Minutes for the Basic Energy Sciences Advisory Committee (BESAC) Meeting July 24-25, 2008 Marriott North Bethesda Hotel and Conference Center North Bethesda, Maryland

BESAC members present:

Simon Bare
Nora Berrah
Sylvia Ceyer
Peter Cummings
Mostafa El-Sayed
George Flynn (Thursday only)
Bruce Gates
Laura Greene
Sharon Hammes-Schiffer

John Hemminger, Chairman Kate Kirby William McCurdy, Jr. Kathryn Nagy John Richards Kathleen Taylor Douglas Tobias John Tranquada (Thursday only)

BESAC members absent:

Sue Clark Frank DiSalvo Michael Hochella Eric Isaacs Bruce Kay

Also participating:

Carolyn Bertozzi, Lawrence Berkley National Laboratory Michelle Buchanan, Oak Ridge National Laboratory Yei Ming Chiang, Massachusetts Institute of Technology George Crabtree, Argonne National Laboratory Patricia Dehmer, Director, Office of Science for Basic Energy Sciences, USDOE Wolfgang Eberhardt, Technische Universitat Berlin Wayne Hendrickson, Columbia University Linda Horton, Oak Ridge National Laboratory Ray Johnson, BESAC Technical Writer Mark Kastner, Massachusetts Institute of Technology Helen Kersch, Basic Energy Science Michael Klein, University of Pennsylvania Harriet Kung, Associate Director, Associate Director for Basic Energy Sciences, USDOE Carl Lindberg, University of Colorado Pat Looney, Brookhaven National Laboratory Emilio Mendez, Brookhaven National Laboratory Michael Norman, Argonne National Laboratory Arthur Nozik, National Renewable Energy Laboratory Julie Phillips, Sandia National Laboratories Geri Richmond, University of Oregon Adam Rosenberg, House Science Committee

John Sarrao, Los Alamos National Laboratory Leslie Shapard, Oak Ridge Institute for Science and Education Stephen Streiffer, Argonne National Laboratory Karen Talamini, Office of Basic Energy Sciences Toni Taylor, Los Alamos National Laboratory

Approximately <u>140</u> others were in attendance in the course of the two-day meeting.

Thursday, July 25, 2008

BESAC Chair **John Hemminger** called the meeting to order at 8:35 a.m. He began the meeting by stating there were several Sub-Committee members sitting with the regular Committee members. These members will be a part of a discussion for later in the day and the Friday morning session. He also stated there was a lot on the agenda that needed to be discussed and requested each speaker stay on schedule as much as possible.

At 8:38 a.m. **Leslie Shepherd** made announcements concerning administrative, safety and convenience announcements. Next, **Hemminger** had the Committee and Sub-Committee members introduce themselves.

At 8:42 a.m. **Hemminger** asked **Patricia Dehmer** to update the Committee on the activities of the Office of Basic Energy Sciences (BES). **Dehmer** began her presentation by stating that **Raymond (Ray) Orbach** could not attend the meeting and that she came in his place. **Dehmer** reviewed the Office of Science organizational structure. She said all three of the Deputy Director positions had been filled. She also stated **Kung** had been named the Associate Director of the Office of Science. She congratulated **Kung** and said the competition for the position was very strong. **Kung's** appointment was effective June 9, 2008.

Next, **Dehmer** provided an overview of the House Appropriations Energy and Water Development (HEWD) Committee General Comments. "The Committee recommendation provides additional funds over the request for the Office of Science and supports the projected doubling of this area of research and development funding over the decade, from 2006 to 2016." **Dehmer** said this is very important and that HEWD wrote a lot of narrative describing what they wanted to see in the future. She also stated this was "very good for the Office of Science."

In research priorities and coordination, **Dehmer** provided an overview, stating the Committee was pleased the Department had taken steps in the right direction, including the completion of 20 planning workshops arranged by SC in consultation with the applied technology programs; integrated budget documentation for six key research and development areas; and the proposal to fund more than two dozen Energy Frontier Research Center (EFRCs). The Committee directs the Department to continue to support and expand these efforts and take the steps needed to ensure that research and development (R&D) integration is implanted at all levels across the Department in planning, budgeting and execution. The Department is directed to provide the Committee with a report detailing progress on these efforts no later than March 1, 2009.

Dehmer did say it was not all good news. Unfortunately, the budget request woefully underfunds many critical applied energy research and development activities in the applied energy technology programs, particularly EERE. This Committee strongly rejects this unbalanced approach by providing robust funding for applied research and development to complement increases in basic science. The Committee directs SC to work with the energy technology programs to identify priority, long-term applied science efforts that should be considered for enhanced investment by the applied technology programs, jointly with the Office of Science as appropriate. The Department is directed to provide the Committee with a report detailing progress on these efforts no later than March 1.

In regard to the Office of Science, the Committee is pleased with the efforts made by the Department to improve energy R&D integration across SC and with the applied energy programs. The Committee is concerned, however, that the integration efforts have been either top-down, being undertaken at the level of Under Secretaries or unique events, such as workshop series and EFRCs. The Department should institutionalize mechanisms for coordination to ensure that these efforts are no longer the exception but the rule and integrate such coordination with the Department's processes for planning, budgeting and execution. With these additional steps, the Committee believes that the Department will make substantial progress in bridging the divide between basic science and applied technology, one of the main motivations underlying proposals for the creation of a new Advanced Research Projects Agency-Energy (ARPA-E).

Next, **Dehmer** provided a summary of the 2009 Energy and Water Appropriations:

- The Sub-Committee legislation would provide **\$27.016 billion** for the Department of Energy. This level is **\$1.124 billion** over the President's budget request.
- Energy and Efficiency and Renewable Energy programs would receive more than \$1.9 billion, which is \$673M over request and \$206 million above FY 2008
- Electricity and Energy Reliability would receive \$166.9 million, which is \$32 million above the budget request and \$28 million over FY 2008. The funding would provide increased investment to support renewable energy integration into the electric transmission grid.
- Nuclear Energy would receive \$803 million, which is \$121 over the FY 2008 funding level
- Fossil Energy would receive **\$876.73 million**, which is \$122 million over the request and \$133 million over FY 2008
- The Naval Petroleum and Oil Shale Reserves would receive **\$19 million**, which is equal to the budget request
- The Strategic Petroleum Reserve would receive **\$205 million**
- The Energy Information Administration would receive **\$110.5 million**, which is equal to the budget request

- Non-Defense EM would receive \$266.4 million, which is \$53 million above the budget request
- The Office of Science would receive more than \$4.649 billion which is \$623 million above FY 2008
- The Yucca Mountain project would receive **\$386.4 million**, the same as current year funding
- The bill would provide **\$380 million** to authorize the \$38.5 billion in loan guarantees
- Weapons Activities would receive \$6.524 billion, which is \$227 million about FY 2008
- Nuclear Nonproliferation would receive more than more than **\$1.909 million**
- Defense Environmental Cleanup would receive more than \$5.771 billion, which is \$474 million above the budget request and \$422 above FY 2008

With the Office of Science fiscal year 2009 budget, several programs that did not receive appropriations this year have received full funding for the coming year (wonderful news). BES received an additional \$284M in requests versus 2008. The House provided \$31M more than requested, but the Senate's request was \$151M less than the requested amount. In addition, Fusion Energy Sciences received a large increase in request versus 2008.

Dehmer discussed the 12-year history of requests versus appropriations for SC programs. BES and ASCR saw large percentage growths, but only BES is now at the ACA level. The others (HEP, NP, FES and BER) are relatively flat over the past 10 years. "We are thankful that BES has done so well."

Approximately one-third of the U.S. primary energy is imported. During the 1950s, there were no imports. While looking at the U.S. Energy Flow (2006) Energy Supply (Quads) chart, domestic production is 71 Quads versus 34 Quads for Imports. Eighty-five percent of primary energy is from fossil fuels, (nuclear accounts for 8%; renewable is 7%). More than 70% of primary energy for the transportation sector and more than 60% of primary energy for electricity is lost.

The overall efficiency of an incandescent bulb is $\cong 2\%$. **Dehmer** showed an example of energy lost during conversion and transmission. The coal needed to illuminate an incandescent light bulb contains 100 units of energy when it enters the power plant. Only two units of energy eventually light the bulb. The remaining 98 units are lost along the way, primarily as heat.

Next, **Dehmer** showed the U.S. Energy Flow in 1950. At mid-century, the U.S. used onethird of the primary energy used today and with greater overall efficiency. Modern CO_2 concentrations in the atmosphere are increasing. The current concentration is the highest in 800,000 years, as determined by ice core data. The concentration now is ~385 ppm. Concentration prior to 1800 was ~280 ppm.

In *Nature* magazine, an article from May 2008 stated the air bubbles trapped in the Antarctic Vostok and EPICA Dome C ice cores provide composite records of levels of

atmospheric carbon dioxide and methane covering the past 650,000 years. Now, the record of atmospheric carbon dioxide and methane concentrations has been extended by two more complete glacial cycles to 800,000 years ago. The new data are from the lowest 200 metres of the Dome C core. This ice core went down to just a few metres above bedrock at a depth of 3,270 metres. The cover shows a strip of ice core from another ice core in Antarctica (Berkner Island) from a depth of 120 metres.

The correlation between CO_2 Concentrations and Temperature is the highest in 300,000 years. The planet is warming because of greenhouse emissions. **Dehmer** said "we have to stop putting CO_2 in the atmosphere." Energy/environment solutions require:

- 1) zero-net-emissions electricity emissions
- 2) Fuel switching
- 3) CCS
- 4) Electric energy storage
- 5) Electricity transmission and distribution
- 6) Fuel switching
- 7) End-use efficiency
- 8) Conservation

Virtually all technologies have shown continuous improvement. But, in general the improvements are not fast or grand enough. In regard to the learning curve for solar cells, the module price has been dropping 20% for every doubling of module production (80% learning curve) since 1976. Extrapolation of this historical trend into the future, plus a projected technological revolution at an annual production level of 150,000 MWp, results in a prediction that \$0.40/Wp would not be reached for another 20–25 years. Reaching \$0.40/Wp sooner to accelerate large-scale implementation of PV systems will require an intense effort in basic science to produce a technological revolution that leads to new, as-yet-unknown technology. This revolution requires a major reduction in the ratio of the PV module cost per unit area to the cell efficiency.

"Grand Challenges in Basic Energy Sciences" by **Fleming** and **Ratner** appeared in *Physics Today* magazine. The article discussed the research focused in five related areas will allow unprecedented control over the microscopic world and could be the key to a sustainable future.

Dehmer concluded her presentation by stating the BESAC "New Era" Sub-Committee is critically important tasks for both the research programs and the scientific User facilities. We must do the following:

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" BRNs 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.
- 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 (ultrahigh brightness with low electron emittance), and temporal structure (nano to atto seconds) for future light sources.

Hemminger thanked **Dehmer** and requested the Committee hold their questions until later in the morning.

At 9:25 a.m. **Harriet Kung**, Associate Director, Office of Basic Energy Science (BES), was introduced and asked by **Hemminger** to provide an update on news from the Office of BES.

Kung's presentation began with the BES staffing, budget updates and BESAC activities. **Kung** said she now has three divisions Materials Sciences and Engineering Division, Scientific User Facilities Division and Chemical Sciences, Geosciences and Biosciences Division. The Office will soon be announcing three additional vacancies and encouraged BESAC members should alert potential candidates. She also announced **Van Nguyen** will begin work August 1 in the Facility Coordination, Metrics and Assessment department (under the direction of **Pedro Montano**).

For FY2008, the Energy Department of Energy Programs Science included verbiage that stated "the amended bill includes an additional \$62.5M for Science. The Department of Energy (DOE) is instructed to utilize this funding to eliminate all furloughs and reductions in force which are a direct result of budgetary constraints. Workforce reductions, which are a result of completed work or realignment of the mission, should proceed as planned. This funding is intended to maintain technical expertise and capability at the Office of Science and may be used for National Laboratory Research and Development including research related to new neutrino initiatives. Funding for research efforts shall not be allocated until the Office of Science has fully funded all personnel requirements."

BES received an additional \$13.5M. Synchrotron and Radiation Light Sources (+\$11,500,000 over a prior FY 2008 appropriation of \$220,092,000, for a revised total of \$231,592,000). Spallation Neutron Source (+\$2M over a prior FY 2008 appropriation of \$164,640,000, for a revised total of \$166,640,000). **Kung** thanked the community and Congress for the response to BES programs.

