**Minutes for the**
**Basic Energy Sciences Advisory Committee (BESAC) Meeting**
**November 20-21, 2008**
**Hilton Washington DC North/Gaithersburg**
**Gaithersburg, Maryland**

**BESAC members present:**

Simon Bare
Nora Berrah
Sylvia Ceyer
Sue Clark
Frank DiSalvo
Mostafa El-Sayed
George Flynn (Friday only)
Bruce Gates
Laura Greene
Sharon Hammes-Schiffer
John Hemminger, Chairman
Michael Hochella
Bruce Kay
William McCurdy, Jr.
Daniel Morse
John Richards
John Spence
Kathleen Taylor (Friday only)
Douglas Tobias (Thursday only)
John Tranquada

**BESAC members absent:**
Peter Cummings
Kate Kirby
Martin Moskovits
Kathryn Nagy

**Also participating:**
Michelle Buchanan, Oak Ridge National Laboratory
George Crabtree, Argonne National Laboratory
Patricia (Pat) M. Dehmer, Deputy Director of Science Programs, Office of Science
Don DePaolo, Lawrence Berkley National Laboratory/UCB
Franz Himpsel, University of Wisconsin-Madison
Michael Hochella, Virginia Polytechnic Institute and State University
Helen Kerch, Basic Energy Sciences
Harriet Kung, Director, Office of Basic Energy Sciences
Ray Johnson, Technical Writer/Recording Secretary
Pat Looney, Brookhaven National Laboratory
David Miller, Idaho National Laboratory
Michael Norman, Argonne National Laboratory
Arthur Nozik, National Renewable Energy Laboratory
Eric Rohlfing, Basic Energy Sciences
John Sarrao, Los Alamos National Laboratory
Jerry Simmons, Sandia National Laboratory
Karen Talamini, Office of Basic Energy Sciences

Approximately 110 others were in attendance in the course of the two-day meeting.

**Thursday, November 20, 2008**

BESAC Chair **John Hemminger** called the meeting to order at 1:01 p.m. He began the meeting by asking each Committee and Sub-Committee member to introduce themselves and their respective affiliations.

At 1:07 p.m. he introduced **Harriet Kung,** Director, Office of Basic Energy Sciences, to provide news from the Office of Science (SC).

**Kung** began her presentation by providing an outline of her presentation. She would be providing a budget update, the status of Energy Frontier Research Center (EFRC) and single-investigator and small-group research (SISGR), a staffing update and what will be happening in the coming months with the new presidential administration.

Since 2004, there have been four major hurdles in the SC budget formulation each year (from **Pat Dehmer's** December 2004 BESAC discussion). Inside the SC (February-April), each Associate Director (AD)-ship determines the program priorities within constraints of the funding guidance provided by the Director of SC. Each AD presents program priorities to the Director of SC. The Director of SC determines program priorities within constraints of the funding guidance provided by the DOE.

Second, once inside the DOE (April – July), the Director of SC and the DOE Assistant Secretaries present their program priorities and cases to DOE. The DOE determines the overall agency priorities. The SC prepares the President's budget. Each SC AD is responsible for preparation of AD-ship budget, with the department deciding what to forward. "This is a very lengthy process. It takes more than one year to influence a budget, with very deliberate and careful planning to influence the outcome," said **Kung**.

Third, (August-December) the DOE budget (with various program elements) is submitted to the Office and Management and Budget (OMB). Each AD defends the program budget at OMB hearing in early September. OMB provides "passback" guidance to DOE in late November. Then, there are discussions between the DOE and OMB to refine final budget numbers. SC prepares the President's budget. Each SC AD is responsible for preparation of AD-ship budget.

Lastly the President's budget is presented to Congress (FY February). In March-September, agencies present their budgets to Congress in formal hearings. Congress appropriates funding for 13 appropriation bills for the next two fiscal years, using the President's budget as a starting point for the Congressional budget and appropriations.

FY 2009 will be a very unusual year for budget planning and execution. For FY 2009 CR, it is expected March 6. For FY 2010, OMB "passback" for Congressional budget preparation is uncertain and does not provide a lot of time. Initiatives for FY 2011 are also uncertain. "We need to be ready to respond immediately. It is critically important to have strongly justified programs for FY 2010 and 2011," **Kung** said.

The SC FY 2009 Budget request was examined. In FY 2007 appropriations, Basic Energy Sciences (BES) had $1,221,380,000. In FY 2008, BES had $1,269,902,000. In FY 2009, the request to Congress was $1,568,160,000, an increase of $298,258,000 (+23.5% increase, based on the past two years). For FY 2009, the request to Congress versus FY 2008 appropriations is $748,827,000 (+18.8% increase) for all of SC.

The summary of FY 2009 BES budget increases includes $160,989,000 for research, with more than $100 million for EFRC. The rest will relate to the Grand Challenges. The facilities have been working under significant restraints, with more than $20M for light sources and $17.9M for neutron sources, $10.1 for NSRCs. For construction, NSLS-II at Brookhaven National Laboratory (BNL) will have more than $53.5 million increases; LCLS + linac operations and instruments will have $33.7 million, which is a significant commitment. Each component is based on strategic planning coming from researchers in the community.

**Kung** proceeded to provide a summary of BES HEWD (House) and SEWD (Senate) marks and impacts.

The House mark includes the Committee recommendation for BES is $1,599,660,000, an increase of $31.5M over the budget request. For research, an additional $17M is provided to accelerate the completion of the LCLS LUSI project for LCLS operations to enable substantially more science to be done in the early stages of the operation of LCLS while it is the only x-ray free electron laser in the world.

