Minutes for the
Basic Energy Sciences Advisory Committee (BESAC) Meeting
September 20 – September 21, 2007
Bethesda Marriott @ Pooks Hill
Bethesda, Maryland

BESAC members present:

Nora Berrah
Sylvia Ceyer
Peter Cummings
Frank DiSalvo
George Flynn
Laura Greene
John Hemminger, Chairman
Eric Isaacs
Kate Kirby
Walter Kohn
Gabrielle Long
William (Bill) McCurdy, Jr.
Ward Plummer
John Richards
John Spence

BESAC members absent:

Sue Clarke
Bruce Gates
Anthony Johnson
Daniel Morse
Martin Moskovits
Mostafa El-Sayed
Kathleen Taylor
Stanley Williams
Mary Wirth

Also participating:

Alexis (Alex) Bell, University of California Berkeley
Patricia (Pat) Dehmer, Associate Director of Science for Basic Energy Sciences, USDOE
Graham Fleming, UC Berkeley and Lawrence Berkeley National Laboratory
Ray Johnson, Recording Secretary
Harriet Kung, Director, Material Sciences and Engineering Division
Dean Miller, Argonne National Laboratory
Pedro Montano, Department of Energy
Raymond (Ray) L. Orbach, Under Secretary for Science and Director of the Office of Science, DOE
Mark Ratner, Northwestern University
Eric Rohlfing, Director, Chemical Sciences, Geosciences and Biosciences Division

Approximately 110 others were in attendance for brief segments during the course of the two-day meeting.

Thursday, September 20, 2007

Chairman John Hemminger called the meeting to order at 8:35 a.m. He promptly asked **Leslie Shepherd** to make administrative, safety, and convenience announcements. Afterwards, **Hemminger** had each committee member introduce themselves.

Hemminger began the meeting by thanking all of those attending the meeting. He also acknowledged all of the hard work from the Sub-Committees who participated in the Grand Challenges Report.

At 8:40 a.m., **Hemminger** introduced **Alexis (Alex) T. Bell** and asked him to provide the Committee with a report on the BES Workshop on Basic Research Needs for Catalysis for Energy.

The workshop was held August 6-9, with Co-Chairs including **Bell**, **Bruce Gates** (UC-Davis) and **Douglas Ray** (PNNL). The BES shepherds were **John Miller** and **Raul Miranda**. The charge of the workshop was to identify the Basic Research Needs and opportunities in catalytic chemistry and materials that underpin energy conversion or utilization, with a focus on new, emerging and scientifically challenging areas that have the potential to significantly impact science and technology. In addition, the workshop should uncover the principal technological barriers and the underlying scientific limitations associated with efficient processing of energy resources. The highlighted areas included the major developments in chemistry, biochemistry, materials and associated disciplines for energy processing and will point to future directions to overcome the long-term grand challenges in catalysis technologies to grow rapidly.

Bell stated this was the first report and workshop fully devoted to catalysis and its impact on fuels production. There were 130 participants (academia accounted for 53; national laboratories 43; government 20; industry professionals 14). Among notables attending included **Rutger VanSanten**, who provided a European point of view; **William Banholzer** from Dow Chemical, who provided feedback concerning the Middle East; and **Anthony Cugani** from DOE, Renewable Energy.

Bell discussed the research drivers – energy security and environmental concerns. With demands and energy on the rise, “by the end of the century we will have to be making some serious changes.” The reserve life at the current consumption rate is 35 years for oil, 60 years for natural gas and 400 years for coal (85% comes from oil, gas and coal, 15% from nuclear and renewable sources).

The growing demand for energy and finite availability of traditional energy feedstocks (oil and gas) motivates the consideration of alternative fossil feedstocks (tar sands, shale, coal) for the short term. Looking longer-term, biomass conversion offers the possibility of a sustainable source of fuel. In the future, the generation of H2 from H2O and H2/CO2 should be considered using non-thermal sources of energy (e.g. photons and electrons).

The conclusions were:

- Changes in the feedstocks from which fuels are produced are likely to occur in this century
- Future fuel-supply technologies must be sustainable
- Novel catalytic technologies will be required for the production of fuels

The implications for researchers:

- Research should be directed at developing a fundamental understanding of how future feedstocks (share oils, tar sands, biomass) can be converted to fuels efficiently
- Basic research aimed at understanding catalyst structure and catalytic phenomena will contribute to the knowledge base used to guide the discovery and development of new catalysts

The Grand Challenges in Catalysts include 1) imaging and simulation of electronic and geometric structures of catalytic materials under reaction conditions 2) Determination of reaction mechanisms and understanding of their kinetics 3) prediction of catalytic activity and selectivity and their response to reaction conditions 4) Understanding of catalytic reaction dynamics

Catalysts particles of uniform size and shape can serve as models. Micro- and meso-porous material can be made with controlled pore size and composition. The control of catalyst structures at the atomic and nanometer length scale and the creation of multi-functional catalysts emulating motifs found in biological catalysts are considered *very* grand challenges. Synthesis of biometric catalysts with applicability for energy applications is also a grand challenge.

For the advanced catalysts for conversion of fossil energy feedstocks, petroleum feeds are becoming heavier and more S-containing, placing an even heavier demand for H2 on refiners. Alternative fossil feedstocks have lower H/C ratios than petroleum and higher S and N contents, raising the demand for H2. For fossil fuel, two challenges are being raised: 1) discover catalysts for the transfer of H atoms from light alkanes (use methane, if possible) 2) discover catalysts for heteroatom removal that minimize product hydrogenation.

Refinery processes are very sensitive to feedstock composition. The changing feedstock requires an understanding the effects of feedstock composition on individual processes. The challenge is to describe complex feedstocks and processes on a molecular basis taking into account catalysts properties.

With structure-oriented lumping (SOL) permits the description of feeds and products at the molecular level, the challenge is to represent dynamics of each reaction step in terms of catalyst properties, including dynamics of transport. This was looked at by **S.B. Jaffe** from Exxon Mobil in 2005.

In the advanced catalysts for conversion of biologically-derived feedstocks, biomass can be converted to fuels by:

- Pyrolysis – complex liquid products requiring further processing
- Gasification – produces CO/ H2 that can be converted further to diesel
- Deconstruction – Produces sugars that can be converted to fuels by enzymatic or non-enzymatic catalysts

The liquid-phases processing of lignocellulose begins with deconstruction cellulose and hemicelluose to release sugars. The challenge is to identify catalyst/solvent systems for the efficient deconstruction of biomass.

The gasification of biomass and production of fuels are filled with chlorine and potassium. The challenges are the development of catalysts for the elimination of char-produced during gasification of biomass and the catalysts for control of product distribution obtained from FTS.

The panelists on the workshop believe there are many important opportunities. Fuel targets can be selected on the basis of energy content, volatility and C rejection as CO2. The challenges include being able to identify catalysts for the selective formation of targeted fuel components and to determine the reaction pathways via which glucose is converted to fuels.

Advanced catalysts for photo- and electro-driven conversion of H20 and C02 finds that all fossil energy feed stocks require H2 to increase their H/C content and to remove heteroatoms. CO2 rejection can be eliminated by using a non-carbon source of H2. The challenges include to provide an inexpensive, non-carbon source of H2 and to recover the C-value of CO2 so as to avoid the need for CO2 emission or sequestration. All of US transportation fuel needs could be supplied by a land area equivalent to about half of that used for agriculture today.

Plants use solar energy to convert H20 and CO2 to sugars with an energy efficiency of <1%. Photo-electrocatalytic systems convert H20 to H2 with an energy efficiency of 1-10%. Electrochemical systems convert H20/CO2 to H/CO with an energy efficiency of ~50%. The challenges include: 1) to understand the relationships of catalyst composition and structure to the elementary processes leading to the generation of H_2 2) To identify catalysts that enable the efficient utilization of e-/h+ pairs for the splitting of H20 and the reduction of CO_2.

In cross-cutting themes: advanced instrumentation in theory, modeling and simulation, the challenge are to develop 1) advanced instrumentation for in situ observation of catalysts 2) reliable theoretical methods for describing the reactions of complex molecules, including the effects of transport 3) simulation strategies for describing the complex systems of reactions occurring during the processing of fossil and bio-derived feedstocks.