BES received \$1,283,402B in fiscal year versus \$1,221,380B for fiscal year 2007. The FY2009 request to Congress versus FY2008 appropriations is an additional \$298,258M. For the Office of Sciences, there is a total surplus of 18.8%.

The FY2009 BES President's Request is \$1,568.2M., including \$719.2M for Facilities Operations; \$325M for MSE Research; \$284.6M for CSGB Research; \$145.4M for Construction and \$20.4M for SUF Research.

The fiscal year 2009 budget highlights include:

- Core research programs
 - \$100,000K for Energy Frontier Research Centers ("a significant piece for Office of Science")
 - Single investigator and small group awards for grand science and energy research
 - Facility-related research such as detectors and optics
 - Scientific User facilities operations
 - Optimal operations of:
 - Synchrotron light sources
 - Neutron scattering facilities
 - Nanoscale Science Research Centers
 - Construction and instrumentation
 - National Synchrotron Light Source-II
 - Linac Coherent Light Source + Linac operations + instruments
 - Advanced Light Source User Support Building
 - Spallation Neutron Source instruments

The current status of the fiscal year budget is that the FY 2009 Senate Mark is \$152,782M less and the House mark is \$31.5M more than the Request. Research in Materials Sciences and Engineering Division and Chemical Sciences, Geosciences and Biosciences Division:

Full funding, including \$100,000,000 for EFRC activities.

- This Committee has long advocated ... open competition for research funding that features head-to-head competition between national laboratories and universities and supports the Department's decision to broadly compete the EFRCs (seeing a lot of teaming and innovative ideas) in this manner.
- The Committee encourages the Department to update and expand upon its Basic Research Needs (BRNs) workshop series in order to ensure that any new science opportunities and challenges relevant to DOE's mission needs can be identified and addressed as they arise.

Funding is provided in the Basic Energy Sciences (BES) for four integrated research and development areas: \$33,938,000 for Electrical Energy Storage, \$10,915,000 for Carbon Dioxide Capture and Storage, \$8,492,000 for Characterization of Radioactive Waste and \$8,492,000 for Predicting High Level Waste System Performance over Extreme Time Horizons. The recommendation includes \$8,240,000 for the Experimental Program to Stimulate Competitive Research (EPSCoR), the same as the budget request.

Facilities Operations & Major Items of Equipment:

- Full funding, including operations of the five Nanoscale Science Research Centers, operations of the Advanced Light Source, the Advanced Photon Source, the National Synchrotron Light Source, the Stanford Synchrotron Radiation Laboratory, the Manuel Lujan, Jr. Neutron Scattering Center, the High Flux Isotope Reactor, the Linac Coherent Light Source (LCLS) at SLAC, and the Spallation Neutron Source (SNS) at their full optimal numbers of hours, as well as additional instrumentation for the SNS and LCLS.
- An additional \$17M is provided to accelerate the completion of the LCLS Ultrafast Science Instruments project and 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.

Constructions:

- The Committee recommendation includes \$159,968,000 for Basic Energy Sciences construction projects, an increase of \$14.5M over the budget request and \$66,703,000 above the FY2008 enacted level.
- \$11.5M is provided for construction of the Advanced Light Source User Support Building (08-SC-01) at Lawrence Berkeley National Laboratory; \$3,728,000 for renovation of the Photon Ultrafast Laser Science and Engineering Building Renovation (08-SC-11) at the Stanford Linear Accelerator Center; \$107,773,000, \$14.5M above the budget request, for continued project engineering and design as well as to initiate construction of the National Synchrotron Light Source II (07-SC06) at Brookhaven National Laboratory; and \$36,967,000 to continue construction of the Linac Coherent Light Source (05-R-320) at the Stanford Linear Accelerator Center.

The Senate report stated "the Committee 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 the Experimental Program to Stimulate Competitive Research (EPSCoR). Of the decrease, \$59,495M of basic solar research is moved to the EERE solar energy research and development program."

The potential impact of FY2009 Senate Appropriation Committee Mark on BES Programs includes:

Research in Materials Sciences and Engineering Division and Chemical Sciences, Geosciences, and Biosciences Division:

To accommodate the move of solar funding to EERE, a number of BES-funded research projects at universities and DOE laboratories may be terminated, which could result in layoffs at DOE labs and the termination of support for principal investigators and students/post-docs at U.S. universities. Such an action may discourage the next generation of talented scientists who are ready, willing and eager to devote their considerable intellectual resources to solving the critical problems associated with the effective utilization of solar energy. This may terminate or impact as many as 300 people.

- The SEWD mark provides for: cost-of-living increases for the ongoing BES research programs; to prevent layoffs at DOE laboratories and universities; and targeted increases identified in the FY2009 budget request that address grand science and energy challenges.
- The SEWD mark makes it difficult to execute the planned initiation of the \$100M (EFRCs) program

Facilities Operations:

- The SEWD mark provides cost-of-living increases for the BES synchrotron radiation light sources, the neutron scattering facilities, electron beam microcharacterization facilities and Nanoscale Science Research Centers. The SEWD mark enables the operation of the facilities at near-optimum levels (~90% of maximum operating hours.)
- The SEWD mark may not provide the full funding for SLAC operations, which will delay routine maintenance activities of the linac that now supports the new Linac Coherent Light Source.

Facilities Research:

The SEWD mark provides funding for some areas of accelerator research for new detector concepts and devices. Areas that may not be supported include accelerator optics and new undulator technology.

The essential role of Basic Science is:

- Today's energy technologies and infrastructure are rooted in 20th Century technologies and 19th Century discoveries—internal combustion engine, incandescent lighting
- Current fossil energy sources, energy production methods and technologies cannot meet the energy challenges we are face
- Incremental changes in technology will not suffice. We need transformational discoveries and disruptive technologies.
- 21st Century technologies will be rooted in the ability to direct and control matter down to the molecular, atomic and quantum levels

With Solar Energy, sunlight provides by far the largest of all carbon-neutral energy sources – more energy from sunlight strikes the Earth in one hour $(4.6 \times 10^{20} \text{ joules})$ than all the energy consumed on the planet in a year. Despite the abundance, less than 0.1% of our primary energy derives from sunlight. The three routes for using solar energy – conversion to electricity, fuels or thermal heat – exploit the functional steps of capture, conversion and storage. They also exploit many of the same electronic and molecular mechanisms. The challenge is reducing the costs and increasing the capacity of converting sunlight into electricity or fuels that can be stored or transported (solar electricity, solar fuels, solar thermal systems). The physical, chemical and biological pathways of solar energy conversion meet at the nanoscale. The ability to create

nanoscale structures coupled with advanced characterization, theory and computational tools suggest that understanding and control of efficient solar energy conversion are key to effective solar energy utilization. Solar research supported by BES emphasizes: photovoltaics exceeding thermodynamic efficiency limits; easily manufactured, low-cost polymer and nanoparticle photovoltaic structures; efficient photoelectrolysis; defect-tolerant, self-repairing systems and bio-inspired molecular assemblies systems for solar fuels production; and new experimental and theoretical tools.

Solar concentrators in use today "track the sun to generate high optical intensities, often by using large mobile mirrors that are expensive to deploy and maintain." Further, solar cells at the focal point of the mirrors must be cooled and the entire assembly wastes space around the perimeter to avoid shadowing neighboring concentrators.

By painting a mixture of two or more dyes onto a pane of glass or plastic, the dyes work together to absorb light across a range of wavelengths, which is then re-emitted at a different wavelength and transported across the pane to waiting solar cells at the edges.

The new development applied the optical techniques developed for lasers and organic light-emitting diodes. A mixture of dyes in specific ratios, applied only to the surface of the glass, allows control over light absorption and emission to substantially reduce light transport losses, resulting in a tenfold increase in the amount of power converted by the solar cells.

The benefits of the innovative development are: (1) static, no tracking needed (2) theoretically unlimited concentration factor (3) no excess heat incident on PVs, pumped at bandgap.

In examining efficient solar hydrogen production by a hybrid photo-catalyst system, solar energy is an attractive source for large scale hydrogen production. Robust, inorganic catalyst systems, such as platinized TiO_2 , have been used to generate hydrogen from sunlight, but efficiency is low because they can only use the UV portion of the solar radiation. Natural photosynthetic systems, such as Photosystem I (PS I), can absorb ~45% of solar spectrum, but are coupled indirectly and inefficiently to a non-robust, oxygen-sensitive hydrogenase to generate hydrogen.

In a novel strategy that combines the best of both worlds, a synthetic molecular wire, consisting of a Fe₄-S₄ cluster and an organic dithiol, is used to covalently link PS I with the Au or Pt nanoparticles. This provides a rapid, efficient pathway for shuttling photogenerated electrons to the inorganic nanocatalyst. Upon illumination, the PS I-Molecular Wire-Nanocatalyst hybrid system generates 8 H₂ per PS I per second over a period of 12-16 hours (with cytochrome c_6 as electron donor).

This represents a new benchmark in the efficiency of hydrogen production by use of modified or hybrid photosynthetic systems. To compare, a genetically engineered PS I-hydrogenase gene fusion generates 0.0045 H_2 per PS I per second, and platinized chloroplasts generate 0.045 H_2 per PS I per second.

"The charge of the BESAC Sub-Committee on New Era of Science that will be presented by **George Crabtree** and **Mark Kastner** later today includes:

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*."

1. 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" BRNs 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 organizational structures that may be required to implement the strategies and supply the human resources (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 (ultrahigh brightness with low electron emittance), and temporal structure (nano to atto seconds) for future light sources.

"The charge of BESAC Sub-Committee on Committee of Visitors (COV), which **Geri Richmond** will present later this morning relates to:

1. For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:

(a) Solicit, review, recommend and document proposal actions

(b) Monitor active projects and programs

2. 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

(b) The national and international standing of the portfolio elements

3. In addition to the above elements, the panel is asked to provide input for the Office of Management and Budget (OMB) evaluation of BES progress toward the long-term goals specified in the OMB Program Assessment Rating Tool. Each of the nine components (or sub-components, if appropriate) of the Chemical Sciences, Geosciences, and Biosciences Division should be evaluated against each of the four PART long-term goals. If a particular long-term goal is not applicable to a specific program component, please indicate so in the evaluation. The OMB guidelines specify ratings of (1) excellent, (2) good, (3) fair, (4) poor or (5) not applicable. In addition to these ratings, comments on observed strengths or deficiencies in any component or sub-component of the Division's portfolio and suggestions for improvement would be very valuable.

At 9:58 a.m., **Hemminger** introduced **Richmond**, COV Chair, to provide an update on COV for Chemical Sciences, Geosciences and Biosciences Division (CGBS) to the BES Advisory Committee.

Richmond said the Committee spent several days on the COV review, which had been broken up into four different groups – AMO Sciences/Gas Phase Chemical Physics; Photochemistry/Condensed Phase Chemical Physics; Catalysis; Heavy Element Chemistry/Separations and Analyses; Geosciences; and Biosciences. The Committee consists of several BESAC members, including **Bruce Gates, Sharon Hammes-Schiffer, Simon Bare, Sue Clark** and **John Richards**.

The major findings of the COV included that across the Division of CGBS, the quality of the decision making processes and the documentation by program managers is outstanding, reflecting the experience and professionalism of these highly talented individuals. This performance is particularly remarkable given the lack of an adequate electronic information system and the uncertainties in the budget.

Overall the quality of solicitation, review, recommendation and documentation were viewed very favorably, including the quality and quantity of reviewers, the in-depth analysis by program managers and the documentation of the process.

Monitoring of active projects and programs suffers seriously from the lack of a comprehensive database that collects such information as publications, presentations, awards, personnel and progress.

There has been an increase in the use of contractors meetings as a tracking and intellectual cross-cutting awareness mechanism, which is enthusiastically supported. **Richmond** said this is "very positive news, excellent ideas and great synergy."

Ambiguities about the decision making process appeared for a number of laboratory reviews. **Richmond** encouraged the CGBS program to direct on-site reviewers to focus on "forward looking," proposed science rather than past accomplishments. She added "lab reviews were based on past performance instead of forward-future thinking."

