE blog



http://science.energy.gov/~/media/bes/efrc/pdf/EFRC_Brochure_05132011.pdf

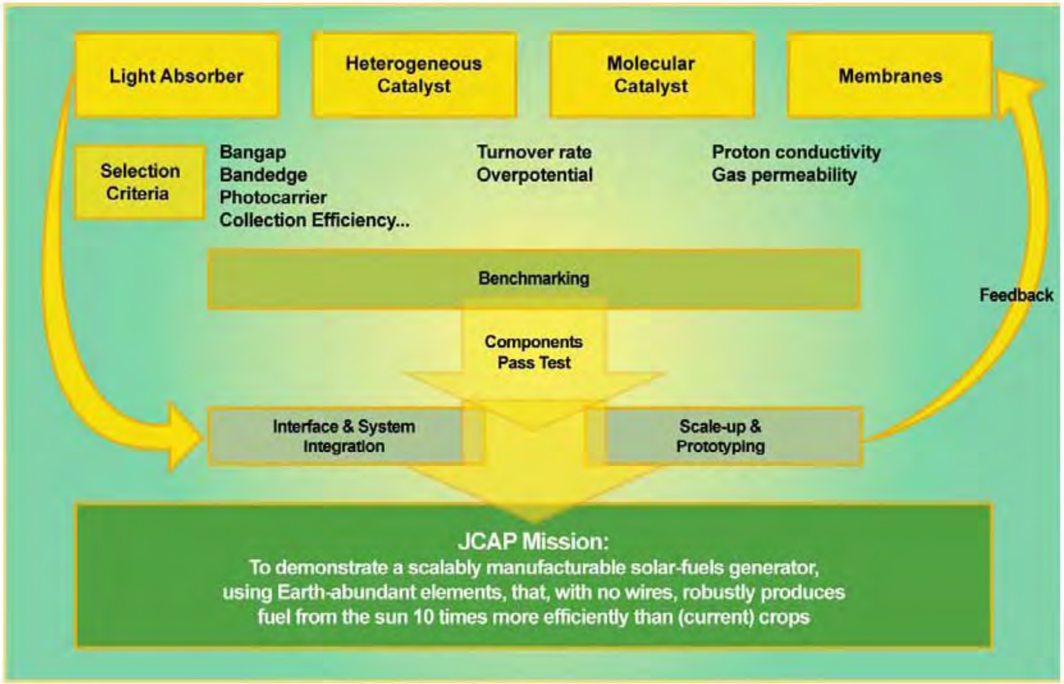
EFRC Brochure

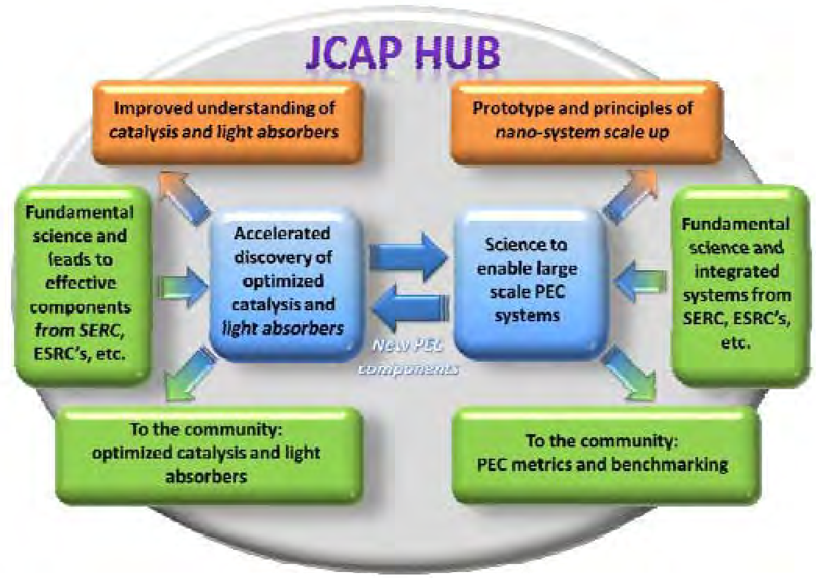
- Contains overview of the EFRC program and a one page summary with early achievements for each center.   Available in print and on-line.

Resources on the www.energyfrontier.us website

- Slides and videos of plenary talks including Secretary Chu's and Pat Dehmer's presentations (www.energyfrontier.us/content/agenda)
- Pat Dehmer's talk is widely used by the EFRCs for education and outreach
- Photo gallery, full schedule, and electronic abstract book
- *Life at the Frontiers of Energy Research* videos (www.energyfrontier.us/video-contest)
- ScienceCinema, the DOE OSTI multimedia search tool, will archive videos

JCAP as an Integrative Hub





JCAP R&D will focus on:

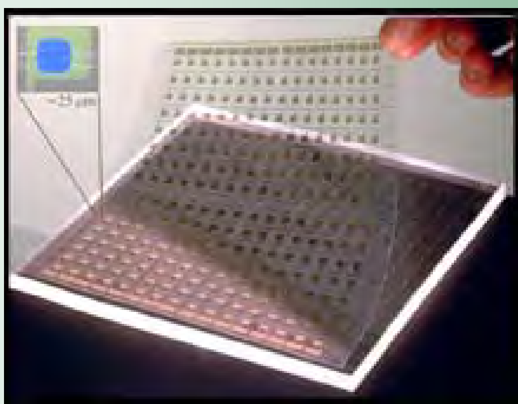
- Robustness of components
- Accelerating the rate of catalyst discovery for solar fuel reactions
- Discovering earth-abundant, robust, inorganic light absorbers with optimal band gap
- System integration, benchmarking, and scale-up