In closing, **Bell** reiterated the Grand Challenges were: 1) understanding the mechanisms and dynamics of catalytic transformations and the 2) design and controlled sythesis of catalytic structures. The priority research directions include understanding:

- Complex transformations of fossil fuel feedstocks
- Lognocellulosic biomass and the chemistries of deconstruction
- Chemistry for conversion of bio-mass-derived oxygenates to fuels
- Photo- and electrochemical conversion of H20 and CO_2

Cross-cutting themes are the advanced instrumentation for in situ characterization of catalysts and catalytic processes and the advanced theoretical methods for the simulation of catalysts and catalytic processes.

Hemminger said the basic research needs have been very important and thanked **Bell** and the group for the tremendous amount of time they have invested in this research and workshop.

Frank DiSalvo complimented **Bell** on “a great report, very interesting.” He added that it overlaps well with the other sciences and questioned if biologists are working with plants will have an effect.

Bell said he was aware of a great volume of work with the biologists.

John Richards that it would be interesting to know how much land how many farmers are selling corn for ethernol. He said it creates social tensions and that we must minimize the land used for these types of activities.

Bell said it we needed to utilize carbon to make fuel for transportation and heating.

Bill McCurdy Jr. congratulated **Bell** on his presentation. He said that a few years ago, the reaction was for catalysts were different and what had been done, if fundamental issues had been applied and the report should include previous information from the report.

At that time**, Hemminger** suggested the Committee move forward with the next presentation and that if there needs to be further discussed and time had been appropriated for later in the afternoon. He also stated that since the Committee met in early in August, **Dehmer** believed it was more important to deliver an overview of the activities and new structure of the BES Division of Material Sciences and Engineering (DMS&E), which would be provided by **Harriet Kung.**

At 9:25 a.m., **Kung** began her presentation with an overview of Materials Sciences and Engineering division for the office of Basic Energy Sciences (BES). Kung presented a presentation outline, which included the program’s vision, reasons for change, new organization structure, team structure overview, projected program evolution, relationships between the Division and with other programs (explaining the unique roles), contact information, new hires and Web site information.

The research themes and highlights included:

- Radiation damage resistance in materials
- Nanomagnetism-scattering
- Superconductivity
- Materials discovery and design
- Nanoscale building blocks for energy applications
- Solar energy utilization

Kung stated the vision is to provide the knowledge base for the discovery and design of new materials with novel structures, functions and properties to drive the frontiers of discovery science and to address grand energy challenges. The three major scientific themes being supported in the Division are 1) scattering and instrumentation sciences 2) condensed matter and materials physics and 3) materials discovery, design and synthesis.

Kung reviewed the current workchart of BES and said the divisions must continue to evolve. Kung is one of three directors reporting to **Dehmer**, with **Pedro Montano** (Scientific User Facilities Division) and **Eric Rohlfing** (Chemical Sciences, Geosciences and Biosciences Division) being the others.

Kung continued by stating what led to the need for change. The emergence of scientific opportunities, to strengthen the focus of scientific themes, to strengthen synergy among CRAs and scientific themes, the balance between discovery science and use-inspired science, the balance between strengths in current research portfolios and future growth opportunities and striving for a more unified Division-wide investment strategy.

The new DMS&E team structure includes three teams, all of whom have a set of central program goals/scope and a close coupling and connection. The Materials Discovery Design and Synthesis team looks at the rational design and synthesis of new materials via physical, chemical and biomolecular routes. Next, the Scattering and Instrumentation Sciences studies photon, neutron and electron interactions with matter for characterization of materials structures and excitation. The third team, Condensed Matter and Materials Physics, looks at understanding and controlling material behavior and discovery of new emergent phenomena. This three-team structure provides scientific focus to capture new opportunities.

Kung continued by discussing members of the Materials Sciences & Engineering Division and their respective responsibilities. **Helen Kerch** is the lead of the Scattering and Instrumentation Sciences team; **Arvind Kini** is overseeing the Materials Discovery, Design and Synthesis and **Jim Horwitz** serving as the lead for the Condensed matter and materials Physics team.

To understand the physical properties of any material, one needs to begin with its structure and dynamics. X-ray, neutron and electron scattering are primary tools for characterizing the atomic, electronic and magnetic structures are excitations of materials. The Scattering and Instrumentation Sciences program is the most comprehensive scattering portfolio in the federal government.

The importance of x-ray and neutron science has been broadly recognized as some 15 Nobel Prizes (14 in x-rays; 1 in neutrons) have been based on research utilizing these tools. This program supported the research of **Clifford G. Shull** at Oak Ridge National laboratory (ORNL) that resulted in the 1994 Nobel Prize in Physics for the development of the neutron diffraction technique. The program has pioneered many instruments and techniques in scattering, spectroscopy and imaging, and it continues to be the nation’s primary supporter of the development, construction and implementation of a wide variety of science-driven techniques and instrumentation for the natural sciences.

The increasing complexity of energy-relevant materials, such as superconductors, semiconductors, magnets, structural and other electronic materials require ever more sophisticated, specific and sensitive x-ray, neutron and electron scattering techniques to extract new and useful knowledge and to develop new theories for the behavior of materials.

Kung added, “We need more sophisticated tools to characterize these processes as we drive to be the frontiers for new techniques.”

Four key areas of research in Scattering and Instrumentation Sciences are:

- Elucidate the mechanisms that control superconductivity and other phenomena in correlated electron systems via scattering probes
    - Determine important correlations (spin, lattice, charge, orbital) that govern superconductivity, magnetism and other phenomena
    - Link structure and excitations to predictability and control
- Develop a structural and dynamical understanding of nanostructured materials
    - Solve the nanostructure problem to provide a complete quantitative chemico-physical characterization
    - Understand the interplay between properties and structure at the nanometer length scale
    - Develop new nanoscience tools and interpretive methodologies
- Understand the behavior of materials using ultrafast diffraction, spectroscopy and imaging techniques
    - See atoms, electrons and molecules at work and understand their functionality
    - Understand how entities form, grow and move under the influence of external fields
- Unify the complementary information obtained through multiple techniques
    - Develop the capability to analyze, visualize and understand data from different experimental probes

At the heart of the CMMP program is the quest to understand how unexpected phenomena emerge when large numbers of constituents interact with one another. These include fundamental building blocks of matter, such as electrons, atoms and molecules, as well as more complex building blocks, such as grain excitrons.

This tremendous range of constituents leads to a spectacular diversity of emergent phenomena. Examples of emergent phenomena targeted by CMMP researchers are ubiquitous in many technology marvels from semiconductor lasers in DVD players to exploiting nanomagnetism in computer data storage.

Studies of new phenomena have also led to significant advances in our understanding of the physical world, (e.g. while the development of ultrapure layered semiconductors made possible the development of high-speed transistors) they have also produced materials that lead to the discovery of completely unexpected new states of matter, such as the fractional quantum Hall state.

Efforts to understand magnets, ferroelectrics, superconductors, polymers, and liquid crystals, exploited in innumerable applications, spurred the development of the elegant, unified conceptual framework of broken symmetry that not only explains how the characteristic behaviors of these materials are related, but also underlies much of modern physics.

The key areas of research in Condensed Matter and Materials Physics were addressed:

- Understand the influence of correlated behavior on the properties of material
    - Determine how electron correlation gives rise to and influences the properties superconductors
    - Characterize the properties of new forms of matter that arise as a consequence of atom or particle correlations
    - Develop predictive models to design materials with complex and targeted emergent behavior
- Structure and properties of materials at reduced dimensionality

- Manipulation of electron spins in quantum structures (beyond Moore's law)
  - Tailor and control the identity, placement, and function of individual atoms leading to a macroscale assembly
  - Understand, control and predict the behavior of basic nanoscale building blocks
  - Coupling of different properties in materials such as electronic excitation with mechanical actuation
  - Develop theoretical framework that bridges the quantum mechanics with statistical mechanics
- Properties of materials under extreme environments
  - New states of matter and phenomena at very low temperature, high pressures, high radiation and very high magnetic fields to improve our understanding of known materials and to produce new, unexpected forms of matter
- Defect-behavior in materials at an atomic scale
  - Predictive models to understand the response of materials subjected to electrical and magnetic fields, chemical and electrochemical environment, and proximity effects of surfaces or interfaces
  - Determine the influence of stress and irradiation on the properties of materials
  - Develop predictive tools to design of materials with specific properties
- Characterization of materials phenomena over a wide-ranging spatial and temporal scales
  - Emphasize the connection between ultra-fast materials science and nanoscience
  - Multi-scale characterization and modeling to link behavior from the sub-nanometer to meter length scale over time scales from fs to seconds

The Materials Discovery, Design and Synthesis: Paving the Scientific Foundations for Innovation and Competitiveness is a program that was established in recognition that discovery and development of new materials has been the engine driving science frontiers and fueling technology innovations.