Overall, the science supported in CGBS consistently reflects a high degree of intellectual depth, scientific breadth and funded scientists are highly regarded both nationally and internationally. **Richmond** said "across the board, the quality of scientists is exceptional. We are currently looking at those currently being funded, not being funded and choosing which ones should be funded."

Evidence for evolution of the portfolio with respect to new investigators and diversity among investigators is substantially anecdotal due to the lack of an electronic information system that can gather the required information. Significant progress has been made in several other areas, including improvement in proposal solicitation, re-evaluation and refocusing of the Energy Biosciences program; an encouraging addition of highly qualified program managers; three new program manager positions; and a systematic program prioritization. We are encouraged by the addition of new staff positions in the Division and see this as an essential component of the new structure and priorities.

The COV recommends, in the strongest terms, the rigorous collection of data on all aspects of proposal solicitation, review, funding recommendation, proposal action and metrics associated with progress including full information on:

- **Reviewers:** Institution, BES funding status, frequency of use, performance metrics, etc.
- **PI's:** Institution, funding profile, annual reports/ contractors meeting abstracts, sponsored publications, patents, presentations, awards, collaborations, project personnel, success stories

The COV also recommends allowing efficient management of the funding process and tracking of progress. The COV believes that an implementation timeline of three years is appropriate. In addition, the COV strongly encourages the collection through a similar database of the demographics of reviewers and of those funded and declined in a manner that is consistent with Federal law. Furthermore, the COV also encourages the enhancement of the representation of women, under-represented minorities and the continued enhancement in the number of new young investigators in project portfolios.

This recommendation parallels repeated calls for similar action, including:

From the 2007 COV Report of the Office of High Energy Physics:

"We recommend that documentation and access to program data continues to be improved and that data is put into electronic form ..."

From the 2007 COV Report of the Office of Nuclear Physics:

"We recommend a more extensive database of the information contained in the university grants, to facilitate tracking of the overall health of the program."

From the 2007 COV Report of the Climate Change Research Division of BER:

"This COV is making recommendations that require additional staff and support, including the development of more complete project dossiers and the development or acquisition of electronic document management and database systems ..."

From the 2005 COV Report of the CGBS of BES:

"COV strongly recommends the development of standardized database software and a coherent BES-wide computer database ..."

From the 2003 COV Report of the Department of Material Science and Engineering of BES:

"The Office of Science information management system is ineffective in many ways. ...Such a database is essential for the program managers to perform their jobs."

From the 2004 COV of the Environmental Remediation Sciences Division of BER: "The COV believes it would be very useful if the research programs supported by BER were to set goals for, and keep records of, funding demographics in terms of underrepresented groups, junior scientists and new investigators ..."

Richmond said she wanted to thank **Eric Rohlfing** (Acting Director of BES), **John Miller** (Acting Direction of CGBS), **Linda Blevins** (Office of Science) and all program managers, staff and associated personnel (especially **Diane Marceau**) for assembling review materials, being available for questions and all organizational aspects of the COV review.

At 10:12 a.m., **Hemminger** said he would like to personally thank **Richmond** and provided time for the Committee to ask questions.

John Spence said the formatting should be the same for DOE and thinks it would make it more efficient if all presentations followed the same formatting.

Martin Moskovits said he believes **Richmond's** Committee got the "right answers and did an excellent job in restricting their message." He added that he was one COV and only had three Committees. He questioned if there would be a post-COV meeting in order to make the exercises more effective.

Hemminger said at the beginning of each COV, there is continuity that addresses administrative concerns. If **Richmond's** proposal is approved, it will be submitted by BESAC and there would be accountability.

Kung said "we are taking this issue very seriously."

Dehmer said **Richmond** was not the first to do an assessment. **Dehmer** said she also did an assessment and said there had been an assessment of all of the COV reports. She added the focus needed to be on issues that were consistent "that come up over and over again" through each of the reports and that a new information management system is needed.

Richmond said "for it to be done right, we need to be patient. The data collection has been revised."

Hemminger asked the Committee for a show of hands to accept the proposal. By an overwhelming margin, it was approved.

At 10:20 a.m., **Hemminger** provided time for an open discussion for **Dehmer** and **Kung**. He began by stating that we do not understand enough of how nature works and scientists need to solve the daunting issues.

Sylvia Ceyer asked if the Office of Science requested funding for EFRC and was it a formal or informal request.

Dehmer said it was not a request from the Office of Science.

John Richards asked if **Dehmer** knew which programs would be effected and questioned why the Senate does not understand how important funding for the programs are for the future of science.

Dehmer stated that the House has been extremely supportive of the Office of Science and that it will take educating the Senate on how current programs will affect the future of science. She said technology has continued to change rapidly and that the Senate has simply not been as receptive as the House.

Laura Green questioned how the appropriations from the House and Senate could be so different. She added the demise of industrial research has been linked to the people responsible at labs and those in charge are "completely blind" to how BES works. "We need to educate the House and Senate."

William McCurdy Jr., asked what is the current relationship with EERE and how is their support been in the past?

Kung said there is a very good relationship with EERE. She said EERE delivers technology through thermal technologies, solar findings and exploratory research.

Martin Moskovits said the U.S. now sees that we are in a crisis and that BESAC is in a "different mode." He questioned how we get the message to the Senate that we are indeed in an energy crisis.

Hemminger said the U.S. has responded in the past with such projects as the Manhattan Project and believes we need to have funding for the EERE.

Arthur Nozik said the managers at EERE are interested in "near-term" successes. He believes the group wants to see science that feeds into technology and that helps move technology forward. He agrees with **Dehmer** and **Kung** that we need to maintain solar research and show a long-term commitment and long-term objectives. It is important to have managers at EERE recognize the importance of the long-term effects it will have on the future of science.

Moskovits said "we need to have a new phenomenon."

Gates said as a community, we have not addressed technological solutions into science. Technology continues to change at a rapid pace, which creates "a disconnect between science and the community." People in the industry have a clear understanding of fundamental science. These are the same people who the time restraints. **Bare** said he believed it was good to be in "crisis mode" because it draws attention to how we respond in our research and the problems we face. It also affects the way we deliver technology and how we get the message across effectively. "We must address the crisis we have before us."

Taylor has done a lot of work with EERE. She said she would like to see EERE to work more directly with science.

McCurdy Jr., said the right response is to "get on with it." We must direct basic research to solar energy conversion. The message basic research is disconnected from what the Senate needs to hear. "We need to get this message across."

At 10:54 a.m. **Hemminger** requested a break.

At 11:11 a.m., **Hemminger** introduced **Adam Rosenberg** to give a brief update concerning the Committee hearing.

Rosenberg said a hearing would take place September 11, 2008. He believes the BESAC Committee could be potentially be "over-reading" the Senate lack of support. He said that although he had heard it numerous times during the morning, he said the message needs to be communicated better for the Senate to have a better understanding and its importance.

At 11:15 a.m., **Hemminger** introduced **Linda Horton**, Oak Ridge National Laboratory (ORNL) to provide an update on National Science Resources Center (NSRC) – Center for Nanophase Materials Sciences (CNMS).

Horton began her presentation by discussing the CNMS is co-located with the Spallation Neutron Source on ORNL's Chestnut Ridge. CNMS integrates nanoscale science with three synergistic research needs:

- Neutron Science Use of unique capabilities of neutron scattering to understand nanoscale materials and function
- Synthesis Science Science-driven synthesis: nanoscale synthesis as enabler of new functionality
- Theory and Modeling Stimulate use of theory and modeling to understand and design new nanomaterials

Next, **Horton** discussed the CNMS research capabilities. It is important to understand, design and control functionality in nanoscale systems – the dynamics, structure and chemistry.

Nanomaterials Theory Institute

• Theory and Modeling for nanoscience

Macromolecular Nanomaterials

• Synthetic polymeric and bio-inspired materials Imaging Nanoscale Functionality

• Unique scanning probe instrumentation; in-situ studies Multi-scale characterization of Nanoscale Functionality

- Neutrons, electron, and X-ray diffraction and spectroscopy
- Raman, optical characterization
- Environmental control, dynamics
- Functional hybrid nanostructures and systems

Nanofabrication Research, Laboratory and Bio-Inspired Nanomaterials

• Controlled synthesis and directed assembly; functional integration of "soft" and "hard" materials

CNMS supports both an Internal Science Program and User Science. The scientific themes are 1) Origins of Functionality at the Nanoscale 2) Functional Polymer Architectures 3) Understanding Emergent Behavior. The Nanofabrication Laboratory also supports underpinning science and technique development. Research staff time, on average, is split equally between the Internal and User Science Programs. **Horton** said "we are currently spending more time on User Programs and are currently working to get a better balance."

There is world class, unique capabilities in polymer synthesis, including synthesis of deuterated polymers for neutron scattering (expertise in organic and polymer synthesis for preparation of well-defined deuterated small molecules, monomers and polymers); SANS studies using CNMS polymers were first published in Macromolecules in 2006; First neutron reflectivity experiments at SNS were on CNMS polymers.

In addition, there are world class capabilities in scanning probes. There are:

- Unique (or nearly so) UHV instrumentation. On-going development of high resolution, low temperature, high-field UHV probes put the science forward in this area.
- Force-based scanning probes
 - Band excitation
 - Bias-induced phase transformation
 - Temperature-induced local phase transition

Next, **Horton** discussed more world class capabilities in theory and modeling of nanoscale systems. There is a partnership with ORNL's leadership class computing capabilities (the development of codes and interface software for these systems). In addition, there is an expertise in a wide range of theory for nanoscale systems.

Nanofabrication and electron microscopy are two more world class capabilities. Nanofabrication is the electron beam disposition. The electron microscopy is a partnership with the Shared Research Equipment Microscopy User Program. CNMS has 66 R&D staff and 15 Postdoctoral Fellows. Sixty percent of R&D staff was selected based on advertised positions. Fifty percent of the staff is new to ORNL programs. Currently, there is only one open position, Theme Lead for Origins of Functionality.

For User Access, the policy is open access, based on scientific and technical quality. All Users submit two pages of proposal text, two calls per fiscal year. The proposals are required to be reviewed by an external peer group. The review guidelines and process are described on the CNMS Web site. There is rapid access of the proposals between calls, with a five day limit. CNMS accepts peer review by other DOE-SC User Facilities. There is flexibility to accommodate spectrum of User needs.

- General Users: Access to existing tools/support/collaboration
- Partner Users: Enhance CNMS capabilities
- Proprietary Users: Access at full cost recovery for sensitive research none to date, rates not yet established

There are no fees if results are published in open, peer-reviewed scientific journals.

The CNMS proposal forms are simple, with a check-off list for instrumentation. There is a Word-fillable form, submitted via email. "We are headed to an all electronic submission system, which SNS is piloting," **Horton** said. Single proposal allows access to CNMS and SHaRE Electron Microscopes. The form offers a check box for interest in neutron scattering. There is also a single electronic proposal for neutron scattering, CNMS and SHaRE access coming. CNMS accepts other facility proposal reviews through Rapid Access Proposals.

There is an open system involving the proposal review committee and criteria posted on the CNMS Web site. The reviewing process includes:

- Feasibility review CNMS staff assesses safety issues and whether we have the capabilities requested
- Scientific review three reviews requested for each proposal and reviewers provide numerical scores on the science and the proposal team plus comments
- Turn-around time from proposal submission to notification of decisions: Eight weeks
- Reviewer feedback is provided to PIs (anonymous)

CNMS has received more than 800 User proposals to date and accepted ~55% as User Projects. CNMS Leveling at more than 200 active User projects. Currently, there are 14 partner User projects. CNMS User population is greater than 300 last year and may reach 400 in FY08.

CNMS Interface with Neutron Scattering Capabilities at SNS and HFIR:

In FY07: Both SNS and HFIR had limited User populations

• 6% of the CNMS Users also used ORNL's neutron scattering capabilities

• Over 20% of neutron scattering Users were CNMS Users

In FY08 to date (9 months):

- 14% of CNMS Users also used ORNL's neutron scattering capabilities
- 15% of neutron scattering Users were CNMS Users (23% for SNS)

Expectations for the Future:

- The numbers of shared Users will continue to increase
- Percentage of CNMS Users who use neutron scattering will increase
- Percentage of neutron scattering Users who use CNMS will decrease as their User population increases

The CNMS impacts beyond User statistics. In FY2007, there were more than 130 refereed journal publications. Approximately 20% in high-impact journals (impact factors are more than five and/or top journal in the field). The journals are evenly divided between the User program and the internal science program. Approximately 40% involve theory and 10% are both theory and experiment.