This funding includes $100M to enhance basic energy research for EFRC activities. This Committee has long advocated. There will be open competition for research funding that features head-to-head competition between national labs and universities. In addition, the House mark supports the Department's decision to broadly compete the EFRCs in this manner. For the construction, the funding includes an increase of $14.5 million over the budget request for continued PED, as well as to initiate construction of NSLS II at BNL.

The SEWD (Senate) mark provides $1,415,378,000 for BES. Of these funds, $145,468,000 is provided for construction activities as requested in the budget. The remaining $1,269,910,000 is for research. Within the research funds provided, $17M is for Experimental Program to Stimulate Competitive Research (EPSCoR). Of the decrease, $59,495,000 of basic solar research is moved to the EERE solar energy research and development program.

The impacts of the Senate mark include the 1) move of solar research from BES to EERE, which would affect approximately 300 researchers. The funding for solar will be minimized. 2) The $152,782K reduction from the President's request would make initiation of the $100M EFRC program more difficult.

**Research** - The BES programs status under CR and beyond was discussed. "For research, everything has been put at the 2008 level. This has caused significant restraints due to the uncertainties," **Kung** said. This includes significant financial concerns on DOE

labs and university programs, leading to possible staffing losses because of the uncertainty of the FY 2009 appropriations. The BES research programs need the FY 2009 funding request to maintain adequate staffing and level of effort after the CR. The new basic energy research direction of the proposed EFRCs and the corresponding effort in single-investigator and SISGR, which have been purposefully identified by numerous major scientific workshops, would significantly enhance the ability of solving the daunting energy and environmental challenges facing the Nation. The accumulated result of three consecutive years (FY 2007-FY 2009) of virtually no appropriations for new areas of basic energy research would be an enormous loss for the U.S. scientific enterprise.

**User Facility Operations** – The supplemental appropriation in FY 2008 has mitigated potential staff layoffs at BES user facilities through the first six months of FY 2009. Under a six-month CR, the operations will run at 80-90% of the optimum level, with a commensurate loss of approximately 300 users. If this should last longer, it will affect staffing and research, which will then have a significant impact on impact and growth. The BES synchrotron light sources and neutron scattering facilities are counting on the FY 2009 under appropriations near the FY 2008 levels.

**Construction and Major Items of Equipment (MIE)** – The FY 2009 request is needed to fulfill construction and MIE commitments. Failures to fulfill such commitments will lead to cost and schedule growth and staff impact at DOR labs due to the planed "ramp-up" of the following projects: NSLS-II, LCLS, ALS USB, and SING –I and SING-II. "We need to articulate the compelling need to basic energy for future prosperity," **Kung** said.

Next. Kung discussed the important dates for the EFRC and SISGR. For ERFC:

- February 23, 2008 – Discussion at BESAC
- April 4, 2008 – Funding opportunity announcement published
- July 1, 2008 – Letters of Intent due (more than 250 letters received)
- October 1, 2008 – Full proposals due (approximately 260 were received)
- February 2009 – Merit reviews
- April 2009 – Awards to be made (pending appropriations)

For SISGR:

- February 23, 2009 – Discussion at BESAC
- April 1, 2008 – Web announcement released
- June – October 2008 – Collect whitepapers (received significant number)
- January 2009 – Notification of PIs of whitepaper decisions
- March 2009 – Full proposal due (tentative)
- June 2009 – Awards made (pending appropriations)

EFRCs are seen are engaging the talents of the nation's researchers for the broad energy agenda. The DOE Office of Science, Office of BES, announced the EFRCs program.

EFRC awards are $2-5 million per year for an initial five-year period. Universities, labs and other institutions are eligible to apply. EFRC will pursue collaborative fundamental research that addresses energy challenges and science grand challenges in areas such as:

- Solar energy utilization
- Catalysis for energy
- Electrical energy storage
- Slid state lighting
- Superconductivity
- Geosciences for nuclear waste and $CO_2$ storage
- Advanced nuclear energy systems
- Combustion of 21$^{st}$ century transportation fuels
- Materials under extreme environments
- Conversion of biological feedstocks to portable fuels
- Others (possible)

This does not involve bricks and mortar construction. This will be reviewed/re-competed after the initial five-year award period and periodically thereafter.

The EFRC application statistics included approximately 260 applications, involving 385 institutions. The applications were from 41 states and the District of Columbia (DC), with investigators coming from 45 states and DC. Of all of the applications received, 71% were from universities; 13 from DOE labs; and 16% from other institutions (for profit, non-profit and individual). There are approximately 3,800 investigators (PIs and co-PIs) with 98% from the U.S. and 2% from 26 foreign countries. There were an average of 15 investigators and 4.8 institutions per proposal.

The ERFC proposal distribution by BRN category: Energy Sources (46%), Cross-cutting (18%), Energy efficiency (11%), Energy storage (11%) and Others (14%). Energy sources include solar energy utilization, advanced nuclear energy systems, bio-fuels, geological sequestration of carbon dioxide. Crosscutting includes catalysis for energy and materials under extreme environments. Energy efficiency includes clean and efficient combustion, solid-state lighting and superconductivity. Energy storage includes hydrogen research and electrical energy storage. The “Others” are not related to BRN or the Grand Challenge Report. All EFRC applications need to address one or more of the grand challenges in the BESAC report *Directing Matter and Energy: Five Challenges for Science and the Imagination.*

**Kung** provided EFRC proposal and PI breakdown by Federal region. The region encompassing Minnesota, Wisconsin, Michigan, Illinois, Indiana and Ohio had 20% of the proposals and 19% of the investigators. California and Nevada had 16% of the proposals and 14% of the investigators. The southeastern region including Florida, Georgia, Alabama, Mississippi, Tennessee, South Carolina, North Carolina and Kentucky has 14% of the proposals and 16% of the investigators.

