BES Update

Solid State Sciences Committee Meeting

Friday, April 11, 2008

Harriet Kung

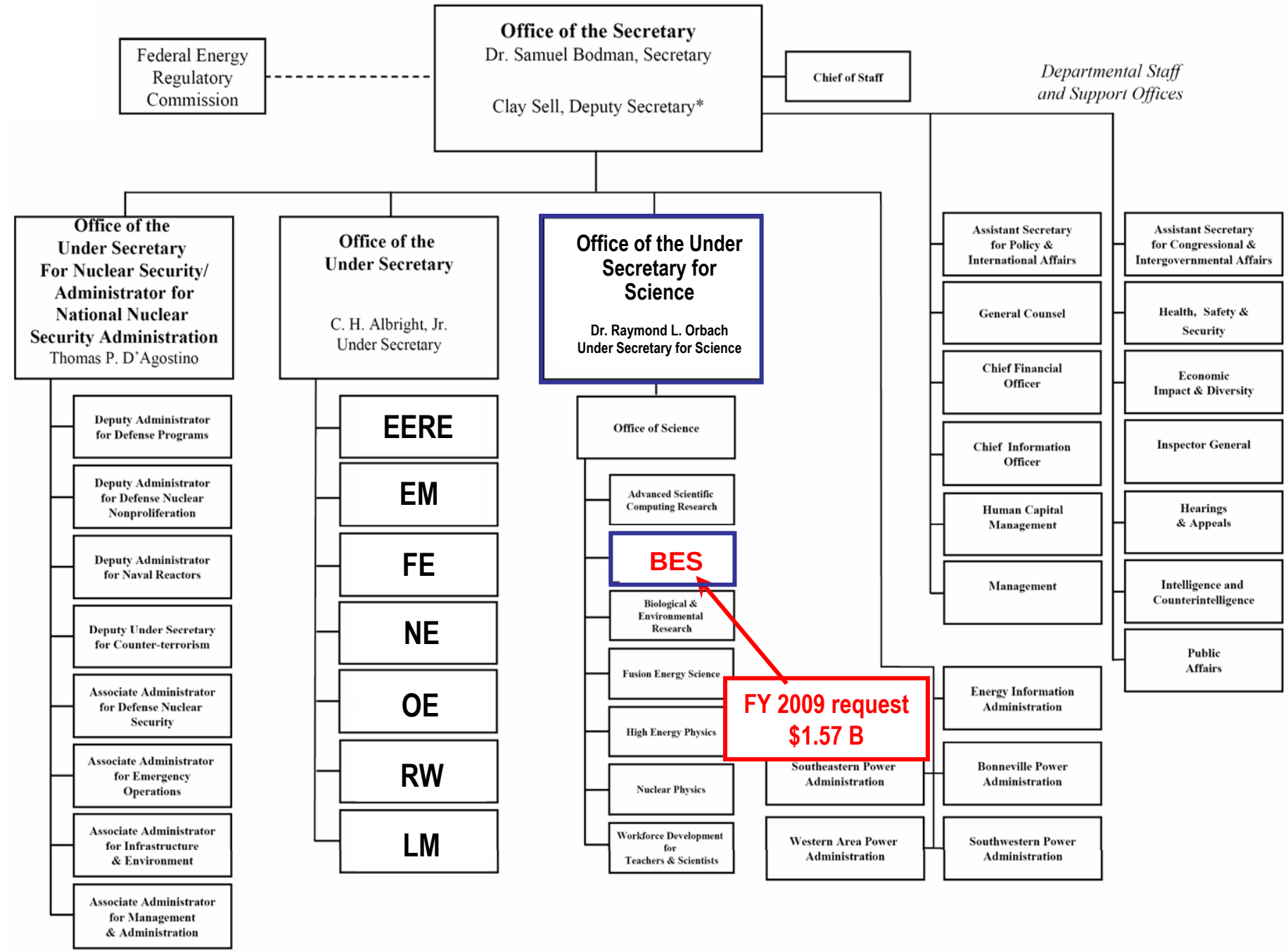
Materials Sciences and Engineering Division