Horton concluded her presentation and asked for questions and comments from the Committee.

Gates asked "What are the goals of the User distribution?"

Horton said "Our goal is have 50-50 time allocation when it comes to Internal versus User Programs. "We expect to see our User numbers come down in the future and have our managers balance that issue better."

Hemminger said "How do you work with other facilities?"

Horton said there is a check-off regarding SNS capabilities. "Users see that they have User capabilities and that they are reviewed by both processes."

Bare asked "How many Users collaborates with the staff?"

Horton said "That is difficult to answer. We make sure that staff members are not listed as a prerequisite. If our staff co-authors or is a co-collaborator, they must follow all rules that are in place."

Kirby asked if there was a mechanism for remote User capabilities to do observations and also if experiments are carried out by the staff?"

Horton said BES provides guidance and are working to make the situation better for experiments using microscopes, allowing Users to see remotely."

Richards asked what the UT-Battelle connection was.

Horton said UT-Battelle has been established to manage and operate the ORNL for DOE.

At 11:52 a.m. **Hemminger** introduced **Toni Taylor**, Los Alamos National Laboratory (LANL), to provide a NSRC update on the Center for Integrated Nanotechnologies (CINT).

Taylor began her presentation by stating LANL is a state-of-the-art facilities that leverages the capabilities of LANL and Sandia National Laboratories and how both work concurrently to develop innovative approaches to nanoscale integration.

CINT Core and Gateway Facilities serve as centers for nanoscience integration. The core facility in Albuquerque is 96,000 square feet and the Gateway facility to Los Alamos is 36,500 square feet. CINT was recently awarded the DOE Secretary's Achievement Award.

The science of nanomaterials integration involves combining diverse nanomaterials together into composite structures and systems from the nano to microscale to discover, understand and design new properties and performance of materials.

CINT's capabilities reside in four science thrusts – Nanophotonics and Optical Nanomaterials; Nanoscale Electronics, Mechanics and Systems; Soft, Biological and Composite Nanomaterials; and Theory and Simulation of Nanoscale Phenomena.

Nanophotonics and optical nanomaterials is the synthesis, excitation and energy transformations of optically active nanomaterials and collective or emergent electromagnetic phenomena (plasmonics, metamaterials, photonic lattices)

Nanoscale Electronics, Mechanics and Systems controls electronic transport and wave functions, and mechanical coupling and properties using nanomaterials and integrated nanosystems

Soft, Biological and Composite Nanomaterials is solution-based materials synthesis and assembly of soft, composite and artificial bio-mimetic nanosystems.

Theory and Simulation of Nanoscale Phenomena involves the assembly, interfacial interactions and emergent properties of nanoscale systems, including their electronic, magnetic and optical properties.

The expertise of the scientists in the theory thrust covers a broad range of capabilities including:

Sasha Balatsky: Electronic properties at the nanoscale Stuart Trugman: Many-body quantum techniques, probes of correlated systems, new numerical methods

Sergei Tretiak: (TD)DFT, excited state structure and dynamics, spectroscopy

Normand Modine: DFT, ab initio MD, organics + tunneling electronics, surface structure of semiconductors

Mark Stevens: MD, charged & biomolecular systems, nanoparticle interactions, self & active assembly

Gary Grest: MD simulations, nanoparticle rheology, self-assembly, polymer membranes **Amalie Frischknecht:** molecular theory and simulation of complex fluids, nanoparticle self-assembly, nanoparticle/polymer composites

Matthias Graf: Visualization

Theory thrust capabilities include:

High performance computing

- parallel computers and codes
- treat complex systems
- quantum to classical methods

Visualization Capability Focus:

- Artificial nanoscale materials
 - the shape and structure of the nanoscale materials such as nanoparticles and nanofoams
 - o SEM depth maps (stereo photogrammetry)
- Visualization of scanning probe data:
 - Spontaneous inhomogeneity in correlated systems such as intrinsic inhomogeneity in the high-Tc cuprates
 - Organic-inorganic hybrids like DNA-CNT

Theory and simulation at CINT connects strongly to other CINT thrusts. Soft materials have classical interactions involve nanoparticle assemblies, energy driven dynamics and assembly and surface/interfacial interactions (SBCN and NPON). Hard materials involve quantum interactions nanoscale inhomogeneity, quasiparticles in nanostructures, low dimensional quantum states, excited states and dynamics and nanodomains (NEMS and NPON).

Theory and simulation at CINT strongly couples to the User program.

- User proposals as screened by thrust leaders for opportunities to couple with Theory/Simulation (suggested at April 2007 review).
- User projects involving theory/simulation:
 - o 2008: 28 (lead), 18 (participant)
 - o 2007: 7 (lead), 9 (participant)

A sampling of User projects involving theory/simulation

- Molecular Transport Junctions
- Complex nanoscale phenomena in doped manganites

- Nano-structural characterization of heavy-fermion thin films
- Electromagnetic Response of Broken-Symmetry Nano-Scale Clusters
- Electronic Differentiation of DNA and Organic/Inorganic Hybrid Nanostructures
- Visualization Applied to Complex Superconducting Materials
- Effects of phonon inelastic scattering in graphene
- Visualization Applied to Molecular Scintillator Design
- Modeling Nanostructured Materials Networks for Energy Conversion and Computation Quantum Invisibility in Nanoassembled Structures

Taylor said there had been great progress in understanding nanoscale inhomogenities in complex oxides: theory and experiment. 3D Tracking of Individual Quantum Dots recently won the 2008 Research and Development 100 Award.

Taylor discussed the novel approaches to understanding the high strength of nanostructures. CINT has partnered with Sandia's MESA to develop Discovery Platform as unique nanoscience tools. CINT has partnered with other materials research User facilities at LANL to provide User access involving scientific interactions, joint User meetings, shared User tracking and Web-based proposal submission capabilities. User access among multiple facilities via joint proposals.

Next, **Taylor** discussed the CINT organizational structure. Currently, there are four thrust leaders – NPON, NEMS, SBCN and TSNP. CINT resides primarily in CINT-focused organizations within Sandia and Los Alamos. More important than the new facilities are the CINT scientists. There are 40 scientific staff members, 2/3 of the time are supporting Users and 1/3 for CINT science. Two positions are open and are to be filled via external searches. Eight positions have been filled externally.

CINT Users have access to capabilities for synthesis, characterization and integration. The core facility has a characterization (TEM, SEM, Low Temp Transport, Scanning Probe Microscopy and Ultra-fast Laser Spectroscopy); Synthesis (Molecular Beam Epitaxy, Chemical & Biology labs and molecular films); and integration wing (E-beam lithography, Photolithography, Deposition and Etch and SEM/FIB). At Los Alamos, Users have access to Biomaterials synthesis, Chemical synthesis, XRD, SEM, UV-vis, ellipsometry, Nano-indentation, Nanoscale optical probes, Microscopies, Physical Synthesis, Pulsed Laser Department, Ultra-fast Spectroscopy, Computer Cluster and Visualization Lab.

User calls have attracted widespread interest. With User projects, 380 researchers are involved in current projects from 34 states and 14 foreign countries. The majority are from academia, host institution and foreign academia.

The CINT proposal evaluation process includes the following steps:

- CINT conducts an internal feasibility screening including ES&H (Pass, revise or fail)
- Proposal is assigned to appropriate external proposal review panel
- Proposal is reviewed by three individuals on panel; Chair normalizes individual scores and resolves discrepancies
- Chair returns a priority score (High = 3.0 to Low = 1.0) for each proposal with feedback comments
- CINT approves proposals based upon score, comments and capability availability

The CINT User proposal review panels are composed of external scientists who serve on rotating appointments; charged with evaluating the technical quality of User proposals; each panel has 5-12 members and is led by a Chair; Master list of reviewers posted on CINT Web site. Current panels are Nanoscale Electronics, Mechanics and Systems (I & II); Nanophotonics and Optical Nanomaterials; Soft, Biological and Composite Nanomaterials; Theory and Simulation of Nanoscale Phenomena; Renewal Proposals

Rapid Access User Proposals provide access to CINT between regular proposal submission cycles for time-critical, focused, high-impact research. Users submits two-page proposal via CINT Web site. The proposal is expedited feasibility screening and management review. Approvals are at discretion of CINT Director/Co-Director. Rapid-Access User projects expire at next available regular proposal submission cycle. All regular reporting requirements apply.

NSRC interactions and teaming are important to CINT's User program in our Outreach program. CINT will play a leading role in nanoscience integration in Users outreach partnering, science thrusts and new tools and SNL/LANL capabilities and facilities.

At 12:33 p.m. **Hemminger** adjourned the meeting for lunch and asked the Committee to return at 1:30 p.m.

At 1:45 p.m., **Hemminger** called the meeting back and to order. The afternoon session began with **Hemminger** introducing **Carolyn Bertozzi**, Lawrence Berkley National Laboratory to provide a NSRC update on the Molecular Foundry.

The Molecular Foundry opened in January 2006. The facility is separated by floors, but is set up for interaction, coming together for sharing ideas. At the facility, each floor is set up for a different facility. Organic and Macro-molecular Synthesis is on the top floor; Biological Nanostructures on the fifth floor; Inorganic Nanostructures in on the fourth floor; Theory of Nanostructures is on the third floor; Nanofabrication is on the second floor and Imaging and Manipulation is on the first floor.

Bertozzi provided an overview of the organization. **Bertozzi** is the Director and has the UEC, Scientific Advisory Board, Scientific Director and Deputy Directors reporting to her. There are six directors, one for each facility. Currently, two positions need to be filled. The Facility Directors are involved in User research.

"If you walked through the Molecular Facility, you would find state-of-the-art instrumentation; on-site Users performing experiments; scientific and technical staff supporting User projects (38 hired, all but 1 from outside LBNL, 7 open positions); and post-docs, graduate students, undergraduates and occasionally high school students," said **Bertozzi.**

At the Molecular Foundry, there is a tri-annual call for proposals (CFP). The outreach programs consists of e-mail announcements; information on <u>http://Foundry.lbl.gov</u>; User meetings; national and international conferences; foundry workshops and seminar series; industrial trade shows; UEC, SAB, former and present Users; foundry scientists' external seminars and word of mouth.

The proposal submission and review process is fairly simple. There is no pre-submission contact with Foundry staff required (although it is welcomed); the proposal is submitted online in response to CFP; internal feasibility and EH&S reviews (one week); external proposal review by expert scientists (three weeks); advisory Council review (two weeks); FTE assignment and User notification (one week). The total review cycle time is approximately seven weeks.

The outcome of the June 12 CFP was very good. There were 118 proposals received, with 112 sent out for external review. Each proposal received at least three reviews. An advisory council meeting is pending. **Bertozzi** anticipates approximately 50% acceptance. The decision will be communicated no later than August 1.

Some of the User proposal statistics, approximately 400 proposals received since operations began. More than 400 researchers have used the Foundry, with more than 32 states and 17 foreign countries represented. Approximately 10% are from the industry.

The Foundry EH&S process is that every proposal undergoes EH&S review before external review and again before work is initiated. All Users must complete required training prior to start of work (much can be completed online before arrival). All Users are trained in the practice of ISM. There are new EH&S classes created for the Foundry including two classes that are required, the *TMF010: Integrating EH&S into Science at the Molecular Foundry* and the *TMF11: Nanoparticle Safety*. In addition, *TMF280: Laser Safety at the Molecular Foundry* and *TMF 230: Cryogenic Safety at the Molecular Foundry*.

"We have scientists that can help Users learn how to use the information." said **Bertozzi.** "The diversity of Foundry User projects comes in all shapes and sizes, such as":

- Synthesize or characterize nanostructures
- Develop new nanoscale materials/devices and methods
- Learn to use nanoscale materials/devices and methods
- Learn to replicate new instruments/techniques
- Long-term collaborative projects
- Materials only/Instrument use only

• Strategic User Partnerships (i.e., Intel, possibly IBM)

There are interactions with other User Facilities including the National Center for Electron Microscopy (NCEM) and the Advanced Light Source (ALS). There have been joint developments of new techniques and capabilities. Joint User meetings have taken place at ALS in 2007 and 2009 and at NCEM in 2008.