Next, **Kung** discussed tackling our energy challenges in a new era of science. Pending appropriations, up to $60M will be available for single-investigator and small-group awards in FY 2009. BES seeks applications in two areas: grand challenge science and energy challenges identified in one of the Basic Research Needs workshop reports. Awards are planned for three years, with funding in the range of $150/$300k/yr for single investigator awards and $500-$1500k/yr for small-group awards. Areas of interests include:

- **Grand challenge science:** ultrafast science; chemical imaging, complex and emergent behavior
- **Tools for grand challenge science:** mid-scale instrumentation; accelerator and detector research (awards capped at $5M over 3-year project duration)
- **Use inspired discovery science:** basic research for electrical storage; advanced nuclear energy systems; solar energy utilization; hydrogen production, storage, and use; geological $CO_2$ sequestration; other basic research areas identified in BESAC and BES workshop reports with an emphasis on nanoscale phenomena.

**Kung** provided a status of the SISGR. There were 879 whitepapers, with 88% coming from universities; 11% from DOE labs and 1% from other institutions. Energy sources accounted for 31%; Grand Science Challenges and Tools (28%); Energy storage (16%); Cross-cutting (15%); and Energy efficiency (10%).

**Kung** proceeded to providing a staffing update of the Office of BES. Currently, "we are very well-staffed. We have been advocating for our staffing and it is due to **Pat Dehmer's** foresight and our future needs." Since July 2008, there have been five new managers hired. Currently, there is one vacancy in Materials Chemistry in the Materials Sciences and Engineering Division. There are two vacancies, Nano-science Centers & E-beam Centers and Accelerator and Detector R&D, in the Scientific User Facilities Division. In the Chemical Sciences, Geosciences and Biosciences Division, there is only one vacancy – in the Physical Bioscience department.

Before concluding her segment, **Kung** looked at six big challenges for BES.

1) Execute well all of our on-going projects/initiatives and transition them to robust operation and programs – TEAM, LCLS, NSLS-II, etc.
2) Make SC – and especially BES – synonymous with energy research. We must increase the understanding of the magnitude of the problems facing society, gain support for a plan of action and lead in executing the plan.
3) Execute the EFRC and SISGR plans to foster, encourage and accelerate high-risk, high-reward basic research to provide the knowledge foundation for transformative energy technologies of the future.
4) Advance the next generation of tools (very high on the agenda).
5) Integrate more effectively our activities in the universities and the DOE labs and with those at the DOE technology programs

6) The BESAC New Era Subcommittee and the Photon Workshop will start the process to furthering strategic planning and developing a communication strategy for long-term basic research support.

"**Pat Dehmer** has lead us to make great strides in putting BES on the map," said **Kung**. "There have been many obstacles to overcome in the past and we need to execute our plans very carefully to be prepared for additional obstacles. We have some of the bets talents in the industry and I am confident that we can be responsible to advancing to the next generation of tools needed for BES."

**Hemminger** asked if there were any questions from the Committee or Subcommittee.

**Mike Hochella** asked if it was possible to hold over the winners in the EFRC?

**Kung** said: "we have a limit of time. We hope that does not happen and we can move forward. We need to make the case clear. Currently, we are not making or considering a "Plan B."

At 1:42 p.m. **Hemminger** introduced **Patricia (Pat) Dehmer,** Deputy Director for Science Programs and requested an update from the Department of Energy (DOE) Office of Science.

**Dehmer** began her presentation by stating that "we are in the middle of an economic meltdown." We are anxiously waiting to see what changes will occur with the new presidential administration.

The stimulus package will probably happen very soon, if not until President Obama takes office. "Currently, there are a lot of rumors out there right now, but honestly, we do not know a thing. We do know that we are in a great flux."

There will be a 10-week transition, with three (principal) team leaders. All three are highly credentialed and are from former President Clinton's administration. These principals are asking for briefings about programs. They want a "high-level view" and all information has to be available. Pat defined the mission of the Office of Science and stated how the group supports major scientific challenges, societal challenges and energy research.

**Dehmer** also looked at the DOE organizational structure. The profile shows a staff of approximately 1,000 (730 in the field and 264 in the headquarters). The budget for FY 2009 is $4,721,969,000, an increase of $748,827,000 over FY 2008.

She said labs must continue to be funded and workshops should continue to take place.

The major programmatic responsibilities are to support fundamental research, support, and scientific users facilities for the nation, oversight of 10 DOE labs and research and

development coordination and integration. “There is a huge degree of commitment from BES.”

The top leadership challenges is to support fundamental research, support of scientific user facilities, oversight of 10 DOE labs, R&D coordination and integration and filling top-level, top management positions.

**Dehmer** asked: “If there is a stimulus bill, what kind of infrastructure can we put into field. What kind of jobs can be created? What kind of clean, green jobs can be created? How much money is needed?

Next, **Dehmer** spoke about “New Science for a Secure and Sustainable Energy Future.” She said it was a very good, well written and interesting and we need to provide feedback by tomorrow. She urged to cover the important points because we cannot get to the next generation without it.

