U.S. DEPARTMENT OF ENERGY

OFFICE OF SCIENCE

Atomic, Molecular, and Optical Sciences

Fundamental Interactions Team
Chemical Sciences, Geosciences, and Biosciences Division
Basic Energy Sciences

Jeff.Krause@science.doe.gov

science.energy.gov/BES/

CAMOS Meeting 4/3/12

DEPARTMENT OF ENERGY

Federal Energy Regulatory Commission

$27.2 B
$26.3 B
$25.7 B

Office of the Secretary
Dr. Steven Chu, Secretary

Daniel B. Poneman,
Deputy Secretary*

Chief of Staff

Departmental Staff and Support Offices

- Advanced Research Projects Agency -Energy
- General Counsel
- Chief Financial Officer
- Chief Information Officer
- Chief Human Capital Officer
- Management
- Public Affairs
- Assistant Secretary for Congressional & Intergovernmental Affairs
- Assistant Secretary for Policy & International Affairs
- Health, Safety & Security
- Inspector General
- Economic Impact & Diversity
- Hearings & Appeals
- Intelligence and Counterintelligence

Office of the Under Secretary For Nuclear Security/ Administrator for National Nuclear Security Administration
Thomas P. D'Agostino

- Deputy Administrator for Defense Programs
- Deputy Administrator for Defense Nuclear Nonproliferation
- Deputy Administrator for Naval Reactors
- Deputy Under Secretary for Counter-terrorism
- Associate Administrator for Defense Nuclear Security
- Associate Administrator for Emergency Operations
- Associate Administrator for Infrastructure & Environment
- Associate Administrator for Management & Administration

Office of the Under Secretary

Dr. Kristina M. Johnson
Under Secretary

- Assistant Secretary for Energy Efficiency & Renewable Energy
- Assistant Secretary for Environmental Management
- Assistant Secretary for Fossil Energy
- Assistant Secretary for Nuclear Energy
- Assistant Secretary for Electricity Delivery & Energy Reliability
- Civilian Radioactive Waste Management
- Legacy Management

Office of the Under Secretary for Science
vacant
Under Secretary for Science

$4.99 B
$4.87 B
$4.90 B

Office of Science
Dr. William Brinkman

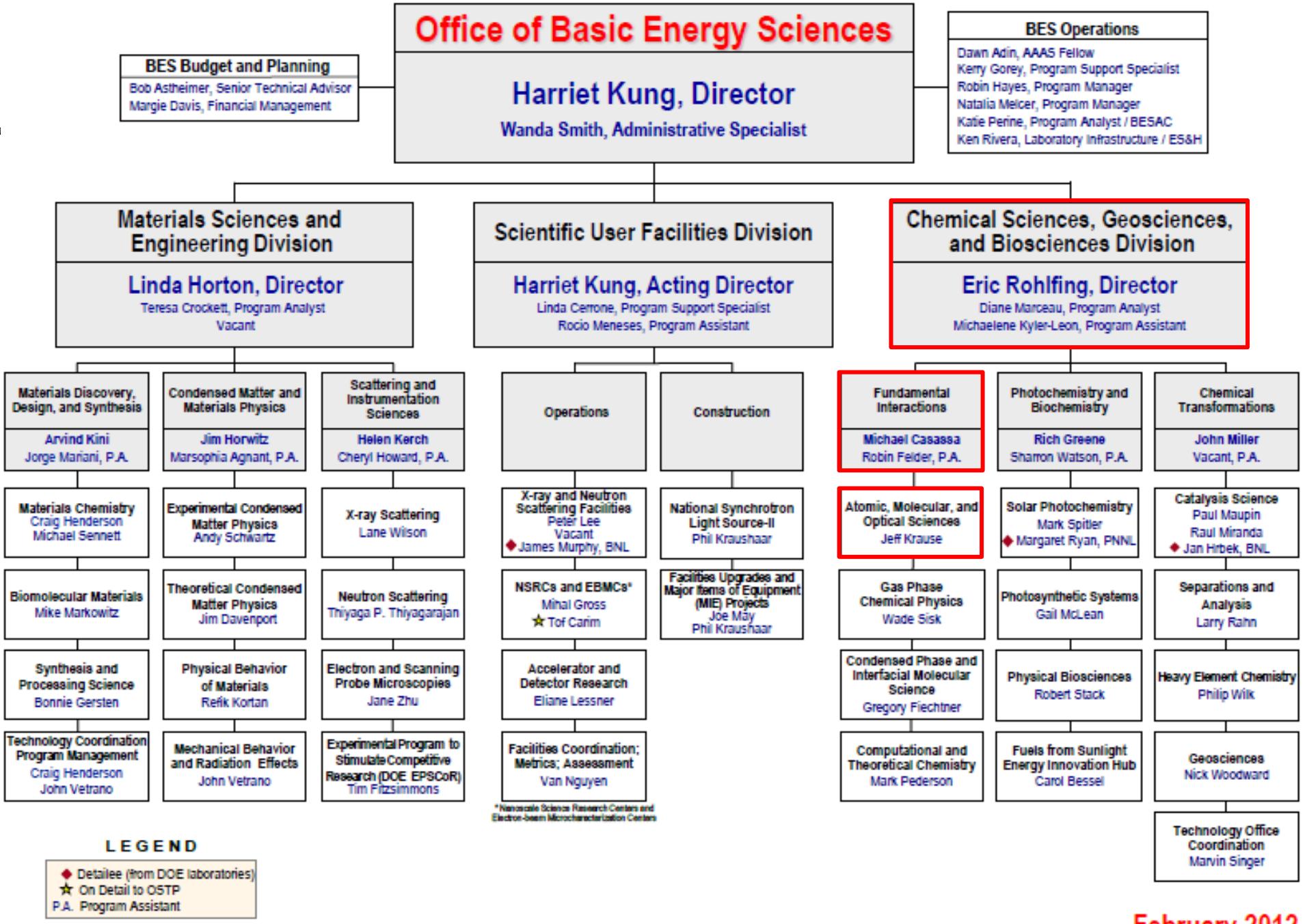
- Advanced Scientific Computing Research
- Basic Energy Sciences — $1.80 B / $1.69 B / $1.64 B
- Biological & Environmental Research
- Fusion Energy Science
- High Energy Physics
- Nuclear Physics
- Workforce Development for Teachers & Scientists

