Minutes for the
Basic Energy Sciences Advisory Committee (BESAC) Meeting
February 21-22, 2008
Marriott North Bethesda Hotel and Conference Center
North Bethesda, Maryland

BESAC members present:

Simon Bare
Nora Berrah
Sue Clarke
Peter Cummings
George Flynn
Bruce Gates
Laura Greene
Sharon Hammes-Schiffer
John Hemminger, Chairman
Eric Isaacs (Thursday only)
Bruce Kay
Kate Kirby (Thursday only)
William McCurdy, Jr.
Kathryn Nagy
John Richards
Kathleen Taylor
Douglas Tobias
John Tranquada

BESAC members absent:
Sylvia Ceyer
Frank DiSalvo
Mostafa El-Sayed
Michael Hochella
Daniel Morse
Martin Moskovits
John Spence

Also participating:
Altaf Carim, Division of Scientific User Facilities
John Galayda, Stanford Linear Accelerator Center
Patricia (Pat) Dehmer, Deputy Director, Science Program, Office of Science, USDOE
John Galayda, Stanford Linear Accelerator Center, Stanford University
Harriet Kung, Acting Director, Associate Director for Basic Energy Sciences, USDOE
Ray Johnson, BESAC Technical Writer
Pedro Montano, Director, Scientific User Facilities Division, USDOE
Randy Ogle, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory
Raymond (Ray) L. Orbach, Director, Office of Science, USDOE
Eric Rohlfing, Director Chemical Sciences, Geosciences and Biosciences Division
Karen Talamini, Office of Basic Energy Sciences, USDOE

Approximately 140 others were in attendance in the course of the two-day meeting.
Thursday, February 21, 2008

BESAC Chair **John Hemminger** called the meeting to order at 9:49 a.m. He welcomed everyone and asked each Committee member to introduce themselves. He thanked everyone for coming and promptly made the announcement that there had been changes in the Office of Science, which had a great impact not only on the office, but also **Patricia (Pat) Dehmer.** He asked **Dehmer** to explain the changes and to also describe her new role as the new Deputy Director for Sciences Programs.

Dehmer displayed a new Basic Energy Sciences (BES) work chart. The changes occurred in late October, with three Deputy Directors - Deputy Director for Field Operations, Deputy Director to

Science Programs and Deputy Director for Resource Management – now reporting to **Raymond (Ray) Orbach**.

Dehmer said there have been significant changes at BES during her past 12 years. Her previous position, Director, Office of Sciences, is currently open, with **Harriett Kung** serving as the Acting Director. One of **Dehmer's** immediate goals is to get the (her former) position filled as soon as possible. She thanked the Committee for all of their efforts during her tenure and also her appreciation in assisting to fill vacant positions.

Hemminger thanked **Dehmer** and stated there was a lot to get accomplished during today and tomorrow's meeting. At 10:00 a.m., **Harriet Kung** was introduced and asked by **Hemminger** to provide an update on news from the Office of BES.

Kung began her presentation by saying that she has been the Acting Director since October 2007. As mentioned, **Dehmer** was appointed Deputy Director for Science Programs, Office of Science, U.S. Department of Energy (DOE).

Kung's presentation included an overview of the execution of the fiscal year (FY) 2008 budget ("not good news"), the FY 2009 budget request ("it is good news and as we continue to be upbeat and optimistic. We need to build a good case for our needs.") and how she is looking forward to tackling our energy challenges in a new era of science. She added, "We have a tremendous journey in meeting the various challenges."

Kung discussed the work chart for the DOE. She said the BES, one of the areas that reports to **Ray Orbach** has a FY 2008 budget of $1.27 billion, almost one third of the science budget.

The DOE funding was examined, comparing the Energy (EERE, NE, FE and OE) to the Office of Science. Over the past four years, there has been a large increase in Energy funding and not such a significant increase in the Office of Science. The budget request versus the appropriation in Energy is widening over Science in 2008.

The FY 2008 Congressional budget appropriations for Office of Science were reviewed. For BES, the FY 2008 enacted appropriation versus the FY 2008 request was a 15.3% decrease. But overall, there were certain areas that received significant increases, such as the Advanced Scientific Computing Research and the Biological and Environmental Research. Fusion Energy Sciences and High Energy Physics received significant decreases.

The impacts of FY 2008 appropriations will affect research, facilities operations and constructions. "We hope 2008 will be a better year," **Kung** said. In research, more than 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 2007. The remaining proposals have been declined. Approximately 250 new awards were anticipated under the BES FY 2008 budget request.

"This is extremely serious to have only 40 awards made versus the number of proposals we received," **Kung** said. "There has been an overwhelming support from the community, which has been greatly appreciated."

Core research in FY 2008 will be flat funded with FY 2007, resulting in reductions due to inflation. **Kung** added "The absolute dollars continue to decrease."

In 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 2007, resulting in a reduction in hours of operation and service to users, possible staff layoffs and other actions to mitigate the funding levels.

"These actions will be disastrous, but we continue to hope for a big turn-around in 2008," **Kung** said.

The construction impact include 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 of 70% below the budget request, resulting in more than a one year delay and several more million dollars in cost increases. Major instrumentation fabrication projects for the Spallation Neutron Source at ORNL and Linac Light Source at SLAC are funded at a level 40% below the respective budget requests. "These reductions have caused major challenges," **Kung** said. "We are currently projecting a year delay in construction."

The results of the FY 2007 solicitations have resulted in a "loss of momentum and opportunity." **Kung** reviewed the FY 2007 request and appropriations, the number of pre-proposal deadlines and decisions, full proposal deadlines and FY awards. In addition, she reviewed additional funding in the FY 2008 request and funding available in the FY 2008 appropriations. Thus far, there have no FY 2008 awards.

Next, **Kung** looked at a retrospective view of a remarkable journey – defining the science directions. *Basic Research Needs to Assure a Secure Energy Future* is a report that started five years ago (February 2003). "This has been a monumental piece of information that recognized the urgency to tackle certain challenges. Current projections estimate that the energy needs of the world will more than double by 2050. This is coupled with increasing demands for "clean" energy – sources of energy that do not add to the already high levels of carbon dioxide and other pollutants in the environment. Those enormous challenges cannot be fully met by existing technologies and scientific breakthroughs will be required to provide reliable, economic solutions for our future energy security."

This workshop report identified the broad basic research directions that will help provide the major scientific discoveries necessary for the major technological changes in the largest industries in the world – those responsible for energy production and use. The findings of this 2003 report "gave birth" to a series of 10 follow-on Basic Research Needs (BRN) workshops over the next five years, which attracted more than 1,500 participants from universities, industry and DOE laboratories. These reports provide in-depth analyses on how the work of the scientific community can further our nation's most challenging missions.

"These BRN workshops provided us with a tremendous foundation and recognized several promising areas," **Kung** said. "There have been three recent studies/workshops conducted since the last BESAC meeting last September."

The three workshops included the *Basic Research Needs for Electrical Energy Storage*. "This workshop identified a number of key areas and projected the doubling of world energy consumption within the next 50 years, coupled with the growing demand for low- or even zero-emission sources of energy," **Kung** said. This has brought increasing awareness of the need for efficient, clean and renewable energy sources. Energy based on electricity generated from renewable sources, such as solar or wind, offer enormous potential for meeting future energy demands. However, practical use of large scale solar- or wind-based electrical generation requires electrical energy storage (EES) systems to level their cyclic nature. In addition, greatly improved EES systems are needed to replace today's hybrid electric vehicles with plug-in hybrids or all-electric vehicles.

The discovery of novel Nanoscale materials with architectures tailored for specific performance offer exciting possibilities for the development of revolutionary three-dimensional architectures that simultaneously optimize ion and electron transport and capacity. New capabilities are also needed to “observe” the dynamic composition and structure at an electrode surface, in real time, during charge transport and transfer processes. New in situ photon- and particle-based microscopic, spectroscopic and scattering techniques with time resolution down to the femtosecond range and spatial resolution spanning the atomic and mesoscopic scales are needed to meet this challenge. Research to formulate a predictive knowledge of structural and functional relationships based upon multi-scale integrating theory-based methods at different time and length scales can effectively complement experimental efforts to provide insight into mechanisms, predict trends and identify new materials.

The *Catalysis for Energy* workshop (January 2008) provided a glimpse of how with domestic reserves of petroleum and natural gas declines, the volumes of imported fuels grow and the environmental impacts resulting from fossil fuel combustion become severe. Our nation must reassess our future chemical energy sources. The catalysis is the essential technology for accelerating and directing chemical transformation and is the key to realizing environmentally friendly, efficient and economical processes for the conversion of fossil and renewable or alternative energy feedstocks.