“This is going to be a difficult year,” **Dehmer** said. “This will be a signature year because of the new administration is going to look at signature projects. We need to make a case for photon science, which is so important for science and technology.”

**Mostafa El-Sayed** asked where the money comes from for nuclear energy?

**Dehmer** said: “she did not have a clue.”

**John Richards** asked if her group was responsible for pension plans. She replied “No.”

**Bruce Gates** asked about the transitional team and if any of them were scientists.

**Dehmer** said she did not recognize all of the names.

With no additional questions from the Committee**, Hemminger** thanked **Dehmer.**

At 2:07 p.m. **Hemminger** began discussing the New Era Subcommittee and the charge to BESAC. The charge included identifying the underlying science drivers that would justify the next generation of facilities/light sources identification. The audience for the output of this Subcommittee is the Office of Science and BES. We need to identify the new types of science that can be done using light sources.

Next, **Hemminger** questioned what are the science drivers? In late October, there was a workshop that brought a strong contingent of people from the science community. **Franz Himpsel** was the Co-chair of the workshop and will put together a report. This will most likely be presented at the late February/early March BESAC meeting and will provide BES and the Office of Science with a better understanding of the fundamental sciences regarding the Photon workshop.

At 2:14 p.m., **Hemminger** introduced **Franz Himpsel**, University of Wisconsin-Madison, to provide an update concerning the BESAC New Era of Science Subcommittee: Photon Workshop Report.

**Himpsel** began his presentation by identifying the charge to the New Era Committee – Identifying future light sources that will be required to help accomplish the scientific challenges described in previous workshops on Basic Research Needs and Grand Challenges. In considering the following "photon attributes:"

- Energy range (from vacuum UV to hard X-rays)
- Coherence (both transversal and longitudinal)
- Intensity (photons per pulse and photons per second)
- Brightness (ultra-high brightness + low electron emittance)
- Temporal structure (nano- to atto-seconds)

The charge to the participants of the Photon workshop included: identifying connections between major new research opportunities and the capabilities of the next generation light sources. Find "killer applications" (things we can't live without) in basic energy research. Emphasize energy-related research and like sciences, which is a big part of light sources. Consider both accelerator-based light sources and novel laser sources for the VUV to x-ray range. Do not consider the design of the light sources, only the required photon attributes (what kind of photons do we need?). Lastly, have a strong coupling of theory and experiment.

There were more than 100 participants at the workshop, which is chaired by **Himpsel** and **Wolfgang Eberhardt**. There were two overview discussions – one by **George Crabtree** (Energy) and the other by **Keith Moffat** (Life Sciences). There were four discussions on next generation light sources:

- Free Electron Lasers **(Pellegrini)**
- Energy Recovery Linacs **(Hofstaetter)**
- High Harmonic Lasers **(Sandner)**
- Next Generation Storage Rings **(Martensson)**

During the two-day workshop, there were nine breakout groups, with extensive discussions taking place, "hashing out" details of the workshop and writing up the highlights, which took 1½ days. The breakout group discussed nanoscale electrons and spins, correlated electrons, catalysis and chemistry, nano-materials for energy applications, life sciences, atomic and molecular physics, matter under extreme environments/environmental science/earth science, novel structural and electronic materials and the crosscutting issues. These breakout groups generated approximately 80 pages of exciting discussions and key specific opportunities.

The findings were five crosscutting challenges amongst three groups:

1) **Designing Materials and Controlling Processes: The Synthesis-Analysis-Prediction-Loop (Group A)**
    a. Materials: Complex materials with correlated electrons, operating devices, batteries, supported catalysts, organic conductors for photovoltaics, lighting, quantum-engineered cluster assemblies
    b. Interfaces: In-situ, buried, nano-structured, bio-inorganic, sequestration, grain boundaries in solar cells and superconductors, damage in nuclear reactor materials
    c. Catalysts: For artificial photosynthesis, splitting water, in realistic situations (presence in gases, liquids)
    d. Static measurements (time resolved in 2, spatially-resolved in 3, both in 5)
2) **Real Time Evolution of Electrons, Spins and Bio-Chemical Reactions (Group B)**
    a. Find efficient and economical ways of harvesting sunlight to produce electrical or chemical forms of energy (photosynthesis, photovoltaics)
    b. Reactions at defects (loss of electrons, radiation damage, in *real time*)
    c. Chemical reaction mechanisms in *real time*
    d. Spintronics: How fast can one switch spins
    e. Movies of proteins in action
3) **Single Nano-Objects (Group B)**
    a. Clusters: From an atom to a solid, tailoring new forms of matter
    Nanocrystals: Beating the size distribution
    b. New materials: Find the electronic structure of a small crystallite
    c. Large protein assemblies: From proteomics to cells
4) **Statistical Laws of Complex Systems (Group C)**
    a. Fluctuations of floppy spins and soft materials at the nanometer scale
    b. Utilize the *full coherence* and high degeneracy of a laser
    c. Utilize a shaped pulse to reach the minimum uncertainty product
5) **Small and Fast (Group C)**
    a. Resolve the coupled motion of electrons and nuclei
    b. Imaging of elementary chemical reactions at the molecular level
    c. Electrons travel nanometers in fem-to-seconds, challenging the limits of combined spatial and temporal resolution

Three different groups described the challenges for future light sources. Group A described the widest range of applications, largest User community and the least aggressive in terms of machine requirements (but clearly beyond available light sources). Group B described new types of experiments, demanding a new kind of light source. There are a sizable number of applications and the potential to become the centerpiece of next generation light sources. Group C is the most aggressive, but also highest risk and lowest number of Users.