Office of Basic Energy Sciences

DOE Office of Science

Harriet.Kung@science.doe.gov

Department of Energy



Office of Basic Energy Sciences

Eric Rohlfing, Director *(Acting)*

Vacant, Administrative Specialist

BES Budget and Planning

Robert Astheimer, Technical Advisor
Margie Davis, Budget Analyst

BES Operations

Linda Blevins, International/Intergovernmental
Richard Burrow, DOE Technical Office Coordination
Don Freeburn, DOE and Stakeholder Interactions
Ken Rivera, Laboratory Infrastructure/ES&H
Karen Talamini, Program Analyst/BESAC

Materials Sciences and Engineering Division

Harriet Kung, Director
Christie Ashton, Program Analyst
Charnice Waters, Secretary

- **Materials Discovery, Design, and Synthesis** — Arvind Kini, Vacant, Prog. Asst.
  - **Materials Chemistry** — Richard Kelley, James McBreen, BNL
  - **Biomolecular Materials** — Arvind Kini
  - **Synthesis and Processing Science** — Tim Fitzsimmons, Bonnie Gersten
  - **Tech. Coordination Program Management** — John Vetrano
- **Condensed Matter and Materials Physics** — Jim Horwitz, M. Agnant, Prog. Asst.
  - **Exp. Cond. Mat. Phys.** — James Horwitz, Doug Finnemore, Ames, Daniel Friedman, NREL
  - **Theo. Cond. Mat. Phys.** — Dale Koelling, Randy Fishman, ORNL, James Davenport, BNL
  - **Physical Behavior of Materials** — Refik Kortan
  - **Mechanical Behavior and Radiation Effects** — John Vetrano
- **Scattering & Instrumentation Sciences** — Helen Kerch, C. Howard, Prog. Asst.
  - **X-ray Scattering** — Lane Wilson
  - **Neutron Scattering** — Lane Wilson
  - **Electron and Scanning Probe Microscopies** — Jane Zhu
  - **Ultrafast Science and Instrumentation** — Jim Glownia
  - **Exp. Program to Stimulate Competitive Research** — Kristin Bennett

Scientific User Facilities Division

Pedro Montano, Director
Linda Cerrone, Program Analyst
Secretary (Vacant)

- **Operations**
  - **X-ray and Neutron Scattering Facilities** — Roger Klaffky
  - **Nanoscience Centers & E-beam Centers** — Altaf (Tof) Carim
  - **Accelerator and Detector R&D**
  - **Facility Coordination, Metrics, Assessment**
- **Construction**
  - **Linac Coherent Light Source** — Tom Brown
  - **NSLS II** — Tom Brown
  - **Spallation Neutron Source Upgrades** — Tom Brown
  - **TEAM** — Altaf (Tof) Carim
  - **Instrument MIEs (SING, LUSI, etc.)** — Tom Kiess
  - **ALS User Support Bldg** — Tom Brown

Chemical Sciences, Geosciences, and Biosciences Division

John Miller, Director (Acting)
Diane Marceau, Program Analyst
Michaelene Kyler-King, Program Assistant

- **Fundamental Interactions** — Michael Casassa, R. Felder, Prog. Asst.
  - **Atomic, Molecular, and Optical Sciences** — Elliot Kanter, ANL
  - **Ultrafast Chemical Sciences**
  - **Gas-Phase Chemical Physics** — Frank Tully, SNL
  - **Condensed-phase and Interfacial Mol. Sci.** — Gregory Fiechtner
  - **Computational and Theoretical Chemistry** — Richard Hildebrandt
- **Photo- and Bio-Chemistry** — Richard Greene, Vacant, Prog. Asst.
  - **Solar Photochemistry** — Mark Spitler, NREL
  - **Photosynthetic Systems**
  - **Physical Biosciences** — Michael Kahn, PNNL
- **Chemical Transformations** — John Miller, T. Russ, Prog. Asst.
  - **Catalysis Science** — Raul Miranda, Paul Maupin, Michael Chen, ANL
  - **Heavy Element Chemistry** — Lester Morss, Norman Edelestein, LBNL
  - **Separations and Analysis** — William Millman, Larry Rahn, SNL
  - **Geosciences** — Nicholas Woodward, Patrick Dobson, LBNL, Marsha Bollinger, AAAS