Furthermore, the workshop examined BRN to maximize the potential for new catalytic discoveries in three specific areas according to source: bio-derived chemicals, heavy fossil-derived chemicals and end-product (such as carbon dioxide and water) reconversion. The grand challenge identified at the core of all of these areas was to achieve detailed mechanistic understanding of catalytic dynamics for complex heavy molecular mixtures, bio-derived species and solid nanostructures and interfaces. Such understanding would allow scientists to build effective catalysts with atom-by-atom precision and convert complex reactants to energy-storing products with molecular precision. The means to resolve this challenge is several-fold: creating new and expanding existing fundamental theories of chemical kinetics that effectively take into account the dynamics and statistical fluctuations of structurally complex and diverse feedstocks; creating and advancing instrumentation that permits real-time high-resolution chemical imaging of reacting species and catalysts; synthesizing new and more complex catalyst structures that exploit multi-functionality and versatility in order to guide reactions through highly selective pathways.

The third workshop was *Materials Under Extreme Environments* (February 2008). Materials are recognized as being central to every energy technology and future energy technologies. This will place increasing demands on materials performance with respect to extremes in stress, strain, temperature, pressure, chemical reactivity, photon or radiation flux and electric or magnetic fields. Therefore, it is not surprising that the failure of materials is a principal bottleneck for developing future energy technologies. New fundamental research of materials under extreme conditions will have a major impact on the development of numerous integrated technologies that can meet future requirements for abundant, affordable and clean energy.

Reaching the intrinsic limit of materials performance is a key challenge. Solutions to this challenge require new understanding regarding the most fundamental atomic and molecular origins of material failure. In particular, ultra-high spatial and ultra-fast temporal resolution characterization tools are needed to observe and follow the initiation and evolution of atomic-scale to cascading macroscale damage events. Complementary advanced computational capabilities to simulate and predict multi-scale damage from atomic to macroscopic dimensions are also needed. Such new understanding of damage and failure will underpin research to discover how atomic and molecular structures could be manipulated in a predictable manner to enable development of new materials having an extraordinary tolerance to function within an extreme environment without property degradation, or even with the ability for self-repair.

The BRN workshops address many elements required for a decades-to-century energy security strategy, such as the following crosscutting issues:

- Research for a secure energy future
- Carbon energy sources

- Energy conservation, energy efficiency and environmental stewardship
- Geologic
- Nuclear fission
- Solar
- Electricity production and grid
- Electric storage
- Hydrogen

The topical grand challenges from the BRN workshops are:

- New materials and functionalities discovery, design development and fabrication, especially materials that perform well under extreme conditions
- Science at the nanoscale, especially low-dimensional systems that promise materials with new and novel properties
- Methods to “control” photon, electron, ion and photon transport in materials for next-generation energy technologies
- Structure-function relationships in both living and non-living systems
- Designer catalysts
- Interfacial science and designer membranes
- Bio-materials and bio-interfaces, especially at the nanoscale where soft matter and hard matter can be joined
- New tools for:
    - Spatial characterization, especially at the atomic and Nanoscales and especially for in-situ studies
    - Temporal characterization for studying the time evolution of processes
    - Theory and computation
    - Synthesis, crystal growth

In *Directing Matter and Energy* (January 2008), this is a new era of science. Together these workshop reports highlighted the remarkable scientific journey that has taken place during the past few decades. The resulting scientific challenges, which no longer were discussed in terms of traditional scientific disciplines, described a new era of science – an era in which materials are designed to specifications and chemical transformations are manipulated at will.

- How do we control materials processes at the level of electrons?
- How do we design and perfect atom- and energy-efficient syntheses of revolutionary new forms of matter with tailored properties?
- How do remarkable properties of matter emerge from the complex correlations of atomic or electronic constituents and how can we control these properties?
- How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?
- How do we characterize and control matter away – especially very far away – from equilibrium?

Addressing these grand challenges are keys to making the transition from observation to control of matter.

Next, **Kung** looked at the world-leading facilities that are driving transformational science and U.S. innovation. The Synchrotron Light Sources help research community extend basic knowledge and advances technology development. Neutron sources provide a unique probe for application in many fields of science and technology. Virtually everything we know about the fundamental structure of magnetic materials – which lie at the heart of today’s motors and generators, telecommunications and video/audio technologies – has been learned through neutron scattering. The DOE Nanoscale Science Research Centers (NSRCs) are designed to be the nation’s premiere user centers for interdisciplinary research the nanoscale, serving as the basis for a national program that encompasses new science, new tools and new computing capabilities.

Additional next generation tools are Linac Coherent Light Source (LCLS) is a revolutionary X-ray free electron laser that will allow probing of chemical and biological structures and examination of chemical reactions in real time at the single molecular level. National Synchrotron Light Source II is a state-of-the-art light source for X-ray imaging, capable of nanometer resolution of structures and features of individual atoms, molecules and crystals. **Kung** also reviewed major items of equipment such as Linac Coherent Light Source Ultrafast Instrumentation (LUSI) and Spallation Neutron Source Instrumentation II (SING II).

Next, Kung reviewed the Office of Science FY 2009 budget request to Congress for BES, which is approximately $300M, a 23.5% increase versus FY 2008 appropriations. For the Office of Science, the FY 2009 request is $748,827M, an 18.8% increase over FY 2008 appropriations. The majority of the request for BES is going toward research ($160,989M).

Kung reviewed the Energy Frontier Research Center Program. These centers are based on the scientific knowledge base of energy-relevant research that has been articulated through the series of 12 workshop reports and have the following distinguishing attributes:

- The research program is at the forefront of one or more of the challenges described in the BESAC report *Directing Matter and Energy: Five Challenges for Science and the Imagination*
- The research program addresses one or more of the energy challenges described in the 10 BES workshop reports in the BRN series
- The program is balanced and comprehensive and supports experimental, theoretical and computational efforts and develops new approached in these areas
- The program provides opportunities to inspire, train and support leading scientists of the future who have an appreciation for the global energy challenges of the 21st century
- The center leadership communicates effectively with scientists of all disciplines and promotes awareness of the importance of energy science and technology
- There is a comprehensive management plan for a world-leading program that encourages high-risk, high-reward research. The Center's management plan demonstrates that the whole is substantially greater than the sum of the individual parts.
- A number of EFRC awards will be initiated in FY 2009 based on an open competition among academic institutions, DOE labs and other institutions. Research activities may be sited at universities, DOE labs or in joint university-laboratory collaborations.
- The EFRC awards are expected to be in the $2-5M range annually for an initial five-year period. Pending Congressional appropriations, it is anticipated that approximately $100M will be available for multiple EFRC awards.
- A Funding Opportunity Announcement (FOA) will be issued in FY 2008 to request applications from the scientific community for the establishment of the initial suite of EFRCs
- As the EFRC program matures, it is anticipated that EFRC competitions will be held every two-to-three years and that renewal submissions will be openly competed with new submissions
- Out-year funding is subject to satisfactory progress in the research and the availability of funding appropriations
- While capital investment in instrumentation and infrastructure are expected as part of the EFRC awards, usage and leverage of existing facilities, including the BES user facilities, is encouraged
- Updates and further will be posted on the FOA through a link on the BES home page – http://www.sc.doe.gov/bes/.

Kung's preliminary thoughts for FY 2009 BES Core Program solicitations include:

- Pending Congressional appropriation, it is anticipated that up to $60M will be available for core research program awards in FY 2009

- Web announcement will be issued in FY 2008 to request applications from the scientific community as part of the Office of Science Financial Assistance Funding Opportunity Announcement
- While no limit is set for each of the awards, funding is primarily aimed at single PI or small-group projects with an initial funding of three years
- Examples of topical areas covered in the solicitations include:
    - Mid-scale instrumentation, ultrafast science, chemical imaging and emergent behavior
    - Basic research for electrical energy storage, advanced nuclear energy systems, solar energy utilization, hydrogen production, storage and use
    - Other research areas identified in the BESAC and BES workshop reports, with an emphasis on nanoscale phenomena
    - Accelerator research and development
- Further updates and information will be available through a link on the BES home page - http://www.sc.doe.gov/bes/)

Following the completion of the 10 BRN workshop reports by BES, **Kung** said "after five years, we are looking to BESAC to assist with two charges to tie together the aforementioned reports." This study has two primary goals: 1) to assimilate the scientific research directions that emerged from these workshop reports into a comprehensive set of science themes; and 2) to identify the new tools required to accomplish the science. This should include the consideration of future light sources with technical characteristics that will address the science questions posed by these BESAC and BES studies. This is predicated by the fact that the coherent interaction between light and matter lies at the heart of quantum control, which is one of the central themes of these reports and defines the new science frontier in the 21st century. Furthermore, the development of the next generation of light sources not only fulfills the Department's core missions, it also part of the unique contribution to the nation's scientific strength.

Kung acknowledged the BESAC members for 2008-09, with a focus on the newest members, **Simon Bare, Sharon Hammes-Schiffer, Michael Hochella, Bruce Kay, Kathryn Nagy, Douglas Tobias** and **John Tranquada.** She concluded by discussing the organization work chart for BES, the vacant positions and the three teams that now fall under Materials Sciences and Engineering Division – 1) Materials Discovery, Design and Synthesis 2) Condensed Matter and Materials Physics 3) Scattering and Instrumentation Sciences.

Hemminger asked the Committee if there were questions for **Kung**. Before she answered questions, Kung again acknowledged **Dehmer's** leadership, dedication and support over the past 12 years and said "Pat's vision is and will continue to be felt in every program. She has provided BES with a great foundation to grow. We have all benefitted significantly."