The findings were four scientific themes:

1) Tailored materials
2) Understanding the phenomena

3) Physics and chemistry at the atomic and molecular level
4) Life sciences and medical applications

There are a substantial number of nuggets with applications in energy and life sciences were developed by the discussion reports and incorporated into the report.

**Himpsel** completed his presentation. **Hemminger** asked the Committee for comments.

**Bruce Gates** requested a better understanding of the different groups – Group A, B and C.

**Himpsel** stated in was the way the New Era Committee chose to break down the information. Designing materials, controlling processes is Group A. Real Time evolution of electrons, spins, bio-chemical reactions and single nano-objects are Group B. Statistical laws of complex systems are Group C.

**Gates** asked **Himpsel** to describe the experiment in Group B.

**Himpsel** said that most techniques used in the experiment are things we might already be doing.

**Daniel Morse** asked if Section A should be the leading section.

**William McCurdy Jr.,** believes the introduction should state what we can do. There is clearly an argument, but it is imperative that we address what is going to happen over the next 15 years.

**Gates** said he thinks that **Himpsel** should write the report, but not assume the final report will be the final version.

**Himpsel** said if he had to re-write the information, he would need to get approvals and discuss all of the suggestions and revisions with everyone who contributed.

At 2:47 p.m., **Hemminger** introduced **George Crabtree,** Argonne National Laboratory, to provide a BESAC New Era of Science Committee Report and challenged the BESAC Committee and Subcommittee members to provide Crabtree feedback on the report. It was also mentioned that **Marc Kastner**, Massachusetts Institute of Technology, was unable to attend the meeting due to a illness.

**Crabtree** began his presentation by thanking all of the New Era Subcommittee members who participated in the project, with many being present at the meeting. **Crabtree, Marc Kastner, Michelle Buchanan, Thomas Mallouk, John Sarrao, Michael Klein, Arthur Nozik, Julia Phillips, Sue Clark, Frank DiSalvo, Don DePaolo, Simon Bare, Wayne Hendrickson, Wolfgang Eberhardt, Franz Himpsel, Michael Norman, Andrea Cavalleri, Carl Lineberger, Yet-Ming Chiang** and **Pat Looney**. **Roger Klaffky, Michael Casassa** and **Jim Horwitz** provided technical support.

The charge included three components that needed to be addressed:

1. **Science** - Summarize the BESAC and BRN reports on Energy and Grand Challenges for Science, identify the most important and crosscutting scientific themes and make the connections between the grand energy and grand science challenges.
2. **Implementation** - Summarize the implementation strategies, and human resources (HR) that will be required to accomplish the science described in these 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. **Light source science** - Identify future light source needs that will be required to help accomplish the scientific challenges described in these workshops. Specifically, consider the photon attributes needed to address future science grand challenges. (This report will come out in late January/early February).

The objective was to present the case for basic research to solve grand energy and science challenges in accessible language. “We hope the report will be taken to DOE,” said **Crabtree**. “Our goal was to not make it too technical.”

The context is energy. There are two transformations – energy is undergoing a transition to greater sustainability. The drivers are finite fossil resources, which are being used faster than they can be made; insecure access; pollution from combustion, greenhouse gas emission. Second, the drivers are “pretty well” appreciated by the audience.

Greater sustainability changes the way we produce, store and use energy.

| **Traditional Energy** | | **Sustainable Energy** |
|---|---|---|
| | | |
| Combustion | | Conversion (not combustion) |
| | | |
| Heat engines, | | Solar, wind, hydroelectric, |
| Steam, internal | | biomass, geothermal |
| combustion, turbines | | |
| | | |
| Transportation | | Electricity/Plug-in hybrids |
| Electricity | | Bio-fuels/transportation |
| Space and water heating | | Geothermal/space and water |
| | | heating |
| | | |
| Materials: commodity fuels | | Materials: needs to be very |
| Cheap, high energy content | | sophisticated, complex, |
| Fossil, biomass | | functional. Photovoltaics, |
| | | catalysts, electrodes, |
| | | membranes for batteries and |
| | | fuel cells |

**Crabtree** looked at the context being energy with traditional combustion and sustainable conversion. We are going to be in between for the foreseeable future. Clean coal $CO_2$ captures sequestration, nuclear waste proliferation and high efficiency, high temperature, extreme environments.

**The Context: Energy and Materials**

| Traditional Energy materials | | Materials for greater sustainability |
|---|---|---|
| | | |
| Coal, oil, gas, $CH_{0.8}$, $CH_2$, $CH_4$ | | Solar cells, water splitting, bio-inspired solar synthesis, electrical storage, fuel cells, membranes and chemistry for CO2 capture, extreme temperature, radiation, corrosively |
| | | |
| Function: combustion | | Function: conversion among light, electrons, chemical bonds: separation, robustness |
| | | |
| Commodities | | Multi-functional materials, complex structures and dynamics, precise nanoscale architectures decades long lifetime |
| Cheap, high energy | | |
| content | | |
| | | |

**Crabtree** said that science is undergoing a transition from observation to control. In the $20^{th}$ century, science included observational tools such as electron microscopy with atomic resolution and scanning probe microscopy. The materials discoveries included high temperature superconductors and carbon nanotubes. In the $21^{st}$ century science, we are directing matter and energy with chemical change and charge, spin and light interactions. The material designs are smart, self-healing materials, nanoscale fabrication and theory and computation, emulating structure and dynamics, lead synthesis.