- Energy Information Administration
- Southeastern Power Administration
- Bonneville Power Administration
- Western Area Power Administration
- Southwestern Power Administration

$ = FY2013 Request
$ = FY2012 Appropriation
$ = FY2011 Appropriation

* The Deputy Secretary also serves as the Chief Operating Officer

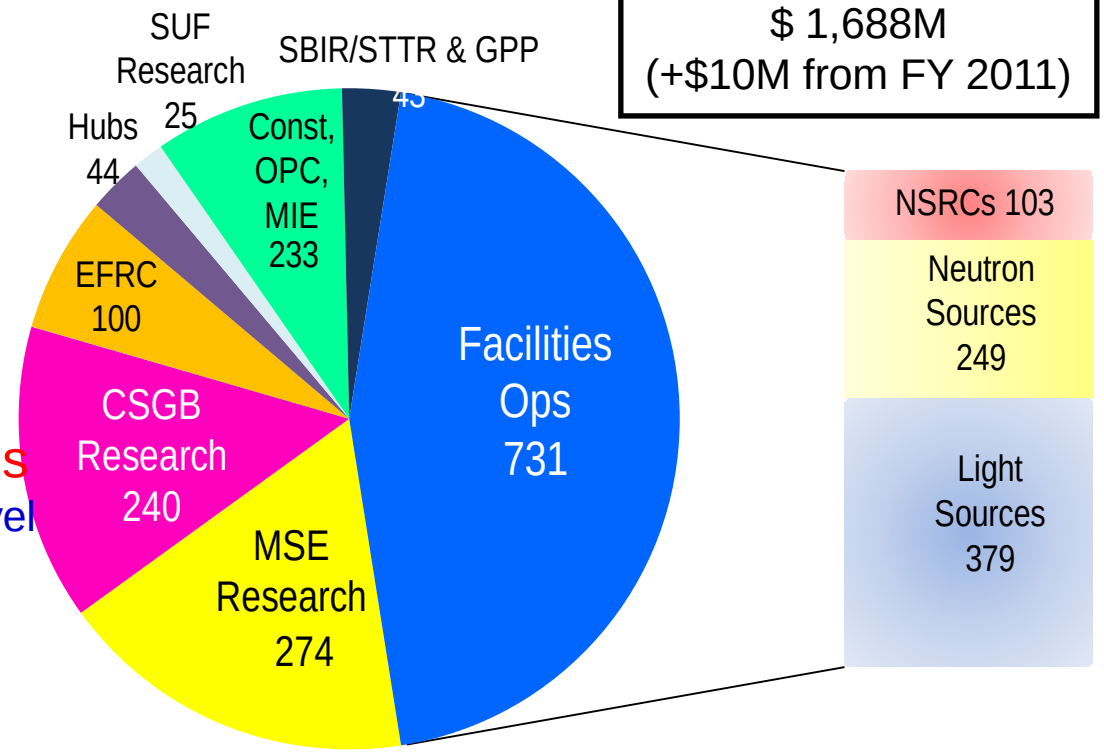
26 May 09


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
Dawn Adin, AAAS Fellow
Kerry Gorey, Program Support Specialist
Robin Hayes, Program Manager
Natalia Melcer, Program Manager
Katie Perine, Program Analyst / BESAC
Ken Rivera, Laboratory Infrastructure / ES&H
Materials Sciences and Engineering Division
Linda Horton, Director
Teresa Crockett, Program Analyst
Vacant
Scientific User Facilities Division
Harriet Kung, Acting Director
Linda Cerrone, Program Support Specialist
Rocio Meneses, Program Assistant
Chemical Sciences, Geosciences, and Biosciences Division
Eric Rohlfing, Director
Diane Marceau, Program Analyst
Michaelene Kyler-Leon, Program Assistant
Materials Discovery, Design, and Synthesis
Arvind Kini
Jorge Mariani, P.A.
Materials Chemistry
Craig Henderson
Michael Sennett
Biomolecular Materials
Mike Markowitz
Synthesis and Processing Science
Bonnie Gersten
Technology Coordination Program Management
Craig Henderson
John Vetrano
Condensed Matter and Materials Physics
Jim Horwitz
Marsophia Agnant, P.A.
Experimental Condensed Matter Physics
Andy Schwartz
Theoretical Condensed Matter Physics
Jim Davenport
Physical Behavior of Materials
Refik Kortan
Mechanical Behavior and Radiation Effects
John Vetrano
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
Experimental Program to Stimulate Competitive Research (DOE EPSCoR)
Tim Fitzsimmons
Operations
X-ray and Neutron Scattering Facilities
Peter Lee
Vacant
◆ James Murphy, BNL
NSRCs and EBMCs*
Mihal Gross
☆ Tof Carim
Accelerator and Detector Research
Eliane Lessner
Facilities Coordination; Metrics; Assessment
Van Nguyen
Construction
National Synchrotron Light Source-II
Phil Kraushaar
Facilities Upgrades and Major Items of Equipment (MIE) Projects
Joe May
Phil Kraushaar
* Nanoscale Science Research Centers and Electron-beam Microcharacterization Centers