Bruce Gates asked with 700 proposals, would there be an assessment of how those proposals could have possibly impacted the science community?

Kung said "we are going to reassess to see if the proposals have the approach of what we have been looking for. We need to stimulate the community and do not want to see the same proposals continue to be resubmitted."

Laura Greene asked with the policy change, will only large centers be funded?

Kung said "no, each center will be looked at on an individual basis."

John Richards asked how does the $630M break down in research funding.

Kung said $580M will go to the two research divisions.

William McCurdy, Jr. questioned the charge to BESAC, but **Hemminger** asked if this question could be further discussed later in the afternoon.

Hemminger added that we do not want to confuse the funding with that of the research centers. He thinks the focus should stay on what the Committee is going to do in the future.

Eric Isaacs asked if there were any discussion in BES on the impact/effect on the scientific community?

Kung said **Ray Orbach** will touch on this subject later in the day.

Simon Bare asked what were the thoughts if these appropriations are not approved?

Kung said that we need to focus on offering support and meeting the criteria. "We need to put the best strategies together to move forward and to offer all of the support that is needed. We are not ready to give up."

Hemminger commented the budget request has been flat over the past three years. Facilities continue to decrease dramatically and to some extent and this is a very disturbing trend. He questioned if there are other facilities that should be turned off and thinks BES management should possibly be thinking about this issue.

Kung said "we are doing a lot of planning and is currently receiving very specific Congressional directional on how money should be appropriated."

Dehmer said "there has been and continues to be a lot of attention on Facilities, but research funding will continue to be cut. Research funding needs to be protected."

At 11:10 a.m., **Hemminger** requested a break.

At 11:30 a.m., **Hemminger** introduced **Eric Rohlfing** and asked him to provide an update on "Committee of Visitors (COV) for Chemical Sciences, Geosciences and Biosciences divisions." **Hemminger** said this information has been "tremendously useful in letting us know what resources we need."

Rohlfing reviewed the outline of his presentation, including the 2008 and 2005 COV, the changes in the division and the COV preparatory work. The 2008 COV Review of the BES Chemical Sciences, Geosciences and Biosciences division plans to meet April 23-25 and **Rohlfing** invited all BESAC members to attend.

Rohlfing shared the charge letter to COV to review the management processes for the Chemical Sciences, Geosciences and Biosciences Division of the BES program. The COV was asked to provide an assessment of the processes used to solicit, review, recommend and document proposal actions and monitor active projects and programs. **Geri Richmond**, University of Oregon, is the COV Chair.

The following is a more detailed breakdown of the charge:

- The panel should assess the operations of the Division's programs in FY 2005, 2006 and 2007 in the following areas: AMO Sciences, Chemical Physics, Photochemistry and Radiation Research, Catalysis and Chemical Transformations, Separations and Analyses, Heavy Element Chemistry, Chemical Engineering and Chemical Energy and Energy Resources
- The panel may examine any files during the review period for both DOE lab and university projects (subject to COI constraints)
- Two major review criteria:

  - Assess the efficacy and quality of the processes used to a) solicit, review, recommend and document proposal actions and b) monitor active projects and programs
  - Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected; a) the breadth and depth of portfolio elements and b) the national and international standing of the portfolio elements
- The COV panel is asked to provide input on the BES OMB Performance Assessment Rating Tool (PART) long-term goals

The COV Organization and Membership is similar to that from 2005, grouped into six panels. There are 36 total members of the COV (16 are currently funded by BES/CSGB and 20 are not).

The demographics of the Committee are:
- 25 men, 11 women
- 27 are from academia, six from DOE labs two are from the industry and one is from another Federal agency
- 13 are from the East, 10 from the Midwest and 13 from the West
- Nine are current or previous BESAC members
- Seven have served on CSGB COVs in 2002 and 2005 (**Rohlfing** added "This is very important for continuity.")

Rohlfing said there were several recommendations and actions from the 2005 COV, but he believed the following were the most significant:
- Program management database
  - Recommendation: Create a BES database for peer review/program management
  - Actions: Modest improvements in SC database (IMSC); more effective use of IMSC
- Improved proposal solicitation
  - Recommendation: Use "Dear Colleague" mailings to community, in addition to normal postings on SC Web site
  - Actions: Department Chair "Dear Colleague" lists developed and used for Chemical Imaging (FY 2006) and Solar Energy (SEU) (FY 2007) solicitations
- Long-term support for basic research and young investigator program
  - Continue "tradition: of long-term support, but also consider implementing a young investigator program
  - Action: A young investigator program is not feasible under current budget constraints. Award for BES PECASE winners coifed ($50k/yr for five years). BES solicitations have allowed more young investigators to be funded.
- Diversity
  - Recommendation: BES should collect demographic data on gender, race and career-stage and efforts should be made to ensure a diverse work force
  - Actions: Sc-wide demographic data collection system "in progress;" CSGB co-sponsored gender and URM equity in chemistry workshops with NSF and NIH
- Re-evaluate and re-focus Energy Biosciences program - integrate it within the Division
  - Recommendation: New program management should re-evaluate and re-focus program on BES missions; program should be better integrated with division
  - Actions: Under new program leadership (Rich Greene), program has been redefined into two components – solar photochemistry and physical biosciences. Significant shifts in the portfolio are underway. Team structure changed to foster improve integration.
- Program management staff
  - Recommendation: Division be given at least three new program manager positions
  - Actions: BES staffing budget n FY 2008 includes three new program manager positions in CSGB
- Portfolio prioritization

- Recommendation: in light of slat funding, prioritize the portfolio in order to continue supporting areas critical to DOE mission at appropriate level
- Actions: Significant prioritization accomplished

Changes in the CSGB division include:

- Organization changes
    - FY 2007: Chemical Physics program split into two parts: Gas-Phase Chemical Physics (combustion related) and Condensed Phase and Interfacial Molecular Science (CPIMS)
    - FY 2008: Created the new Photo- and Biochemistry Team from the Energy Biosciences program, plus the Solar Photochemistry program (from fundamental interactions); associated modest program name changes
- Significant program changes (portfolio optimization)
    - FY 2006-2008: Phase out of the Chemical Energy and Chemical Engineering Program
    - FY 2005-2007: Investment in ultrafast chemical science, principally in AMOS program
    - FY 2006: investment in chemical imaging across division
- Staffing
    - Significant changes in division staff since the last COV
    - Significant (but transient) understanding during upcoming COV

Rohlfing showed the organization chart from February 2005 and showed how it had changed over the past three years.

The CSGB budget distribution for FY 2007 appropriations was $221 million.

Solicitations with impact during the COV period:

- Notice 04-20, Basic Research for the Hydrogen Fuel Initiative
    - Published in FY 2004; awards made in FY 2005
    - Large, BES wide initiative that provided ˜$21M in new funds across BES; supplemented by ˜$3M in FY 2006
    - ˜38 awards assigned to several programs in CSGB; under renewal review in FY 2008 as an integrated program across BES
- Notice 05-30, Basic Research for Chemical Imaging
    - Published in FY 2005; awards made in FY 2006
    - Modest, CSGB only initiative that reprogrammed ˜$3M within CSGB
    - ˜17 awards in nearly every program in the division
- Notice 06-15, Basic Research for Solar Energy Utilization
    - Published in FY 2006; 27 awards made across BES with modest funding (˜$8M) in FY 2007
    - 14 awards in CSGB in Solar Photochemistry and Biosciences programs
- Notice 06-17, Basic Research for Hydrogen Fuel Initiative
    - Published in FY 2006; 13 awards made across BES with modest funding (˜$4M) in FY 2007
    - Six awards in CSGB in Catalysis Science program

The COV preparatory work includes a meeting on November 7 between **Geri Richmond** and Division. This was an opportunity for Chair to meet with the entire division to understand the structure and programs. Geri used this successfully as Chair of the 2007 COV for NSF Chemistry Division. She believed it was important to understand the differences between NSF and BES. The visit included divisional overview presentation, presentation on COV information and informal discussions between Geri and program managers/team leads in each program.

The next steps for COV is the completion of the membership drive, which was finished in December 2007; plans for COV Web site – now operational and will be updated with current information; additional teleconferences with Chair and with Chair/Panel leads before COV. Information for the 2008 COV: Prior to COV – via password-protected Web site (ORISE)

- COV roster (soon to be updated for second read assignments)
- Charge letter
- Reports from 2002 and 2005 COVs (links to BES Web site)
- Review procedures (links to BES Web site)
- Core research activity descriptions (links to BES Web site, with updated versions for COV)
- Published solicitations during COV period (links to SC Grants Web site)
- Logistical details (agenda, travel, lodging, etc.)

Information for the 2008 COV: During COV

- BES and Division overview presentation
- Topical overviews by team leads – topics to be determined (TBD), but most likely solicitations, lab reviews, etc.
- Program overview presentations
- Spreadsheet for each program showing every project (university and lab) that was active during three-year review period
- Selection of university and lab review files (new awards, renewals, declinations), plus access to all files (constrained by COI)
- COV report template (including OMB PART assessments)

At 12:00 p.m., **Hemminger** adjourned the meeting for a lunch.

