



U.S. DEPARTMENT OF  
**ENERGY**

OFFICE OF  
**SCIENCE**

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# **Atomic, Molecular, and Optical Sciences**

**Fundamental Interactions Team  
Chemical Sciences, Geosciences, and Biosciences Division**

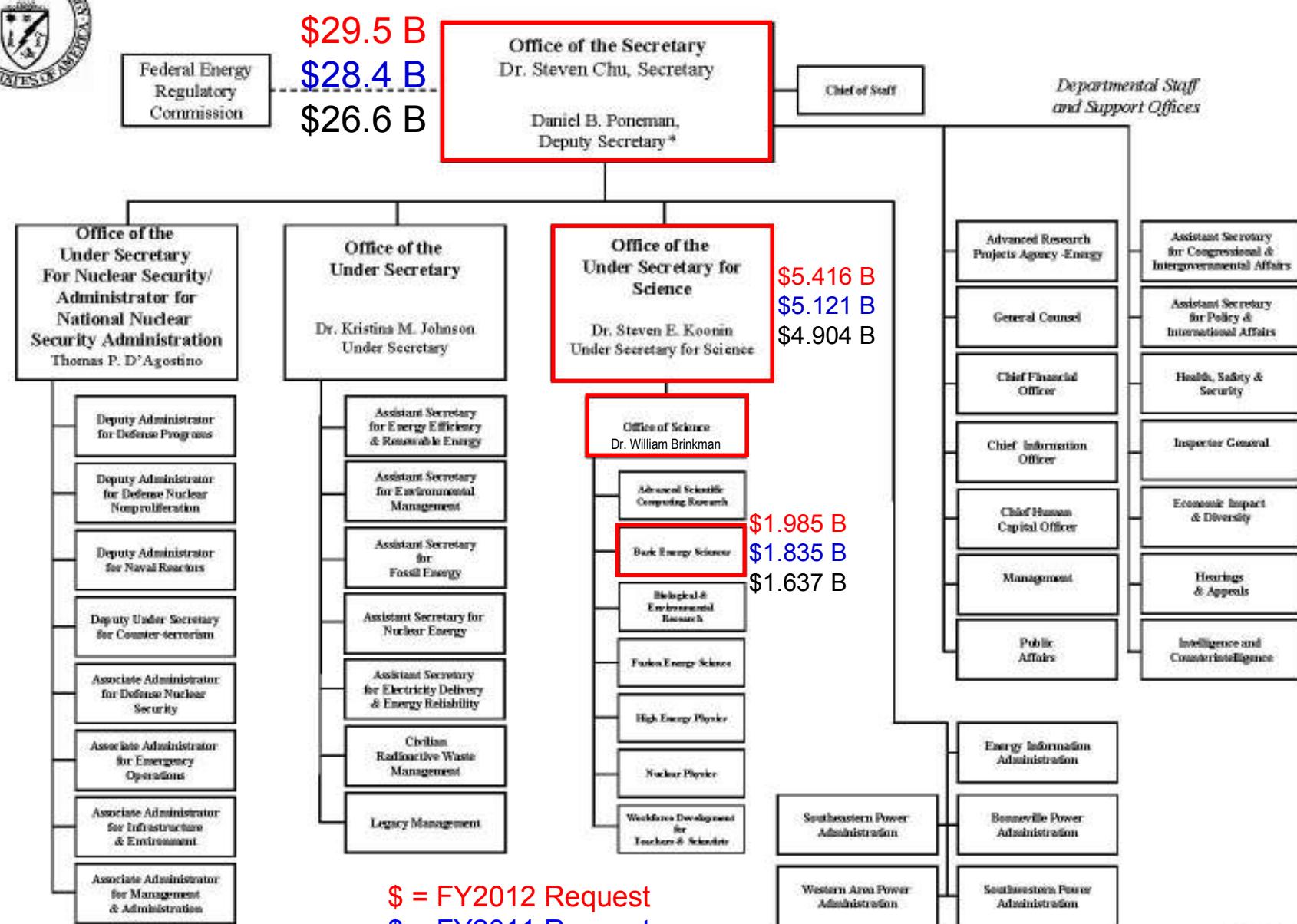
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**CAMOS 4/5/11**



# DEPARTMENT OF ENERGY



\* The Deputy Secretary also serves as the Chief Operating Officer

\$ = FY2012 Request  
\$ = FY2011 Request  
\$ = FY2010 Appropriation

26 May 09

# Office of Basic Energy Sciences

## BES Budget and Planning

Bob Atheimer, Senior Technical Advisor  
Margie Davis, Financial Management

## Harriet Kung, Director

Wanda Smith, Administrative Specialist

## 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  
Charnice Waters, Secretary

#### Materials Discovery, Design, and Synthesis

Arvind Kini  
Jorge Mariani, P.A.