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 Molecular 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 Chemistry
Philip Wilk
Geosciences
Nick Woodward
Technology Office Coordination
Marvin Singer
LEGEND
◆ Detailee (from DOE laboratories)
☆ On Detail to OSTP
P.A. Program Assistant
February 2012

FY 2012 BES Budget Appropriation

- **Research programs**
  - Energy Innovation Hubs
    - Battery and Energy Storage Hub (+$20M)
  - Energy Frontier Research Centers
  - Core Research
    - Plan to initiate new projects in materials and chemistry by design
- **Scientific user facilities operations**
  - All facilities operate below optimum level
    - Synchrotron light sources
    - Neutron scattering facilities
    - Nanoscale Science Research Centers
- **Construction and instrumentation**
  - National Synchrotron Light Source-II ($159M) and NEXT instrumentation ($12M)
  - Spallation Neutron Source instruments ($12M)
  - Advanced Photon Source upgrade ($20M)
  - Linac Coherent Light Source-II ($30M)

FY 2012 Approp:
$ 1,688M
(+$10M from FY 2011)



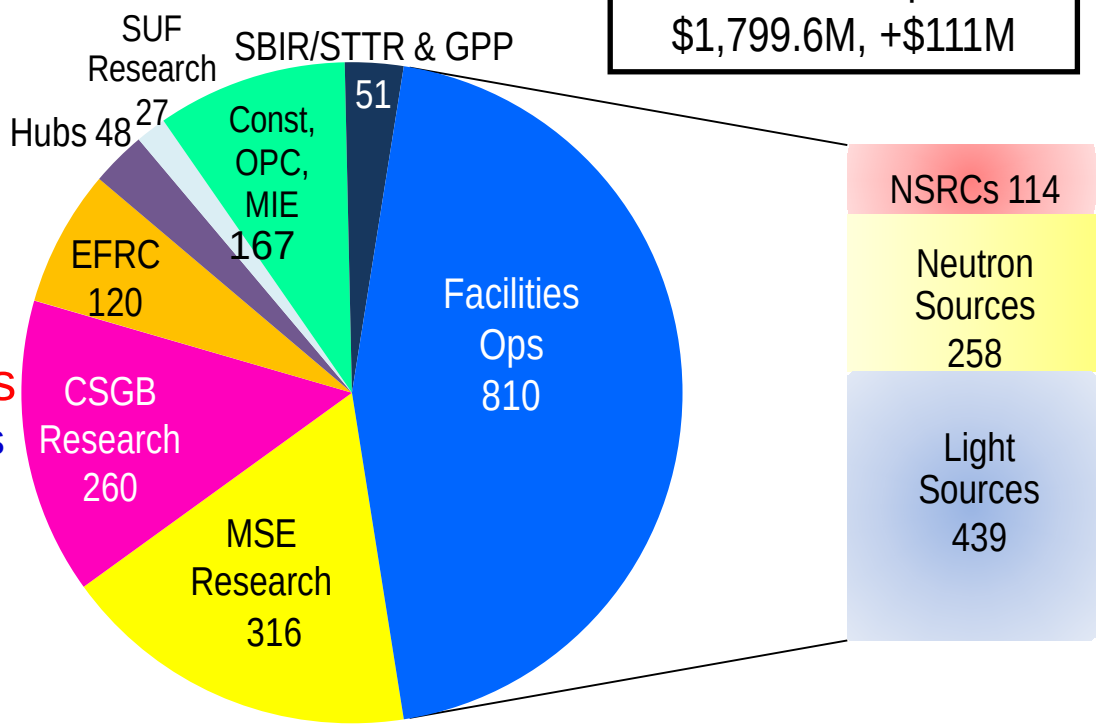
FY 2012 Appropriation

- "In order to increase transparency and accountability across all Science activities, the Department is directed, not later than September 1, 2012, to create a performance ranking of all ongoing multi-year research projects across the six major Science research programs, including those at universities, national laboratories, Energy Frontier Research Centers, Energy Innovation Hubs and other recipients, by comparing current performance with original project goals. The report shall include an inventory of the number and dollar amount of awards that have been terminated in fiscal years 2011 and 2012 before their multi-year awards have concluded.
- "The conferees direct the Department to provide to the House and Senate Committees on Appropriations, not later than February 10, 2012, a budget scenario for fiscal years 2013 and 2014 with the Office of Science funded at the fiscal year 2012 level, highlighting funding levels for each major program and project, including activities, such as ITER, with scheduled changes in funding requirements."