Some examples of User projects include the design and construction of protein nanotubes, which asks the question "can rings be engineered to self-assemble into tubes?" Six cysteined were engineered into each ring face and the rings self-assemble into covalent nanotubes.

Another example of User projects is the carbon nanotube heterojunctions, which asks the question "why do SWCNT heterojunctions show quantum dot-like behavior?" A model of SWCNT heterojunction assisted with the prediction of localized states at interface. The defects that accommodate junction led to localized states.

The Foundry has four internal research themes - Combinatorial Nanoscience, Synthesis and Characterization of Nanointerfaces, Multimodal in situ Nanoimaging and Spectroscopy and Single-digit Nanofabrication.

Combinatorial nanoscience "has been with us since the early 1990s," said **Bertozzi.** "This is how nature finds new sciences. Combinatorial synthesis of bioinspired polymers includes the following User applications: protein mimetics, nanostructured materials, drug carriers, sensor elements and biomineralization templates. Combinatorial robotic nanoparticle synthesis includes automated nanocrystal synthesis (Fall 2008); Synthesis and highly oriented assemblies of GeTe nanocrystals (User project) and electrical and thermal transport in nanocrystal thin films (two User projects).

One of the future initiatives is Fluid cell *in situ* TEM, a joint venture with NCEM. The impact on the User community includes soft matter and organic-inorganic interfaces and inorganic nanostructures.

Hemminger asked if there is anything in the planning stages whether we should create a strategic program to become a long-term User.

Bertozzi said that there has been no action taken yet.

John Richards asked if international Users are easy to deal with or if they had any issues regarding visas?

Bertozzi said "international Users have not had any problems with visas. She said most are Europeans."

At 2:32 p.m. **Hemminger** introduced **Stephen Streiffer**, Argonne National Laboratory for an update on NSRC – Center for Nanoscale Materials.

Streiffer provided an outline of his presentation, which included an introduction to the CNM group, the facilities and capabilities, the science highlights, budgeting and staffing, User access and statistics and interactions with stakeholders and partners.

NSRC is an integrated facility for Nanoscience research. The CNM groups include NanoBio interfaces, which creates bio-inspired materials and processes for energy transduction; Nanofabrication and devices, which discovers new paths for nanostructured materials, including below 10nm; Nanophotonics provides an understanding and control of optical energy pathways; X-ray microscopy creates images of the nanoworld with hard X-rays; theory and modeling towards the 'virtual fab lab'; and electronic and magnetic materials and devices, which provides an understanding and controls charge and spinbased materials for energy and information support.

The Nanoscale Materials facilities encompass 88,000 square feet and opened in September 2006. There is an area for EMMD, NanoBio, Nanophotonics, X-ray, NanoFab, as well as laboratory space.

Key Facilities and Capabilities

- Materials Synthesis
 - Colloidal nanoparticle synthesis using wet methods
 - o Complex oxide molecular beam epitaxy
 - PECVD nanocrystalline diamond
 - Polymeric templating
 - Spin coating
 - Peptide/DNA synthesis methods
 - o Centrifugation
 - Thin films by sputtering and evaporation
- Nanofabrication Research
 - Electron-beam lithography (JEOL 9300, Raith 150)
 - Focused ion beam processing (FEI Nova 600)
 - Nanoimprint patterning methods (Nanonex NX-3000)
 - Reactive ion etching
 - Optical lithography
 - Wet etching and chemistry
 - o Metrology
- Characterization
 - Proximal Probes: AFM, NSOM, UHV VT-STM
 - o SEM (JEOL JSM7500F)
 - Magnetometry and electrical characterization
 - o Optical microscopy and spectroscopy
 - Thermal analysis (TGA, DSC, rheometry)
 - o Diffractometry
- Dedicated Hard X-Ray Nanoprobe Beamline at the APS
- Computational Nanoscience
 - o 1152 node cluster with compute capacity of approximately

o 10 Tflops, ~11M CPU hr/yr

The CNM and APS partnership at Sector 26-ID is the Hard X-Ray Nanoprobe is jointly staffed and managed by CNM and APs, with four CNM staff and two APS staff members.

Early Nanoprobe results are coherent diffraction across nanoscale grains in a Nb thin film and diffraction maps across strained SOI. The path to Nanometer focuses on X-rays with multi-layered lens. The goal is 6 nm with complete MLL. The scientific highlights for the User are optical probe of grapheme sheets and the role of nanoparticles in alloy corrosion. For the staff, a novel synthesis of Ag nanoplates and ordering in polymer systems.

Recent awards were given to **Dr. Libai Huang** and **Dr. Tiffany Santos**. **Huang** won the Young Investigator Award and **Santos** won Best Poster Award.

The FY08 CNM Budget Request is \$20.8M. The actual FY08 Budget was \$17.7M which was divided amongst staff (\$10.2 million); building operations (\$3.3 million); materials and supplies (\$1.5 million); maintenance and upgrades (\$1.4 million) and capital equipment (\$1.4 million. **Streiffer** said "we have not been staffed the way we would have liked."

Next, **Streiffer** reviewed the CNM staff. In the hiring process, the positions are competed and hiring committees evaluate candidates and make recommendations to the Director. The staffing profile includes:

- 23 PI's, 12 post docs, 16 technical & support staff, 10 administrative staff
- 15 PI's, 3 technical/support staff new to Argonne
- All scientific and tech. staff serve as Scientific Contacts responsible for users
- PI's spend approximately 50% of their time on users

The staffing progress is limited by the FY08 budget. Currently the following positions need to be filled:

- Group leader, Theory and Modeling (candidates being interviewed)
- Group leader or senior scientist, X-ray Microscopy
- Several positions in Nanofab
- Limited User access to certain capabilities (nanoimprint, thin film deposition)

Streiffer reviewed the staff criteria and said they are constantly looking forward to the "best and brightest. The goal is to ensure user productivity and satisfaction in a safe environment; execute innovative, world-leading research in the area of nanoscience; develop and implement world-class instrumentation for nanoscience; and ensure scientific/technical integration within and across groups.

The User proposal process includes:

- Proposals submitted at http://nano.anl.gov
- Review & selection are based on scientific and technical quality
 - An external Proposal Evaluation Board (PEB) is used to evaluate proposals
 - Feedback is provided to the User
- Access for non-proprietary work is free
- Cost-recovery charged for proprietary work
- Registration is required to submit a proposal
- Proposals are submitted on-line
 - Abstract, 250-max words (two page maximum)
 - Research description is prompted by six standard questions
 - o Capabilities, safety issues, timeframe, general contact information
- Nanoprobe proposals may be submitted either through CNM or APS

Current CNM Users

- Instituting three calls-for-proposals per year synchronized with APS; next deadline Oct. 31, 2008
- 201 accepted proposals since 7/06 (88% acceptance rate), 149 active proposals
- Last CFP 7/11/08: 113 submissions
- 236 publications from May 2006 to July 2008 (166 staff + 70 user)
- 709 registered Users
- 42 States and Puerto Rico
- 22 other Countries
- The facility has received 113 submissions, 75 from the academic community.

In Coupling to Theory and Modeling, research topics include Chemical Reactivity at the Nanoscale; Bio-inorganic Nanostructures and Nanophotonics. Users provide support for experiment and theory by receiving access to CNM resources and facilitation of access the INCITE program on Argonne Leadership Computer Facility.

CNM Oversight and Proposal Evaluation

- Scientific Advisory Committee
 - Provides advice to CNM on all matters from science to user policy
 - Chair, Prof. Bob Burhman, Prof. Vicki Colvin, Prof. Heinrich Jaeger, Prof. Janos Kirz, Prof. George Schatz, Prof. Michael Therien
 - o Last meeting April 2007
 - Recent discussions with committee in April 2008 (capital equipment proposals)
- User Executive Committee
 - Provides advocacy for CNM Users to CNM management, organizes annual users meeting, elected by user community to staggered three-year terms
 - Chair, Prof. Gayle Woloschak (NU); Past Chair Prof. Paul Evans (UW, Madison), Prof. Yi Ji (U. Delaware); Dr. Nicolai Moldovan (ADT, Inc.);

Prof. Teri Odom (NU); Prof. Greg Wurtz (U. North Florida), Dr. Dillon Fong (Argonne)

- See <u>http://nano.anl.gov/executive_committee.html</u>
- o Full committee last met February 19, 2008
- Recent discussions with committee in April 2008 (capital equipment proposals); at Users' meeting in May 2008; June 2008
- Proposal evaluation Board
 - External peer reviewers covering CNM themes
 - Two or more reviews per proposal

User Engagement, Input and Feedback is received at annual users; meetings, workshops (40 since 2000), staff lectures, meetings and seminars; end-of-experiment surveys and the BES annual facilities questionnaire.

Recent (and Future) Cross-NSRC Collaborations

- Staff participation in NSRC-Hosted Workshops
 - Bode, CFN Users' Meeting Workshop on Electrical Nanoprobes, May 19, 2008
 - Streiffer, CNMS 3rd International Workshop on Piezoresponse Force Microscopy, September 23-25, 2008
- DOE Experimental Program to Stimulate Competitive Research (EPSCoR) Program Review July 22-24, 2008
 - Hosted by ORNL, <u>https://www.orau.gov/epscor2008</u>
 - Presentation on DOE's Nanoscience Centers by Kathleen Carrado Gregar, Manager, User and Outreach Programs, CNM
- NSTI Nanotech 2008, Boston, June 1-5, 2008
 - o http://www.nsti.org/Nanotech2008
 - All of the NSRCs shared a booth at the Expo: http://www.nsti.org/Nanotech2008/exhibitors.html
- NSRC Brochure: Production through Argonne's Media Services
- ESH Working Group
 - NSRC Guidance Document on Safe Handling of Nanomaterials
 - Argonne hosted the Symposium on Safe Handling of Nanomaterials, July 7-9, 2008

El Sayed asked about the circumstances if Users are hurt while at the facility. He questioned if they have to sign anything concerning liability?

Streiffer said that legal framework is in place and that all Users have to sign a liability form.

At 3:09 p.m., **Emilio Mendez**, Brookhaven National Laboratory was introduced by **Hemminger** to provide an update on NSCR – Center for Functional Nanomaterials (CFN).

Mendez began his presentation with thanking the other Nanomaterial Centers. Each nanocenter "has their own personality and would like to share some exciting news and the future growth plans at Brookhaven." The goal is to become a world-class hub of nanoscience research. There is equal attention given to staff-driven research and User-driven research. The mission is to "contribute to the solutions to the country's research challenges." The CFN is the "youngest" of the five centers, opening for operations March 21, 2008.

The facility has state-of-the-art nanoscience-research equipment. It has a comprehensive suite of tools and a balance between equipment requiring straightforward training with equipment demanding extensive training and expert knowledge.

For the User program, **Mendez** said he wants CFN to become a resource for the nanoscience community of the Northeastern U.S. and beyond. The characteristics of the program includes free access to facilities and expertise for non-proprietary research academia, companies, national laboratories; based on peer-reviewed proposals; three proposal cycles per year (regular access, rapid access); full-cost recovery for proprietary work; suitable to a wide range of Users' needs from straightforward, one-time measurements to complex, extended experiments.

The evolution of User proposals has hit its stride in Cycle 3 2008. There have been 39 continuations and 37 new proposals. Thus far, CNF has received 306 proposals since 2006.

Some examples of User projects include "Fabrication of Kinoform Lenses for Hard X-ray Focusing" and "Electrospun Single Crystal MoO3 Nanowires for Sensing Probes." The scientific themes are electronic materials/photovoltaics; interface science and catalysis; and soft and biomaterials. The cross-cutting programs are the electron microscopy and theory and computation. These themes and programs are relevant to the energy challenge, address important scientific questions, are synergistic with BNL's core programs and take advantage of BNL facilities.

The basic scientific questions and approaches being addressed are:

Scientific Questions

- What is the active phase in a catalysis system under reaction conditions (time, pressure, temperature)?
- What determines reactivity (S/V ratio, electronic structure, active site)?
- How can photovoltaic physical processes be optimized? (Light collection, exciton diffusion and recombination)?
- How to better capture the solar spectrum?
- How to assemble nano-objects in large well-ordered 3D structures?
- How does addressable recognition compete with non-specific interactions?