The messages are that greater energy sustainability requires designed functional materials of greater complexity. These materials come from advances in basic research. Specifically, new complex materials and precise control of chemical charge, tools that penetrate the ultra-small and ultrafast and understanding based on theory, modeling and computation. The intersection of the need for materials of greater complexity and the transition from observational to control science creates a tipping point for energy sustainability.

The vehicle for these messages to occur is to imagine a secure, sustainable energy future. We need to focus on the vision of desirable outcomes. It defers the question of technical barriers. Lastly, it presents science as a problem solver and a source for future technological and economic growth.

The recommendations are to be brief, high level and easy to read; target the decision to fund science; and implementation details left to later discussion with BES.

**Crabtree** concluded his presentation asking for feedback and that "word-smithing." He also questioned if we have the right content and are the main messages correct.

At 3:00 p.m., **Hemminger** declared a break and requested all Committee and Sub-Committee members return by 3:30 p.m. and be prepared to offer Crabtree advice on how to make the report stronger, whether it was by "word-smithing," the recommendations, introduction, conclusion or evidence.

At 3:37 p.m., **Hemminger** called the meeting back to order. He told the Committee and Subcommittee that this time is an opportunity to review **George** and **Mark's** report. **Hemminger** said he would like to "review the report in segments and make sure that are hitting the target." He questioned if the main message needs to be "re-targeted and if the wording and message needed to be made clearer."

**John Richards** said the report makes it clear we need to explore new technology instead of technology that has already been developed.

**Bruce Gates** said the major goal is for basic research. He believes we are meeting the challenge.

**Laura Greene** stated she was "happy with the report and how issues were addressed," but thought one of the issues was the structuring. She believes that super-conductivity still needs to be researched and that there is still a lot that we do not understand. We also should not stress the Manhattan Project because it was and still is controversial. She also suggested making the report more "inviting."

**Douglas Tobias** believes the Manhattan Project is a good example because of its enormity. He believes what is missing it is aimed not at something we can take credit for, goals we can get accomplished in a certain timeframe (2-6 years).

**Nora Berrah** said the funding is very important.

**Hemminger** questioned the age of the readers and if they would understand the examples that are provided.

**Frank DiSalvo** questioned if we are confusing the message and who is ultimately responsible for getting these things accomplished? DOE? "We are still looking at needing oil and gas for another 30-50 years. We need to discuss the breakthroughs and how future oil and gas can be clean as possible."

**Hemminger** requested clarification from **Kung** or **Dehmer** regarding BES's involvement.

**Kung** said DOE will work with development and training in research programs. There is a need to highlight the importance of workforce development.

**Bare** referenced coal and questioned if coal is really clean. We should focus on carbon. He liked the how the technical hurdles are equally handled in this report. The timeline should focus on things that we can accomplish quickly.

**Hemminger** said putting a timeline with years on it is dangerous. He recommended stating phrases like "short-term" or "long-term." We want to invent technology we can export to the rest of the world. "We not only have to convince the U.S., but those all over the world, such as the Chinese."

**Sharon Hammes-Schiffer** said we should focus on the "short-term with the greatest payoff."

**Sylvia Ceyer** said there should be a greater emphasis on basic science and examples of fundamental research for the readers.

**William McCurdy, Jr.,** asked: "what is the overall message or are we just skimming." It is like the Apollo and Manhattan Project. The impact of this report at the beginning somehow gets lost by the end."

**Mostafa El-Sayed** said we need new discoveries, more research and fresh ideas.

**Bruce Gates** said the statement that says coal is clean needs to be changed to say this is a huge challenge.

**Sharon Hammes-Schiffer** questioned the overall structure and said after looking at the first two pages and then the last page, she believes the last page needs to be stronger. The bullets need to be shorter, increase the rate of discovery and the nature of the discovery. She suggested a team with different backgrounds. She said you do not always know what will come out of fundamental research.

**Bruce Kay** said he did not believe the people doing the work and working on the team is stressed enough.

**Nora Berrah** encouraged young scientists to come together. We need to stress the importance of the young generation and how they are needed. But, the report affords them. She believes the report lacks the urgency of addressing the issue. She also believes that the facts are provided in the report, but needs to be presented in a more exciting way to show the potential and discoveries. She believes this is too "low-key."

**Daniel Morse** said nuclear is mentioned a couple of times. He questioned if the report says if nuclear is just around the corner. Are we adequately defining the other sectors against the nuclear argument?

**DiSalvo** said: “in talking scale, we need to have a number of nuclear or bio-fuel be the answer. What is the scale needed and what is the rationale? He suggested including a section on how we are going to address these issues as well as solar.”

**Crabtree** said with nuclear energy, we need new reactors, which will require new materials.

**Gates** said that something in the report needs to state something about regulations efficiencies in the field. We need to recognize that we need to do, but that isn’t enough. We need to quantify it.

**Hemminger** said we need contribution from all energy sources. The origin is based on what do you do with existing technologies and how can you make it better.

**Richards** said **Pat Dehmer** was passionate this morning about BES and the Office of Science. He said we need to state what we are going to export instead of import. The Manhattan Project was a 10-year project. The DOE has a stellar history of collaboration. We need to make the point the Office of Science does huge, grand scale projects.