Numerous recent Nobel prizes- quantum Hall effect and fractional quantum Hall effect (Physics 1985, 1998), buckyballs (Chemistry 1996), and conducting polymers (Chemistry 2000) – were made possible by new materials. The material discoveries have also enabled generations of technology breakthroughs, from integrated circuits, lasers, optoelectronic communications, to solid-state lighting. Virtually, further advances in these technologies have been limited by the performance of materials.

Scientists from different disciplines – materials science, physics, chemistry, biology – have learned to combine different atomic constituents in different ratios and configurations to achieve structures with novel functionalities.

Understanding and controlling the hierarchical assembly of fundamental building blocks (atoms, molecules, clusters, and colloids etc.) in ways to synthesize materials with "designer" properties defines a grand challenge for materials research, (i.e. shifting the paradigm of materials discovery from serendipity to rational design).

The key areas of research in materials discovery, design and synthesis are to:

- Develop scientific strategies to precisely fabricate and engineer macroscopic materials with nanometer scale precision – "atom-by-atom" synthesis of materials
  - Organization principles regulating the assembly of atoms, molecules and clusters to form functional macroscopic structures
  - Predictive modeling of parameters associated with nucleation and growth processes
- Establish a fundamental understanding of thermodynamic, kinetic and dynamical aspects of self-assembly to produce both equilibrium and non-equilibrium material structures
  - Understand and emulate the self-, directed-, hierarchical- and dynamic assembly processes that are so pervasive in nature
  - Design and synthesize self-repairing materials

    - Exploiting interplay between multiple properties develops into new and unique functions (emergent behavior)
- Produce materials with precisely controlled defects for exploiting defect-controlled material properties
    - Tailoring the number and distribution of defects
    - Understanding fundamental principles and forces responsible for defect formation and concentration
    - Design of defect-tolerant and self-healing (of defects) materials
- Develop multi-component, multi-functional materials that can lead to properties and phenomena that are not achievable in individual components alone (e.g., inorganic, organic, polymeric, biological)
    - New combinations of components that have traditionally been considered incompatible with one another (e.g., biological and inorganic)
    - New properties and functions in such materials
- Develop entirely new classes of materials and innovative material architectures that can revolutionize energy conversion, storage and transfer
    - Can we synthesize novel material architectures in which the dynamics of energy and electron flow can be manipulated in a controlled fashion?

Kung moved into reviewing all of the workshops that had been held since October 2002 through August 2007. She said there had been significant benefits to holding each of the workshops and that these type of learning opportunities need to continue. All workshop reports are accessible at www.sc.doe.gov/bes/reports/list.html.

The programs that have recently been held and upcoming activities include:

- National Academy of Sciences
    - A Decadal Assessment and Outlook for the Field of Condensed Matter and Materials Physics (Spring 2007)
        - Review of the field of CMMP; make recommendations on how U.S. research might realize the full potential of CMMP research
    - Materials Discovery and Crystal Growth (Summer 2008)
        - An assessment of the status of U.S. capabilities in the discovery of new materials and in crystal growth
    - Biomolecular Materials and Processes (Winter 2007)
        - An assessment of the compelling science at the interface between biology and materials, and identification of future research opportunities.
    - Frontiers of Science at the Interface of Physical and Life Sciences (Winter 2008)
        - A more comprehensive assessment of the scientific opportunities at the broader interface between physical and life sciences
        - Identification of complex, large-scale problems which, when successfully pursued, will produce scientific breakthroughs in both
- Council for Division of Materials Sciences and Engineering-Sponsored Panel Studies
    - Ultrafast Materials Science (Fall 2007)
        - **Toni Taylor** (Los Alamos) and **Tony Heinz** (Columbia) panel co-chairs
        - Study focused on conveying new and perhaps under recognized (by the broad materials community not engaged in these activities) research at the intersection of ultrafast, optical and measurement science, condensed matter physics and nanoscience to observe and control dynamic emergent behavior in materials under non-equilibrium conditions
        - October 2007, Bishops Lodge, Santa Fe, New Mexico
        - Panel study publication to appear as comprehensive review article in Materials Science and Engineering R: Reports ("Complex Material Behavior at Ultrafast Timescales: Dynamics under Non-equilibrium Conditions")
    - Long Range Interactions (Fall 2007)
        - **Roger French** (DuPont& U Penn) and **Adrian Parsegian** (NIH) panel co-chairs
        - Panel aims to develop a comprehensive framework and language of long-range interactions in nanoscale science, acknowledging the different types of forces and different fields of science which have independently pursued them. Primary

forces include electrodynamic, electrostatic, and polar interactions that often exist in nanoscale assembly, colloid science, and solvation in electrochemical systems.
    - October 2007, Doubletree Hotel Annapolis, Md.
    - Panel study publication to appear as comprehensive review article in the Reviews of Modern Physics in February 2008

Kung said she looked forward to the output of the report. She also added there are some potential growth areas in the program evolution.

- Seeing Atoms and Electrons at Work
    - How do atoms and electrons give the functionality we need to catalyze a chemical reaction, divert a crack, pin a grain boundary, form a nanocrystal, and avoid electron-hole recombination?
    - What are the microscopic forces that lead to structural phase transitions in the picosecond time scale? How do nanoscopic magnetic structures form, grow, and move under the influence of external fields? How do intense electric and magnetic fields control electronic and structural materials properties?
    - What are the microscopic mechanisms in the slow dynamics of spin glasses and ferrofluids; the structure and topological details in the growth of thin films and interface roughening, sintering, phase separation, shear thickening in concentrated colloidal solutions?
- Discovery of New Emergent Phenomena
    - New materials and materials under conditions that are far from their equilibrium environment
    - Consequences of proximity effects that arise due to surfaces, interfaces and the interaction of materials with dissimilar properties
    - Control of the material defect structure, including type, density and distribution, including studies on single crystals, brittle materials and the controlled introduction of defects using radiation
    - Theoretical framework for the prediction of emergent properties and/or the explanation of the new phenomena
- Defining the Language of Self-assembly
    - Establish a fundamental understanding of thermodynamic, kinetic and dynamical aspects of self-assembly to produce both equilibrium and non-equilibrium material structures
    - Learn from Nature, then go beyond -- Emulate the self-, directed-, hierarchical-, and dynamic assembly processes that are so pervasive in nature
    - Achieve the atom-by-atom connectivity control and architectural diversity of materials in Nature
    - Design and synthesize self-repairing and adaptive materials
    - Harness the synthetic power of biology – Reprogram biological apparatus to grow very large crystals of predetermined shapes
    - Design and synthesize materials in which the interplay between multiple properties develops into new and unique functions (emergent behavior)
- Materials under Extreme Environments
    - Conduct experiments on the scale of the fundamental interactions; atomic scale, in-situ, real time characterization
    - Establish theoretical and simulation framework for predicting and extrapolating performance; capturing complex multi-scale phenomena and predicting beyond accessible regimes
    - Design and synthesis of transformation materials via control of atomic structure and complex damage evolution
    - Extreme environments for materials design and synthesis: photon/particle flux, chemical reactivity, thermo-mechanical and electromagnetic fields

Kung continued be stating the DMS&E portfolio is a significant source of federal support for fundamental scientific research in the following energy mission relevant topics:

- Radiation Effects

- Aqueous and Galvanic
- High Temperature Gaseous Corrosion
- Mechanical Behavior of Structural Materials at Very High Temperatures
- Strongly Correlated Electron Systems (including 5f systems)
- Photovoltaic

Kung added that there is a strong linkage to the relationship of DMS&E and other programs, including:

- Intra-DOE:
  - Energy Materials Coordinating Committee (EMaCC)- involves 19 DOE program offices that support materials research
  - Other SC and DOE Programs:
    - BES: CSG&B and DSUF
    - SC: ASCR and FES
    - EERE: Hydrogen, FreedomCAR and Vehicle Technologies, Solar Energy Technologies, Solid-state Lighting, and Industrial Technologies
    - OETD: Superconductivity, Utility-scale Energy Storage
    - FE: Hydrogen from Coal
    - NE: NGNP, GNEP and NHI
- DOE NNSA Defense Program
  - Strategic Science Alliance
- Interagency: MatTec Working Group on Structural Ceramics, MatTec Working Group on Metals, NNI NSET subcommittee, Interagency Working Group on Hydrogen and Fuel Cells; participated by other DOE programs, NSF, DoD/DARPA, NIST, NASA, DOT

At the end of her presentation, **Kung** reviewed a number of relevant Web sites for DMS&E programs:

www.science.doe.gov/bes/dms/DMSE.htm and click on List Manager

For core research programs:

- http://www.science.doe.gov/bes/dms/DMSE.htm (Division of Materials Sciences & Engineering)
- http://www.science.doe.gov/bes/dms/Staff_Contacts/staff_contacts.htm (Staff Contact)
- http://www.science.doe.gov/bes/dms/Publications/EMaCC/emacc.htm (EMaCC for info on materials research within DOE)

For SBIR/STTR:

- http://sbir.er.doe.gov/sbir

For upcoming hires in FY08

- 1 Program Manager for Materials Chemistry/Biomolecular Materials
- 2 Program Managers for Condensed Matter Physics (Theory and Experiment)
- 1 Program Manager for Neutron Scattering
- 1 Program Assistant for MDDS Team

Laura Greene said **Kung's** presentation is very inspiring. She added the success of her vision for the department is to coordinate all findings with Eric and Pedro's departments (essential to the success to collaborate).

Kung added that there is already discussions and strategies of growth between the departments and is leading to some new directions.

At 10:17 a.m., **Hemminger** requested a short break.

At 10:28 a.m., **Hemminger** introduced **Eric Rohlfing** and requested he abbreviate his presentation to end by 11:00 a.m. to stay on schedule.

Rohlfing began his presentation by presenting an outline of his presentation, the CSGB Division goals and the mission relevance. The CSGB division goals are to support experimental and theoretical research for the fundamental understanding of chemical transformations and energy flow in systems relevant to the DOE mission.

Current science opportunities include:

- Chemical processes and energy transfer over an enormous range of spatial and temporal scales – from atoms to kilometers and attoseconds to millennia
- Experimental tools for probing with chemical specificity, at the molecular scale, and on the time-scale of bond breakage and formation
- Theory, modeling, and computation from detailed quantum calculations to multi-scale modeling of real-world systems
- Synthesis of chemical systems from molecules to supra-molecular assemblies to nanostructured materials

The DOE mission relevance is to generate, use and store energy and mitigating the environmental consequences of energy use

- Improved catalysts for clean and efficient production of fuels and chemicals
- Better separations and analytical methods for energy processes, environmental remediation, and waste management
- Efficient combustion systems with reduced emissions of pollutants
- Chemistry and physics to improve geological repository performance
- New chemical, biological, and biomimetic paths to the conversion of solar energy to electricity and fuels

Rohlfing presented a current diagram of the three divisions he oversees – Fundamental Interactions, Photo- and Bio-Chemistry and Chemical Transformations.

The evolution (since FY2006) has seen the Split of Chemical Physics program into two parts: Gas-Phase Chemical Physics (combustion related) and Condensed Phase & Interfacial Molecular Science (CPIMS); created the new Photo- and Biochemistry Team from the Energy Biosciences program plus the Solar Photochemistry program (from Fundamental Interactions); and modest name changes.

- Fundamental Interactions Team

Structural and dynamical studies of atoms, molecules, and nanostructures and the description of their interactions with external stimuli (photons, electrons, etc.) at full quantum detail

- Photo- and Biochemistry Team

Molecular mechanisms involved in the capture of light energy and its conversion to chemical and electrical energy through chemical and biological pathways

- Chemical Transformations Team

Characterization, control, and optimization of chemical transformations, from catalysis to geochemistry

Rohlfing said the fundamental interactions area “gives a good flavor of what we are doing within the division.” The fundamental interactions team includes programs such as the AMO Sciences, Gas-phase Chemical Physics and condensed phase and interfacial molecular sciences. Crosscutting, division-wide areas are the theoretical and computational chemistry and the ultrafast chemical sciences. The synergy within the team and across the division is the gas-phase chemical physics & CPIMS closely coupled (formerly one program), AMOS intersects strongly with chemical physics in molecular systems, theory/computation very strong in team and across division, ultrafast chemical science growing theme across division, particularly in AMOS and the interfacial chemistry in CPIMS connects with catalysis and geochemistry; condensed phase chemical physics relevant to radiolysis and HEC. The relationship to science missions are AMOS tied strongly to application of current and next generation light sources (lasers, synchrotrons, LCLS) and gas-phase chemical physics has significant impact on clean & efficient combustion processes; management of Combustion Research Facility and SNL.

The Chemical Transformations team consists of programs in catalysis science, heavy element chemistry, separations and analyses and geosciences. The synergy within and across division is the long-standing connection between HEC and separations science analytical (chemical imaging) tools developed in S&A are applied widely nanoscale science is pervasive – connecting catalysis, separation science, geochemistry catalysis intersects with bio-catalysis and photo-catalysis in Photo- and Biochemistry. The relationship to science opportunities include chemical imaging and nanoscale science are central themes across team, catalysis directly connected to energy efficiency, production, and utilization of fuels, HEC and separations an important aspect of fundamental research for next-generation nuclear energy systems, Geosciences provides a fundamental understanding of environmental contaminant fate and transport and for predicting the performance of repositories for radioactive waste or CO2 sequestration

Biofuels research has been a great success story for science and DOE. The BES Energy Bioscience program has a goal of having new knowledge and an understanding**.** Fundamental molecular understanding (i.e., science grand challenges) of mechanisms that govern plant and microbial metabolism and growth that may be only peripherally connected to today’s problems in energy technologies. New tools and techniques for advanced modeling, imaging and structural analyses of plant and microbial energy transduction systems.

Rohlfing stated the current strategic planning is strongly influenced by the basic research needs, such as fundamental interactions, chemical transformations and photo- and biochemistry. The strategic planning for the future includes:

- Contractors’ meetings as tools for strategic planning and cross-fertilization between programs
  - CPIMS – tradition of “visitors” from other program – Catalysis, Geosciences
  - Solar Photochemistry – in 2008 will include visitors from Natural Photosynthesis
  - Initiate new biosciences meeting in 2008 (tentatively Physical Biosciences)
  - HEC and Separations – tradition of joint contractors’ meetings
  - Analysis meeting in 2008 will feature FY2006 projects in chemical imaging across the Division

- Chemical Sciences Council
  - On hiatus since 2006; will be reconstituted in 2008 (this will have the same focus as before, to sponsor one workshop per year)
  - Include biochemistry/biophysics expertise (Energy Biosciences never had a council)
  - Renew focus on workshops (one per year) intended to assess current status and future potential in areas of interest to the Division
- Geosciences
  - Earth Sciences Council workshop on geofluids (Dec 2007)
  - Joint contractors’ meeting with FE on CO2 sequestration (March 2008)

Next, the external relationships with BES, SC and DOE were discussed, with BES coordinating with Materials Science & Engineering (BES-wide programs in solar, nuclear, hydrogen and joint funding of “center” activities – PULSE at SLAC; SERC at LBNL (pending FY08 solar funds) and the Scientific User Facilities (Light sources: extensive synchrotron use by AMOS, Catalysis, Geosciences; development of LCLS experimental program

(AMOS); Nanoscale Science Research Centers: strong connections with developing thrusts in catalysis, theory/modeling, nanophotonics, bio-nano hybrids, among others; and Neutron sources (modest, but increasing use, particularly in Geosciences)

SC coordination with BER on biofuels (Physical Biochemistry) and on environmental chemistry, including EMSL at PNNL (Chemical Physics, HEC, Geosciences); ASCR on theory/modeling/simulation including SciDAC & TMS Nano (Theory/Comp, Chemical Physics; Geosciences; HEC); OFES (and NNSA) on high-energy density and ion physics (AMOS)

DOE technology office coordination with EERE Freedom Car & Vehicle Tech programs – combustion, including CRF (Gas-phase Chem Phys); EERE HFI and Industrial Technologies programs – catalytic processes (Catalysis); FE Stage III Sequestration Storage Tests – CO2 sequestration (Geosciences); RW & EM – radioactive waste storage; fate and transport of contaminants (Geosciences); BES-wide activities: EERE Hydrogen Program (Catalysis, S&A, Solar Photochem); EERE Solar America Initiative (Solar Photochem, Natural Photosynthesis); NE Advanced Nuclear Energy Systems (HEC, S&A, CPIMS).