#### Condensed Matter and Materials Physics

Jim Horwitz  
Marsophia Agnani, P.A.

#### Scattering and Instrumentation Sciences

Helen Kerch  
Cheryl Howard, P.A.

#### Materials Chemistry

Dick Kelley  
Vacant  
• John Schlueter, ANL  
• Darryl Sasaki, SNL

#### Exp. Cond. Mat. Phys.

Andy Schwartz  
• Doug Finnemore, Ames  
Vacant

#### X-ray Scattering

Lane Wilson

#### Biomolecular Materials

Mike Markowitz

#### Theo. Cond. Mat. Phys.

Jim Davenport  
■ Kim Fems, PNNL

#### Neutron Scattering

Thiyaga P. Thiyagarajan

#### Synthesis and Processing

Bonnie Gersten

#### Physical Behavior of Materials

Refik Kortan

#### Electron and Scanning Probe Microscopies

Jane Zhu

#### Tech. Coordination Program Management

John Vetrano  
Vacant

#### Mechanical Behavior and Radiation Effects

John Vetrano  
■ Richard Wright, INL

#### DOE EPSCoR\*

Tim Fitzsimmons  
■ Helen Farrell, INL  
■ John Schlueter, ANL

## Scientific User Facilities Division

### Harriet Kung, Acting Director

Linda Cerrone, Program Support Specialist  
Rocio Menees, Program Assistant

#### Operations

#### Construction

## Chemical Sciences, Geosciences, and Biosciences Division

### Eric Rohlffing, Director

Diane Marceau, Program Analyst  
Michaelene Kyler-King, Program Assistant

#### Fundamental Interactions

Michael Casassa  
Robin Felder, P.A.

#### Photochemistry and Biochemistry

Rich Greene  
Sharon Watson, P.A.

#### Chemical Transformations

John Miller  
Vacant, P.A.

#### Atomic, Molecular, and Optical Sciences

Jeff Krause  
Vacant

#### Solar Photochemistry

Mark Spitzer  
◆ Margaret Ryan, PNNL

#### Catalysis Science

Paul Maupin  
Raul Miranda  
◆ Jan Hrbek, BNL

#### Gas-Phase Chemical Physics

Wade Sisk

#### Photosynthetic Systems

Gail McLean

#### Heavy Element Chemistry

Vacant  
Larry Rahn  
■ Norm Edelstein, LBNL

#### Condensed-Phase and Interfacial Mol. Science

Gregory Fiedhner

#### Physical Biosciences

Robert Stack

#### Separations and Analysis

Larry Rahn

#### Computational and Theoretical Chemistry

Mark Pederson

#### Fuels from Sunlight Energy Innovation Hub

Carol Bessel

#### Geosciences

Nick Woodward  
■ Jennifer Blank, LBNL

#### Technology Office Coordination

Marvin Singer

## LEGEND

◆ Detailee (from DOE laboratories)

■ Detailee, ½ time, not at HQ

● Detailee, ¼ time, not at HQ

◆ On detail from EM

P.A. Program Assistant

\* Experimental Program to Stimulate Competitive Research

\*\* Nanoscale Science Research Centers and Electron-beam Microcharacterization Centers

\*\*\* National Synchrotron Light Source II

\*\*\*\* Major Item of Equipment projects

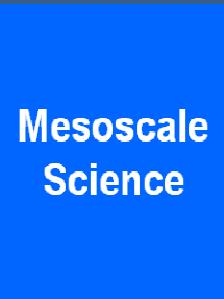
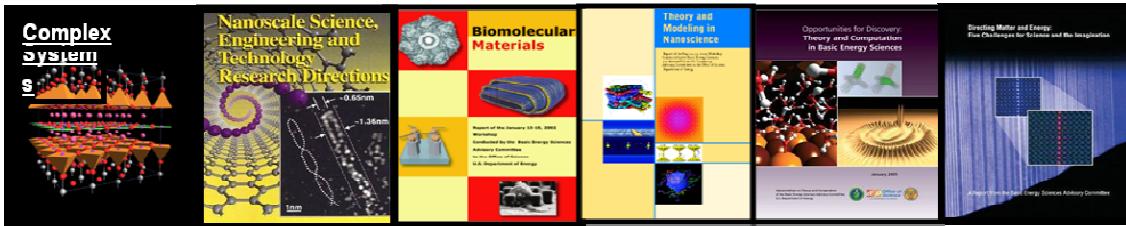
March 2011