**Bare** said the BRNs are in the recommendations, and suggested putting some history in the foreword. The Grand Challenges came out of the BRNs. We must use strong, enthusiastic words. He suggested an appendix on all of the workshops.

**Hemminger** said an appendix had previously been discussed.

**Ceyer** said: “We need to be concerned about making the report too long. She also stated the blue boxes were repetitive because the information is stated in other areas of the report.”

**Gates** thinks there is a substantial issue with using the word “material.” He said we need to make it clearer and define what exactly we mean when we say material because it could be confusing to the reader. He suggested using more specific examples and talk in terms that people understand.

**Michael Hochella** said we are at a critical crossroads. He thought it was a great document and written at the right level. The mission is the urgency and the drama.

**Bare** questioned if the bullet points at the beginning of the report “sell the document.” The science should sell it.

**Hemminger** believes putting the urgency at the beginning and on the last page is a good idea.

**Hammes-Schiffer** said: “We need to present to our audience that we are talking about extinction.”

**Dehmer** said we should be careful in the report not to come across as "hysterical."

**Hochella** believes we will never run out of energy if we use it wisely. Energy conversion is the key. The report should discuss the immediacy. Things that are predicted in the 1950s are happening faster than predicted.

**Gates** questioned the bullet points at the beginning hold the truths that the report must maximize basic energy research will meet the needs.

**Tobias** said the emphasis and tone is very positive. It is necessary to use existing technology. Basic Research Science is not the only way to fix the problem.

**Hemminger** said no one has said we shouldn't say Applied Sciences. We need to focus on the basic fundamentals of science. In order to solve the problem long-term, we need transformational discoveries.

**DiSalvo** added research is a worthwhile investment.

**McCurdy Jr.** said the report has a nice balance in the conclusion and the contents in the report.

**DiSalvo** said: "it goes back to scale, we have 400 nuclear reactors and 100 are in the U.S."

**Hemminger** said: "In general, the people who have read the report are happy, but some details need to be worked on. We need to have some 'word-smithing.' We need to add some material not currently included in the report. We need to make sure the size of the report does not 'balloon.' The information does not need to be too 'expansive.'" He recommends the Subcommittee and Committee members work together this evening to gather and look at all of the comments discussed and come back in the morning and make suggestions on how to make the report stronger and then we can get additional feedback."

At 5:01 p.m., **Hemminger** asked for public comment.

**David Miller**, Idaho National Laboratory, just returned from a conference and said it was discussed repeatedly that regulators are now starting to be concerned over environmental omissions. "This is a complicated problem and time is of the essence." **Miller** also said there are many rumors in the field that there will be a significant reorganization of the DOE.

**Jerry Simmons**, Sandia National Laboratory, said the Apollo and Manhattan Projects each had a specific goal. He believes what is missing is a metric that will succeed. "The stretch goal will be very tricky. We must present our projects as concrete, even if they are tentative."

With no additional public comment**, Hemminger** adjourned the meeting at 5:07 p.m.

**Friday, November 21, 2008**

At 8:32 a.m., **Hemminger** called the meeting to order. He introduced **Karen Talamini** who requested all BESAC members must sign and provide the "Conflict of Interest" form before the end of the day's meeting.

At 8:34 a.m. **Hemminger** introduced **Simon Bare** to provide an update on the upcoming Committee of Visitors (COV) of the BES division of Materials Sciences and Engineering. The 2008 meeting will be held March 30-April 2, 2009 in Germantown, Maryland. **Bare** provided an outline of his presentation, reviewing the 2990 COV charge, organization and membership. This charge is for FY 2006 – 2008. He will also review the 2006 COV, the recommendations and actions. The charges are usually for a three-year period. He will also look at the changes to DMSE and the COV preparatory work.

The COV charge includes:

- The panel should assess the operations of the Division's programs in FY2006, 2007, and 2008 in these areas:
    - Materials Chemistry and Bio-molecular Materials, Synthesis and Processing Science, X-ray and Neutron Scattering, Electron and Scanning Probe Microscopy / Ultrafast Science, Experimental and Theoretical Condensed Matter Physics, Mechanical Behavior and Radiation Effects / Physical Behavior of Materials
- 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 OMB Performance Assessment Rating Tool (PART) long-term goals

"We need to make sure we have the right people for the right projects," **Bare** said.

**Bare** will be serving as the chairman of the COV. The panel members will be represented by those funded and not funded by BES/Division of Materials Sciences and Engineering (DMS&E), originating from universities, national labs and the industry, gender diversity, prior COV experience, geographic diversity and those from Experimental Program to Stimulate Competitive Research (EPSCoR) states.

There are six proposed panels for the 2009 COV organization and membership. The first panel will be to discuss Electron and Scanning Probe Microscopies & Ultrafast Science and Instrumentation**. Frances Ross** from IBM and the 2006 COV has been invited to be the panel lead. The second panel will discuss Physical Behavior of Materials and Mechanical Behavior and Radiation Effects, with **Robert Hull** from RPI being panel lead. The third panel will discuss Materials Chemistry and Bio-molecular Materials, with **Sam Stupp** from Northwestern University being invited to serve as the panel lead.

The fourth panel will be lead by **Rob Dimeo** from NIST to discuss X-ray and Neutron Scattering Science. The fifth panel will have **Brian Maple** from UCSD serving as the panel lead for Experimental and Theoretical Condensed Matter Physics. The sixth panel will discuss Synthesis and Processing Science, with **Ivan Bozoviv** from Brookhaven National Laboratory serving as panel lead.

