Minutes for the
Basic Energy Sciences Advisory Committee (BESAC) Meeting
July 31 – August 1, 2007
Hilton Rockville Executive Meeting Center
Rockville, Maryland

BESAC members present:

Nora Berrah
Peter Cummings
Frank DiSalvo
George Flynn
Bruce Gates
John Hemminger, Chairman
Eric Isaacs
Anthony Johnson
Walter Kohn
Gabrielle Long
William McCurdy, Jr.
Martin Moskovits (Monday only)
Ward Plummer
John Richards
John Spence
Mary Wirth

BESAC members absent:

Sylvia Ceyer
Sue Clarke
Mostafa El-Sayed
Laura Greene
Kate Kirby
Daniel Morse
Stanley Williams
Kathleen Taylor

Also participating:

Leon Balents, University of California, Santa Barbara
Linda Blevins, Basic Energy Sciences
Michelle Buchanan, Oak Ridge National Laboratory
Phillip Bucksman, Stanford University
George Crabtree, Argonne National Laboratory
Donald DePaolo, University of California, Berkeley
Patricia Dehmer, Associate Director of Science for Basic Energy Sciences, USDOE
Graham Fleming, UC Berkley and Lawrence Berkley National Laboratory
Kristen Balder-Froid, Lawrence Berkley National Laboratory
Jay Groves, Lawrence Berkley National Laboratory
Russell Hemley, Carnegie Institute of Washington
Ray Johnson, Recording Secretary
Pedro Montano, Department of Energy
Daniel Nocera, Professor of Chemistry, Massachusetts Institute of Technology (MIT)
Teri Odom, Northwestern University
Lynn Orr, Stanford University
Richard Osgood, Columbia University
Julia Phillips, Sandia National Laboratories
Mark Ratner, Northwestern University
Jeff Wadsworth, Oak Ridge National Laboratory

Approximately 120 others were in attendance for brief segments during the course of the two-day meeting.

Tuesday, July 31, 2007

Chairman John Hemminger called the meeting to order at 9:08 a.m. **Hemminger** began the meeting by thanking all of those attending the meeting. He stated he believed the next two days would be very informative and important in getting feedback on the workshops. He also thanked all those who participated in the Grand Challenges Report, a tremendous amount of work went into completing the project. Afterwards, he asked each of the Committee members to introduce themselves.

At 9:15 a.m., **Hemminger** asked **Patricia Dehmer** to update the Committee on the activities of the Office of Basic Energy Sciences (BES). **Dehmer** began by stating she had some good news and bad news to share concerning the fiscal year FY07 and FY08 budget. The execution of the FY07 budget was not as good news as what had been anticipated.

Prior to FY1977, fiscal years ended on June 30. For the past few years, there have been as many as six months pass before until appropriations are completed.

For FY06, the Office of Science had appropriations of $3,632 million. On January 31, 2007, the U.S. House of Representatives passed an appropriations level of $3,796 million for FY07, when $4,102 million had been requested.

For Basic Energy Sciences (BES), there was a request to Congress for $1,250,250,000 for FY07 and $1,498,497,000 for FY08. The FY08 President's budget request and the material presented in the spreadsheet **Dehmer** provided, assumed the requested level for FY07, as the timing of FY07 appropriations did not allow their inclusions. **Dehmer** stated that the reduction in funding level received was an enormous hit for the Office of Science, resulting in across-the-board cuts.

There were four major solicitations for FY07 – *instrumentation*, *basic research for solar energy utilization*, *basic research for the hydrogen fuel initiative* and the *basic research for advanced nuclear energy systems* - totaling $84 million. The FY07 appropriations under H.J.R 20 were cut to $10.6 million, with $7.1 million going to solar energy utilization and $3.5 million going to hydrogen fuel initiatives.

Proposals received in response to all four solicitations are being held for consideration of funding in FY08. Additional awards will be made only after the FY08 funds that are requested for these activities are appropriated by Congress and signed into law by the President.

For good news, **Dehmer** told the Committee members the FY08 budget is currently being well-received and the execution of the FY07 budget is anticipated.

Dehmer discussed the revised timelines for BES solicitations. For FY08, requested appropriations exceed FY07 appropriations by approximately $79 million.

"There is talk in Washington that President Bush is going to veto the appropriations, which will send the Bill back for further review, said **Dehmer**. "Currently, continuing resolutions and getting appropriations after October 1 is a goal. At the present time, we are simply waiting on Congress to act."