The five NSRCs are in operations and serving users

Center for Nanoscale Materials
Argonne National Laboratory

Molecular Foundry
Lawrence Berkeley National Laboratory

Center for Functional Nanomaterials
Brookhaven National Laboratory

Center for Integrated Nanotechnologies
Los Alamos National Laboratory &
Sandia National Laboratory

Center for Nanophase Materials Sciences
Oak Ridge National Laboratory

The FY 2008 Congressional Budget Appropriations for Office of Science

	FY 2006 Enacted Approp.	FY 2007 Enacted Approp.	FY 2008 Request	FY 2008 Enacted Approp.	FY 2008 Enacted Approp. vs. FY 2007 Enacted Approp.		FY 2008 Enacted Approp. vs. FY 2008 Request	
Basic Energy Sciences	1,134,557	1,250,250	1,498,497	1,269,902	+19,652	+1.6%	-228,595	-15.3%
Advanced Scientific Computing Res.	234,684	283,415	340,198	351,173	+67,758	+23.9%	+10,975	+3.2%
Biological & Environmental Res.	451,131	483,495	531,897	544,397	+60,902	+12.6%	+12,500	+2.4%
High Energy Physics	716,694	751,786	782,238	688,317	-63,469	-8.4%	-93,921	-12.0%
Nuclear Physics	367,034	422,766	471,319	432,726	+9,960	+2.4%	-38,593	-8.2%
Fusion Energy Sciences	287,644	318,950	427,850	286,548	-32,402	-10.2%	-141,302	-33.0%
Science Laboratory Infrastructure	41,684	41,986	78,956	64,861	+22,875	+54.5%	-14,095	-17.9%
SC Program Direction	159,118	166,469	184,934	177,779	+11,310	+6.8%	-7,155	-3.9%
Workforce Development	7,120	7,952	11,000	8,044	+92	+1.2%	-2,956	-26.9%
Safeguards & Security	73,630	75,830	76,592	75,946	+116	+0.2%	-646	-0.8%
Subtotal, SC	3,473,296	3,802,899	4,403,481	3,899,693	+96,794	+2.5%	-503,788	-11.4%

Impacts of FY 2008 Appropriations to BES Programs

Research:

- Over 700 proposals in response to BES initiatives in solar energy utilization, hydrogen research, advanced nuclear energy systems, and mid-scale instrumentation were received. Only 40 awards were made in FY 07; the remaining proposals have been declined. Approximately 250 new awards were anticipated under the BES FY 08 budget request.
- Core research in FY 08 will be approximately flat funded with FY 07, resulting in reductions in effort due to inflation.

Facilities Operations:

- The operations of the Intense Pulsed Neutron Source at Argonne National Laboratory have been permanently terminated, and the facility is being placed in shut down mode.
- The operations of all remaining BES user facilities – the synchrotron radiation light sources, the neutron scattering facilities, the electron beam microcharacterization centers, and the nanoscale science research centers – are flat funded with FY 07, resulting in reduced hours of operation reduced service to users, possible staff layoffs, and other actions to mitigate the funding levels.

Constructions:

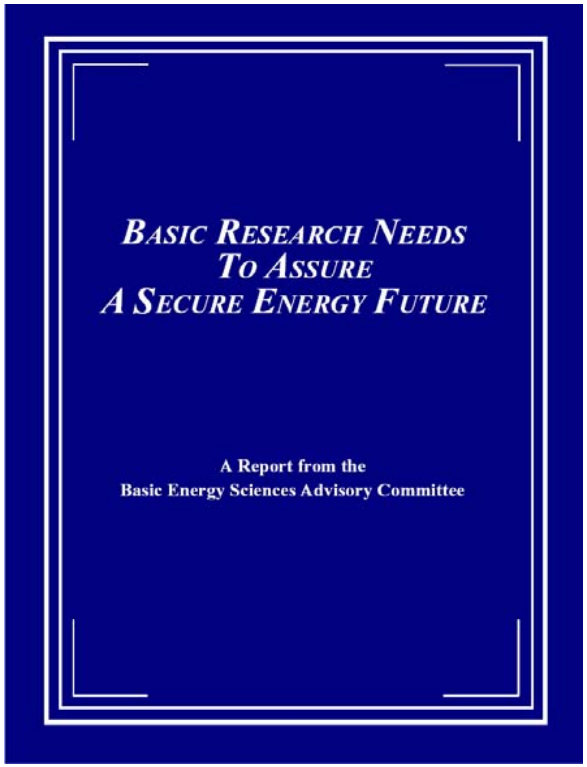
- The National Synchrotron Light Source-II at BNL is funded at a level that is 33% below the budget request.
- The Advanced Light Source User Support Building at LBNL is funded at a level 70% below the budget request, resulting in more than one year delay and several million dollars cost increases
- Major instrumentation fabrication projects for the Spallation Neutron Source at ORNL and Linac Coherent Light Source at SLAC are funded at a level 40% below the respective budget requests.