Other external relationships with Federal agencies include the NSF division, program interactions, interagency working groups and joint with NSF CHE and HIH NIGMS (Biochemistry).

Due to the lack of time, **Rohlfing** was asked by **Hemminger** to abbreviate his presentation. His entire PowerPoint presentation is available on http://www.sc.doe.gov/bes/besac/Meetings.

Rohlfing began taking questions from the Committee. **Berrah** said **Pat, Eric** and **Harriet** have produced a report that provided a clear picture and that it extremely important for the (respective) groups to continue to work together. **Hemminger** agreed the report was "splendid" by the way it brought biology and photosynthesis into the forefront. **Isaacs** thought the vision was great and liked the reorganization of chemistry and how material synthesis was identified as a key area for growth. He questioned "how do you drive a cultural divide in the community to make sure you reinvigorate those involved in this area?"

Kung said how this is implemented should be discussed by the Committee. "We should inspire people to take the field more seriously. It is apparent we need new materials and that we need to continue to push the message to the community. We are in the initial steps of moving in the right direction and that this is the best way to implement these programs for longevity."

Kohn just attended "Energy and the Environment," a conference in Beijing China. He stated that "global warming was on everyone's mind and that coal was the number one source for energy in the country."

Rohlfing closed his presentation at 11:07 a.m.

Next, **Hemminger** requested **Graham Fleming** and **Mark Ratner** provide an overview and discussion of the BESAC Grand Challenges Report. **Hemminger** requested all questions and comments concerning **Fleming** and **Ratner's** report should be held until later in the afternoon when the Committee will discuss the Report.

Fleming provided an overview of the BESAC Grand Challenges Report. His presentation, "Controlling Matter and Energy: Five Challenges for Science and the Imagination" included a look at the true grand challenges. He said the challenges must be scientifically deep and demanding ("it needs to be difficult or it will not be a challenge"), be clear and well-defined, be relevant to the broad portfolio of BES and promise real dividends in devices or methods that can significantly improve the quality of life and a secure energy future for the United States. **Fleming** stated this material had not yet been reviewed or approved by BESAC. **Fleming** said he and **Ratner** collected suggestions for grand challenge questions from members of BESAC & the Grand Challenge subcommittee. Some of the many examples:

- Create complex functional materials that can be fully disassembled and re-assembled
- Design and build self-regulating, self-repairing molecular devices
- Enhance our predictive understanding of strongly-correlated electronic materials
- Build devices that fully integrate living and nonliving components?
- Interact finite mass nuclei and electrons, far outside the Born-Oppenheimer approximation caused by high energy and high frequency incident radiation and particles

The process of addressing these grand challenges was taking a look at the following subjects and asking the following questions:

- Can we go the last micron? Can we wire up the biological world for energy and information transfer?
- Can we control transition states in chemical reactions/phase transitions to create novel compounds/materials?
- What is the state of matter between solid and plasma? Can we understand high energy density matter?
- Can the atomic structure of proteins be solved rapidly without need for crystallization?
- Can movies be made of molecular reactions?
- Can we design and execute reactions at solid surfaces with the same predictability and control of molecular reactions in solution?

Fleming said that certain scientific areas were re-occurring. 1) we go to the very small 2) we go far from equilibrium 3) we encounter strongly correlated systems and systems with emergent properties 4) we want to define the limits of material properties 5) we want to manipulate energy and information ever more rapidly and efficiently 6) we want to recreate in synthetic systems properties and capabilities we find in nature.
As an underlying set of concepts emerged, **Fleming** and **Ratner** began “connecting themes.” Our ideas suggested that we are on the threshold of a transition from observation science to control science at a much deeper level than is currently possible. These two ideas lead to constructing five large challenges: correlations coherence emergent properties, information and energy exchange, BES grand challenges science, self-assembly regulation repair and systems far from equilibrium fluctuations.

The five grand challenges for science and the imagination include:

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

From the August BESAC meeting, the response to input from the BESAC Committee was to enlist science writer and editor **Art Robinson** and science writer **Lynn Yarris**; rewrite Executive Summary & Chapter 1; make extensive revisions to Chapter 7 and incorporated section on theory as; attempted to weave theory throughout chapters 2 through 6; rewrite Introduction to each chapter with attention to uniformity and accessibility; abbreviate science chapters and remove repetition; change and remove figures to improve value as illustrations of key points; shorten sidebars and simply text wherever possible; held two editorial meetings at Boston/MIT and LBNL in August, with all chapters leaders participated; Made extensive revisions to Chapters 3 & 4.

Looking at the first Grand Challenge, (How do we control materials and processes at the level of electrons), Fleming said that we need to make quantum systems work for us.

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

The second grand challenge is: How do we design and perfect atom-and energy-efficient synthesis of new forms of matter with tailored properties? **Fleming** said we must look at "directing the 'un-glueing' and 're-glueing' of electrons' by:

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

The third challenge is to look at how do remarkable properties of matter emerge from complex correlations of atomic and electronic constituents and how can we control these properties? Fleming said we must uncover the fundamental rules of correlations and emergence and learning to control them.

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

The fourth challenge is can we master energy and information on nanoscale? **Fleming** said we are creating new technologies with capabilities rivaling those of living systems.

- Tap the existing world of biological nanotechnology by constructing interfaces between living cells and synthetic technology
- Fabricate devices with functionalities approaching those of living systems, but with different hardware implementation
- Nano-macro junctions: covering the gap from a few tenths to a few hundred nanometers (photonic, electrical and magnetic, mechanical)
- Defects and the end of Moore's law
    - adaptive probabilistic computing
- Energy transduction at the nanoscale

    - stochastic processes, signals & noise)
- Ad hoc networking among nanoscale devices

Lastly, the fifth challenge is how do we characterize and control matter away – especially very far away - from equilibrium? **Fleming** said we are making non-equilibrium systems work for us by nanoscale thermodynamics, molecular transport junctions, fluctuations, exploring rough landscapes, jamming and science of life.

These five ideas must run through each of the chapters.

At 11:31 a.m., **Fleming** introduced **Ratner** to discuss what is needed. **Ratner** said the transition from observation science to control science envisaged in the five Grand Challenges requires a three-fold attack: new approaches to training and funding, development of instruments that are more precise and more flexible than those used for observation science and creation of theories and concepts beyond those we currently possess.

Ratner looked at the overall challenge in making the leap from observation science to control science. He acknowledges **Ward Plummer** had been "incredibly helpful" to the group in looking at the things we want to do (i.e. designing materials to have the properties we want and directing synthesis to achieve them) require the ability to see functionality at the relevant time, length and energy scales. He continued by saying we will need to develop and disseminate new tools capable of viewing the inner workings of matter – transport, fields reactivity, excitations and motion. This new generation of instruments will naturally lead to devices capable of directing matter at the level of electrons, atoms or molecules.

Ratner said we needed to look at the next generation of instruments. We must interrogate matter at a level much deeper than the macroscopic average to observe and control the properties of individual molecules or microscopic domains of materials. He continued by saying the biggest challenge lies ahead and that we are combining sub molecular spatial resolution with femtosecond time resolution.

In addition, he looked at what machines could have the broad impact of synchrotons. We need higher time resolution, to improve imaging methods and have new and improved detectors. We must balance how we get all of these things accomplished.