PostEDBARY

- ***Science for Discovery – Directing and controlling matter and energy***
  - 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
- ***Science for National Need – Bringing forefront scientific knowledge and state-of-the-art tools to solving grand energy challenges***
  - Hydrogen Economy
  - Solar Energy Utilization
  - Superconductivity
  - Solid-state Lighting
  - Advanced Nuclear Energy Systems
  - Clean and Efficient Combustion of Fuels
  - Electrical Energy Storage
  - Geosciences
  - Catalysis for Energy
  - Materials under Extreme Environments
- ***National Scientific User Facilities – the 21st century tools of science***
  - Maintaining and renewing 3<sup>rd</sup> generation light sources, including complete construction of NSLS-II
  - Expanding neutron scattering capabilities and user base
  - Ensuring operation excellence and scientific impact of nanoscale research tools
  - Planning and executing a strategy to maintain U.S. leadership in photon science- 4<sup>th</sup> generation source



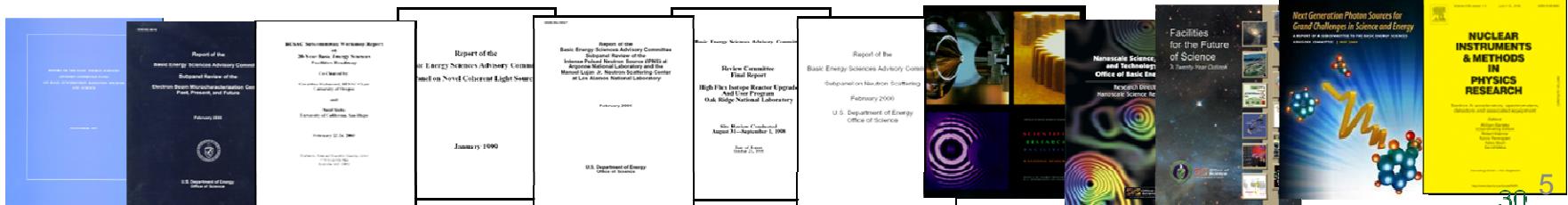
## ▪ Science for Discovery



## ▪ Science for National Needs



## ▪ National Scientific User Facilities, the 21<sup>st</sup> century tools of science



# FY 2012 BES Budget Request

+24% from FY10

## ■ Research programs

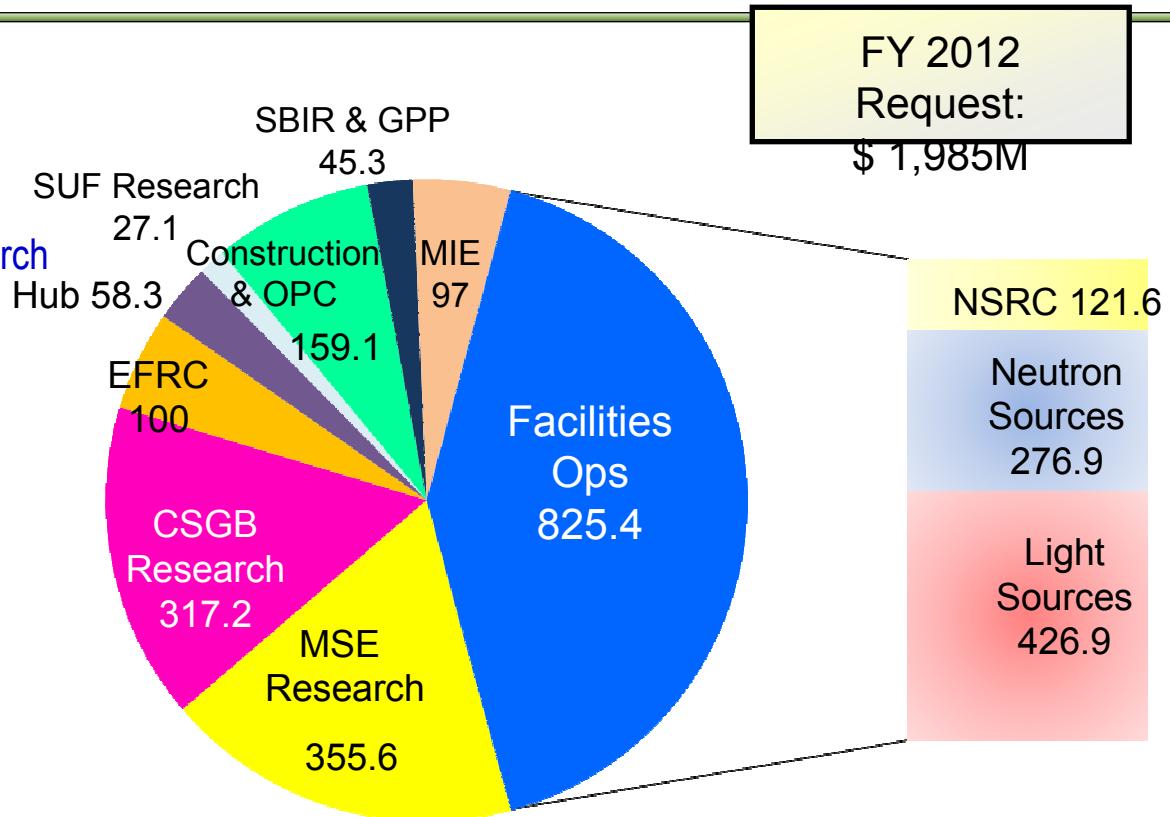
- Energy Innovation Hubs
- Energy Frontier Research Centers
- Core Research: increases in basic research for energy; materials by design; nanoelectronics; methane hydrates

## ■ 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





<b>Non-carbon Sources</b>	<b>(Dollars in thousands)</b>
Solar Electricity from Photovoltaics	+ 8,000
Advanced Nuclear Energy Systems	+ 8,000
Materials under Extreme Environments	+15,000
<b>Carbon Capture and Sequestration</b>	
Carbon Capture	+ 8,000
Carbon Sequestration	+ 8,000