FY 2013 BES Budget Request

- **Research programs**
  - Energy Innovation Hubs (+$5M)
  - 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 (+$42M)
    - Synchrotron light sources
    - Neutron scattering facilities
    - Nanoscale Science Research Centers
  - Instrumentation for clean energy, joint with EERE (+$15M)
  - NSLS-II Early Operations (+$22M)
- **Construction and instrumentation**
  - National Synchrotron Light Source-II
  - NSLS-II instrumentation (NEXT) ($12M)
  - Advanced Photon Source upgrade ($20M)
  - Linac Coherent Light Source-II ($64M)

FY 2013 Request:
$1,799.6M, +$111M



President's FY 2013 Budget Request (Feb. 14)

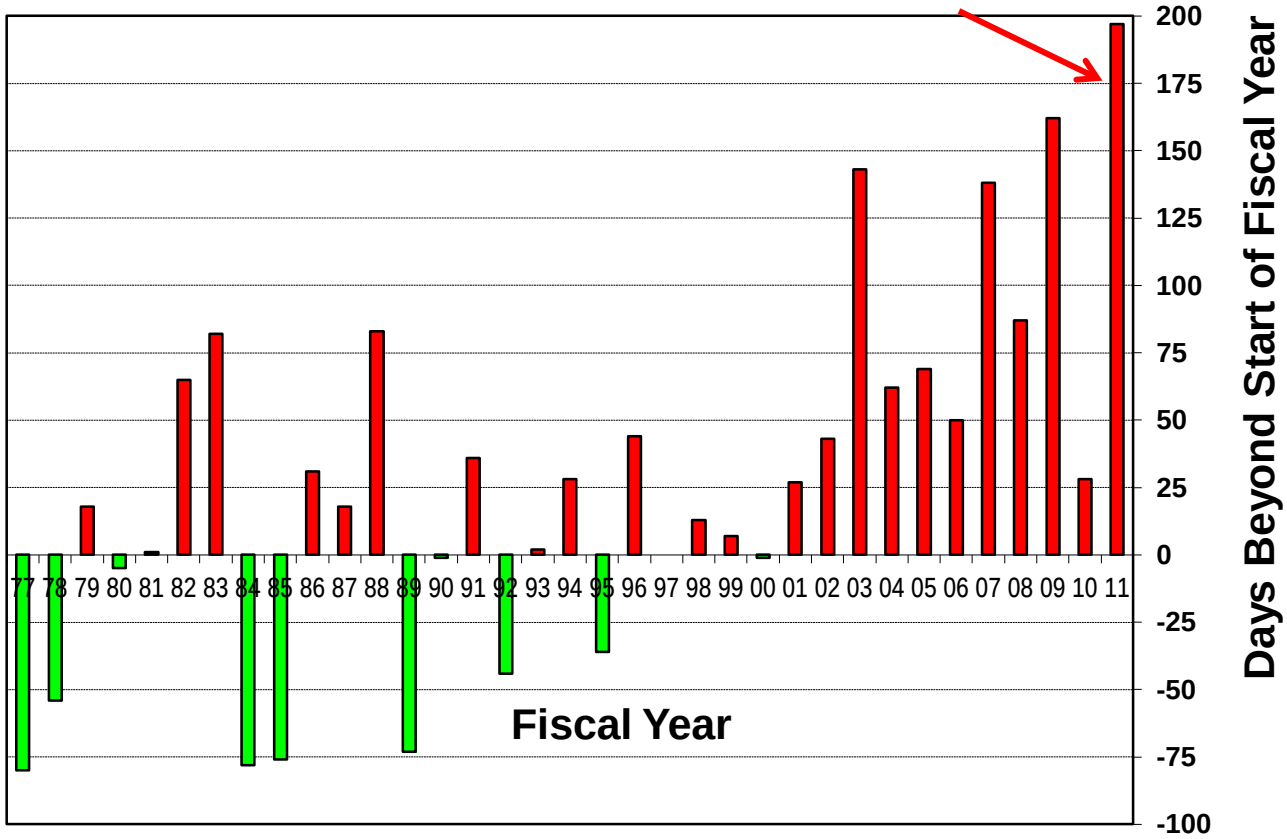
BES: $1,689 M (Increase of 6.6% compared to FY12 enacted)

AMOS: $22.070 M (Increase of 4.7% compared to FY12 enacted)

"AMO sciences research will emphasize the development and application of new ultrafast x-ray and optical probes of matter, including experiments at the Linac Coherent Light Source and BES synchrotron light sources and theoretical and computational methods for the interpretation of ultrafast measurements."

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 and budget execution.