At 1:40 p.m., **Hemminger** called the meeting back to order. The afternoon session began with **Hemminger** said the Committee should come up with a name to call the next charge to BESAC. The next charge is "follow-on" of the idea of BES and Office of Science described in the Grand Challenges. "We set up a sub-Committee of BESAC and looked at Chapter 7 to see which issues need to be further addressed." **George Crabtree** and **Marc Kaster** will Co-Chair the BESAC Sub-Committee Charge. The charge is to be completed over the next five years.

As discussed during **Kung's** presentation, **Crabtree** said the new BESAC Sub-Committee charge is "following the completion of the 10 BRN workshop reports by BES in the past five years and recent Grand Challenges study under the auspices of BESAC, BESAC is now embarking on a study to tie together the following reports: 1) to assimilate the scientific research directions that emerged from these workshop reports into a comprehensive set of science themes; and 2) to identify the new tools (implementation strategies) required to accomplish the science. Included in this should be the consideration of future light sources with technical characteristics that will address the science questions posed by these BESAC and BES studies.

Crabtree said this new charge "sets the stage for the main science drivers, what needs to be accomplished and the cross-cutting issues.

The charge is broken down into three components:

1) Summarize the range of scientific research directions that emerged from the 2002 BESAC report, *Basic Research Needs for a Secure Energy Future*, the follow-on BES BRN reports, and the BESAC report *Directing Matter and Energy: Five Challenges for Science and the Imagination.* Identify key cross-cutting scientific themes that common to these reports. In doing so, also make the connections between the themes that resulted from the "use-inspired" BRN workshops and those that resulted from the consolidation of the fundamental challenges that face our disciplines.
2) Summarize the implementation strategies and human resources that will be required to accomplish the science described in the aforementioned reports. These strategies may include new experimental and theoretical facilities, instruments and techniques. Consider

possible new organization structures that may be required to implement the strategies and supply the human resources. **Crabtree** added "There needs to be continued support between theory and experiments."

3) Identify future light sources needs that will be required to help accomplish the scientific challenges described in these workshops. Specially, consider the energy range (from vacuum UV to hard X-rays), coherence (both transversal and longitudinal), intensity (photon per pulse and photon per second), brightness (ultra-high brightness with low electron emittance) and temporal structure (nano to atto seconds) for future light sources.

Hemminger said he looked again at previous reports and workshops, especially Chapter 7 in the Grand Challenges Report. He said "we need BESAC membership to bring ideas to the table." He said everyone is busy, buts says he would like everyone to be a part of the Sub-Committee.

John Richards asked if this was being driven separately from BESAC.

Hemminger said we are going to make recommendations to implement strategies.

Laura Greene asked if it was a BES charge or DOE driven.

Hemminger said we are an advisory committee and should be providing advice or drivers on what BES should be doing.

John Richards asked if there was a timeframe or schedule to get this accomplished.

Hemminger said we typically have a BESAC meeting in late July-early August. By the next meeting, we hope to have significant progress and allow BESAC to provide feedback. There would also be a workshop possibly needed in the spring. If we follow that, we could possibly have a draft.

Eric Isaacs asked **Hemminger** if he could clarify more if we are to expand on Chapter 7.

Hemminger said we are simply helping BES to capture the attention of the next administration.

Kung said it should assist in justifying.

Bruce Gates said "we need to find the right volunteers to produce a working draft, and then the Committee could move quickly.

Hemminger agreed.

William McCurdy, Jr., said in #2 and #3 in the Sub-Committee charge, the last one has been an on-going question for years since there are many ways of looking at this information. He questioned how this is different from what is in the Grand Challenges Report.

Hemminger said there are cross-cutting, scientific themes and issues. It would assist the community to look at areas such as the multi-scale model.

Crabtree said we need to identify these cross-cutting areas.

Eric Isaacs said "we need to create a report that supports our efforts or find a way to implement our goals."

Bruce Gates said "there are new opportunities in looking at where something ends and where other things begin." He advised the Committee to "not look at the conceptual, but to look at what overlaps and match those with what is in the end report."

Dehmer said “we are making #1 more complicated than it needs to be.” “It is mind-numbing to explain task media files. The data needs to be compressed and be very pragmatic, make materials by design, and added “it should not take a lot of people too much time. Simply get to the main themes.”

Nora Berrah asked if the new centers **Harriett Kung** discussed this morning connected to this exercise.

Hemminger said this report will have multiple purposes.

At 2:30 p.m., **Hemminger** declared a break.

At 3:00 p.m., **Raymond (Ray) Orbach** was introduced and thanked all members of BESAC. He said “everyone would probably agree that we have some Grand Challenges. “I am probably going to use some strong language during my presentation because we are entering into a crucial period. We are still unable to satisfy getting certain things accomplished.”

Orbach said President Bush has great confidence in BESAC. He is still willing to back us and that is a positive situation for us to be in.” He added the President supports science work and that we need to work with the American public for them to understand it is in their best interest.

In looking at Office of Science FY 2009 budget request to Congress, the 23.5% increase over the FY 2008 appropriation is a *very* important appropriation. There is a significant amount of money being put into Fusion Energy Sciences and a large increase for Science Laboratories Infrastructure because our labs are aging rapidly. “Our budget is huge, 8/10 of a billion dollars,” **Orbach** said. We have some messages that need to be delivered and to have to bring our labs up to make them a pleasant environment.”

For BES, FY 2009 budget request is $1,568M. The FY 2007 appropriations were $1,221M and the FY 2008 appropriations were $1,270M.

There is a “heavy investment” in core research. Research activities are supported in FY 2009 in areas of condensed matter and materials physics, chemistry, biosciences, and geosciences with increased support in areas of solar energy utilization, electric-energy storage, basic research for the hydrogen economy, advanced nuclear energy systems and other energy-related research. “There is a major change in how we fund research, but we are getting positive feedback from the current administration,” **Orbach** said. To accelerate the rate of scientific breakthroughs in these areas, Energy Frontier Centers will be initiated to address Grand Challenges for Basic Energy Sciences. (FY 2007=$445.6M; FY 2008=$451.6M; FY 2009=$629.9M)

Facility operations are increased in FY 2009 to provide for optimal operations of the four light sources, three neutron sources and five Nanoscale Science Research Centers. (FY 2007=$547.9M; FY 2008=$555.8M; FY 2009=$593.5M)

The National Synchrotron Light Source II (NSLS-II) Project has FY 2009 supporting Project Engineering Design, as well as other project costs and construction for NSLS-II. NSLS-II will provide the world's finest capabilities for X-ray imaging and enable the study of material properties and functions at the nanoscale. (FY 2007=$25.0M; FY 2008=$49.7M; FY 2009=$103.3M). **Orbach** added “This has been reduced in magnitude.”

The Linac Coherent Light Source (LCLS) Project will continue construction and other project costs. Funding is also provided in FY 2009 to fully support operation of the SLAC Linac. (FY 2007=151.7M; FY 2008=$127.9M; FY 2009=$152.7M)

Instrumentation fabrication and other construction projects for major scientific user facilities and other construction activities (FY 2007=$39.8M; FY 2008=$43.8M; FY 2009=$49.3M). **Orbach** said this is a strong statement for our economy.
In addition, others included SBIR/STTR and GPP/GPE. (FY 2007=$11.4M; FY 2008=$41.1M; FY 2009=$39.5M). **Orbach** added, "We are very clear on what we want to build and operate."

Next, **Orbach** The Scientific Opportunities in BES were identified in The "Basic Research Needs" Workshop Series. He said the *Basic Research Needs for a Secure Energy Future* (BESAC) was an extraordinary collection and so important to the various areas-topics they cover, which include:

- *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*

Orbach said the Grand Science Challenges are "very exciting and interesting with all of the developments over the past couple of years. Congratulations to finding the following new and exciting research opportunities."

- 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

The FY 2009 Budget Request: A New Era for Science

- Energy Frontier Research Centers (~$100M/yr) - Innovative basic research to accelerate scientific breakthroughs needed to create advanced energy technologies for the 21st century. The awards to be $2M-$5M per year for an initial five-year period (then we will look at the progress).
- The Office of Science seeks to engage the nation's intellectual and creative talent to tackle the scientific Grand Challenges associated with determining how nature works, leading the scientific community to direct and control matter at the quantum, atomic and molecular levels, and harness this new knowledge and capability for some of our most critical real-world challenges.
- With Energy Frontier Research Centers, we will pursue fundamental basic research in areas such as: Solar Energy Utilization, Catalysis for Energy, Electrical Energy Storage, Solid State lighting, Superconductivity, Geosciences for Nuclear waste and CO2 Storage, Advanced Nuclear Energy Systems, Combustion of 21st Century Transportation Fuels, Hydrogen Production, Storage and Use and lastly, Materials Under Extreme Environments.

Orbach added, "We have moved funding opportunity announcement that will now tell what *you* want to do versus the old way of the RFD stating it." U.S. universities, DOE laboratories and other institutions are eligible. "This will allow universities to compete with labs, which in the past would not been permitted. This is a wonderful opportunity for the community to have their voice heard."