<b>Transportation and Fuel Switching</b>	
Energy Systems Simulation - Combustion	+ 15,000
Batteries and Energy Storage Hub	+ 34,020
<b>Transmission and Energy Storage</b>	
Electric Power Grid-Enabling Materials Sciences	+ 4,000
Power Electronics	+ 3,500
Batteries and Energy Storage Hub	(same as above)
<b>Efficiency</b>	
Advanced Solid-state Lighting	+ 8,000
Energy Efficiency – Enabling Materials Sciences	+ 4,000



<b><i>Light Source Construction, Upgrade &amp; Expansion</i></b>	<b>(Dollars in thousands)</b>
National Synchrotron Light Source-II (NSLS-II)	151,400
Advanced Photon Source Upgrade	20,000
Linac Coherent Light Source Expansion	30,000
Instrumentation for NSLS-II (NEXT)	12,000
<b><i>Neutron Source Instrument &amp; Upgrade</i></b>	
Spallation Neutron Source Instrument-II (SING-II)	11,500
Spallation Neutron Source Power Upgrade (PUP)	5,500
<b><i>Electron Microscopy &amp; Microcharacterization</i></b>	
Transmission Electron Aberration-Corrected Microscopy II (TEAM II)	18,000
<b><i>Facilities Instrumentation for Energy</i></b>	
Light Sources	24,000
Neutron Sources	8,000
Nanoscale Science Research Centers	15,000



- 1st Continuing Resolution, (through Dec. 3, 2010) **SC @ \$4,903M (FY 2010)**
- 2nd Continuing Resolution, (through Dec. 18, 2010) **SC @ \$4,903M**
- 3rd Continuing Appropriations Act (through Dec. 21, 2010) **SC @ \$4,903M**
- 4th Continuing Appropriations Act (through March 4, 2011) **SC @ \$4,903M**

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- Further Continuing Appropriations Amendments (through March 18, 2011)  
**SC @ \$4,826 M**
- Additional Continuing Appropriations Amendments (through April 8, 2011)  
**SC @ \$4,826 M**
- House Year-Long Continuing Resolution **SC @ \$4,017 M (-18%)**
- Senate Year-Long Continuing Resolution **SC @ \$4,725 M (-4%)**
- Both bills failed in the Senate.