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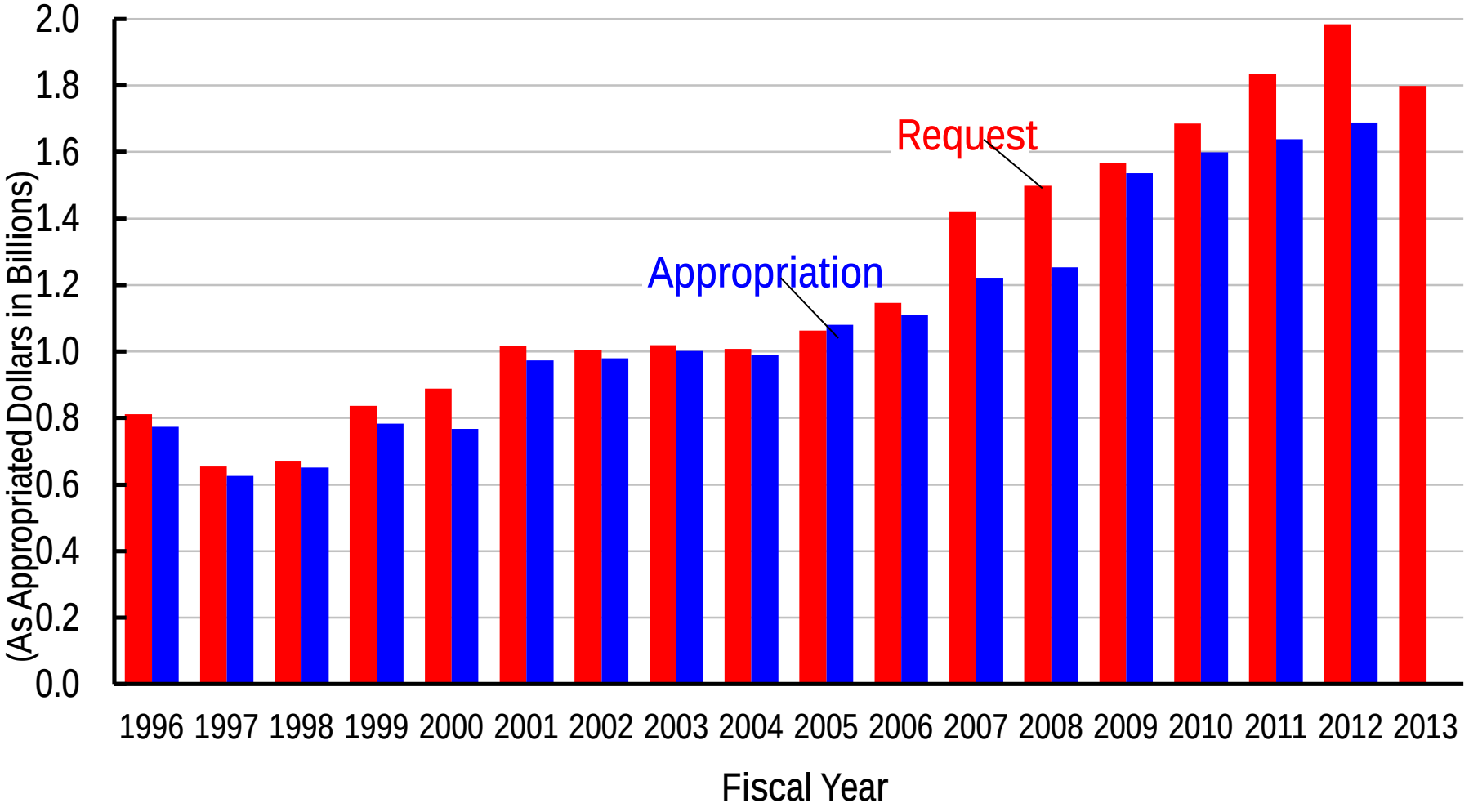
History of BES Request vs. Appropriation



AMOS Portfolio

- 62 Principal Investigators at 35 Universities
- 5 Programs at National Laboratories with 28 Principal Investigators
- 1 Center Grant (KSU) with10 Principal Investigators

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

FY 2010	FY 2011	FY 2012*	FY 2013**
$23,011K	$22,598K	$20,370K	$22,070K

*Not yet finalized
** President's Request

AMOS Program Composition (by Funding)

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

- **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.