The FY 2009 budget request is a new era for science. World-leading facilities are driving transformational science and U.S. innovation, such as Spallation Neutron Source ($177.6M) and the High Flux Isotope Reactor ($58.8M). These two facilities together provide capabilities unavailable anywhere else in the world for study of the position and motion of atoms in materials – from liquid crystals to superconducting ceramics, from proteins to plastics and from metals to cell walls.

Four Synchrotron Light Sources - Advanced Light Source ($51.1M), Advanced Photon Source ($116.5M), National Synchrotron Light Source ($40.1M) and Stanford Synchrotron Radiation Laboratory ($33.0M) - are extraordinary tools for determining protein structures, probing the physical properties of new materials, and studying chemical reactions.

Five DOE Nanoscale Science Research Centers ($101.2M) provide unmatched capabilities for fabrication, synthesis and characterization of matter at the nanoscale.

The next generation tools, which are being constructed and remarkably successful include the LCL Source ($56.0M), a revolutionary X-ray free electron laser that will allows probing of chemical and biological structures and examination of chemical reactions in real time at the single molecule level and the National Synchrotron Light Source-II ($103.3M) – a state-of-the-art light source for X-ray imaging, capable of nanometer resolution of structures and features of individual atoms, molecules and crystals.

The BES Challenge
The Past and Present:

- The President's Request for BES in FY 2007 was $1,421M. The appropriation for BES in FY 2007 was $1,250M. (We lost $171M.)
- The President's Request for BES in FY 2008 was $1,499M. The appropriation for BES in FY 2008 was $1,270M. (We lost $229M.)
- The President's Request for BES in FY 2009 is $1,568M. The appropriation for BES in FY 2009 is an answered question.

"We have lost more than $400M over the past two years," said **Orbach**. He added that he did not know if the appropriations will go up or down in 2009. They will be looking for sources to cut unless we are able to justify our needs."

The future has many questions that need to be answered. The President's Request for FY 2009 is $298M more than the FY 2008 appropriation, the largest dollar increase for any of the Office of Science programs. BES could easily, again, become a "donor" program. This possibility, a "three peat" for BES, could doom BES to a flat- to declining budget for years to come. Compounding the danger is the widespread attitude in the scientific community that the proposed increases for the physical sciences under the ACI and America COMPETES act are "a done deal".

The goal for BES must be a world-class, vigorous and productive program, which balances key portfolio components together to create a uniquely DOE program:

- Fundamental research
    - in support of a mission-driven basic research
    - 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 U.S. 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 and we must make a case for long-term basic research, which is an investment in our future
    - The community and BESAC need to continue to develop a strategy to communicate the long-term BRN 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.

The Office of Science Challenge
The Past and Present:

- The President's Request for SC for FY 2007 was $4,102M. The appropriation for SC for FY 2007 was $3,813M, a loss of $289M.
- The President's Request for SC for FY 2008 was $4,404M. The appropriation for SC for FY 2008 was $3,903M, a loss of $501M
- The President's Request for SC for FY 2009 is $4,722M. The appropriation for SC for FY 2009 is still a question, but we have lost $790M over the past two years for research.

The Future:
The President's Request for FY 2009 is $819M more that the FY 2008 appropriation, a huge dollar increase. As mentioned earlier, SC could easily, again, become a "donor" program. If we are to avoid this scenario we need to actively and publicly make the case for <u>long-term</u> basic research rather than short-term applied research. It is now up to us to make the case.

Orbach concluded his presentation with a quote from President George Bush in his January 28, 2008 State of the Union Address. This statement was not in his original address and he personally added it. So now, it is up to the Committee:

"To keep America competitive into the future, we must trust in the skill of our scientists and engineers and empower them to pursue the breakthroughs of tomorrow . . . This funding is essential to keeping our scientific edge."

Laura Greene said "you tell us that we need to keep trying to reach the public and give us advice on how to educate the public and provide an outreach for the outside community to have a good feeling toward science. Can you provide guidance to the Committee what else we can do to make an impact?'

Orbach said that we should go to our Congressmen and Senators and tell them how important science is to our future. You have a tremendous opportunity to speak to political figures in ways that impact the scientific community. We need to take advantage of the intellectual strength of our nation. Pat, Harriett and I cannot do it alone."

John Spence asked if **Orbach** gets support from societies?

Orbach said "yes, they have been wonderful, but there is a naivety from some societies and we need to keep making the case over and over again. We have the American public who needs to hear an explanation so these initiatives and long-term research projects can jump-start the economy."

Orbach completed his questions with a thought," How long will foreign countries bail us out if we do not have economic stimulus?"

At 3:45 p.m. **Hemminger** began his BESAC Grand Challenges Report: *Directing Matter and Energy: Five Challenges for Science and the Imagination*. He began by stating the report was put together by several Sub-Committee members and co-chaired by **Graham Fleming** and **Mark Ratner**. He asked the Committee why are these Grand Challenges now? It is because of necessity and opportunity. In regard to necessity, it is critical that we continue to find the issues that we do not know much about. We recognize that the U.S. needs to do more short-term research to fix the current problems. In regard to opportunity, transformational science and understanding how nature works will lead to some new and exciting opportunities. **Hemminger** told a side story of how he was recently asked what was the most impactful thing to happen in his lifetime. He said because of all of the opportunities, he hopes it has not happened yet.

Hemminger said that we have continued to evolve over the past few centuries. "In the 21st century, control of matter and energy is going to go from observational science to controlling what happens. How do you change? We simply watch and look at nature versus getting nature to do what we want it to do."

In the Grand Challenges report, it was stated "During the 20th century, scientists developed increasingly sophisticated technologies and instrumentation for the study of quantum effects. Our understanding of these phenomena has reached the point where we are ready to move beyond simple observation and take the steps that will enable us to direct and control matter and energy at the quantum level."

Hemminger said that humanity's top problems over the next 50 years are energy, water, food, environment, poverty, terrorism/war, disease, education and population. In 2003, there are 6.3 billion people in the world. In 2050, it is projected there will be 8-10 billion.

In looking at energy, the environment and global change, technology, energy and society are inextricably intertwined. The U.S. overall energy needs to continue to grow and outpace our domestic supply. Until the mid-1950s, the U.S. was self-sufficient with energy. Now, our consumption and production has continued to grow further and further apart.

"The world energy needs will grow significantly in the 21st century," Hemminger said. "We need to look at potentials of U.S. renewable energy sources, such as wind, biomass, solar, hydroelectric and geothermal. The costs, ¢ (kw-hours) is $.25-.$.50 for solar, versus less than $.08 for oil, nuclear, wind, gas and coal (potentially the least expensive)."

In reviewing climate changes, we do not understand certain criteria about what has happened in the past to have the effect on our climate and its changes. **Hemminger** offered the example of abrupt climate change in the Younger-Dryas Central Greenland temperatures. There is an historic correlation between CO2, concentration and temperature.

There are Four Broad Energy Goals in the DOE Strategic Plan – Priorities, Operating Principals, Vision and Strategic Themes. With Priorities, scientific and technological innovation, nuclear security, energy security and environmental stewardship must be reviewed.

With Operating Principals, we need to:

- Ensure safe, secure and environmentally responsible operations
- Act with a sense of urgency
- Treat people with dignity and respect
- Make the tough choices
- Keep our commitments
- Embrace innovation
- Always tell the truth
- Do the right thing

In Vision, the results in our lifetime must ensure energy security, national security, science-driven technology revolutions and one DOE-keeping our commitments.

With Strategic Themes:

- Promoting America's energy security through reliable, clean and affordable energy
- Ensuring America's nuclear security
- Strengthening U.S. scientific discovery, economic competitiveness and improving the quality of life through innovations in science and technology
- Protecting the environment by providing a responsible resolution to the environmental legacy of nuclear weapons production

- Enabling the mission through sound management

There are Four Broad Energy Goals in the DOE Strategic Plan

1) Energy Diversity - Increase our energy options and reduce dependence on oil, thereby reducing vulnerability to disruptions and increasing the flexibility of the market to meet U.S. needs.
2) Environmental Impacts of Energy - Improve the quality of the environment by reducing greenhouse gas emissions and environmental impacts to land, water and air from energy production and use.
3) Energy Infrastructure - Create a more flexible, reliable, and higher capacity U.S. energy infrastructure.
4) Energy Productivity - Cost-effectively improve the energy efficiency of the U.S. economy.

Next, **Hemminger** detailed the five Grand Challenges for Science and Imagination.

1) How do we control materials and processes at the level of electrons? Making quantum systems work for us.

- Attosecond optical pulses, high intensity excitation
  - Failure of Born-Oppenheimer Approx.
  - Conical intersections
- Control of spins (spintronics)
- Quantum computing and the use of coherence in devices
- Quantum simulators

2) How do we design and perfect atom and energy-efficient synthesis of new forms of matter with tailored properties? Directing the “un-gluing” and “re-gluing” of electrons.