**BES: \$1,985 M (Increase of 24.1% compared to FY10 enacted)**

**AMOS: \$24 M (Increase of 4.2% compared to FY10 enacted)**

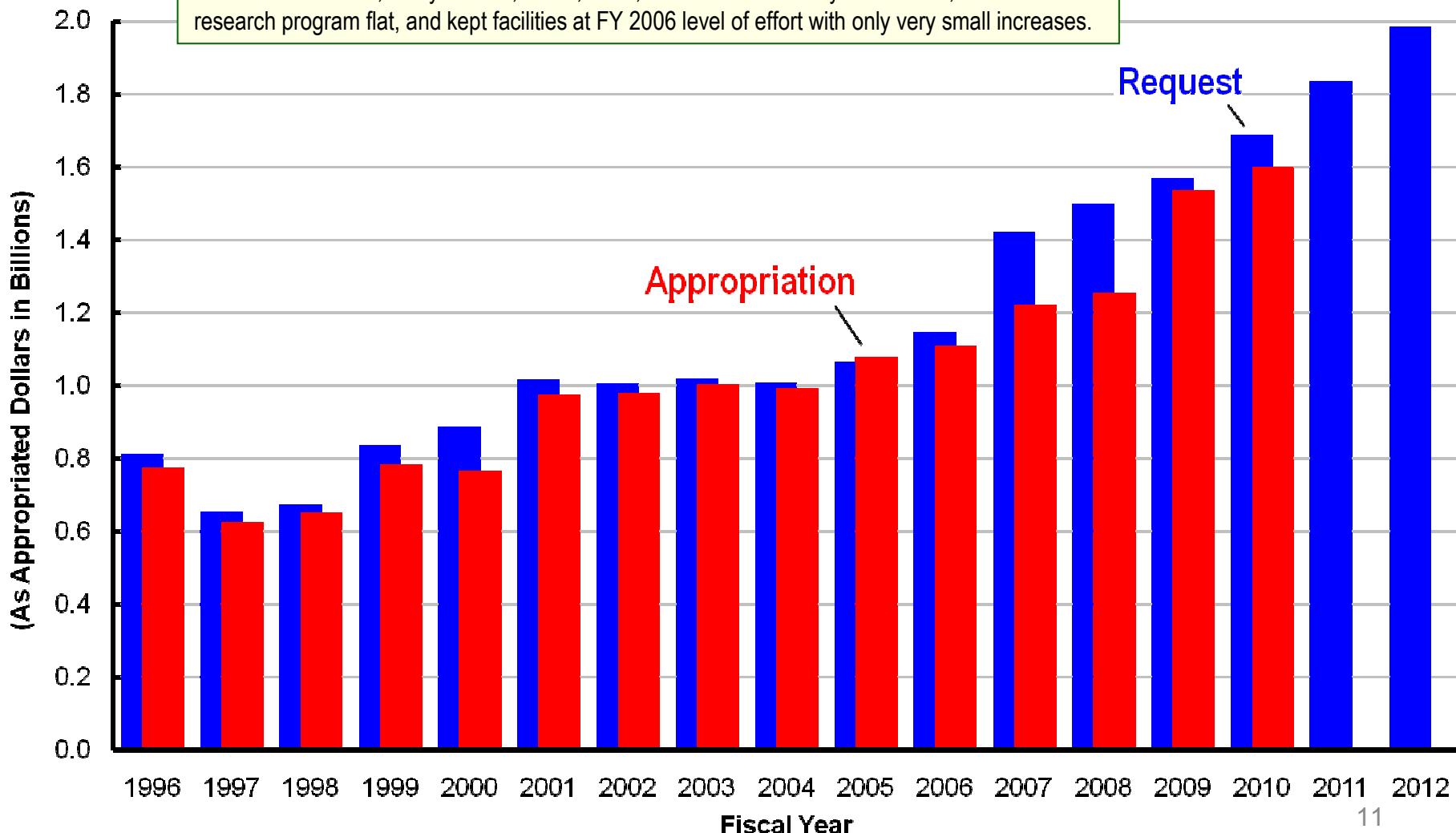
“In FY 2012, research will emphasize the development and application of new ultrafast x-ray and optical probes of matter, including some of the first experiments to be performed on the Linac Coherent Light Source; theoretical and computational methods for the interpretation of ultrafast measurements; and the use of optical fields to control and manipulate quantum mechanical systems.”