Ratner continued by looking at the Grand Challenges and Theory. Theoretical challenges described in this report cannot simply be reduced to ever larger computations. In many cases, we do not know how to formulate theory well enough to compute anything. We need to create a culture for high-risk, high-reward theoretical exploration of grand challenge topics (coherence, correlations, inter-conversion of energy and information, non-equilibrium phenomena). Furthermore, we need to attract the brightest, most theoretically inclined minds to basic energy sciences. These individuals will discover/produce the new laws and concepts necessary for understanding and controlling matter and energy with precision.

Energy scientists of the future are needed to sustain efforts over long periods of time, offer new support and training structures and support interdependent science.

Looking at the next generation, their training and the support of interdependent science, innovation in BES is critical to the nation and requires the engagement and support of our most creative scientists. We must sustained efforts over long periods, have an awareness of the technological, industrial and policy implications and be firmly anchored in one or two areas and be able to communicate effectively across physics, chemistry, engineering and biology.

Ratner said **Dehmer** had been tremendously helpful in keeping the project on target and said **Hemminger** had made this "a mission" with lots of time spent assisting with the project. **Ratner** continued by saying the Grand Challenge Science is "these capabilities will transform BES, play a critical role in securing our energy future and produce applications not yet imagined which we actually have to think about."

Ratner asked the Committee for their assistance on the Title of the report, the Cover Art (which does not convey what we are trying to say); the Executive Summary (must have the most important text); Chapter One (the chapter that non-scientists will read and discuss) and Chapter 7 (provide recommendations).

Ratner concluded his presentation and asked the Committee for comments.

Cummings said the report was "coming around very nicely." He jokingly asked if one of the photos could be replaced without the clouds.

Kohn asked for comments on the Title. He did not think the word "controlling" has a "conversational" undertone and is "Non-active."

Fleming said agreed with **Kohn** and maybe they should consider the word "directing" instead of "controlling."

Kohn agreed with the change. He also suggested that they could use "controlling and directing." He added the cover does not "strike him as visually stimulating" and seems "empty and dull."

Flynn said he had the impression that there was a request for the Committee's assistance that these are not mutually exclusive categories. He believes Chapter 7 should be moved behind the Executive Summary. "If you are talking to a Congressional staffer, the material in Chapter 7 is aimed at BES.

Ceyer said there is no information from Chapter 7 in the Executive Summary.

DiSalvo said to be careful not to point out that we can exceed what Biology can do. The Grand Challenges are incredibly daunting and we should foster and nrture creativity.

Hemminger thinks the Executive Summary is missing creativity and needs to be strengthened in the "wording," with **Fleming** agreeing.

McCurdy suggested the Committee stat out the afternoon (after lunch) to come to an agreement and then "drill down" the individual sections.

Hemminger announced a break for lunch at 12:03 p.m. and requested all Committee members to reconvene at 1:15 p.m.

At 1:29 p.m., **Hemminger** called the meeting back into session and quickly introduced **Orbach** to discuss the budget appropriations from the President, House and Senate.

Orbach presented the budget "as we currently know it." The 2007 appropriations were very difficult because it grew out of a continuous resolution,

"If we have another year-long of continuing resolutions, it will have an effect on research funds," **Orbach** said. "We have lived through two difficult years and 2008 will be a serious year for us due to the huge amounts riding on the FY08 budget. Currently we will be held to the '06 budget until it is approved."

Office of Science

FY 2008 Budget Request Status

Office of Science

FY 2008 Funding Status

(budget authority in thousands of dollars)

	FY 2007 Approp.	FY 2008					
		Request	Req. vs. 07	House	House vs. Request	Senate	Sen. vs. Request
Basic Energy Sciences	1,250,250	1,498,497	+248,247	1,498,497	——	1,512,257	+13,760
Advanced Scientific Computing	283,415	340,198	+56,783	340,198	——	334,898	-5,300
Biological and Environmental	483,495	531,897	+48,402	581,897	+50,000	605,320[a]	+73,423
High Energy Physics	751,786	782,238	+30,452	782,238	——	789,238	+7,000
Nuclear Physics	422,766	471,319	+48,553	471,319	——	471,319	——
Fusion Energy Sciences	318,950	427,850	+108,900	427,850	——	427,850	——
Science Lab Infrastructure	41,986	78,956	+36,970	151,806	+72,850	88,956	+10,000
Science Program Direction	166,469	184,934	+18,465	178,290	-6,644	184,934	——
Workforce Development	7,952	11,000	+3,048	11,000	——	11,000	——
Safeguards and Security	70,225	70,987	+762	70,987	——	70,987	——
Total, Science	**3,797,294**	**4,397,876**	**+600,582**	**4,514,082**	**+116,206**	**4,496,759**	**+98,883**
Less: Earmarks	——	——	——	-70,145[a]	-70,145	-49,150[a]	-49,150
Total, Science except earmarks	3,797,294	4,397,876	+600,582	4,443,937	+46,061	4,447,609	+49,733

[a] The House report did not specify which program(s) earmarks were to be funded in. Senate earmarks are funded within the Biological and Environmental Research program.

Office of Science FY08 Funding status is as follows:

- FY 2007 Appropriations were $3,797,294 billion
- Request of $4,397,876 billion
- Request versus FY07 - +600,582 million

The President requested a 16% increase. The budget is supposed to “kick in October 1, but will probably not take place until at least mid-October. The Congressional action will hopefully happen by early November.

House

- $4,514,082 for total science
- House versus request +116,206 million

Senate

- $4,496,759 for total science
- +98,883 Senate versus request

In November, 2003 DOE’s Office of Science proposed a portfolio of 28 prioritized new scientific facilities and upgrades of current facilities spanning scientific disciplines to ensure the U.S. retains its primacy in critical areas of science and technology well into the next century. **Orbach** added, “We need to look ahead and prioritize a list of the facilities we need.”

The *Facilities for the Future of Science: A Twenty-Year Outlook* was the first long-range facilities plan prioritized across disciplinary lines ever issued by a government science funding agency anywhere in the world by creating a roadmap.

Significant progress has been made in implementing the plan and deploying many of the planned facilities. We have just finished an update on where we are at now in 2007.

Priority

<u>Near-Term</u>

Priority	Office	Facility
1	FES	International Thermonuclear Experimental Reactor
2	ASCR	UltraScale Scientific Computing Capability
Tie for 3	HEP	Joint Dark Energy Mission
	BES	Linac Coherent Light Source
	BER	Protein Production and Tags
	NP	Rare Isotope Accelerator
Tie for 7	BER	Characterization & Imaging
	NP	Continuous Electron Beam Accelerator Facility 12GeV Upgrade
	ASCR	Esnet Upgrade
	ASCR	NERSC Upgrade
	BES	Transmission Electron Achromatic Microscope
12	HEP	BTeV

Mid-Term

13	HEP	Linear Collider
Tie for 14	BER	Cellular Systems Analysis & Modeling
	BES	SNS 2-4 MW Upgrade
	BES	SNS Target Station II
	BER	Whole Proteome Analysis
Tie for 18	NP	Double Beta Decay Underground Detector
	FES	Next Step Spherical Tokamak
	NP	RHIC II

Far-Term

Tie for 21	BES	National Synchrotron Light Source Upgrade
	HEP	Super Neutrino Beam
Tie for 23	BES	Advanced Light Source Upgrade
	BES	Advanced Photon Source Upgrade
	NP	eRHIC
	FES	Fusion Energy Contingency
	BES	High Flux Isotope Reactor Guide Hall II
	FES	Integrated Beam Experiment

Orbach said the importance of the ACI is critical and that we need to build light sources in the U.S. He said “We need to partner with other countries due to the expense.”

Orback continued by comparing the facilities portfolio with Europe’s Roadmap. The DOE Science plan:

- Is a “bottoms up” and “top down” approach
- Includes prioritization across fields of science
- 28 facilities made the cut

- While some facilities are international, most would be entirely funded by the U.S.

ESFRI Roadmap:

- Is not a priority list
- Aim is to facilitate discussion to allow for coherent planning
- 35 facilities made the cut
- Each facility supported by at least one European Member and has great potential at pan-European level

The charge is a major achievement. The 21st Century Light Sources is an assessment of the needs driven by new scientific opportunities.