Results of FY 2007 Solicitations

Solicitation:	Instrumentation	Basic research for solar energy utilization	Basic research for the hydrogen fuel initiative	Basic research for advanced nuclear energy systems
FY 2007 Request	$19.6 million	$34.1 million	+ $17.5 million	$12.4 million
FY 2007 appropriations under H.J.R 20	—	$7.8 million	+ $3.9 million	—
FY 2007 Congressional Budget released	February 6, 2006			
Announcement of intent to issue solicitations	February 16, 2006			
Posting solicitation on SC website	March 7, 2006	March 21, 2006	April 20, 2006	October 12, 2006
Preproposal deadlines	May 17, 2006 106 preproposals	June 5, 2006 656 preproposals	July 6, 2006 502 preproposals	Nov. 22, 2006 209 preproposals
PIs notified of preproposal decisions	June 30, 2006 59 encouraged	August 11, 2006 346 encouraged	Sept. 12, 2006 249 encouraged	January 5, 2007 126 encouraged
Full proposal deadlines	August 30, 2006 58 received	Nov. 14, 2006 309 received	Dec. 12, 2006 229 received	March 14, 2007 118 received
FY 2007 awards*	— none —	May 22, 2007 27 awards	May 15, 2007 13 awards	— none —
Additional funding in the FY 2008 Request	+ $19.6 million	+ $32.2 million	+ $23.1 million	+ $12.4 million
Funding available in the FY 2008 Appropriations	0	0	0	0
FY 2008 awards*	None	None	None	None

The First "Basic Research Needs …" Workshop

Basic Research Needs to Assure a Secure Energy Future (October 2002)



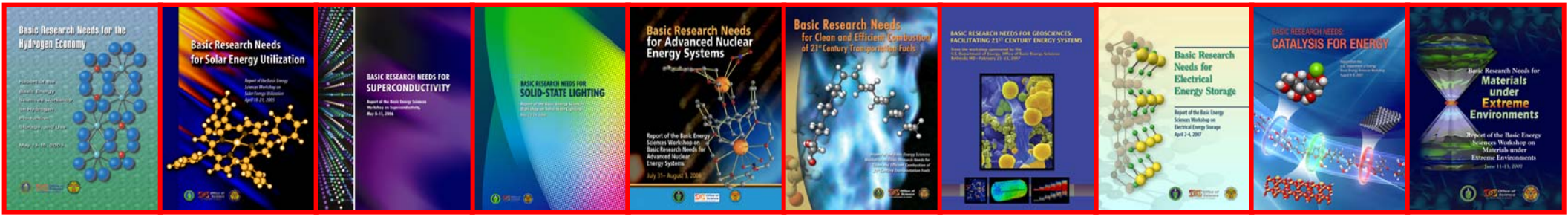
- The report identified basic research directions required for major technological changes in the largest industries in the world—those responsible for energy production and use.
- The reports highlighted the remarkable scientific journey that took place during the past few decades. The resulting scientific challenges are describe a new era of science — an era in which materials functionalities are designed to specifications and chemical transformations are manipulated at will.
- In this new era of science, we design, discover, and synthesize new materials and molecular assemblies through atomic scale control; probe and control photon, phonon, electron, and ion interactions with matter; perform multi-scale modeling that bridges the multiple length and time scales; and use the collective efforts of condensed matter and materials physicists, chemists, biologists, molecular engineers, applied mathematicians, and computer scientists.
- The findings inspired 10 additional workshops over the next five years, which together attracted more than 1,500 participants.