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

Scientific Discovery to Commercialization of Low Cost Solar Cells

Basic Science

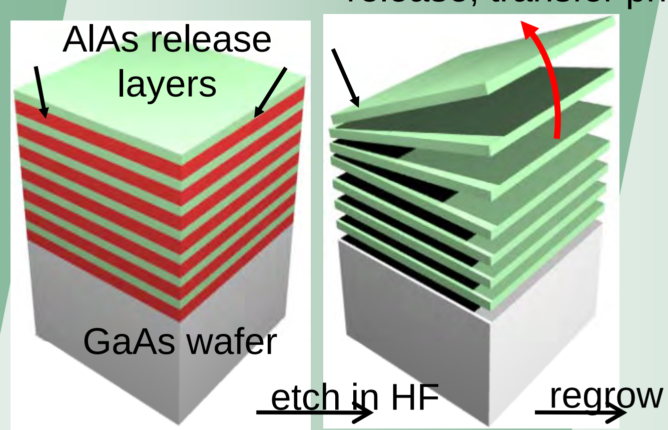


Basic research focused on materials-centric aspects of a micro-transfer printing process for single crystalline silicon and other semiconductors, dielectrics and metals.

Applied R&D

EERE Solar America Initiative: Established new materials strategies & manufacturing methods for low-cost, high performance photovoltaic modules

GaAs epi-stacks for solar microcells



Manufacturing/ Commercialization

SEMPRIUS

John Rogers, Ralph Nuzzo (co-founders)

Micro-Contact Printed Solar Cells

Industrial collaborations

ARCH Venture Partners

gvc Global Venture Capital

Illinois VENTURES LLC

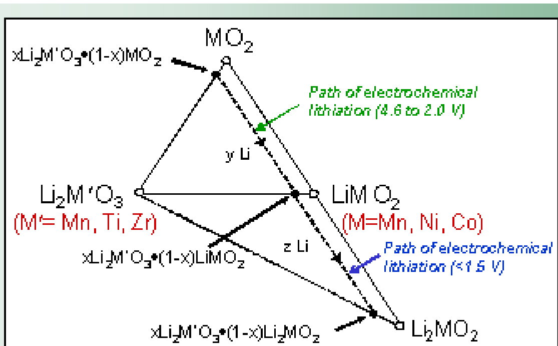
IQT IN-Q-TEL

Applied Ventures, LLC the Venture Fund of APPLIED MATERIALS

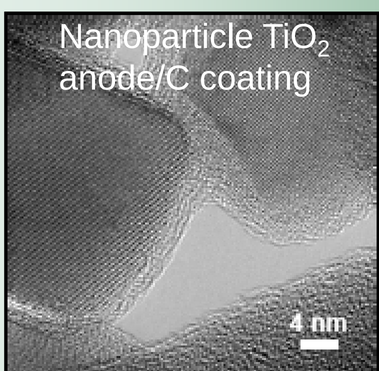
INTERSOUTH PARTNERS

Scientific Discovery to Commercialization of High-Energy Lithium Batteries

Basic Science (BES)



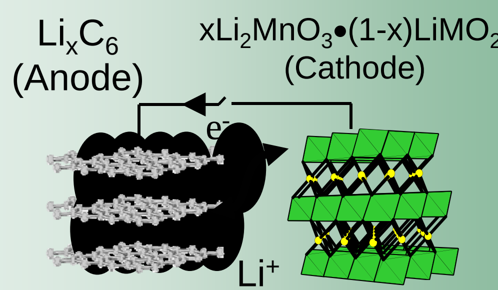
Discovered new composite structures for stable, high-capacity cathodes



EFRC research

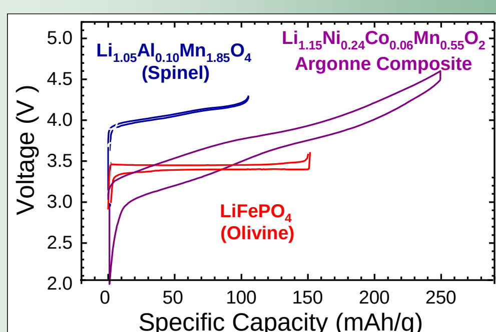
Tailored electrode-electrolyte interface using nanotechnology

Applied R&D (EERE & others)



Created high energy Li-ion cells…

…with double cathode capacity, enhanced stability



Manufacturing/ Commercialization

ENVIA SYSTEMS

BASF The Chemical Company

TODA KOGYO CORP.