- The BES suite of storage-ring-based light sources is one of the largest and most scientifically productive complex of user facilities in the world, serving more than 8,500 users each year
- The Linac Coherent Light Source at SLAC, the first hard x-ray, linac-based light source, will be added to this complex in FY 2009. It will be fully operational a year or two later
- The National Synchrotron Light Source – II at BNL, an advanced ultra bright storage-ring-based light source, will be added to the complex a few years later, in approximately 2015
- By 2015, with LCLS and NSLS-II newly operating, the youngest of today's BES light sources will be approaching its 20th birthday. Now is the time for DOE and the scientific community to begin the process of strategic planning for the 21st century light sources that will be as impactful as today's light sources and address the scientific needs of the community in the 21st Century
- The scientific opportunities and mission needs – as developed over the past five years in ten Basic Research Needs workshops and in the BESAC Grand Challenges study – are the major drivers for the specifications of new and upgraded light sources.

The BESAC Charge is to consider the characteristics of the next generation light sources that will address the scientific and technological challenges put for in the Basic Research Needs workshops reports and the BESAC Grand Challenge study and that will enable new and innovative ways of probing our material world in the 21st Century.

The characteristics to be specified are the standard ones used to describe light sources: wavelength, flux, brightness, emittance, coherence, pulse length, potential instrument suite, availability and reliability of the entire system, and user accessibility. The charge excludes consideration of the many specific pre-proposals or proposals for light sources that are currently being discussed in the community. However, the capabilities of various types of light sources (including lasers, storage-ring-based and linac-based light sources, or other types of light sources) should be evaluated against the preferred characteristics of the new light sources. Both upgrades and new facility concepts may be considered in this context.

The work of the BESAC subcommittee should be reported to BESAC at its summer 2008 meeting.

Orbach asked the Committee for questions and comments.

Greene asked if there is anything we can tell our universities/communities to work with our representatives.

Kohn said newspapers in China are reporting that the country is going to pass the U.S. in global omissions. Looking ahead 20 years, he asked **Orbach** how he sees China and their role.

Orbach said China will be a major player, thinking toward and their future we need to figure out how to work together with China, Europe, Japan and other countries to achieve common goals.

Plummer said we need to be "super-smart" in looking ahead to create future "geniuses."

Orbach said we are doing a good job with existing science. "But, we have a problem in fusion and high energy. We must have the tools for our best and brightest, if not, they will go elsewhere. We have begun encouraging middle school teachers to keep enthusiasm up amongst students, especially young women.

Berrah said to take advantage of the broad pool of talent, DOE must provide money for this. We must make it attractive to the younger generation and start now so our talent will be "home grown."

Orbach said we are now in the process in DOE having an education budget and focus on diversity and the inclusion of young women.

Ceyer said the next generation of light sources, detectors and questioned if we have the capabilities.

At that time, **Hemminger** requested the Committee cut off discussion and requested a 15-minute break.

At 2:43 p.m., **Hemminger** called the meeting back to order to discuss the Grand Challenges Report. He requested that all comments be constructive concerning the report and wants all Committee members to later break out in small groups to discuss individual chapters and then provide a synopsis on suggestions on how to make the Executive Summary and each chapter stronger.

He requested **Bill McCurdy** and **Walter Kohn** work together on Chapter 2; **Frank DiSalvo** work on Chapter 3; **Eric Rohlfing** and **Eric Isaacs** on Chapter 4; **John Richards** on Chapter 5; **Peter Cummings** on Chapter 6 and **Ward Plummer** on Chapter 7.

Isaacs began the discussion by asking who the target audience is for the document. He questioned if it was Congress or the scientific community.

Hemminger responded by stating he thinks there is a wide-range audience for the report, including the "scientific community and peers"

Dehmer believes the report has to inspire students who will be reading the report and believes the Executive Summary needs to be able to reach a wide audience.

Hemminger said he believes the content in Chapter 7 should stay in the chapter and not be moved closer to the front of the report.

Plummer read the document and "thinks about education and the people (audience) we want to bring in." He believes the content of Chapter 7 should be moved to the beginning of the document and believes that if we do not get the "geniuses back into field, we are not going to be successful."

McCurdy believes that between the last draft that was reviewed and the current one, we are closer to have "the flavor" and that something good is happening with the changes. He questioned if Chapter 7 is being written as recommendations for BES?

Berrah said Chapter 7 in its current format is "very good, very specific" and that she agrees with the recommendations. She would like to see needs to have new technology and training. She also suggested the title be "Controlling and Directing."

Isaacs likes the current title. He also likes some of the images, but not the smaller ones. He said Chapter 1 is really good, but needs to address physical science instead of chemical science.

Fleming asked **Isaacs** to be more specific with the areas he mentioned.

Flynn liked Chapter 7 in its discussion of Howard Hughes energy section. He also stated “if you do not bring in the private sector, should there be a suggestion to the energy industry to establish.”

Ratner said it was written for the Office of Science.

Flynn thinks it is “completely appropriate” to tell BES or DOE is a good idea.

Ceyer likes the title “For the Imagination” for the title.

Richards questioned the logic of the sidebars and found them hard to following and understanding them.

Cummings agrees the title is good.

Kohn said in the report, you find words like “controlling,” “directing” and “controlling and directing.” He thought he needs to be consistent throughout.

Long said the focus of the Challenges has been magnificent.

McCurdy agreed the sidebars were hard to follow. He suggested paying attention to figures that appear throughout the report may not be consistent. “It is the little things that add up to make sure the report is as good as it can be.”

Fleming said he and **Ratner** felt strongly the five areas are interconnected and the repetition was deliberate. “We intended to look at the same topics with different perspectives.”

Hemminger said he thinks the Executive Summary still needs to be strengthened.

At 3:15 p.m., **Hemminger** asked the groups to have a discussion for an hour and to bring a list of suggestions back to **Fleming** and **Ratner** to make the report stronger and which items need to be incorporated into the report.

At 4:50 p.m. **Hemminger** asked the Committee members to reassemble and provide their comments. The challenge is to give **Fleming** and **Ratner** a coherent list of changes to the individual sections.

For Chapter 2, **McCurdy** said certain figures and sidebars are not understandable or comprehendible and have made suggestions to present to them. He also said a diagram appears twice in the report.

For Chapter 3, **DiSalvo** and **Long** said they thought the chapter needs a lot of work. They did not feel there is logic, figures or an explanation why this is a Grand Challenge. They said they had made 3 ½ pages of comments they would forward to **Fleming** and **Ratner**.

For Chapter 4, **Greene** would like to discuss the changes with **Fleming** and **Ratner** and said there are definitely changes to be made, but discussions need to take place.

For Chapter 5, **Richards** said he was writing all the changes and would present them to **Fleming** and **Ratner** before dinner.

For Chapter 6, **Cummings** and **Ceyer** said there were only minor changes to be made.

For Chapter 7, the figures were not comprehendible.

Hemminger said we need specifics if you are going to request changes.

At 5:15 p.m., **Hemminger** opened the floor to public discussion. With there being no other public input, **Hemminger** adjourned the meeting.

Friday, September 21, 2007

At 9:12 a.m., **Hemminger** called the meeting to order and announced **Fleming** and **Ratner** are still incorporating changes and told the Committee how much he appreciated their hard work, comment and suggestions for the report.

Hemminger introduced **Dean Miller** to provide a workshop summary on "Future Science Needs and Opportunities for Electron Scattering: Next Generation Instrumentation and Beyond." The workshop was held March 2007 and addressed basic science needs will require advances in our capabilities to characterize and study materials. The "Basic Research Needs" workshops have uniformly called out the need for advances in characterization.

The workshop vision was to identify priority research directions for electron scattering and instrumentation development needed to meet basic science research needs. The charge was to identify emerging basic science and engineering research needs and opportunities that will require major advances in electron-scattering theory, technology and instrumentation (including microscope columns and detectors) in order to be addressed and to establish high priority directions for the development of specific capabilities to meet those research needs.

The report is still in draft stage, but the Committee should expect the final version soon.

The workshop strategy was to identify major scientific challenges that motivate advances in electron scattering methods and identify electron scattering capabilities needed (instrumentation, techniques) to meet those challenges.

There were 60 participants from DOE national labs (29%), academia (26%), industry (18%), federal government 918% and international (9%).