The 10 "Basic Research Needs …" Workshops

10 workshops; 5 years; more than 1,500 participants from academia, industry, and DOE labs

Basic Research Needs to Assure a Secure Energy Future (BESAC)

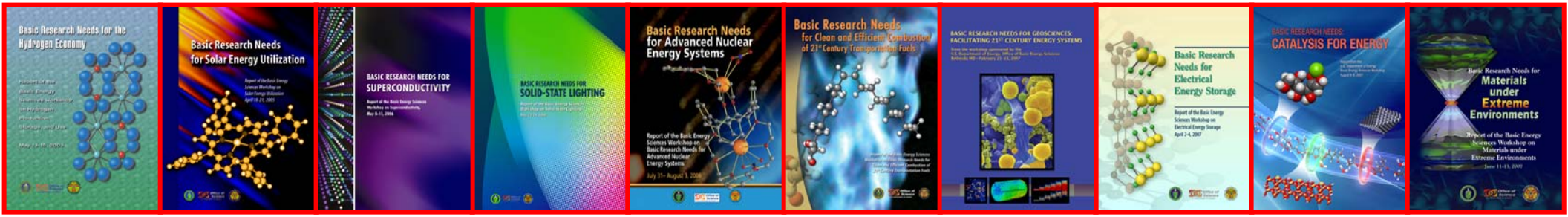
- Basic Research Needs for the Hydrogen Economy
- Basic Research Needs for Solar Energy Utilization
- Basic Research Needs for Superconductivity
- Basic Research Needs for Solid State Lighting
- Basic Research Needs for Advanced Nuclear Energy Systems
- Basic Research Needs for the Clean and Efficient Combustion of 21st Century Transportation Fuels
- Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems
- Basic Research Needs for Electrical Energy Storage
- Basic Research Needs for Catalysis for Energy Applications
- Basic Research Needs for Materials under Extreme Environments



Important Recurring Themes from the Workshops

Control of materials properties and functionalities through electronic and atomic design

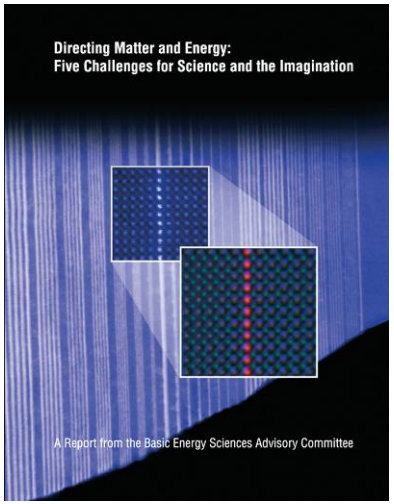
- New materials discovery, design, development, and fabrication, especially materials that perform well under extreme conditions
- "Control" of photon, electron, spin, phonon, and ion transport in materials
- Science at the nanoscale, especially low-dimensional systems
- Designer catalysts
- Designer interfaces and membranes
- Structure-function relationships
- Bio-materials and bio-interfaces, especially at the nanoscale
- New tools for spatial characterization, temporal characterization, and for theory/modeling/computation



One Additional Workshop: Science Grand Challenges

How does nature execute electronic and atomic design? How can we?

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



- **Control the quantum behavior of electrons in materials**

  Imagine: 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**

  Imagine: Create and manipulate natural and synthetic systems that will enable catalysts that are 100% 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**

  Imagine: 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**

  Imagine: 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**

  Imagine: 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.