Approach

• Atomic-scale precision in model systems

- In-situ observation of dynamic processes. under reaction conditions
- Nanostructured PV devices based on low-cost (organic) materials
- Assembly methods for large-area patterning at nm length scales
- Exploitation of properties of DNA and proteins
- Development of new techniques and tools

The liquid-solid phase transition of nanoparticles, DNA-guided crystallization of nanoparticles, epitaxial grapheme on Ru are just three of the projects **Mendez** discussed.

Next, **Mendez** discussed the organizational chart. Currently there are 19 scientists, six post-docs and 10 support employees. For 2010, the CFN has 30 scientific staff, 12 post-docs and 13 support funded. Currently, there are 46 full-time employees, with nine scientists and technicians hired in the last 12 months. The immediate CFN staffing plan in management is to hire an Associate Director, User and External Programs. For the scientific staff, electron microscopy, ultrafast spectroscopy, organic materials synthesis, materials processing, soft-matter theory and NSLS end station need to be filled. For technical and administration support, materials preparation, information technology and User program.

CNF has had interaction with other DOE facilities and NSRCs:

- National Synchrotron Light Source (NSLS) at BNL
 - CFN-owned/maintained end station for small-angle X-ray scattering
 - CFN-owned LEEM/PEEM facility at NSLS beamline
 - Contribution to NSLS's users' catalysis consortium with high-p.
 - XPD synchron
 - o proposal cycles and (planned) coordinated proposal system
 - o integration of CFN's stockroom with NSLS's
- NSLS II
 - Participation in planning of catalysis beamline, and (probably) others
- Other NSRCs
 - Visits to NSRCs for familiarization with other facilities
 - Exchange of ideas and experiences with NSRC directors (monthly phone calls, BESAC meetings)
 - Coordination of acquisition of new instrumentation
 - o (Planned) CFN users referral to complementary facilities in NSRCs

CNF is engaging the scientific community by holding workshops, conducting visits and lectures, participation in Stony Book University, focused collaborations and energy frontier research centers and international (institutional) collaborations.

The challenges include hiring and finding top science candidates with optimum profile for a User-oriented research center; at the facilities, completing suite of instruments for state-of-the-art facility; the budget presents the challenge of planning in uncertain times; and the User program faces managing growth of User base and attracting industrial Users. Mendez completed his presentation by providing a summary of his presentation:

- User-oriented research center striving to become world-class resource
- Uniqueness from synergy between advanced equipment and expert staff
- In full operations since March 21, 2008
- Staff's research focused on energy-related materials & processes
 - o photovoltaics
 - o interface science and catalysis
 - soft and bio nanomaterials
- Blooming high-quality User program
- Thriving research program
- Planned facilities enhancement
- Staffing plan well under way

At 3:52 p.m., Hemminger asked the Committee for questions for Mendez.

Berrah said there should be a roadmap for nanocenters and questioned what type of new research could be done in this new era.

Gates said it would be helpful to have a synthesis from the directors concerning the overlap, the gaps and the optimization of what is working successfully and what have been the challenges.

Richards questioned of all nanocenters, how much has the DOE put into the program?

Mendez said thus far, approximately \$340 million, with an annual budget of \$88 million.

Bertozzi said she has felt "staff-limited with the budgets being flat. We are not able to take full advantage of our infrastructure."

At 4:00 p.m., **Hemminger** declared a break.

At 4:17 p.m., **Hemminger, Crabtree** and **Kastner** provided the Committee with an overview and recap of the BESAC New Era of Science Sub-Committee discussion and the Basic Research Needs for Workshops.

Hemminger began the presentation by stating the agenda for the Sub-Committee over the next two days. On Thursday, the discussion (including the BESAC Committee and the Sub-Committee) would include providing the background for the New Era Report; discussing the bullets for BRN Energy and the Grand Challenge Charge; and the bullets for the Implementation Charge. On Friday morning, the discussion (with the BESAC Committee and Sub-Committee) would include reviewing the bullets and outline for the Light Source Science Charge and a timetable for completing the Report. On Friday afternoon, the Sub-Committee would hold a closed door meeting to complete the bullet point draft of the report; logistics for completing the Report; and assignments for the next interaction.

Hemminger thanked everyone who agreed to be on the Sub-Committee and believes it is extremely important for BES. He said "this Sub-Committee can have a large impact on how things move forward with the issues involved. As the Sub-Committee moves forward, they will get 'buy-in' from the scientific community, with a report that BESAC Committee members will review and accept in order to have a clear understanding."

At 4:22 p.m., **Hemminger** introduced **Crabtree**, who opened by thanking the BESAC and Sub-Committee on the great comments he had received thus far during the day. He said he would incorporate the remarks into the Report.

Crabtree then discussed the Charge for the New Era Report. Following the completion of the 10 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: to assimilate the scientific research directions that emerged from these workshop reports into a comprehensive set of science themes and 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.

The charge will:

- 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" BRNs workshops and those that resulted from the consolidation of the fundamental challenges that face our disciplines.
- Summarize the implementation strategies and 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.
- 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 (ultrahigh brightness with low electron emittance), and temporal structure (nano to atto seconds) for future light sources.

Crabtree followed by discussing the expected outcomes:

- Compelling reasons and innovative methods for organizing support of energy and discovery science, e.g. EFRCs, collaborative networks and summer institutes
- Compelling energy and discovery science drivers for next-generation light sources
- Compelling message on the need for science in solving energy
 - Use inspired basic research
 - Grand Challenge science

The Report should also have two layers of impact – add value to the scientific enterprise and explain the value of energy and discovery science.

Crabtree said that the expected outcome of this meeting is to have a bullet point outline of promising messages for the report and a plan for a Workshop on Light Source Science to solicit input from the community.

Kastner continued by discussing the current political landscape of historical carbon emissions with two pathways for the future and the stabilization wedges. With historical carbon emissions, our current predicted path will most likely lead to at least a tripling of atmospheric CO2relative to its preindustrial concentration, while keeping emissions flat would keep us on track to avoid a doubling of CO2. With stabilization wedges, the wedges are divided into seven "equal" parts. The seven wedges are needed to build a stabilization triangle. One wedge avoids one billion tons of carbon emissions per year by 2054. Environmentalists say "just do it." The industry says "We don't know how and need to do more research."

There has been a decline in Federal Energy R&D.

- U.S. federal spending on energy R&D is well below the historical average
 - Declined from 10% of US R&D in 1980 to 2% in 2005
 - Since 1980, every major developed country except Japan has decreased its energy R&D investment as well
- Private R&D has also declined, although it picked up considerably in 2007 and 2008 because of venture capital

In comparing energy R&D to other sectors, the private energy sector invested only 0.23% of its revenue in R&D from 1988-2003. The biotech industry invests <u>39%</u> of its revenue, pharmaceuticals invest <u>18%</u>, and semiconductors invest <u>16%</u>. With respect to established industries, the electronics industry invests <u>8%</u> of sales on R&D and the auto industry invests <u>3.3%</u>. The overall US industry average R&D investment is <u>2.6%</u>. Experts recommend increasing R&D to significantly higher levels.

Historical precedents (based on 2002 dollars) are the Manhattan Project (\$25 billion over five years); Apollo Program (\$185 billion over nine years); Reagan defense buildup (\$445 billion over eight years); Doubling NIH (\$138 billion over five years) and War on Terror (\$187 billion over the first three years).

Energy R&D is a good investment. In 2001, DOE reported that its 20 most successful projects saved 35 times their total cost. In 1997, PCAST report estimated that energy R&D could result in a 40:1 return on federal investment. I huge R&D investment is necessary. The International Energy Agency (IEA) estimated this year that stabilizing CO₂ emissions at current levels by 2050 will require a total worldwide investment of \$17 trillion (\$400 billion per year) in R&D and implementation. With reducing emissions to 50% below 2005 levels (the goal that the G-8 leaders committed to in July 2008) will require a total investment of \$45 trillion (\$1.1 trillion per year).

Recent proposals include the Boxer-Lieberman-Warner Climate Security Act would only provide only \$436 million per year in R&D funding (18% of the current level); it does not approach any of the above recommendations. Funding R&D from a cap-and-trade system (most likely source of resources) is not ideal, because it will be variable and probably back-ended, while R&D needs to be front-ended. Ideally, R&D funding should come from a mixture of cap-and-trade revenue and baseline appropriations.

Kastner said "we need to tell stories to get the funding that is needed. The solar energy issue is the tip of the iceberg. This is fundamental science that needs to take place. It is crucial to make a good case for basic energy research. Our report should point out critical science that must be done if aggressive goals of CO_2 reduction and energy supply expansion are to be met. In addition, the report should make clear what tools and manpower are needed for that science." He also added there seems to be more "D" (development) than "R" (research) happening at the present time. He concluded by stating that he believes the "payoff will be huge."

Hemminger then asked the Committee and Sub-Committee for questions and comments.

Eberhardt believes it is a question of skill and that it is "off the scale from their core business."

Moskovits said he thinks the industry needs to do some research and will invest in it because it now affects *their* business. He added "Until recently, the issue was not a problem. It is a known fact the industry does not do industry research. It was not funded, even when it was lesser expensive. We need to educate government officials that we are in a transition era. We need to capitalize our areas of science as soon as breakthroughs occur. We could not convince government that this was important 10 years ago.

Green said it is "difficult to address. This is a tremendous challenge and we have to show a systematic change that has put us far behind over the past 30 years. We need to show the steady decline over the years and provide examples and cite projects such as the Reagan project and Manhattan project. In addition, we must show that money has been given in the past to these projects and that they no longer exist."

Gates said in the fossil fuel industry, there are resources to keep us going for decades, if not centuries. If there is not a restraint, there is no reason for the industry to change. "We must accept that industry does not do fundamental research."

Bare said "we have to do our own fundamental research. People want to grasp on to something as a potential answer. The general public is finally getting a grip on the importance. The younger generation has a better understanding.

Tobias asked if there was a time scale. Are there ways of increasing efficiencies to show breakthroughs that may lead to something meaningful?

Crabtree said time scale has been an issue.

Nagy said "in the interest to boost the economy, we need to supplement these companies to sell the basic energy research to Congress."

Cummings said he believes that it is inexcusable that we are not giving more than .23% versus what we were giving 10 years ago.

Richards said nuclear energy could be utilized. He questioned why this has not "come up because it does not require all of the mechanics like other options."

Kung said some of the applied nuclear programs are being looked at as an alternative.

Looney said the Apollo and Manhattan Projects were National Security Projects.

Gates said "there is more on the agenda that needs to be looked at than the 'new' in sciences. We have a very pragmatic issue on the outset. There is a danger this document could be misread. We need to make sure for the basic energy sciences to work in the community that we include light sources."

Crabtree said "we want to appear that we are solving problems and providing answers. We need to get the attention of the public. In looking at the bullets for this project, what do we need to include?" The audience is Congress and we want to make sure they understand and the report. It also important that all levels of science understands this report.

Hemminger said "we need to write the reports to provide insight to decision makers. It must excite the science community or it is not going to work. It is written to appeal only to Congress, it will not be successful."

Kung agreed. "It needs to be understood by not only Congress, but ensure the scientific community. The general public will appreciate the value of research. We must excite the public."

Berrah said we should have a general summary that includes economy and security into the basic energy research. She agreed that we "need to grab the attention of Congress, show how industry is not investing into future sciences and have documentation that

shows we have a significant problem and how it affects not only the economy, but energy and security."

Richards said "we have environmentalist who think we should work with what we've got. We need to find a way to get them to understand and know how to relate to their arguments, concerns and criticisms."

Crabtree said he agrees and thinks this is an excellent idea and will incorporate it into the report.

Hemminger said the charge is to define the science drivers for what BES needs to be doing for the future. "The science driver is light source technology, which has a lot in common with our fundamental research."

Spence said we need to be careful with light source because it is a rapidly changing field.

Tranquada said we should not be fighting with environmentalists. The wedge area is correct, but it is going to take time. Environmentalists think we need to get started now. The economics is the major problem.

Wayne Hendrickson said "this century is the century that we can build the foundation that is a compelling, optimistic approach. Scientists are now ready to take on these challenges."

McCurdy Jr. said he was not comfortable with the charge. He said it is important that the scientific discussion and the arguments for BES is a different argument and we have such a short period of time to fulfill the charge.

Flynn said it is critical to understand the audience of this report. "We must pinpoint if it is Congress, the scientific community or the general public?"