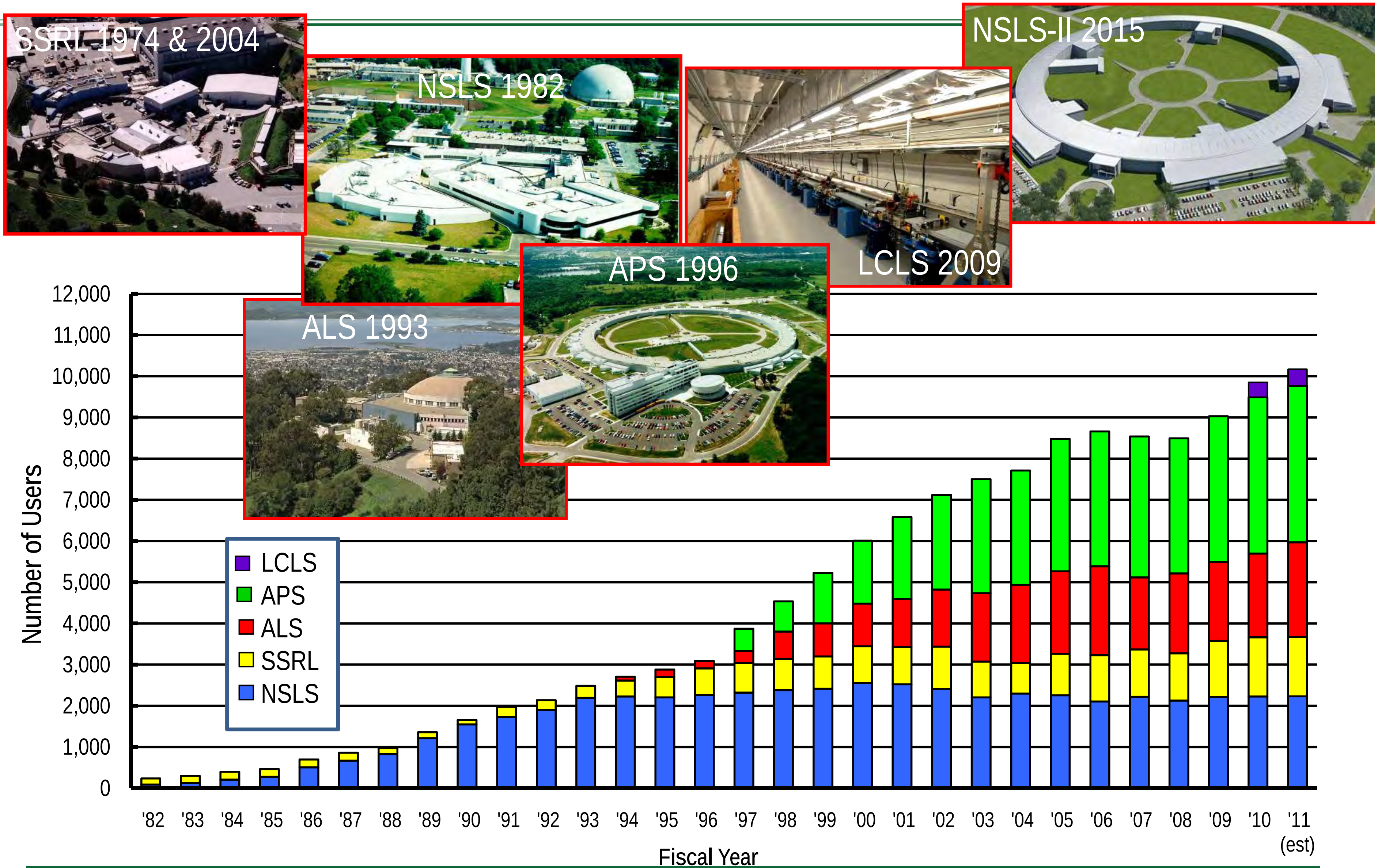
LG Chem

GM

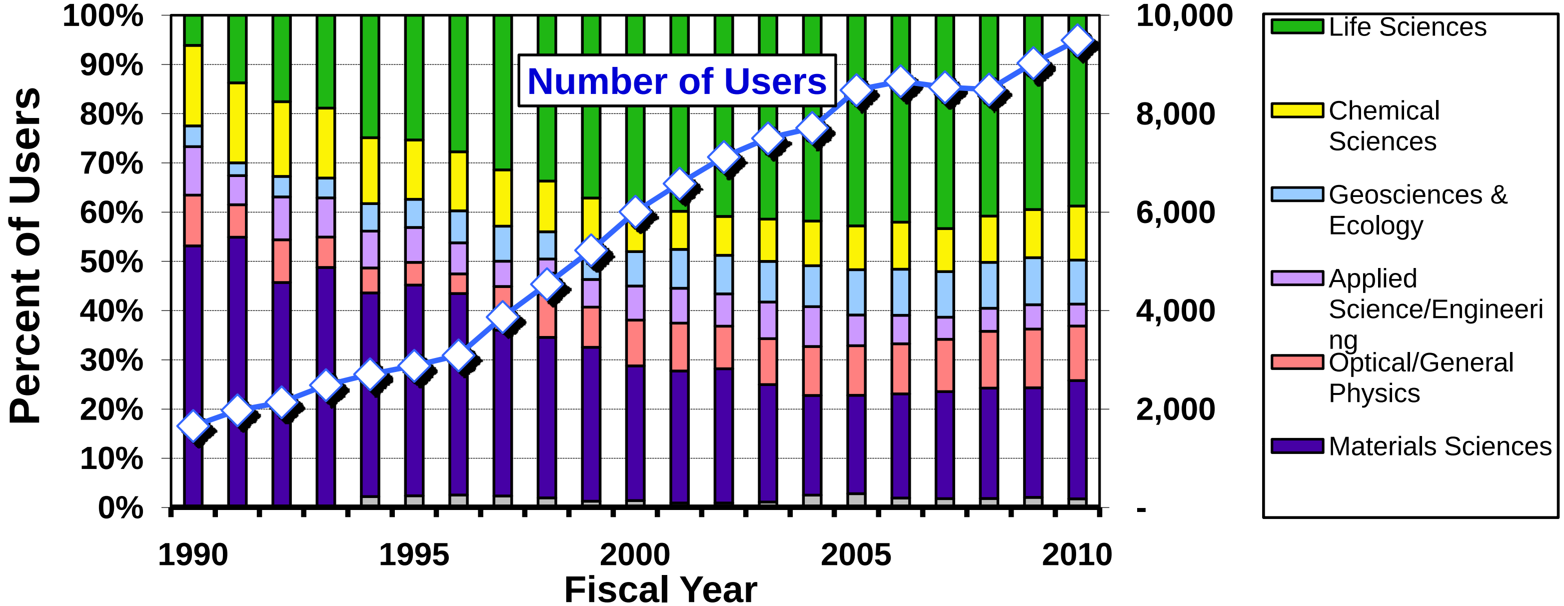
VOLT

Licenses to materials and cell manufacturers and automobile companies