- Design for a particular electronic structure by finding the optimum combination of crystal structure and elements that yields (e.g. a specified band structure)
- Design for self regulation and even self repair of catalysts
- Low cost efficient solar cells
- Designing molecular logic
- Contra indicated properties (e.g. transparent conductors)
- Meta materials: perfect lenses, invisibility cloaks in the visible range

3) How do remarkable properties of matter emerge from complex correlations of atomic and electronic constituents and how can we control these properties? Uncovering the fundamental rules of correlations and emergence and learning to control them.

- Create successor to current semiconductors from strongly correlated materials (e.g. multi-ferroics combine and couple electric and magnetic action—electrical control of magnetism)
- Quantum correlated liquids
  - Quantum spin liquids: artificial photons, fractional quasi particle (error free quantum computing)
- Strongly correlated atoms --quantum emulators & simulators (e.g. tests of the Hubbard Model for cuprites)
- Soft matter
- Biology

4) Can we master energy and information on the nanoscale? Creating new technologies with capabilities rivaling those of living systems.

- Tap the existing world of biological nanotechnology by constructing interfaces between living cells and synthetic technology
- Fabricate devices with functionalities approaching those of living systems, but with different hardware implementation

- Nano-macro junctions: covering the gap from a few tenths to a few hundred nanometers (photonic, electrical and magnetic, mechanical)
- Defects and the end of Moore's law - adaptive probabilistic computing
- Energy transduction at the nanoscale - stochastic processes, signals and noise
- Ad hoc networking among nanoscale devices

5) How do we characterize and control matter very far away from equilibrium? Making non-equilibrium systems work for us (most systems are non-equilibrium).

- Nanoscale thermodynamics
- Molecular transport junctions
- Fluctuations; Design, complexity, robustness
    - energy-capture and energy-storage capabilities
    - mitigate environmental damage
- Molecular Exploring rough landscapes
- Jamming
- Science of life

In addition to the five Grand Challenges, there are some connecting themes, with an underlying set of concepts emerging – correlations coherence emergent properties, self-assembly regulation, BES Grand Challenge science, information and energy exchange and systems far from equilibrium fluctuations. We are on the threshold of a transition from observation science to control science at a much deeper level than is currently possible.

As stated earlier, **Hemminger** said he is still waiting and looking to understand what is the most impactful thing that has happened in his lifetime. These are strategies that BES should be moving toward.

The new BESAC Sub-Committee Charge, which will be co-chaired by **George Crabtree** and **Marc Kastner**, is stated below:

Following the completion of the 10 Basic Research Needs (BRNs) workshop reports by BES in the past five years and the recent Grand Challenges study under the auspices of BESAC, BESAC is now embarking on a study to tie together the aforementioned reports. This study has two primary goals: (1) to assimilate the scientific research directions that emerged from these workshop reports into a comprehensive set of science themes; and (2) to identify the new tools required to accomplish the science. Included in this should be the consideration of future light sources with technical characteristics that will address the science questions posed by these BESAC and BES studies.

1) Summarize the range of scientific research directions that emerged from the 2002 BESAC report *Basic Research Needs for a Secure Energy Future*, the follow-on BES BRNs reports, and the BESAC report "*Directing Matter and Energy: Five Challenges for Science and the Imagination.*" Identify key cross-cutting scientific themes that are common to these reports. In doing so, also make the connections between the themes that resulted from the "use-inspired" BRN workshops and those that resulted from the consolidation of the fundamental challenges that face our disciplines.
2) Summarize the implementation strategies and human resources (HR) that will be required to accomplish the science described in the aforementioned reports. These strategies may include new experimental and theoretical facilities, instruments and techniques. Consider possible new organizational structures that may be required to implement the strategies and supply the HR.
3) Identify future light sources needs that will be required to help accomplish the scientific challenges described in these workshops. Specifically, consider the energy range (from vacuum UV to hard X-rays), coherence (both transversal and longitudinal), intensity (photon per pulse and photon per second), brightness (ultra-high brightness with low

electron emittance), and temporal structure (nano to atto seconds) for future light sources.

In review, **Hemminger** restated the five Grand Challenges:

- How do we control materials processes at the level of electrons?
- How do we design and perfect atom– and energy–efficient synthesis of revolutionary new forms of matter with tailored properties?
- How do remarkable properties of matter emerge from the complex correlations of atomic or electronic constituents and how can we control their properties?
- How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?
- How do we characterize and control matter away—especially very far away—from equilibrium?

The Implementation Strategies include:

- Grand Challenge Science: the people and the tools required
- HR
  - Attracting and educating the next generation of students and young faculty
  - Stable funding for senior investigators
  - Team science
- Theory
- New laboratory-based instrumentation
- New facilities

As **Hemminger** closed his presentation, he asked the Committee if they had questions or comments.

Dehmer asked what type of response are you getting from the science audience?

Hemminger said the feedback has been good, but is not certain if the general public has a complete understanding.

Bruce Gates asked if we started over with another group of people, does he believe the Grand Challenges would be the same?

Hemminger said from a mechanism standpoint, we had a good core sub-Committee that reached out to their science community. He believed it would not be much different because the Challenges are robust.

Simon Bare commented if there was a way of taking a portion of the report, not popularize it, but make it easy to make our case? **Bare** said he thinks a small group should be formed to go out and speak to larger groups.

William McCurdy, Jr., said he believed the Grand Challenges will continue to tell the same story to the general public.

Hemminger said there will always be the question “If we do this, can we do that.”

Peter Cummings said we need more time to take a long-term look at these problems.

Hemminger said if we do a similar presentation, you must be “prepared to truthfully answer the questions. The audience is very smart and you must give intellectual and intelligent answers to their questions and be straightforward.”

Laura Greene recommended that someone be hired with structural design background. She believes this person should be someone who "truly understands how to communicate. The outreach needs to be impressive and results need to be measured."

Hemminger responded that he was not convinced the science message was getting lost.

Greene asked how do we communicate these messages outside of this room (to an external audience)? We need assistance in communication a core message we are trying to get across.

At 4:45 p.m., **Hemminger** asked for public comment.

Alan Hurd (Los Alamos National Laboratory) said the IPNS was closed in January 2008. He wanted to commend the facility for several great neutron projects that came from the facility. He believes neutron scattering is more important than ever, especially in correlated systems. Europe, Japan and China are building new sources and believes IPNS showed them the way.

Greg Exarhos (Pacific Northwest National Laboratory) thanked **Hemminger** for his presentation and said we can see evidence that there is a lot of work to do.

With no further public comment, **Hemminger** adjourned the meeting at 4:53 p.m.

Friday, February 22, 2008

Hemminger called the meeting to order at 8:32 a.m. He began the meeting by telling the Committee we would continue straight through the agenda with no breaks due to inclement weather. He promptly introduced **John Galayda** and asked for an update on Linac Coherent Light Source (LCLS).

Galayda provided a short overview to his presentation including:

- LCLS project status
    - History
    - Cost and schedule
    - Commissioning
    - Construction status
- LUSI project status
- First experiments
- LCLS performance enhancements future

There have been significant research opportunities since the first proposal was written in 1992. He briefly described the timeline of events:

1994 - National Academies Report
1996 - Design Study Group
1997 – BESAC Report
1998 - LCLS Design Study Report
1999 – BESAC Report
2000 - LCLS- the First Experiments
2001 – DOE Critical Decision
2002 – LCLS Conceptual Design
DOE Critical Decision
$36 million for Project Engineering
2003 – DOE Critical Decision – 2A
$30M in 2005 for Long Lead Procurements
2004 – DOE 20 year Facilities Roadmap
2005 – Critical Decision 2B Define Project Baseline
Critical Decision 3A Long-Lead Acquisitions

2006 – Critical Decision 3B Groundbreaking
2009 – First Light
2010 – Project Completion

The construction is greater than 75% complete. After FY 2010, the budget for TEC is $352M, OPC is $68M and TPC is $420M.

Next, **Galayda** provided a project overview, including a look at the location of the experiment hall, e-beam transports, conventional facilities, and the location of Linac with logistics to Argonne National Laboratory. He also discussed the injector commissioning goal were met and produced the specified currents.

With coherent effects in optical transition radiation diagnostic, total light energy is disproportionate with charge. The likely cause is coherent optical transition radiation from the electron beam. This is indicative of charge clumping on submicron length scale.

All undulator magnets have been accepted from the vendors. Thirty-nine (39) are at SLAC, one is at Argonne. The assembly of the undulator girders is on the project path for undulator commissioning. Several parts are, or are near, the limited factor.

There have been two experiments involved with this project – the XES Near and Far Hall Hutches and Beam line Layout. The soft X-Ray imaging has a collaboration forming and DOE funding is being sought. With high energy density science, the prospects for funding are encouraging.

The schematic of AMO instrument has a schedule of carrying design to completion in May 2008; build/buy and assemble July-December 2008; Assembly and Testing February-June 2009; and Ready for First Light July 2009.

LUSI Project Description
Prime performance parameters

- X-ray pump probe instrument (XPP)
  - 4-24 keV operation with pump laser
  - 2-d detector with 1024x 1024pixels
    - Large dynamic range, moderate pixel size
- Coherent x-ray imaging instrument (CXI)
  - 4-24 keV operation with focused beam
  - 2-d detector with 760 x 760 pixels
    - Moderate pixel size, central hole
- X-ray photon correlation spectroscopy (XCS)
  - 4-24 keV operation
  - 2-d detector with 1024 x 1024pixels
    - Very low noise, small pixel

Next, **Galayda** discussed the LUSI Status.