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

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

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

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

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

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

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AMOS Portfolio Composition

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

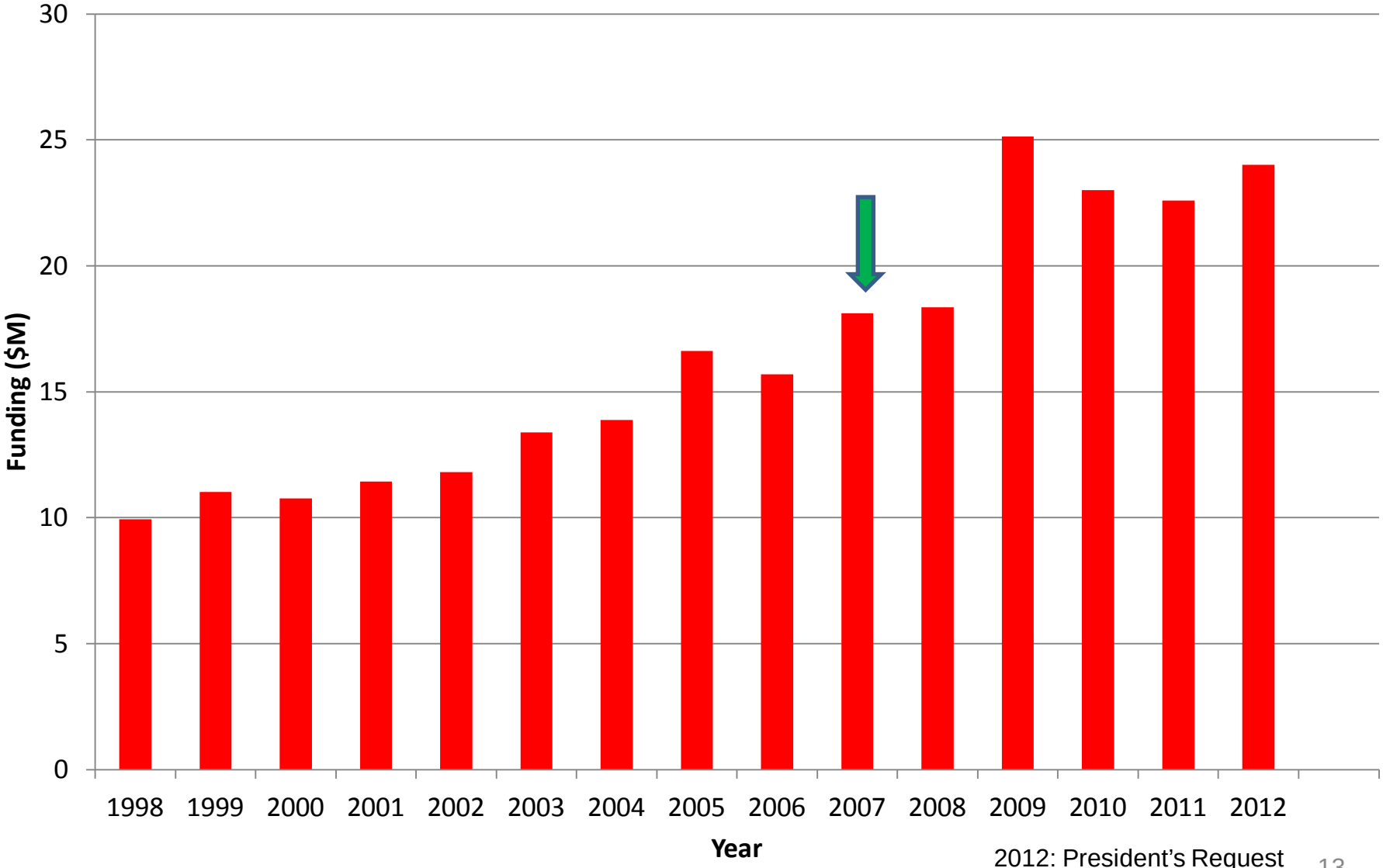
By topic (DOE Lab Programs):

3 programs focus on ultrafast science

1 program combines studies of ultrafast science and correlated dynamics

1 program focuses on nanoscience

Program Evolution: Funding



2012: President's Request

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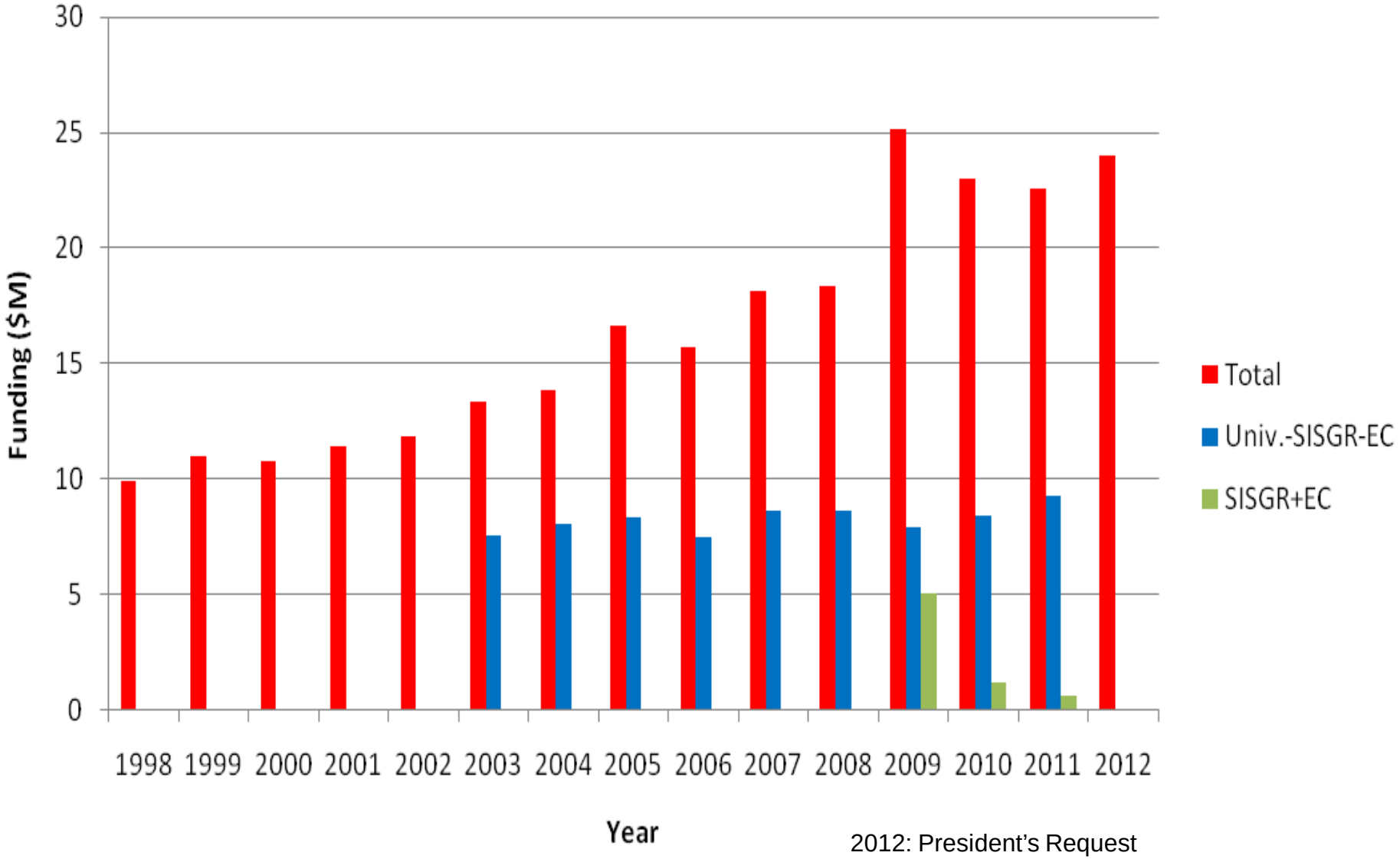
Funding: Lab vs. University