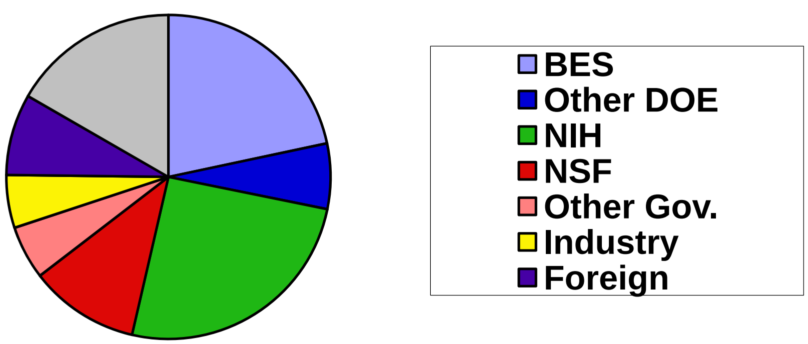
X-ray Synchrotron Light Sources



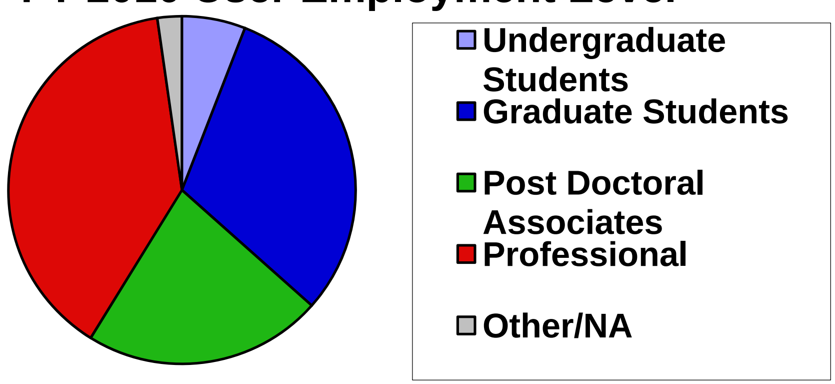
Characteristics of Users at the Synchrotron Light Sources