As stated earlier, the Committee recommendation for BES FY08 is $1,498,497,000, the same as the budget request and an increase of $248,247,000 over the current fiscal year. For purposes of reprogramming during FY08, the Department may allocate funding among all operating accounts with BES, consistent with the reprogramming guidelines outlined in **Dehmer's** report.

FY08 BES Budget – House Mark

For *research*, the Committee's recommendation includes $1,093,219,000 for materials sciences and engineering and $283,956,000 for chemical sciences, geosciences and energy biosciences. The Committee recommendation funds 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 Intense Pulsed Neutron Source and the Manuel Lujan, Jr., Neutron Scattering Center at their optimal number of hours, additional instrumentation for the recently-completed Spallation Neutron Source (SNS) and the science research portion ($59,500,000) of the hydrogen initiative at the requested levels. Given the long-term nature of the hydrogen as an energy transfer medium, with timescales for deployment similar to those for fusion energy, funding for hydrogen research in the Office of Science is particularly appropriate. The Committee previously directed the National Nuclear Security Administration to make available, for existing stocks, sufficient heavy water to meet SNS needs, and the Committee renews this direction for FY08. Also, included within this account is $8,240,000 for the Experimental Program to Stimulate Competitive Research (EPSCoR), the same as the budget request.

Given the dismal operating record of the High Flux Isotope Reactor (HFIR) in FY06 with 89.5% unscheduled downtime and the lack of major research accomplishments from its operation, the Committee will be watching to see that the steps taken by DOE to put HFIR back-on-track are successful.

For *construction*, the Committee recommendation includes $121,322,000 for BES construction projects, the same as the requested amount. The Committee recommendation provides the recording funding of $51,356,000 to continue construction of the Linac Coherent Light Source (05-R-320) at the Stanford Linear Accelerator Center; $366,000 to complete construction of the Center for Functional Nanomaterials (05-R-321) at Brookhaven National Laboratory; $45,000,000 for continued project engineering and design of the National Synchroton Light Source II (07-SC-06) at Brookhaven National Laboratory; $17,200,000 for construction of the Advanced Light Source User Support Building (08-SC-01) at Lawrence Berkeley National Laboratory; $950,000 for PED of the Photon Ultrafast Laser Science (08-SC-10) and Engineering Building Renovation at the Stanford Linear Accelerator Center; and $6,450,000 to begin renovation of the Photon Ultrafast Laser Science and Engineering Building Renovation (08-SC-11) at the Stanford Linear Accelerator Center.

Given the extremely poor record of the Department in correctly estimating and controlling costs for major projects, particularly construction, the Committee compliments the Office of Science for completing the Spallation Neutron Source almost on schedule and on budget.

FY08 BES Budget – Senate Mark

The Committee recommends $1,512,257,000 for BES, an increase of $13,760,000 from the budget request. The Committee fully funds facilities within this account, including the four Nanoscale Science Research Centers and provides $15,992,000 for the Manual Lujan, Jr., Neutron Scattering Center. The committee provides $17,000,000 for the EPSCoR.

The details of the FY08 Congressional Budget Request for BES includes comments from **Dehmer** that research construction was flattened for the current year and that “everything new that was going to happen has been put off until next year.” For FY06, there was no funding available for such areas as solar energy utilization, advanced nuclear energy systems, ultrafast science, mid-scale instrumentation, chemical imaging, complex systems/emergent behavior and electrical energy storage. For FY07, The President’s request includes funding in the aforementioned areas and core research and hydrogen, totaling $536,001,000. The FY08 President’s request includes additional funding for core research (7.2%), hydrogen (19.0%) and solar energy utilization (17.3%).

Dehmer continued by stating “we must cope with what Congress does and we are looking forward to a better year in 2008, with requests currently sitting on the Hill.”

Dehmer continued her presentation by providing an overview of the “Basic Research Needs” (BRN) Workshops. These workshops began in 2002 and the 10th and final workshop will take place in Bethesda, Maryland August 5-10. She continued by saying these workshops have been “impactful beyond our expectations and have been received with great enthusiasm.” She also challenged the Committee to go back to the beginning of the workshops (2002-present) and try to assimilate information from all of the workshops.

Past and future BRN workshops have addressed many elements required for decades-to-century energy security strategies. They have involved thousands of people, with the research for a secure energy future (supply, carbon management, distribution and consumption) being the main theme.