Bare said there were major recommendations upfront and that BES came back with the following actions in 2006:

- Program management database
    - Recommendation: Create an effective information management system
    - Action: BES to work with SC management to improve current system
- Workload of program managers (under-staffed)
    - Recommendation: aggressively expand recruiting of program managers and support staff
    - Action: BES-wide staffing plan developed. Several new positions allocated in FY07
- BRN workshops
    - Recommendation: planning and resources for BRN's should continue and be expanded
    - Action: DMS&E will lead the electric energy BRN and staff will participate in future FY07 & FY08 workshops
- Laboratory and university support
    - Recommendation: balance of support between these two entities should be determined by open competition
    - Action: BES uses standardized peer review process
- Multi-investigator awards
    - Recommendation: BESAC should be used as a sounding board for development of university-based multi-investigator programs
    - Action: Number of multi-investigator grants at universities has increased. BES agrees that exploring this implication would be an important topic for BESAC.

The vision of the DMS&E is to provide the knowledge base for the discovery and design of new materials with novel structures, functions, and properties to drive the frontiers of discovery science and to address grand energy challenges. The three major themes are:

1) Scattering and Instrumentation Sciences

2) Condensed Matter and Materials Physics
3) Materials Discovery, Design and Synthesis

Next, **Bare** reviewed what led to the need for change at DMS&E. There were emerging scientific opportunities, the need to strengthen the focus on scientific themes, strength synergy among CRAs and scientific themes, the balance between discovery science and use-inspired science, balance between strengths in current research portfolios and future growth opportunities and striving for a more division-wide investment strategy.

The new DMS&E structure has each team having a set of central program scope and goals. There will be a close coupling and connection between the teams, discussing the three following topics: Condensed matter and materials physics (control and understanding of materials behavior and discovery of new emergent phenomena); materials discovery design and synthesis (rational design and synthesis of new materials via physical, chemical and bio-molecular routes); scattering and instrumentation sciences (study of photon, neutron and electron interactions with matter for characterization of materials structures and excitation).

**Bare** continued by looking at the Materials Sciences and Engineering division work chart. **Helen Kerch** is the acting division director. There are also several new program managers. In the coming weeks, there is a list of preparatory work and items that need to be completed. The completion of panel leads should be completed by the end of November. The completion of panel members will be completed by mid-December. The group will establish a password protected website for all members to access and share information by the end of January 2009. There will be an all-day visit to BES by **Bare** to meet with program managers in February 2009 to fully understand the structure of the DMS&E and the different programs. The COV will be held March 30 - April 2, 2009, with all BESAC members invited to attend.

**Hemminger** thanked **Bare** for his presentation and said there is an excellent argument for additional staffing.

At 8:47 a.m., **Hemminger** said **Crabtree** had met the Committee and Subcommittee members to get their comments and suggestions.

**Crabtree** began his presentation by thanking all Committee and Subcommittee members for their time and input to the New Era October Report. Some of the major revisions will include replacing importing expensive fuels with exporting valuable technology; enhancing science for clean coal and advanced nuclear, in addition to fully sustainable technologies; include biomass to fuel, a technically easier task than $CO_2$ to fuel, which is mentioned in the report and an important partial contribution like clean coal and nuclear; a clearer distinction between fundamental science and engineering needs to be made clear; strengthening prose on first and last pages, scale and urgency and make it more exciting and forceful; “use-inspired basic science” to project societal benefit.

In addition, it was recommended **Crabtree** indicate the scale such as identifying the problems by number of power plants or area for solar required. Scale requires contribution from all energy sources; state the uniqueness of BES for solving this big problem, utilizing university-lab resources, large interdisciplinary dream teams and facilities; add inside cover references to BRNs and Grand Challenge reports; add an introductory "about this report" to the beginning; remove repetition from boxes; and refers to laser success story.

**Crabtree** also requested that all Committee and Subcommittees members provide edits via hard copy or by email.

The recommendations were that there is a big problem that needs game changing solutions, producing entirely new technologies for the economy through an effort commensurate with the size of the problem. The solution is through control science and high-risk/high payoff directions. The dream teams are interdisciplinary, focus on the challenges and perform science holistically. Lastly, we must attract and nurture new talent for sustained effort.

**Hemminger** said the Subcommittee worked hard to incorporate the changes into the report.

**DiSalvo** said that science is really important and the report will emphasize the long-term nature of the problem.

**Richards** said: "good things happen when good things come together." We need technology and science. He suggested being careful about making BES look like revolutionaries."

**Hammes-Schiffer** said the report needs to state the foundation, solid science and that a lot of hard work needs to be done. She also suggested adding a statement or phrase concerning the sense of urgency. "We need to start now to initiate new science and new programs.

**Spence s**uggested adding a slide and image regarding atomic scale, with 3-D atomic resolution.

**DiSalvo** said it could be a good idea to include a slide show or video on the BES Web site. "It could be interesting and provide some new opportunities."

**Hochella** said we should get "controlled science" across better.

**McCurdy Jr.** said that we talk about technology and believes the draft "should state science will inspire technology."

**Hemminger** said we have had an opportunity to provide feedback and now believes that it is important to move forward with the report. We now need to help the Subcommittee come up with a final draft.

BESAC members accepted the motion.

**Hemminger** asked for public comment.

With no further comment, **Hemminger** adjourned the meeting at 9:15 a.m.