FY 2010 Source of User Support



FY 2010 User Employment Level



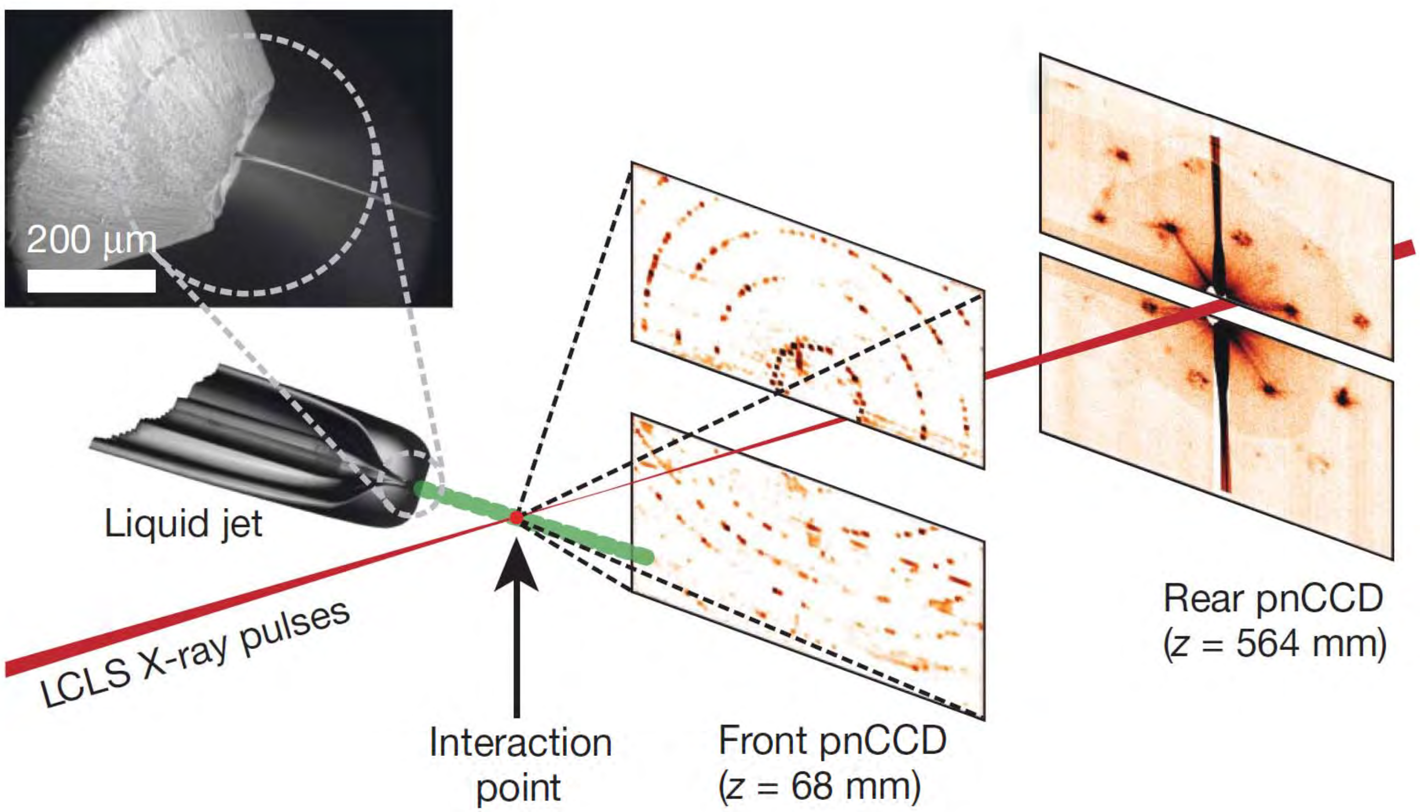
Expect the unexpected from new tools

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

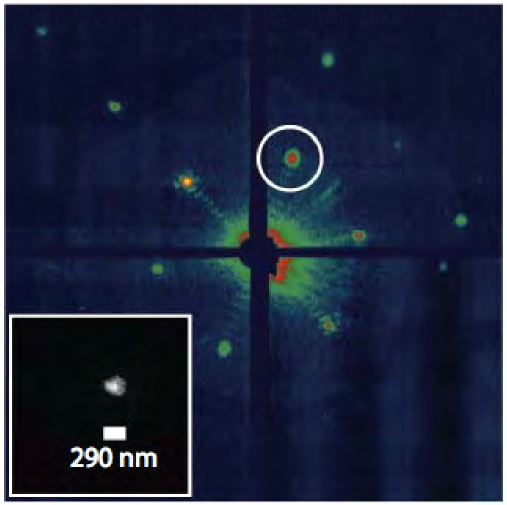
Femtosecond X-ray Protein Nanocrystallography



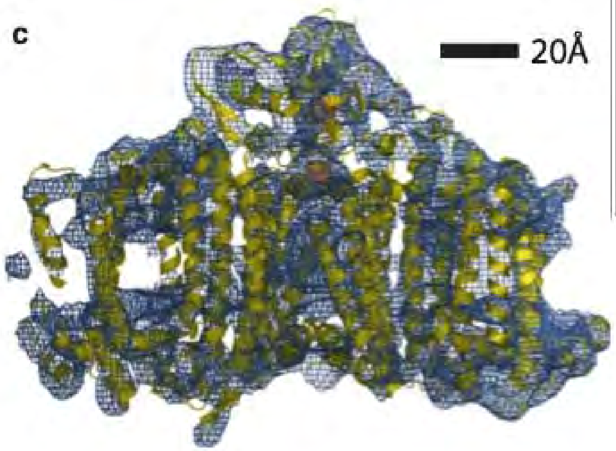
Nanocrystals flow in their buffer solution in a gas-focused, 4-µm-diameter jet at a velocity of 10m/sec perpendicular to the pulsed X-ray FEL beam that is focused on the jet.

Chapman, H. N., et al. **Nature**, Feb 3rd, 2011.

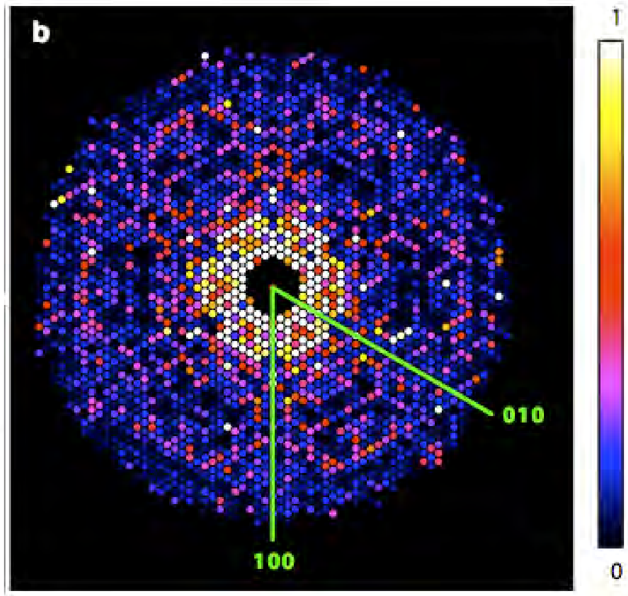
Femtosecond X-ray Protein Nanocrystallography