- Instrument scientists are on board

- Successful DOE Conceptual Design Review (last summer)
- CD1 approved
- Continuing Resolution: FY2008 budget reduced from $10M to $6M
- 2009 Budget requested $15M, will surely be delayed by Continuing Resolution (CR) Schedule impact being assessed
- CD2 review scheduled for May 2008
- LUSI-LCLS Interface Working Group recent business:
    - Conventional facilities
        - Details of hutch design, rack placement, etc.
- Controls/Data acquisition
    - Details of data flow, storage, interface to detectors
- Precisely defining LUSI/LCLS interfaces

Galayda discussed the submission of proposals, with **J.R. Schneider** at SLAC recently joining the facility. SLAC will announce within the year an opening for the permanent head of LCLS Science Program. Until then, the submission of proposals includes Pre-proposal workshops May 2008; Initial Call (Amo, XPP) June 2008; The first round of proposals are due August 2008; notification will be October 2008 and the schedule setting will be during the first quarter 2009.

A Conventional Facilities update was given, with **Galayda** stating construction completion was ahead of the 28 month duration. The first activity, survey network/monument placement took place in January of this year. Lastly, the anchors and stands in beam support hall are ready to be set.

Galayda closed his presentation by discussing opportunities and challenges facing LCLS. LCLS has unfathomed scientific potential and a clear field for many years to come. LCLS can define and stay at the forefront of ultrafast science with X-rays. The opportunities hinge on the priorities during the next 5-10 years. He also stated LCLS has gone through a reorganization and it reflects on how LCLS will operate in the future.

At 9:15 a.m., **Altaf Carim** was introduced and thanked everyone for their interest and support with the program. He provided a summary of “Nanoscale Science Research Centers (NSRCs) - Operational Review and User Access.”

Carim provided an overview of his presentation stating he would first provide an introduction and background, discuss policies and results for User Access and lastly, the process and outcomes with operations reviews.

Carim said the characteristics of the NSRCs are “basic information with what we are intended to accomplish. As you will see, there is a broad spectrum of activity.”

- Research facilities for synthesis, processing, analysis and characterization of nanoscale materials
- Provide specialized equipment, unique tools and dedicated scientific and support staff that are difficult for individual institutions to put in place and maintain
- Operated as user facilities and available to everyone. Access determined by peer review of proposals. No cost for Users precompetitive, non-proprietary work leading to publication; cost recovery for proprietary work.
- Co-located at DOE national laboratories with existing major user facilities (synchrotron radiation light sources, neutron scattering facilities and other specialized facilities) to leverage and provide complementary characterization and analysis capabilities

The five NSRCs are in operations and serving users. The facilities are located at the Center for Nanoscale Materials at Argonne National Laboratory, the Center for Functional Nanomaterials at Brookhaven National Laboratory, the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory, the Center for Integrated Nanotechnologies at Los Alamos National

Laboratory and Sandia National Laboratory and the Molecular Foundry at Lawrence Berkeley National Laboratory.

NSRCs provide new types several new kinds of capabilities, including X-ray synchrotron beam lines with nanoscale resolution. These are unique instruments to study individual nanostructures, offers quantitative structure, strain and orientation imaging and sensitive trace element and chemical state analysis. In addition, "Discovery Platforms" are modular micro-laboratories for nanoscience that are standardized and batch fabricated and provides access to a wide range of diagnostic and characterization tools.

Next, **Carim** provided definitions for users. Users are <u>researchers who propose and conduct peer-reviewed experiments at a scientific facility.</u>

- The primary type of user is a Badged User, i.e., a researcher who conducts experiments within the facility (majority of users)
- There are two other types of users who conduct experiments:
    - Remote User - a researcher who has been granted authority to remotely produce data (this excludes persons who can "look at data")
    - Off-Site User - a researcher to whom the facility provides custom-manufactured materials, tools or devices that the facility has unique or unusual capabilities to fabricate (only applies to NSRCs; starting 2007).

For both types of these users, only one user is to be counted per proposal regardless of the number of co-investigators and only if no individual is counted in any of the other user categories under the same proposal.

- For annual totals, an individual is counted as one user at a particular facility no matter how often or how long the researcher conducts experiments at the facility during the fiscal year

Starting FY 2007, there have been 774 total users – 626 Badged Users, 40 Remote Users and 108 Off-site Users. "We need to see what other users can be accommodated," **Carim** said.

With User Access, **Carim** said there are two types of users – General Users and Partner Users. General Users have access based on peer merit review of submitted proposal, evaluated by external Proposal Review Committee or equivalent. It includes on-site (Badged), remote and off-site users. Partner Users have access based on peer merit review of submitted proposal, evaluated by external Proposal Review Committee and/or by Scientific Advisory Committee. Partner Users enhance capabilities of and/or contribute to operation of facility, with benefits to the general user community, are defined and have a limited period of reserved time or preferential access. The large majority of time must remain available to General Users. A very limited amount of time may be allocated directly at the discretion of the NSRC Director or management for rapid access. Collaboration with facility scientists is an important potential benefit to users, but is not required. Facility staff may provide input on feasibility and time needed but do not select or approve proposals.

User agreements, authorities, intellectual property and related issues are extensively discussed among DOE-BES, DOE-General Counsel and NSRCs. Existing authorities and types of user agreements available for non-proprietary, essentially non-collaborative work and proprietary, non-collaborative work (full cost recovery). New authority and user agreement template has been developed for pre-competitive (non-proprietary), collaborative work. Existing authorities are available on case-by-case basis for proprietary and collaborative work (CRADAs, WFO, etc.).

The NSRC review process includes many steps:

- Review date determined and charge letter sent to facility director

- Facility prepares Review Documents (RDs) and submits to BES; additions/revisions if necessary
- Reviewers selected by BES and sent charge letter and RDs
- Agenda drafted by facility and finalized with input from BES
- On-site review
- Reviewers' individual, written reports received and collated by BES
- Program Manager debriefs BES management
- Review results communicated to Facility Director:
    - Letter with discussion of findings, BES observations, recommendations, and/or action items
    - Attached BES summary of reviewer reports
    - Attached verbatim (anonymized) full text of reviewer reports
- Formal facility response to review results and recommendations

With operations budget, **Carim** said NSCRs have been offered considerable latitude in defining how much of their annual budget is allocated to capital equipment in these early transitional years. BES entertained requests in FY 2007 for additional capital funds for relatively large, specific equipment items (at $0.2M - $2M each) based on science that would be enabled and on value to users. Funds available permitted two such requests to be supported: an automated nanoparticle synthesizer at the Molecular Foundry (LBNL), and a 160-node computational cluster at CNMS (ORNL). These requests and their consideration were distinct from the operational reviews.

BES reviews operating facilities on a three-year cycle. For the NSRCs, there is an on-site meeting, with individual evaluations submitted by external peer reviewers. There are additional evaluations of review documents by mail reviewers and fundamental review criteria (from charge letter to the facility). The same review criteria are stated in charge letters to reviewers.

In reviewing the documents, a companion document entitled "Review Policies for the Nanoscale Science Research Centers: Criteria, Process, and Documentation" was supplied to each NSRC as an attachment to the charge letter. In addition, a summary Review Document is required for Facilities Operation and Overview; a template is provided as part of the above document. This includes (as major sections) an executive summary, facility overview, instruments and laboratories, user access, impact, future directions and BES annual data submissions and survey results for prior three fiscal years. Furthermore, additional review documents are required for each existing or proposed scientific thrust area, following BES guidance at: http://www.sc.doe.gov/bes/Guide_for_Lab_Rev_Docs.pdf.

As stated earlier, Reviewers are selected by BES and sent charge letters and RDs. There are 44 total reviews received from 34 distinct reviewers. Some reviewers also participated recently or concurrently in reviews of research programs supported by other divisions of BES at the same laboratory and were asked specifically to comment on program distinctness and duplication. Thirty-three (33) of the reports were from on-site reviewers and the remaining 11 were based on evaluation of the review documents by mail. All reviewers were asked to comment on ES&H, but reviewers with specific expertise were included and asked to focus on this area.

Recognizing that this is an initial (baseline) review of a new facility that has only been in operations for approximately a year, we would like each reviewer to provide an individual evaluation addressing the following issues:

- Quality and quantity of the research performed at the facility in terms of number and impact of research publications, presentations and other outputs
- Appropriateness and quality of the facility staff research and development (R&D) program
- Satisfaction of the user community with the facility support and staff
- Overall availability of quality instrument time and capabilities to the user community
- What is the user demand at the facility?