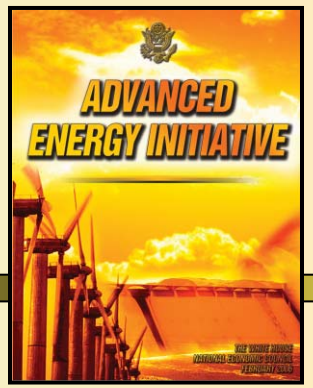
How Nature Works ··· to ··· Materials by Design ··· to ··· Technologies for the 21st Century

Grand Challenges	Discovery and Use-Inspired Basic Research		Applied Research	Technology Maturation & Deployment
How nature works	*Materials properties and functionalities by design*			
▪ 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	▪ 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	▪ 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	▪ 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



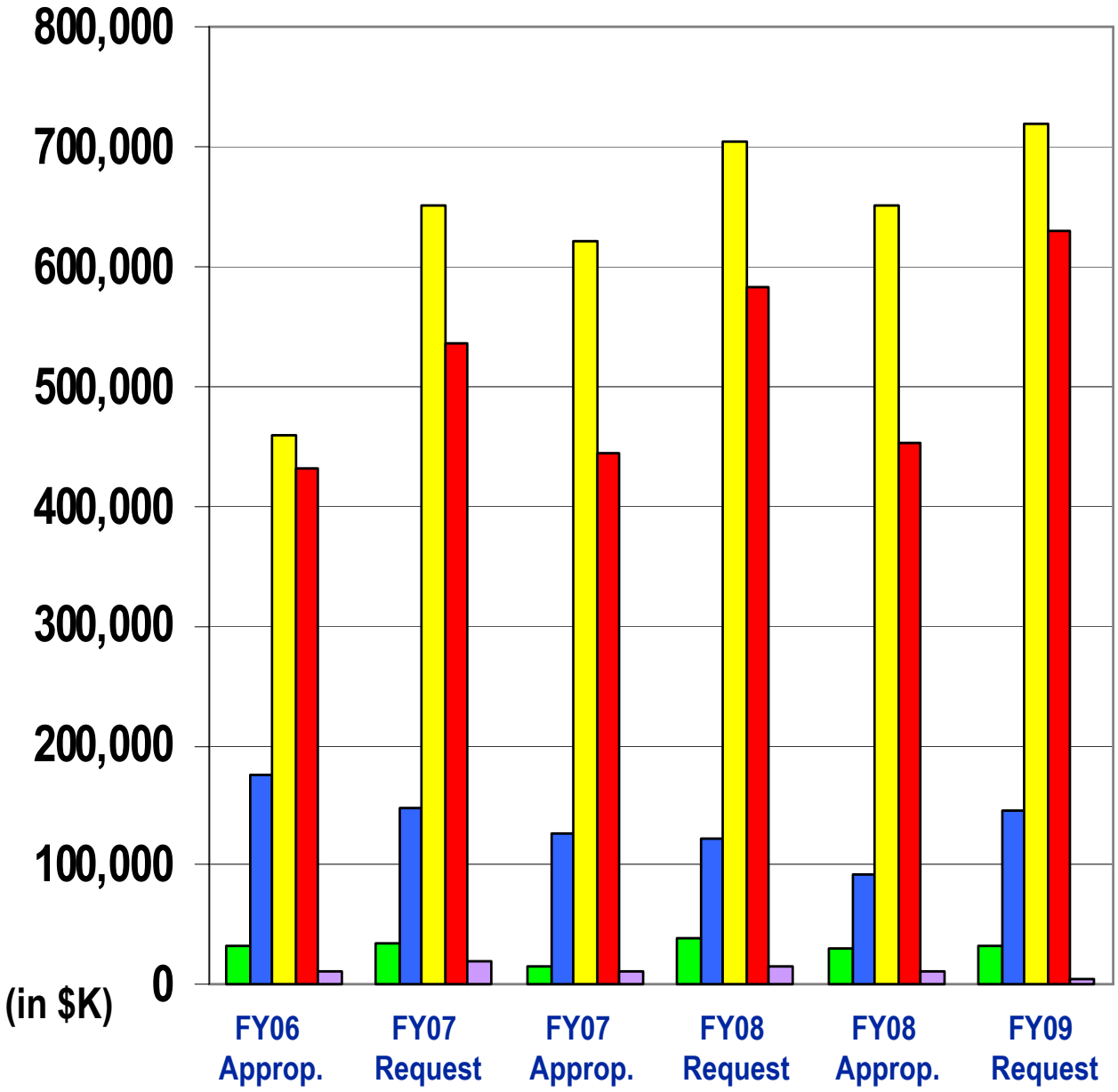
The Office of Science FY 2009 Budget Request to Congress