At 5:33 p.m., **Hemminger** asked for public comments. There was none, but before adjourning the meeting for the day, he asked to Committee and Sub-Committee to work on a homework assignment. He stated that **Crabtree** had put together a short report with a list of bullets. **Hemminger** requested each BESAC member and Sub-Committee member make comments to the existing bullets, bullets for the Grand challenges Report and cross-cutting issues. He asked that each member question what is missing in the existing report and come up with a format and send their comments to **Crabtree** and **Kastner** before the Friday morning session.

At 5:40 p.m., **Hemminger** adjourned the meeting for the day.

Friday, July 25, 2008

Hemminger called the meeting to order at 8:37 a.m. He began the meeting by thanking everyone for staying for this very important second day. He also acknowledged and welcomed Carl Lindberg, former BESAC Chairman.

At 8:39 a.m., **Hemminger** introduced **Harriet Kung** to provide an update on New Funding Opportunities.

Kung said the DOE Office of Science and Office of BES has announced the Energy Frontier Research Centers (EFRCs) program. EFRC awards are \$2–5 million per year for an initial five-year period. Universities, laboratories and other institutions are eligible to apply. Energy Frontier Research Centers will pursue fundamental research that addresses both energy challenges and science grand challenges in areas such as:

- Solar energy utilization
- Catalysis for energy

Solid state lighting

- Electrical energy storage
- Advanced nuclear energy systems
- Combustion of 21st century transportation fuels

Geosciences for nuclear waste and CO₂ storage

- Hydrogen production, storage and Use
- Materials under extreme environments
- SuperconductivityMaterials underConversion of biological feedstocks to portable fuels

EFRCs are based on the scientific knowledge of energy-relevant research that has been articulated through the series of 11 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* (http://www.sc.doe.gov/bes/reports/files/GC_rpt.pdf).
- The research program addresses one or more of the energy challenges described in the 10 BES workshop reports in the *Basic Research Needs* series (<u>http://www.sc.doe.gov/bes/reports/list.html</u>)
- The program is balanced and comprehensive, and, as needed, supports experimental, theoretical and computational efforts and develops new approaches 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 FY2009 based on an open competition among academic institutions, DOE labs and other institutions. Research activities may be sited at universities, at DOE labs or in joint university-lab collaborations.
- The EFRC awards are expected to be in the \$2–5 million range annually for an initial five-year period. Pending Congressional appropriations, it is anticipated that approximately \$100 million will be available for multiple EFRC awards.
- A Funding Opportunity Announcement (FOA) was issued on April 4, 2008 to request applications from the scientific community for the establishment of the initial suite of EFRCs
- 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 information on the FOA will be available through a link on the BES home page (<u>http://www.sc.doe.gov/bes/</u>)

Next, **Kung** discussed the Funding Opportunity Announcement (FOA) Number: DE-PS02-08ER15944. The issue date was April 4, 2008 (Amendment No. 002, June 19, 2008). The application due date is October 1, 2008 at 11:00 p.m. The Letter of Intent (LOI) was due July 1, 2008. Part IV, Subsection B.1. of the EFRC FOA, "LOI" asks for the following:

- name and mailing address of the lead institution
- listing of the other institutions that are expected to be involved in the planned application
- planned title of the EFRC
- name and email address of the EFRC Director and Principal Investigator(s)
- estimate of the total cost of the project over the five-year project period and/or an estimate of the cost in each year of the project
- 5–6 page narrative containing the following:
 - an overview of the strategic plan, including the long-term vision and goals for the proposed EFRC, as well as the objectives for the initial five-year period of the project
 - o an overview of the research plan

Kung said "The submission of LOI is very strongly encouraged as they will be used to organize and expedite the merit review process. However, failure to submit such letters will not negatively affect a responsive application submitted in a timely fashion."

The following is a summary of the 251 FOA LOIs

- 205 LOIs are from universities in 42 U.S. states and D.C.
- 29 LOIs are from 12 DOE labs (no more than three may be submitted from a specific institution)
- 14 LOIs are from private institutions and 3 LOIs are from individuals

- The 251 LOIs indicated a total funding request of more than \$900 million per year
- The EFRC research areas cover all 10 BRN workshop areas with particular interests in solar, electrical energy storage, nanoscale materials for energy applications, interfacial charge transport, et al.
- Many LOIs describe EFRCs with substantial breadth, making statistical categorization into BRN categories inappropriate

In reviewing single investigator and small group research, **Kung** said we are "tackling our energy challenges in a new era of science." Pending appropriations, up to \$60M will be available for single-investigator and small-group awards in FY2009. BES seeks applications in two areas: grand challenge science and energy challenges identified in one of the BRN workshop reports. Awards are planned for three years, with funding in the range of \$150-300k/yr for single-investigator awards and \$500-1500k/yr for small-group awards (except as noted below). Areas of interest include:

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

This opportunity is being handled as part of the normal BES process for seeking new applications from universities and DOE labs. For universities, it falls within the broad annual announcement for the Office of Science, DE-PS02-08ER08-01 (and the FY2009 equivalent). Potential university applicants are strongly encouraged to follow the BES guidelines for grant applications (<u>http://www.sc.doe.gov/bes/grants.html</u>). These guidelines include an initial contact with a suitable BES program manager(s) and submission of a pre-application, which is evaluated by BES for encouragement or discouragement of a full application. Appropriate BES program manager(s) contacts are listed for each of the areas of interest. DOE labs are welcome to respond to this opportunity. Additional guidance has been given to the DOE labs regarding the submission of a full proposal.

El-Sayed asked what about the breakdown of the appropriations.

Kung said "60% goes to DOE labs and 40% goes to universities." She added, "Some of the challenges we face are with the Senate and House appropriations, but we plan to move forward with our focus being on EFRC."

Gates asked "How is the scientific community responding?"

Kung said "We have seen a broad range from the community responding to team arrangements that encompass labs and universities. The focus is one basic science that covers multiple subject matters."

Kirby asked how proposals would be evaluated.

Kung said it will take three-to-four months to review before an award. "We will have a clear sense of the '09 budget."

Hemminger asked if people are responding to the fundamentals of technology.

Kung said "yes, there has a great response to the FOA process."

At 9:02 a.m., **Hemminger, Crabtree** and **Kastner** lead a discussion on BESAC's New Era of Science Sub-Committee Discussion – "Facilities and Light Source of the Future."

Kastner began the presentation by stating "there are a number of cross-cutting issues that show up in multiple reports. We need to identify these issues and then discuss the roadblocks in finding the solutions to the energy problems plaguing the U.S. It is hard to identify how we get certain things accomplished. The second part is to do what BESAC is set up to do. How should we address the challenges that need to be addressed? This is an implementation strategy. We have a clear recognition to communicate the message of the importance of light sources to decision makers. Without these breakthroughs, we can't get to get where we want we need to be."

Kastner continued by saying "it has been brought to our attention through budget appropriations of the importance. We do not need to have five or six reports. We have a timeline issue to have something that is effective. We need to have a quality preliminary report that addresses the 'show-stopper' issues of the BRNs and Grand Challenge Report and the implementation strategy and solutions. This is the strategy that **Hemminger** would like the Sub-Committee to move forward with. Yesterday, we had a reasonable amount of input. Today, we would like to hear some implementation strategies to get these things accomplished."

Gates said "we need to make sure the report is about energy. We should hire a science writer to create a condensed report to make statements about cross-cutting issues. The introduction is crucial and needs to be written concise, positive way and stress the importance of research."

The following are the Charges concerning "BESAC's New Era of Science."

Charge 1

1. Materials by design

• Materials discovery by design -- move beyond serendipitous materials synthesis, especially by extracting design principles through theory/modeling to accelerate

discovery; actual materials by design still seems a stretch, especially for emergent, correlated phenomena, but we need to do much better than random walk.

- Determination and design of structure-function relationships for controlled synthesis of nanoscale and supramolecular structures
- New materials by design and advanced search techniques for solar photoconversion. The number of materials presently used or under study for solar photoconversion to electricity and fuels is extremely small (hundreds) compared to the total number of possibilities (tens or hundreds of millions). The ability to conduct both advanced theoretical analyses plus extremely rapid and high throughput combinatorial synthesis of new materials with specific properties (such as high solar conversion efficiency, long-term stability and made from abundant and inexpensive elements) will be a major advance in energy science and technology. The targeted materials and systems include organic, inorganic and hybrid solar cells; photoelectrodes and molecular-based structures for solar water splitting and CO2 reduction with H2O to produce solar H2, alcohols and hydrocarbons (artificial photosynthesis); and water oxidation catalysts and other important chemical transformation catalysts.
- Synthesis by design instead of serendipity
- Develop the knowledge and ability to design and fabricate, through controlled synthesis, materials, interfaces and structures with tailored properties
- Design and virtually synthesizing new materials
- Designer interfaces and membranes

2. Materials synthesis

- Determine and control the origin of mistakes in structure during polymer synthesis, to get compositionally and structurally pure material
- Determine the limits (and their origin) to controlled fabrication of integrated nanosystems with reproducible properties. Can we achieve the level of control needed to fabricate integrated nanosystems with the same level of reproducibility as found in today's integrated circuits?
- Predicting self assembly
- New materials discovery, design, development and fabrication, especially materials that perform well under extreme conditions
- Bio-materials and bio-interfaces, especially at the nanoscale
- Synthesis and crystal growth

3. Understanding defects

• Controlling and exploiting defects and interfaces for performance - for a number of functional responses, performance arises from manipulating and controlling defects (e.g., pinning vortices in superconductors) and interfaces (e.g., enhanced strength and radiation resistance in structural nanocomposites); we need to be able to do this reliably and repeatedly, especially because reaching semiconductor purity (where defects are relatively irrelevant) is unachievable for most complex materials

4. Multi-scale/Emergence

- Fundamental rules of correlation and emergence in systems ranging from many-body atomic and molecular processes to condensed matter
- Multi-scale emergence of macroscopic damage from nanoscopic defects
- Understand and exploit the atomic/microscopic basis of macroscopic complexity (emergent structures and behavior)
- Multi-scale characterization, understanding and control of matter, spanning atomic spatial and time scales (elementary process thermodynamics, mechanisms and kinetics) to macroscopic spatial and process time scales, in gas, liquid and condensed phases and at interfaces and in confined environments.

5. Modeling

- New paradigms for describing complex matter and processes at conditions far from equilibrium, beyond the Born-Oppenheimer approximation
- Perform modeling that enables reliable predictions about materials performance at long (possibly geologic) timescales and in extreme environments
- Integrate the physical characterization and modeling of materials systems
- Providing insight into nanoscale experimental measurements with theory and modeling
- Understanding function and impact of dynamics and fluctuations
- Virtual characterization of new materials
- Structure-function relationships

6. Self-healing

- Self-repair of systems for converting solar radiation to solar electricity and solar fuels (solar photoconversion). Since all solar energy converting systems require large initial capital investments, the lifetime of their peak performance must be approximately 20-30 years in order to be considered as cost effective energy options. The ability of these systems to self-repair the damage incurred from long-term exposure to the natural but relatively severe outdoor environment will be a major advance in energy science and technology. Understanding and utilizing the lessons of self-repair in biological systems may prove to be very useful to meet this objective.
- Self-healing of defects induced by extreme environments such as sunlight and high temperatures

7. In situ characterization

• Develop in-situ, real-time spectroscopies of functional response and couple them directly to synthetic approaches

- In-situ characterization of energy transduction processes, and in materials under extreme conditions, with spatial resolution on the scale of molecular dimensions or better and time resolution on the scale of atomic and molecular processes
- In situ characterization of energy conversion processes: photovoltaic, electrochemical, photosynthetic, etc.
- Provide real-time imaging of physical processes at the atomic/molecular scale, for example of the structural changes in arbitrary biomolecules when they interact with photons
- New tools for spatial characterization, temporal characterization and for theory/modeling/computation

8. Catalysis

- Designer catalysts
- Design and controlled synthesis of catalyst structures
- Catalysis of energy conversion reactions: water splitting, oxygen reduction, reduction of CO2 to fuel, etc.
- Understanding the mechanisms and dynamics of catalyzed reactions at the atomic and molecular scale
- Understand the catalytic deconstruction of cellulose and lignin at the molecular level
- Design and understand reactions that remove oxygen and increase the hydrogencarbon ratio
- Understand in detail how multi-electron transfer reactions, such as photosynthesis, occur