Single shot diffraction pattern



Reconstructed 3-D Structure

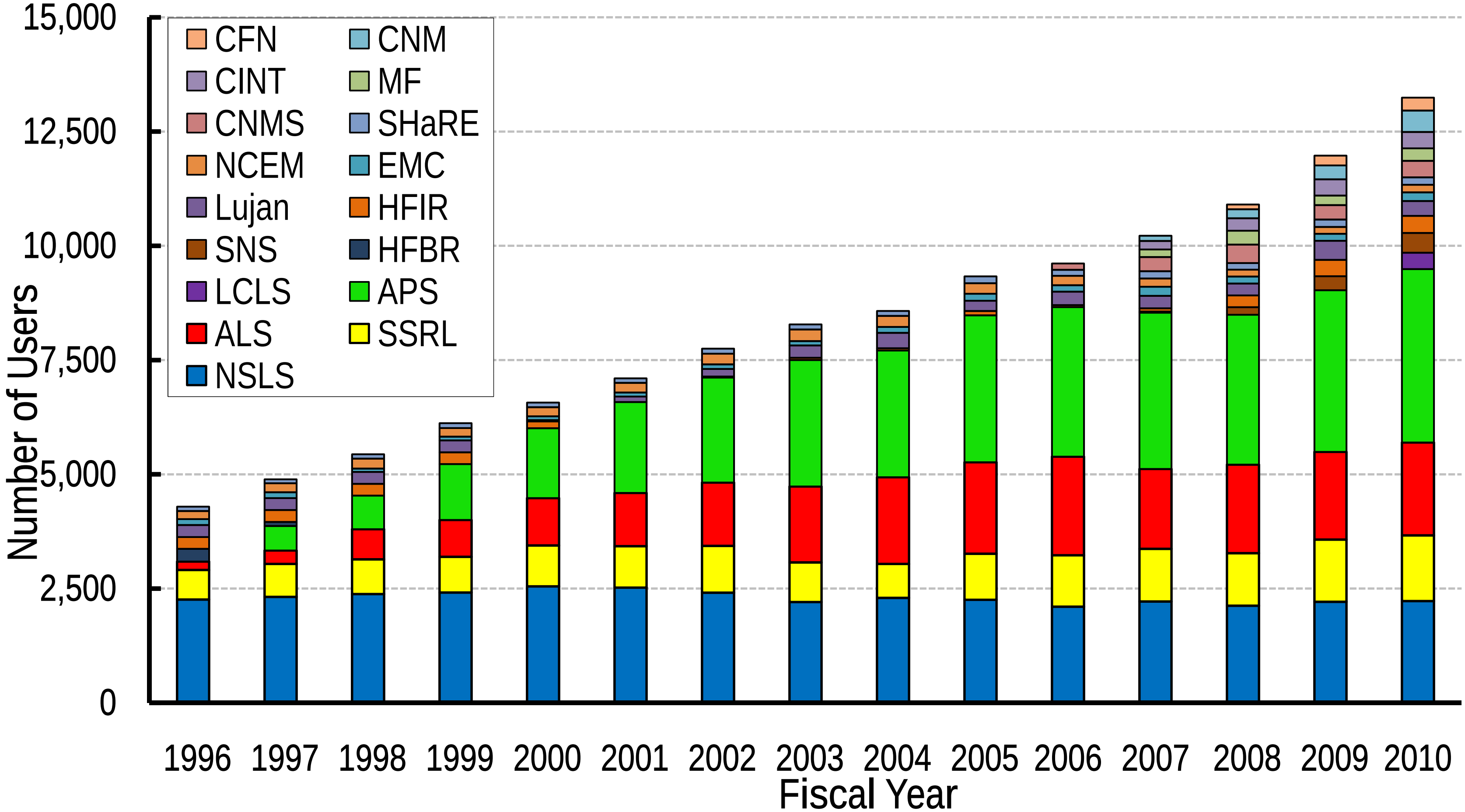


Combined 3D diffraction pattern

- Photosystem I plays key role in photosynthesis.
- Difficult to crystallize and use standard x-ray crystallography to obtain structure.
- Single shot images from LCLS of nanocrystals used to build up full 3-D diffraction pattern.
- Low resolution (~9 Å) shows structural details (*e.g.*, helix density).
- High resolution image subsequently taken

Chapman, H. N., et al. **Nature**, Feb 3rd, 2011.