**The Continuing Resolution for FY 2011 proposed by the House cuts BES funding by 22%, to FY 2008 levels.**



## BES Appropriations versus Requests

FY 07 and FY08 appropriations were below the President's Requests by \$170M and \$230M, respectively. Impacts included declination of 700 proposals for new research awards; premature termination of IPNS; delay of USB, LCLS, LUSI, and SING-II of one year or more; held core research program flat, and kept facilities at FY 2006 level of effort with only very small increases.



## FY 2008 and FY 2010 Budget Comparison

	FY 2008	FY 2010	FY 2010 vs. FY 2008
EFRCs	...	100,000	+100,000
Hubs*	...	...	.....
ALL Other BES Research	451,517	563,428	+111,911
SNS Power Upgrade Project ORNL	...	2,000	+2,000
NSLS -II (OPC + Construction)	49,727	141,000	+91,273
LCLS + Other Construction	63,538	15,240	-48,298
Other MIEs	30,543	23,000	-7,543
Facility Operations, including LCLS	646,333	749,728	+103,395
GPP/GPE	11,098	4,572	-6,526
SBIR/STTR	30,646	37,532	+6,886
<b>Total, BES</b>	<b>1,283,402</b>	<b>1,636,500</b>	<b>+353,098</b>

In addition to rigorously managing existing core research and user facilities, BES has made bold investments in key areas, as shown above, to ensure that the portfolios continue to serve DOE's mission and maintain world leadership for decades to come.

\* Solar Fuels Hub was funded in EERE in FY 2010 and continued in FY 2011 under the CR.

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**Experiments and theory to understand structural and dynamical properties of atoms, molecules, and nanostructures.**

**Emphasis:**

- Fundamental interactions with photons and electrons for characterization and control.
- Interactions of matter with ultrafast light pulses and x-rays.
- First-principles quantum descriptions of properties and dynamical processes: chemical bond breaking and forming, high-field interactions, collisions, electron correlation, and ultracold chemistry.
- Nanoscale structures with novel light-matter interactions.

**Relevance and Impact:**

- Underpins science conducted in many other BES programs; advances DOE's energy and facilities missions
- Studies of matter and chemical processes at the level of electrons and on ultrafast time scales, using novel ultrafast optical probes, including ultrafast x-rays from table-top sources, 3<sup>rd</sup> generation synchrotrons (ALS and APS), and 4<sup>th</sup> generation sources (LCLS).
- PIs: 3 NAS members; 60 APS fellows; recent MacArthur, Rabi, Wood, Schawlow, Zewail, Davisson-Germer, Langmuir, Plyler, and Frederic Ives awards

**Key Relationships:** LCLS, APS, ALS, BES research programs

- u **36% Theory, 64% Experiment (University), 30%/70% (University+Labs)**

- u **Intense Field and Ultrafast X-Ray Science (48%U, 57%U+L)**

*Goal: Discover, understand, and exploit fundamental phenomena associated with interactions of intense electromagnetic fields and matter on ultrashort time scales.*

- u **Correlated Dynamics (38%U, 33%U+L)**

*Goal: Characterize, understand, and control strongly correlated dynamics involving electrons, atoms, and molecules.*

- u **Ultracold Molecules (11%U, 5%U+L)**

*Goal: Discover, understand, and control fundamental interactions involving ultracold molecules.*

- u **Nanoscale Science (3%U, 5%U+L)**

*Goal: Discover, understand, and exploit novel phenomena in light-matter interactions in nanoscale structures.*

- 62 Principal Investigators at 35 Universities
- 6 Programs at National Laboratories with 34 Principal Investigators

Overall Budget (57% is invested in DOE labs, 43% in Universities)

FY 2009	FY 2010	FY 2011*	FY 2012*
\$24,269K	\$23,011K	\$26,118	\$24,011K

\* President's Request

Of ~96 current PIs and co-PIs:

**By type of work:**

33% are theorists; 67% are experimentalists

35% work in group programs at DOE labs; 65% are university PIs

**By topic (University PIs, Primary Area):**

52% are involved in ultrafast science

36% study correlated dynamics

7% study ultracold molecules

5% focus on nanoscience

**By topic (DOE Lab Programs):**

3 programs focus on ultrafast science

1 program focuses on correlated dynamics

1 program combines studies of ultrafast science and correlated dynamics

1 program focuses on nanoscience