- Evaluate the proposal review process for effectiveness and fairness in the allocation of time and resources
- Evaluate the fairness in the distribution of time and capabilities among users (i.e., facility staff versus outside users)
- Evaluate the appropriateness of the instrumentation to satisfy the present and future needs of the user community
- Evaluate the performance and cost effectiveness of the operation of major capabilities (i.e. cost of operating a specific signature instrument or cluster of related instruments in relation to its demand by users and its scientific productivity)
- Evaluate what is an appropriate level of research and development funding for efforts related to improving operations, instrumentation, sample preparation, upkeep, etc.
- How does the facility see its role in the nanoscience community as a whole, and in the scientific community at large?
- What is the expected future capability of the facility?

The agenda is drafted by the facility and finalized with input from BES. The typical operations review agenda is 2.5 days for NSRCs. The review includes time for plenary talks, breakouts, small groups, tours, posters and the executive session.

The results are reviewed and communicated to Facility Director. A letter is sent with discussion of findings, BES observations, recommendations and/or action items. An attached BES summary of the reviewer's reports and an attached verbatim (anonymized full text of reviewer reports are also included. The major areas of interest in review of NSRCs include:

- Quality (and quantity) of science
    - Research accomplishments and output
    - Number and nature of thrusts
- User program
    - Number of Users
    - Diversity of Users: new Users, non-host lab and geographical
    - Accessibility, ease-of-use and user satisfaction
- Environmental, safety, and health (ES&H) aspects
- Management and organization
    - Present management
    - Management structure
- Overlap/interaction with other BES, DOE, and non-DOE programs
    - Subject matter overlap
    - Staff sharing
    - Utilization by programs at laboratory
    - Collocated user facilities
- Advisory committees

Assessments of quality of individual scientific thrust areas and NSRC programs as a whole were largely positive, but did vary considerably. No concerns were expressed about quantity of output, though several comments noted that it was "too early to tell." Sample quotes from reviews:

- "In my view, the quality of the research is simply stellar."
- "High-quality research… impressive record of publications in prestigious journals."
- "Overall, this is an exciting research theme involving outstanding scientists working on cutting-edge research problems."
- "The general ideas are in the main stream of research, without major novel ideas being advanced."
- "Being realistic it seems that at some moment the decision will have to be made which areas to strengthen and which to abandon."

Some examples of NSRC science includes using DNA to guide controlled 3-D crystallization of nanoparticles, assembly of and charge transport in quasi-1D nanocrystal arrays (CNM) and producing defined protein nanotubes.

In general the user programs reviewed extremely well. Processes and demand were found to be robust, and access was regarded as fair and straightforward. A few reviewers were concerned, at some sites, about the low number of non-collaborative users thus far. Some sample quotes:

- "The review process is clear, fair and credible. The user program is first-rate."
- "(The) staff is dedicated to providing a productive environment for the user community... It will be important to pay close attention to both the efficiency of… staff as the user workload increases and ability of users to operate in a more independent, less collaborative mode."
- "There appears to be relatively little user program activity beyond the collaborative model… staff believe that users who simply want a particular material or device to be produced will increase sharply in the near future."
- "I am more than a little concerned about the establishment of a "club" atmosphere."

In most reviews, there was considerable focus on Environmental, Safety and Health (ES&H) aspects from a reviewer specifically tasked with this. Overall, the reviews very strong and positive, with many specific positive remarks. Remaining issues largely concern off-hours activities and ease and uniformity of training, with a few other very specific comments at individual centers.

The review outcomes in other areas included:

1) Management and organization
- NSRC Directors and management teams were widely praised in all reviews
- For several NSRCs, concerns about management or other organizational structure were raised
- Organizational changes are underway to respond to these concerns

2) Overlap/interaction with other BES, DOE, and non-DOE programs
- The NSRCs employ a variety of different staffing models. Review results included an emphasis on most NSRC staff having a large commitment (e.g., fraction of their time) in the center, to maximize ownership and clarify priorities. Adjustments have been made or are underway where necessary
- Subject matter and/or staff overlap between the NSRC and other BES-supported research programs was an issue in some limited cases; these are being addressed by BES-SUF, the BES research divisions and laboratories as needed.

3) Advisory committees
- Proposal Review Committees and equivalents were functioning well
- In some cases, Scientific Advisory and/or other management-level Committees were underutilized or disengaged; BES accordingly recommended actions to remedy this.

In closing, **Carim** provided a summary of NSRC review results to date, although he stressed these were initial baseline reviews, undertaken in some cases before the facility reached full operations and before any NSRC was fully staffed or had reached steady-state operations. As expected, scientific thrusts varied in strength and coherence within each NSRC and across NSRCs. The facilities were strongly encouraged to constrain scope and focus efforts where necessary. User programs are "off to a strong start across the board", with enthusiastic and productive users at all facilities. Oversubscription rates (proposal declinations) are moderate now but steadily rising and management of community expectations in this transitional environment is challenging. Each NSRC has taken concrete steps to address review recommendations, some complete and others still underway. The response to the prior review is one explicit component of each triennial review.

Nora Berrah asked if there was a structure to working at the centers and asked if he been in touch with BER.

Carim said yes, proposals should be accessed to all users and that he had been in touch about review reports and had received a strong reaction from the community.

Hemminger said there are many high profile staff opportunities and asked how the staffing was progressing.

Carim said CNS is fully staffed. The other three are more than 50%, but agreed there are still many high-level openings. There have been some scientists that have come from other laboratories and also some young scientists. He added that he had been pleased with the staffing process, but feels there are still some great opportunities out there for the right person.

At 10:25 a.m., **Randy Ogle** was introduced and asked to provide an update on "DOE Nanoscale R&D Environment, Safety and Health." Ogle said there is great potential, good funding and big (ES&H) questions. He began his presentation by summarizing the history of the project, dating back to the 1950s. One of the highlights was finally receiving funding from former President Clinton in 2000. The National Nanotechnology initiative is steering U.S. activities, funding R&D and funding environment, safety and health R&D, largely toxicity testing.

Thus far, what do we know about Nanoparticle safety? The human experience with nanoparticles in air -- we have evolved in an atmosphere of Nanomaterials. The size and material characteristics relate to ES&H. The potential effects include increased toxicity, flammability, and reactivity (Controlling Nanoparticle exposures is straightforward), Risk is a function of the degree of hazard (e.g., toxicity) and exposure and lastly, the perception and communication are very important.

According to the *San Francisco Chronicle*, Nanotechnology could revolutionize science, technology, medicine and space exploration, but could also ravage the environment, eliminate jobs and lead to frightening new weapons of war. Those are two extreme takes on the hottest, and potentially most controversial, new technology since biotech and PCs.

Ogle said "there has not been a lot of new, emerging information over the past 3-4 years regarding toxicity." There are a number of factors that include:

- Depends on chemistry, morphology, surface charges, etc.
- Probably relates to particle surface area especially for insoluble/low soluble
- Benign residence
- Free radicals (in vitro)
- Increased inflammatory response (in vivo)
- Translocation to target organs (rodents)
- Allergic asthma symptoms
- Aggravate symptoms of pneumonia
- Cardiac effect - two days later

The size is important. Surface area as dominant characteristic contributing to toxicity is plausible. Controlling the nano-hazards can happen by agglomeration a function of time, enclosed reactors, ventilation, encapsulated in processes, among others.

The R&D safety within DOE and specifically in the NSRC includes Integrated Safety Management (ISM) followed from inception in the NSRCs; NSRCs are designed to accommodate the planned R&D; ES&H and projected R&D staff designed individual labs and controls and used experience, benchmarking, and best available control technologies.

The NSRCs collaborated on design and execution, including environmental, safety, and health issues. In addition, they shared construction safety experiences and information on Nanosafety. In 2003, Operations/ES&H people began informal teleconferences with BES-ES&H, developing guidelines for Nanosafety and initiated informal communications with NIOSH. Today, there is chartered (by NSRC Directors) activity and members are involved in consensus standards development.

Next, **Ogle** provided a look at general Nanoscale safety at the NSRCs. NSRC laboratories are User facilities, with safety programs and training tailored to Users. ES&H for R&D includes substantial interactions with subject matter experts and planning and said “the NSRC research staff is integral.” There are interactions with NIOSH and Environmental Protection Agency (EPA). To the extent possible, hazards are engineered out of the proposed R&D activities. The currently accepted approach to nanotechnology and other new technologies is known as prudent avoidance (avoid unnecessary exposures).

Nanoscale Safety at the Center for Nanophase Materials Sciences (CNMS) is similar at all NSRC Labs. Safety envelopes are set for each lab, with limits on hazardous activities are preset and can be modified through “work planning.” CNMS strictly controls access to labs. HEPA systems are used for all free-nano activities. CNMS ES&H has used the NSRC sampling methods to affirm safety (emissions) for current activities. Guidance has been provided to CNMS staff on waste handling and lastly, Nanoscale safety training has been developed and is available to all nanotech researchers.

Today, Nanoscale R&D is common in DOE research and at DOE labs. The DOE labs have a common safety program, the Integrated Safety Management (ISM). In 2005, DOE issued a Nanoscale R&D policy statement. Currently, DOE facilities are implementing the Nanoscale R&D policy as DOE tracks the progress.

Ogle completed his presentation by stating said he does expect a lot of requirements from OSHA or EPA.

Hemminger asked for public comment. With no additional remarks, **Hemminger** adjourned the meeting at 11:05 a.m.