(dollars in thousands)

	FY 2007 Approp.	FY 2008 Approp.	FY 2009 Request to Congress	FY 2009 Request to Congress vs. FY 2008 Approp.	
Basic Energy Sciences	1,221,380	1,269,902	1,568,160	+298,258	+23.5%
Advanced Scientific Computing Research	275,734	351,173	368,820	+17,647	+5.0%
Biological and Environmental Research	480,104	544,397	568,540	+24,143	+4.4%
High Energy Physics	732,434	689,331	804,960	+115,629	+16.8%
Nuclear Physics	412,330	432,726	510,080	+77,354	+17.9%
Fusion Energy Sciences	311,664	286,548	493,050	+206,502	+72.1%
Science Laboratories Infrastructure	41,986	66,861	110,260	+43,399	+64.9%
Science Program Direction	166,469	177,779	203,913	+26,134	+14.7%
Workforce Dev. for Teachers & Scientists	7,952	8,044	13,583	+5,539	+68.9%
Safeguards and Security (gross)	75,830	75,946	80,603	+4,657	+6.1%
SBIR/STTR (SC funding)	86,936	——	——	——	——
Subtotal, Office of Science	3,812,819	3,902,707	4,721,969	+819,262	+21.0%
Adjustments*	23,794	70,435	——	-70,435	——
Total, Office of Science	3,836,613	3,973,142	**4,721,969**	+748,827	+18.8%

* Adjustments include SBIR/STTR funding transferred from other DOE offices (FY 2007 only), a charge to reimbursable customers for their share of safeguards and security costs (FY 2007 and FY 2008), Congressionally-directed projects and a rescission of a prior year Congressionally-directed project (FY 2008 only), and offsets for the use of prior year balances to fund current year activities (FY 2007 and FY 2008).

BES Budget Requests & Appropriations



	FY 2009 Request (in $K)
Construction	145,468
Major Items of Equipment	34,000
Facility Operations	719,247
GPP/GPE	4,948
Research	629,958
SBIR/STTR	34,539
TOTAL	1,568,160

Summary of FY09 BES Budget Increases

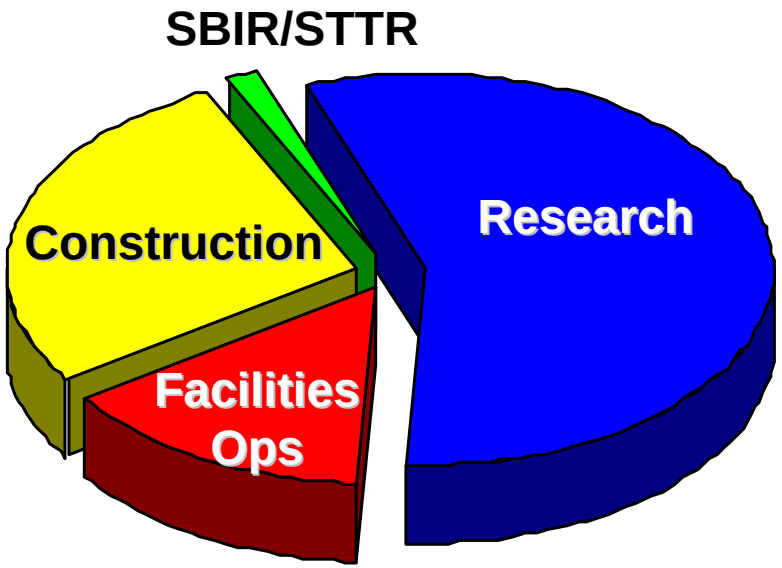
Research (~$100M devoted to EFRCs)	160,989
Facility related research (Accelerator & Detector, E-beams)	10,354

Facilities	
Light Sources	20,708
Neutron Sources	17,924
NSRCs	10,106
IPNS D&D	-4,000

Construction	
NSLS-II	53,546
LCLS + linac operations + instruments	33,778
PULSE	-3,664
ALS USB	6,546
SNS instruments	1,144
TEAM	-6,687
CFN	-863

GPP/GPE	-6,150
SBIR/STTR	4,527

TOTAL ($K)	298,258



Energy Frontier Research Centers

Tackling our energy challenges in a new era of science

Energy Frontier Research Centers will bring together the skills and talents of multiple investigators to enable research of a scope and complexity that would not be possible with the standard individual-investigator or small-group award.