BES User Facilities Hosted Over 13,000 Users in FY 2010



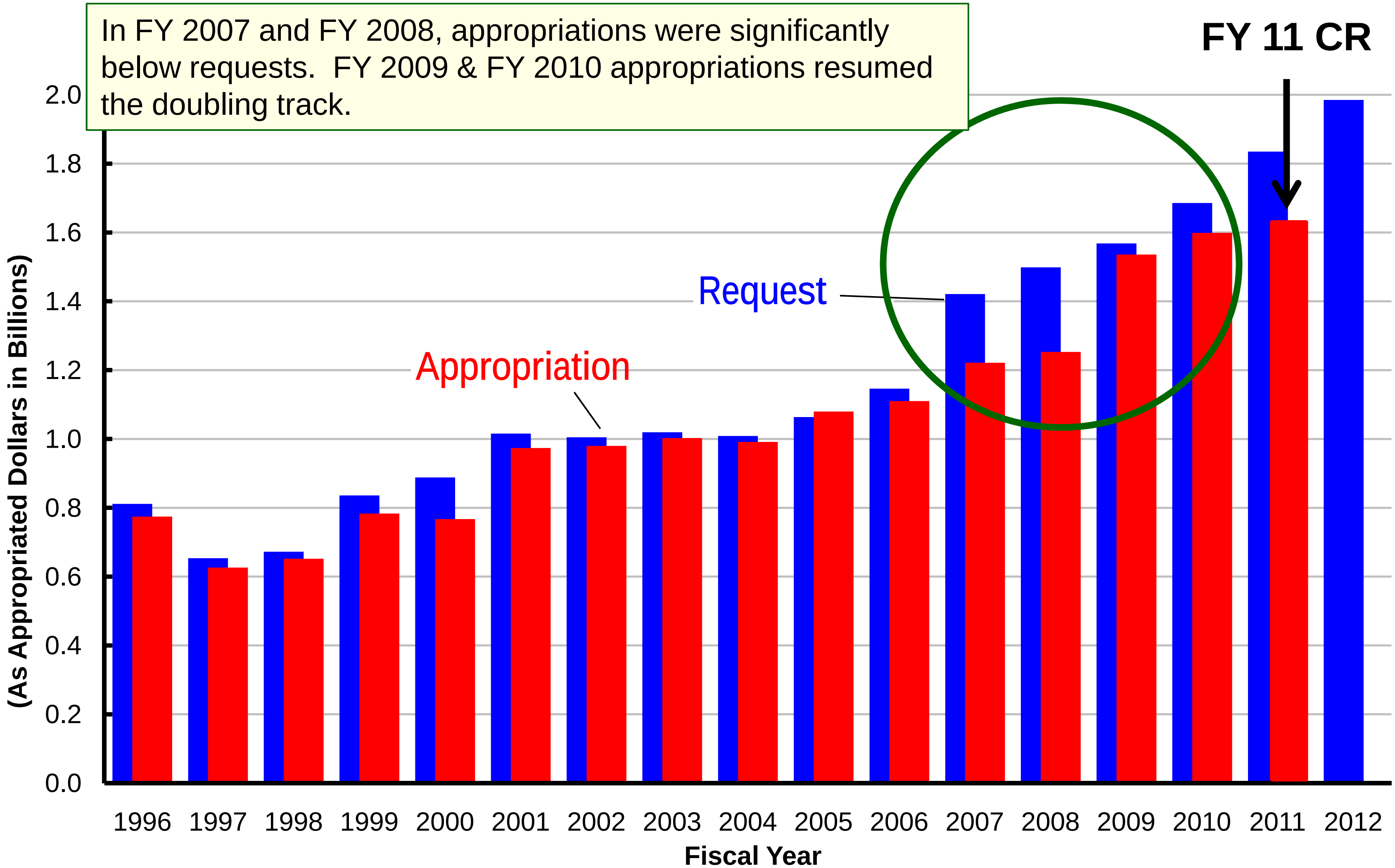
More than 300 companies from various sectors of the manufacturing, chemical, and pharmaceutical industries conducted research at BES scientific user facilities. Over 30 companies were Fortune 500 companies.

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
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

BES Budget: Past, Present, and Future

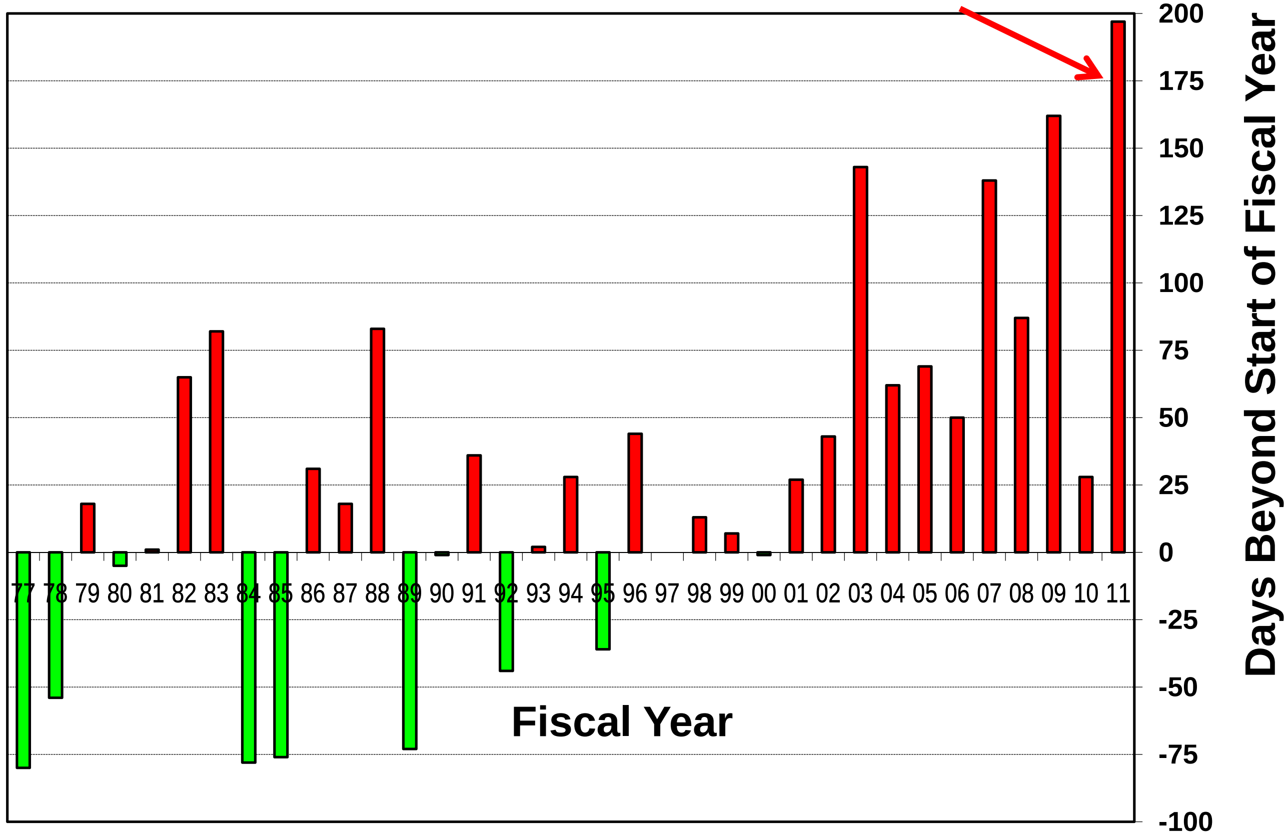
History of BES Request vs. Appropriation



FY 2009 excludes funding from the Recovery Act.