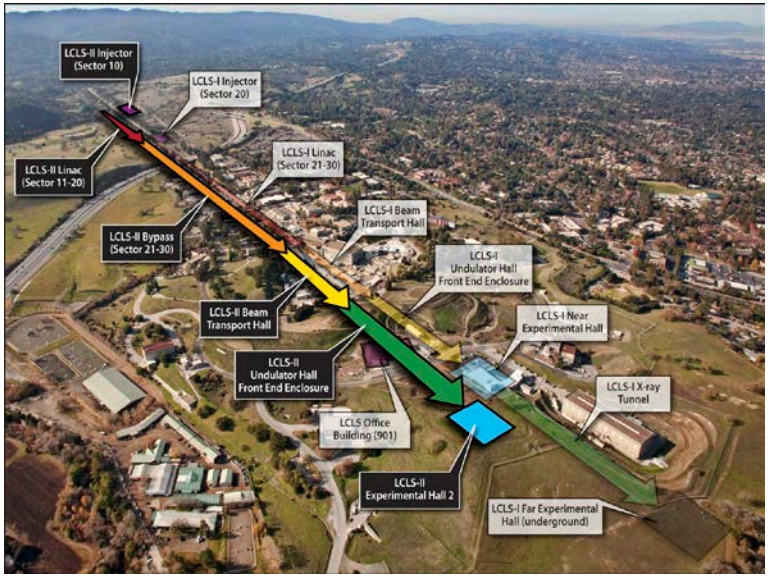


2012: President's Request

Linac Coherent Light Source-II

Expansion of Highly Successful LCLS:

- New experimental hall with room for 4 experimental stations, nearly doubling capacity
- Simultaneous operation of experimental stations
- Enables US to remain at international forefront for XFEL science



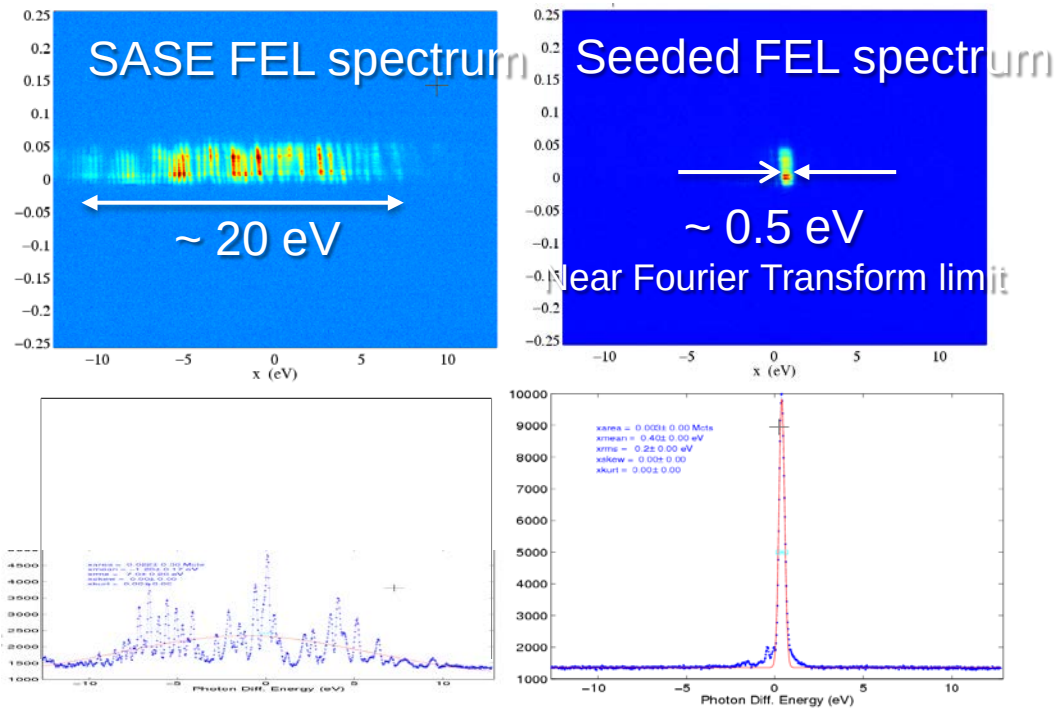
Capabilities:

- Expanded x-ray energy range (250eV – 13keV)
- X-ray polarization control
- Control pulse length down to ~1 femtosecond
- Multiple, independently controlled x-ray beams
- Factor of 20 increase in intensity

CD-1 Cost Range: $350M - $500M (Line Item Construction); FY 2012 $30M, FY 2013 Request $64M for R&D, design, long lead procurement, and construction

Apr 2010	CD-0, Approve Mission Need	(Complete)
Oct 2011	CD-1, Approve Alternative Selection and Cost Range	(Complete)
Mar 2012	CD-3a, Approve Long Lead Procurements	
Jan 2013	CD-2, Approve Performance Baseline	
Jun 2013	CD-3b, Approve Start of Construction	
Sep 2019	CD-4, Approve Start of Operations	

First Demonstration of Hard X-ray Self Seeding at LCLS: Enhanced Coherence



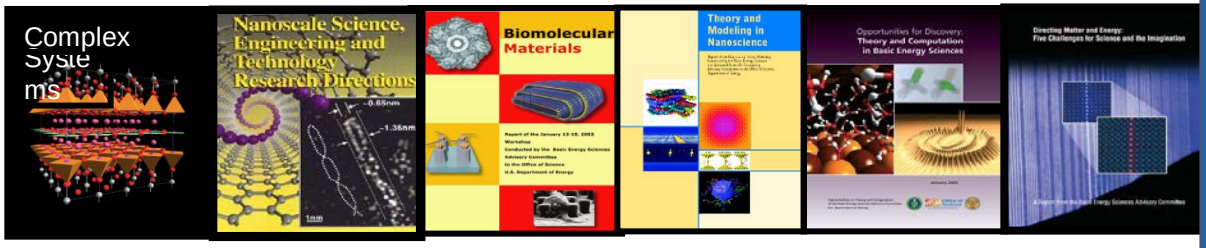
SASE and Seeded spectra recorded on single shots. The left panels are SASE with 150 pC, 3kA peak current, un-seeded. The FWHM of the SASE spectrum is 0.2 % Bandwidth. The right panels are the seeded beam with the same electron beam parameters. The FWHM of the seeded beam is 0.5 eV ($5x10^{-5}$ bandwidth)

- Concept developed by Geloni, Kocharyan and Saldin, DESY 10-053 (2010).
- The mean seeded FEL power is 8 GW with a 2.5 GW SASE background at 8 keV for 40 pC bunch charge.
- Peak seeded power is in excess of 15 GW, comparable to SASE but with a spectral bandwidth reduction by the factor of 40.
- Next steps include system optimization of the LCLS undulator beamline including additional undulators which should increase seeded power and reduce intensity fluctuation.

SLAC-Argonne-TISNCM Collaboration

BES Strategic Planning Activities

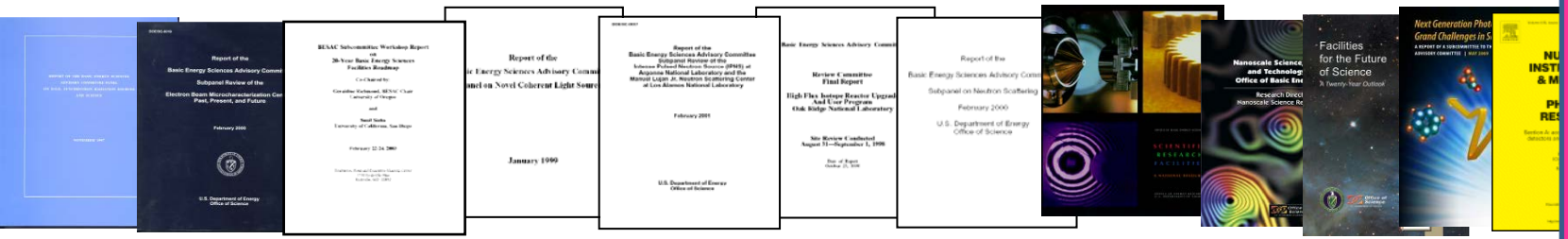
- *Science for Discovery*



Mesoscale Science

- *Science for National Needs*

- *National Scientific User Facilities, the 21st century tools of science*



Detector R&D