9. Interfacial Processes

Catalysis and chemical transformations at surfaces, energy flow at interfaces

Other

- Understanding and control of the interaction of photons and electrons with matter.
- Quantifying transport mechanisms at the nanoscale
- Control of photon, electron, spin, phonon, and ion transport in materials
- Science at the nanoscale, especially low-dimensional systems

Charge 2

Magnitude / Organization of funding support

- Investments consistent with the magnitude of the challenge --this year's EFRCs (\$5M/yr for five years) are a good step in the right direction; we need to make these real and not be a one-time phenomena and then build networks of EFRCs to ensure appropriate competition and collaboration
- Integration of support mechanisms across scientific disciplines

Collaboration

- Create "centers" that enable scientists from institutions all over the world to come together to work on specific grand challenge problems. These would involve virtual connectivity enabling world-wide communication/collaboration on the specified problem and a physical place where groups could gather for specific projects and workshops/seminars.
- Energy or scientific grand challenge networks, composed of top scientists at multiple institutions with collaborative focus on a single grand challenge
- Develop mechanisms such as networks, collaborative access and data sharing to facilitate access to unique capabilities and to great synergy in addressing the science and energy challenges
- Sustained investment in focused multi-disciplinary teams, including theory and experiment, in the full range of disciplines necessary to address energy and science grand challenges
- Science institutes at national labs to integrate and support science projects generated from the academic community
- How can we improve the efficiency of interaction between the science drivers and the instrumentation developers?
- Very often the science drivers are not the ones who design and build the best and most novel instrumentation and vice versa. A more efficient interaction between these groups of scientists would certainly be beneficial.
- Programs for integration of User scientists into facility development for training and innovation
- Implement programs that will improve the coupling of state-of-the-art theory and experiment

Single Investigator

• Maintain a focus on serendipitous discovery by entrepreneurial single investigators to ensure the seed corn of the future continues to be cultivated; endeavor to bring a greater fraction of early career investigators to the portfolio

Workforce development

- Energy or science grand challenge summer schools for top students, post-docs and early career scientists with comprehensive introduction to a multidisciplinary grand challenge
- Five-year energy fellowships for promising early career scientists
- Investment in mechanisms to develop a work force needed to address energy and science grand challenges, including fellowships for students, post-docs, and scientists at various career stages
- DOE/SC should take the lead in a large scale public education program to make all citizens cognizant of the great issues related to energy and the environment. This should be done in the pre-college educational system starting in elementary school through high school, as well as in the general arena of public information and education.
- Scientific and technological progress in meeting our energy challenges requires a scientific workforce which is highly inter-disciplinary in physics, chemistry and biology. DOE should establish and support programs at research universities that promote interdisciplinary studies and academic programs related to energy science and technology. These would include special and prestigious energy fellowships for undergrads, graduate students, post-docs, and faculty. Within DOE and the Office of BES itself, the traditional stove-piping of materials sciences, chemical sciences and biosciences should be eliminated and cross-disciplinary programs should be coordinated to maximize productivity from limited resources. DOE should encourage and reward inter-national lab cooperation, collaboration and jointly-funded programs.

Basic-applied translation

- Lower barriers to translation of scientific breakthroughs to technologies and products, specifically in areas germane to energy. This involves both a change in the operation of DOE (closer interaction between SC and the technology offices) and the development of a structure that rewards scientists both for scientific breakthrough and for translating those breakthroughs to societal impact.
- A very important structural element required for success with DOE research programs to bridge the cultural and communications gap between the programs and their managers at the DOE Office of Science and those of the various DOE Energy Technology Offices. The basic energy science generation by SC should underpin and lay the foundation for present and future energy technologies. There should be a smooth and efficient path for transferring new science into new and/or improved technologies. The present situation is far from optimum and is inhibiting progress in improving present energy technologies and establishing new and better energy technologies for the future. Correction of this issue will result in better funding and political support for the SC basic energy science programs.

Equipment / Infrastructure

• Invest in physical infrastructure (competitively), on a scale comparable to the current crop of nanocenters: Energy Discovery Centers, focused on multidisciplinary coupling of synthesis, characterization and theory--in a sense these would be a response to the

"beyond nano" need articulated in the Complex Systems workshop report (http://www.sc.doe.gov/bes/reports/files/CS_rpt.pdf)

• Investment in developing equipment, particularly at the mid-scale level, to address energy and science grand challenges.

Charge 3

Space and time resolution

- Imaging of functionality at the best possible spatial and temporal resolution. This is certainly at the heart of many of the scientific challenges described in the previous reports.
- Attosecond pulses --- what is the best strategy to study and control ultrafast electronic processes (chemistry, information technology)
- Attosecond pulses have severe limitations because of their inherent energy bandwidth
- The study and control of these phenomena requires not only the temporal resolution, but also sufficient energy resolution to discern the electronic states. Is there an optimum for information?
- Femtosecond X-ray pulses at full high-brightness for single-particle diffraction studies in life science and nanoscience
- Attosecond time resolution to see chemical reactions
- Sub-nm X-ray focusing to enable spatially resolved probing of complex molecules

Imaging

- Light-based imaging techniques in the VUV to X-ray range can certainly have a large impact. What can be achieved and what does that require in terms of a light source, optics and detectors.
- Competition with scanning probes and electron microscopy

Coherence

- X-ray coherence at 1Å wavelength (FEL) for a broad range of science
- Coherent control of atomic positions by the electric field of light to "catalyze" chemical reactions

In situ

- Study of processes under real conditions so far, mostly idealized model systems are being investigated, whereas the real processes are occurring under totally different conditions (under a high pressure atmosphere, in liquids (water) for biological systems). How can we get closer to make observations of processes under real operating conditions?
- Develop the capability to 'catch materials at work' -real-time studies of 3-d materials interactions, in analogy to LCLS' "watching chemical bonds break and form"-- this would necessitate relatively high energy X-rays (for macro samples) and a relatively

high repetition rate- likely coherent (for dynamic events) and high fluence (for single shot measurements rather than averaging)

Theory

• Integration of theory efforts into next generation facilities

Capacity

• Facilities with sufficient capacity to support photon needs for studies at the cutting edge of science, but not necessarily at the technological limit of brightness or coherence

Greene said we "should hire a science writer. We need to work closely with this person to get key points across in the report. We have to stress the importance of funding at universities, how research has changed and the importance of basic research. It is a matter of global survival. We already have the information. It just needs to be funded to continue the research.

Spence asked if there are mechanisms in place to give collaborators the funding the funding they need? Kung responded "yes."

Moskovits asked who the audience was for this report. "There is a presumption that we have to convince people of the importance of basic research." He said he would like "to have a greater clarity who will be reading this report and who we are trying to impress. It would be helpful to have a well-structured, brief introduction about energy responsibility from the DOE and how to solve the current problems." In addition, **Moskovits** said it would be "worthwhile to engage the industry and government and take the message with credible fundamental roadmaps of major light sources and how do we 'connect the dots.""

Kirby agrees with **Moskovits** that we know who is going to "convey the message." She questioned if those participating in the report (Sub-Committee) should engage in this process.

Ceyer asked if we are over-emphasizing the need of collaborative structures.

Berrah said "in order to have feedback, national labs have to collaborate with each other. Science will benefit and have more impact if thoughts are pulled together. I strongly encourage more scientists from different labs to work together."

Hammes-Schiffer said the "collaborative structure needs to include the younger generation. It is important for collaboration to be broad and bring in young minds. If not, we are going to lose a whole generation of scientists."

Bare asked "what is this report supposed to do?" He said he was sure it would be great like the others, but questioned the strategy of taking this report, getting it published and getting the word out that we are truly in a crisis. "We should concentrate on getting this report to newspapers, NPR, labs and universities presidents. The message must be worthwhile and impactful. It needs to be understandable and we should be able to communicate it to different audiences."

Hemminger said "In the past, BESAC has not been active in getting the reports to the next level." He suggests convincing a small number of Committee/Sub-Committee of what we are going to do with the report.

El-Sayed said "what we are going to do with this report is going to determine how it is written."

Hemminger said "this is not a topic that we are going to determine today and need to have additional discussions. We need to focus on what will help the Sub-Committee most."

McCurdy Jr. said "Until we get a focus of how and who we are going to present this information, I recommend that we make the connection to science themes to resolve issues to the energy crisis. We need to communicate our change in culture and how things will be different in the next 10 years."

Eberhardt said we have to foster the collaboration between disciplines of science.

Morse said he agrees with McCurdy's comments that it is time to stop addressing the scientists and address the people. "We are addicted to oil and that is the challenge we must show."

Eberhardt asked how do we get more young people to go into the field of science?

Crabtree said "the appeal to energy is greater than the appeal to science."

Nagy suggested DOE should provide more funding and have five years of fellowships.

Richards said "it is important to have academic and national lab positions. Both of these have to be well-funded for young people to have an eventual career."

Berrah said we must keep our students interested, but the financial situation is not keeping people in their respected fields. "We must have better salaries, more post-doc

opportunities which should be funded for five years and creatively think about funding mechanisms.

Taylor said "we have great science and have the ability to solve problems. We must continue to find great scientists. You must choose the right people. DOE must have a mission to do this and make sure it gets done."

Moskovits said "we must integrate workforce development. We must start early and excite young people. This is not a new problem. Reports have predicted for years that there will be a shortage of scientists, but I do not believe it has happened." He suggested the greatest impact is that of "beginning faculty" (science people early in their careers). They are the future of their department. They will be the ones who are responsive to the current set of problems. He questioned what the problem is concerning funding for young faculty. Many universities do not want between young faculty members. He believes there is potential to find a new set of radical new ideas through these collaborations.

Gates said there is not enough money and the consequences of that are "professors are dying on the vine." If funding is available, people will continue to work and have an interest.

Crabtree asked if the Committee/Sub-Committee could change their focus to looking at the Tools of Light Sources and beyond.

McCurdy Jr. said this is a difficult topic. He said "we do not have to start from scratch. There have been intense discussions at the labs to reach far enough to do much with the science in our plan. You must collect the information that is already out there."

Berrah said we cannot forget the detectors. "We have not done this in the past because of the expense. We are far behind and it is time to be more effective and efficient."

El-Sayed said "imaging should be a higher priority."

Morse asked "How do we present and decide the allocation of personnel and tools. Are we looking more at the personnel or the tools?"

Dehmer said "Every time we have this discussion, I suggest the initiative have more of a balance. Workshops and excellent research have come from this balance. It is easier to sell a facility than it is to sell research. It is an on-going challenge to maintain a balance."

Gates said the same challenges exist in the laboratories.

Dehmer said "I have worked very hard to increase the people who are doing research. I want to encourage the academia workforce to attract more students, but it takes the entire Federal system to buy into this. Facilities are now funded at 50% versus 25% just 15 years ago, yet it is 10 times harder to get support for personnel than a facility."

Kirby said graduate fellowship programs give you more independence and prestige concerning picking your project as a scientist. "We need to raise the amount of money that a graduate fellowship would provide. A DOE fellowship would attract a great group of young minds. I would also like to see it at the post-grad level."

Berrah said Light Source has had a great impact. "I do not see this should be an issue of adding this into the document."

Morse said young researchers see what we need to do, yet sometimes believe it is not for them.

Bare said "the students will go where the money is, whether it is in industry or wherever. Light Sources have great potential in research areas. We can't forget a community of Light Source users."

Cummings asked if we could partner with a group from Siemens to attract young scientists at the high school level. "I would recommend a \$150,000 gift to high school students. These types of gifts will get the attention of DOE."

Morse said two of the things that the U.S. is lacking are science perks and shared facilities, which is already happening in Japan and Singapore. "We need to collaborate more to meet expectations."

Cummings said he think the audience of this report has to be the public.

Ming Chiang suggested more one-on-one partnerships.

Gates said the industry is putting substantial attention to energy-related research. Industry needs to encourage faculty to work in energy areas. "We are at a time to form a contingency to say everything is ready for us to make a case."

Hemminger said "we need to work on new ways to couple experiments and theory. We have had a lot to say over the past two days. I think it is apparent that we can count on the BESAC Committee and Sub-Committee to discuss these issues with George and Mark in greater detail. I hope everyone stays engaged in this very important report.

At 10:58 a.m., **Hemminger** asked for public comment.

Hemminger adjourned the meeting at 11:00 a.m.