Workshop participants identified major scientific challenges that were categorized into 7 research themes:

High Performance Materials: Understanding the Nanoscale Origin of Macroscopic Properties.

- Understanding Individual Atoms, Point Defects and Dopants
- Interfaces at Arbitrary Orientations
- Crystals Interacting with Liquids, Vapors, Soft Materials

- Mapping Fields In and Around Matter
- Small Particles – Large Impact
- Materials in Extreme Environments: The Behavior of Matter Far from Equilibrium

The research opportunities present many common technical challenges, such as atomic scale (including resolution), in situ (studying material in their natural environment), and real time.

In order to understand materials behavior, we need to understand the defects that control materials behavior, yet often we cannot characterize them adequately:

- A few atoms can dominate material behavior and
- Dislocation motion often governs mechanical behavior

The key challenges include defects and interfaces, the key challenges include 3D atomic-scale structure and chemistry for a variety of reasons, “real” systems, not “special” interfaces, real time dynamics and in situ probes for unique properties

With environments, growth processes and hard/soft materials, materials behave differently in growth environments 0- understanding growth processes, especially self-assembly via organic or bio, presents a challenge. The key challenges are:

- In-situ observation of growth processes - at atomic resolution in growth environment
- In-situ high-spatial resolution chemical analysis
- Simultaneous imaging of hard/soft components
- Dynamics - *Fast* detection schemes, detectors, and sources

In small particles: nanomaterials and catalysis, nanomaterials and processes challenge our ability to understand them, with the key challenges being:

- Quantification - nanocrystallography at atomic resolution (automated w/ real time modeling and simulation)
- Atomic scale 3D imaging and diffraction
- *In situ*: controlled environments for simultaneous imaging and spectroscopy during reactions
- Dynamics: real-time observation

With mapping of electric and magnetic fields, we are poised for significant advances in magnetics, electronics superconductivity. The key challenges are:

- Magnetic structure and atomic scale crystal structure simultaneously
- 3D magnetic structure – quantitative
- Dynamics - in situ measurement of real-world systems

The priority research directions are technical developments identified as critical needs to address the scientific challenges:

Environmental and “*in situ”* Instruments
- Dynamic Experiments: Time Resolved and Time sliced Instruments
- Detectors: “Count every electron and make every electron count”

- New Electron Sources
- Multi-Mode Excitation: Combining probes and signals
- Virtualization & Community Software - the QTEM & the “virtual TEM”

In addition, we should build a suite of dedicated resources, each of which specializes in a different in-situ environmental geometry, to quantitatively stude materials ranging from subnanometer to atomic resolution: Gaseous environment, fluidic environment and E/M field environment.

The instruments for dynamic experiments involved building a suite of dynamic instruments covering the three ranges of spatial-temporal resolution.

Many proposed advances can build from the successes of TEAM:

The Transmission Electron Aberration-Corrected Microscope project (TEAM) is demonstrating DOE-BES’ role in innovation for electron scattering. TEAM recently reached a major milestone: 0.5Å resolution in both TEM and STEM. The TEAM framework, including aberration correcting optics, provides a foundation on which to develop *in situ* and dynamic TEAM capabilities.

The broad impact anticipated is:

- Scientific opportunities prevalent:
    - CMMP 2010: Condensed-Matter and Materials Physics: The Science of the World Around Us
    - “Basic Research Needs” workshop series
- Pathways toward priority developments are already being explored:
    - CMMP 2010: Condensed-Matter and Materials Physics: The Science of the World Around Us
    - “Basic Research Needs” workshop series
- Meet the Challenge: Characterization on the scale of fundamental interactions:
  Atomic scale, in situ, real time

Miller closed his presentation by asking for questions and comments:

Isaacs complimented **Miller** on a “very nice presentation” and asked to what extent does he think we need to develop some of the workshops?

Miller said a lot can be accomplished by researchers.

Isaacs said these sources are being developed for the next generation of sources.

Berrah asked what other sources are being used?

Miller said there is a variety being proposed, at certain stages of development, some things are best handles in laboratories.

Hemminger said outside of U.S. participants, there was a 10% international presence.

Miller completed his presentation be saying we have standards of how to manipulate data and improving quantitative techniques.

At 9:50 a.m., **Hemminger** asked **Fleming** and **Ratner** to provide an update on the edits that was incorporated into the report.

Fleming said he was "delighted by the constructive comments and that many will help to clarify what exactly we want to say." He added that he had accepted also all changes to the Executive Summary and believes it is now very straightforward. In Chapter 2, he also accepted most comments, but believes a few of the comments he received need to be further discussed and will plan to spend time "hashing out" some of the details. In Chapter 3, there also needs to be further discussion about some of the comments and edits. In Chapter 4, he accepted most all of **Laura Greene** and **Eric Issacs** comments and will continue making a few more of their edits and incorporating them into the report. In Chapter 5, he accepted all of **John Richard's** comments. In Chapter 6, **Sylvia** and **Peter** provided excellent suggestions and he accepted all of them. In Chapter 7, **Ward Plummer** made one comment and said he liked the 7.1 section and got rid of 7.2.

Fleming continued by stating that Chapter 3 had many thoughtful comments from **Frank DiSalvo**, but the chapter does not distinguish what is happening now. He added that it will depend on how soon we want the finished document because they would be losing one of the authors. "If we need to send this to be approved, we need to know how much more time we have to make changes." He also said the sidebars should not be in Chapter 3, but instead will consider moving them to Chapter 5.

Ratner said he would also like more input on the title of the document, the cover and a list of acknowledgements for the report.

Fleming said if more comments were going to be given, they needed to receive the edits by the end of the day.

Ratner said he was pleased with the title and that it works better than having a lengthy one. He said they would consider changing the word "controlling" to "directing." He agreed the photo of the cover is "dreadful."

Plummer preferred a static structure, not the future and feels the current cover has already appeared in the past.

Dehmer said we should look at the cover at how it relates to a broad spectrum of people and make sure it communicates a message. "You want people to look immediately and get a sense of what the report is about."

Plummer suggested putting the Chapter 7.3 graphic on the cover.

Hemminger said the current cover should be "interesting and colorful enough to where it immediately catches our eye. There are images out there that surely can be more 'eye-catching.'"

Ratner said **John Spence** will work on the cover.

Hemminger said **Fleming** and **Ratner** will receive other photos, something more contemporary.

Hemminger also said he would like to see the report go to the printer by the end of the month. Chapter 3 still needs to have significant changes and **DiSalvo** will assist with the edits.

Fleming said that he and **Ratner** will not be able to receive any changes after another 2 ½ weeks, if not sooner. He also said he will need to get permission to use all of the photos in the book. He also suggested making an appendix instead of acknowledging each photo with a caption.

Hemminger said he was pleasantly surprised the Committee has nailed down five Grand Challenges and that there has been very little argument and debate. He added that when the process started, it was said that the Committee would never be able to agree on just five challenges. He said BESAC should move forward with the report being sent to the Co-Chairs for final approval and asked for a show of hands if everyone agreed, which was unanimously accepted.

DiSalvo said this exercise has been very important and it needs to be continuous. He wants to see more grand challenges and what we can do to keep people excited.

Dehmer said that after 2002, we have five years of follow-up workshops and at that time, did not understand the impact. She suggested moving forward with more workshops.

Cummings added that a series of workshops will keep the momentum going.

Hemminger said he would like to discuss the charge that was presented by **Orbach** during the Thursday meeting. He believes the essence of the charge is that we should go back and look at the basic research needs and the current report and how we can accomplish what is in the report. **Hemminger** said he and **Dehmer** are currently looking at this and how to improve the process of the charge. This will acquire a substantial amount of time and input.

McCurdy asked for further clarification.

Hemminger said he sees what **Orbach** says in a component, not a full charge. He wants to look at the science drivers and that the Committee needs to be careful in not getting involved with specific proposals.

Dehmer said that she and **Hemminger** had debated back and forth if this is a one- or two-step process. Given everything BESAC and BES are looking at, what are the new science drivers for new tools and needed characteristics? She said she would like to report back to **Orbach** by next summer and that meetings will be held during the winter months.

Hemminger once again thanked the Committee for their attention to the project and asked for public comment. There was none and he adjourned the meeting at 10:29 a.m.