History of the Energy and Water Development Appropriation

FY 2011 – a new record!

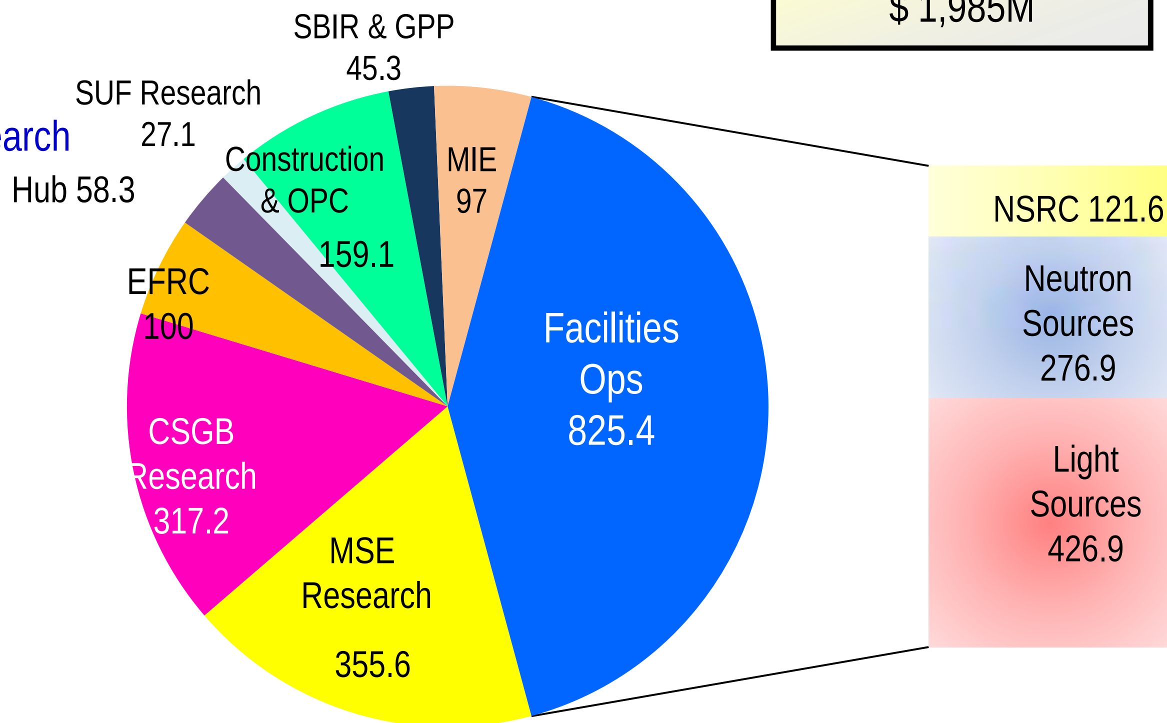


The budget uncertainty associated a significant delay in the appropriation creates havoc with agency planning.

FY 2012 BES Budget Request

- **Research programs**
  - Energy Innovation Hubs
  - Energy Frontier Research Centers
  - Core Research: increases in basic research for energy; materials by design; nanoelectronics; methane hydrates
- **Scientific user facilities operations**
  - Synchrotron light sources
  - Neutron scattering facilities
  - Nanoscale Science Research Centers
  - Instrumentation for clean energy
- **Construction and instrumentation**
  - National Synchrotron Light Source-II and instrumentation (NEXT)
  - Spallation Neutron Source instruments & power upgrade
  - Advanced Photon Source upgrade
  - Linac Coherent Light Source-II
  - TEAM-II

FY 2012 Request:
$ 1,985M



U.S. DEPARTMENT OF ENERGY | Office of Science

Accelerator Support in the Office of Science Programs

Basic Energy Sciences (~$500+M, overwhelmingly operations of facilities)

National Synchrotron Light Source
Stanford Synchrotron Radiation Laboratory
Advanced Light Source
Advanced Photon Source
Linac Coherent Light Source
National Synchrotron Light Source-II
Spallation Neutron Source
Manuel Lujan Jr. Neutron Scattering Center

Nuclear Physics (~$250M, overwhelmingly operations of facilities)

Continuous Electron Beam Accelerator Facility
Relativistic Heavy Ion Collider
Holifield Radioactive Ion Beam Facility
Argonne Tandem Linear Accelerator System

High Energy Physics (~$500M, with very substantial advanced R&D)

Tevatron Collider + improvements/upgrades
Large Hadron Collider
Advanced technology R&D

Short-term, Mid-term, and Long-term Activities

	HEP	BES	NP
Maintain and upgrade flagship user facilities	✓	✓	✓
Develop concepts, techniques, and materials for future facilities	✓	✓	✓
Maintain core competencies and a trained workforce in accelerator science	✓	✓	✓
Steward accelerator science and technology development broadly	✓		