The DOE Office of Science, Office of Basic Energy Sciences, announced the Energy Frontier Research Centers (EFRCs) program. Pending appropriations, up to $100M will be available in FY2009 for EFRC awards that are $2–5 million/year for an initial 5-year period. Universities, labs, nonprofits, and for-profit entities are eligible to apply.

Energy Frontier Research Centers will pursue fundamental research that addresses both energy challenges and science grand challenges in areas such as:

- Solar Energy Utilization
- Catalysis for Energy
- Electrical Energy Storage
- Solid State Lighting
- Superconductivity
- Bioenergy and biofuels
- Geosciences for Nuclear Waste and CO_2 Storage
- Advanced Nuclear Energy Systems
- Combustion of 21st Century Transportation Fuels
- Hydrogen Production, Storage, and Use
- Materials Under Extreme Environments

EFRC Funding Opportunity Announcement was published on April 4, 2008.
See: http://www.sc.doe.gov/bes/EFRC.html

Single-Investigator and Small-Group Research

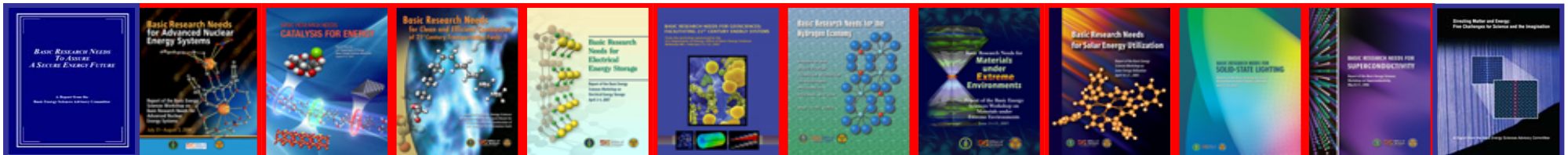
Tackling our energy challenges in a new era of science

- Pending appropriations, up to $60M will be available for single-investigator and small-group awards in FY2009.
- BES seeks applications in two areas: grand challenge science and energy challenges identified in one of the Basic Research Needs workshop reports.
- Awards are planned for three years, with funding in the range of $150-300k/yr for single-investigator awards and $500-1500k/yr for small-group awards (except as noted below)
- Areas of interest include:

  Grand challenge science: ultrafast science; chemical imaging, complex & emergent behavior

  Tools for grand challenge science: midscale instrumentation; accelerator and detector research (awards capped at $5M over 3-year project duration)

  Use inspired discovery science: basic research for electrical energy storage; advanced nuclear energy systems; solar energy utilization; hydrogen production, storage, and use; other basic research areas identified in BESAC and BES workshop reports with an emphasis on nanoscale phenomena
- For full details see: http://www.sc.doe.gov/bes/SISGR.html



Looking Ahead: The Plan

- **The goal must be a world-class, vigorous, and productive program, which balances key portfolio components that together create a uniquely DOE program:**
  - **Fundamental research**
    - in support of a *mission-driven basic research* and
    - in support of *discovery science* that enables the mission; this also includes the support of a critical mass of principal investigators – "the great discovery machine"
  - **Forefront scientific user facilities for the Nation**
- **A robust, scientifically compelling plan for BES must be developed that is supported by:**
  - The scientific community, the Administration, Congress and the public and addresses the long-term realities of the Nation's energy needs.
- **The scientific community is critically important:**
  - The community needs to continue to develop a strategy to communicate the long-term basic research needs for tackling the 21st century energy challenges.
  - The community needs to make the case for the science, and its benefits to the Nation, to Congress and the public. Funding is not an entitlement.

Source: R.L. Orbach BESAC Presentation 2/21/08