Next, **Dehmer** presented a charge from **Raymond (Ray) Orbach** to **John Hemminger.** First, to summarize the science themes that emerged from the BESAC report, *Basic Research Needs for a Secure Energy Future* and the follow-on *BES Basic Research Needs* reports and relate those science themes to the Grand Challenges identified by BESAC.

Secondly, to identify the tools and facilities that will be required to accomplish the science described in the workshops, from the first to the last. Think broadly about tools – include X-ray, neutron and electron scattering; proximal probes and other microscopes; time resolved tools; theory and modeling; computational “end station,” i.e., community codes; and any tools and facilities that may be important. It is also more relevant to specify the broad characteristics of tools and facilities than to define the details of a given tool or facility at this time.

Lastly, identify other impediments to the successful implementation of this program of research in BES, including human resources and workforce development.

Dehmer said she has discussed these items with **Hemminger** and believes they should be “framed in a way that everyone can understand.” She also believes that light sources must be better formatted and we must make sure that roadmaps are accessible.

With the general counsel meeting before the beginning of the BESAC meeting, she reported that more than half of the Committee members are conflicted concerning light sources discussions. She added that according to what was mentioned, every school in California is in conflict.

Finally, **Dehmer** stated BESAC should continue its triennial evaluations of the BES divisions using a Committee of Visitors (COV). The established routine of evaluating one BES division per year is working well, and the resulting COV reports have been extremely helpful to **Orbach** and to BES.

Based on several COV recommendations, **Orbach** is currently working on a system that will allow the collection of demographic data; however, the implementation of that recommendation is not straightforward because it requires the establishment of databases that can store and software that can collect personally identifying information. “We are working with our general counsel and our information technology colleagues within and outside the department on this issue.”

Dehmer then began discussing the Office of BES organizational work chart. There has been a reorganization of the research components into three teams – Materials Sciences and Engineering Division (**Harriet Kung**, Director), the Scientific User Facilities Division (**Pedro Montano**, Director) and Chemical Sciences, Geosciences and Biosciences division (**Eric Rohlfing**, Director). Currently, there are two openings, Physical Scientist in the Materials Sciences and Engineering division and a Chemist in the Chemical Sciences, Geosciences and Biosciences division. She stated there had been success in hiring more than a dozen new employees, with 10 additional employees budgeted for 2008.

In the Office of Science, the organizational work chart has three new deputies for each group. All positions “fit tightly under each group.” The Office of Science has been significantly restructured, with many job openings. **Dehmer** said she and **Dennis Kovar** have been assisting **Orbach** throughout the restructuring, but she is ready to get the vacant position filled.

Hemminger opened the floor for comments. **Walter Kohn** asked **Dehmer** how the topics for the workshops were identified. **Dehmer** stated that each had a basic science component and was based on a recognition that they needed to be addressed and believed it was important to have attention brought to the topic. She continued by stating: "People from the scientific community were interested in hearing suggestions. We will continue to have workshops as the topics need to be addressed and when voices need to be heard."

Eric Isaacs requested a discussion with general counsel on what Committee members can do without being in conflict with guidelines. He said there has been a "huge amount of noise about the future of light source and a lot is being driven by the fact that we can do things technologically that we could not do 10 years ago."

Dehmer said Committee members should stay informed and their role is to know what the major "science drivers" are.

At 9:52 a.m., **Hemminger** requested a break.

At 10:05 a.m., **Hemminger** called the meeting back into session and made three announcements regarding **Graham Fleming's** update to the BESAC Grand Challenge Science. First, **Hemminger** stated the information that **Fleming** would be providing had not been reviewed or approved and requested the information be limited in its distribution. There will be modifications and the Committee does not want the information to fall into the wrong hands and send a mixed message to the community. Second, there are aspects of the report that impact the work BES performs. The Committee needs to find ways to solve some of these challenges that impact DOE. Lastly, **Hemminger** requested each presenter try to stay on schedule due to the large number of presentations throughout the day. He also stated the number of questions asked after each presentation will be limited and that time will be allotted at the end of the day for additional questions on all subjects.

At 10:10 a.m., **Hemminger** introduced **Fleming** to provide an introduction and executive summary of the BESAC Grand Challenges Science Report. **Fleming** began his presentation by stating that although the report is still in its draft stage, he is hoping to have it finalized by the September BESAC meeting.

Fleming has worked closely with his Co-Chair **Mark Ratner**, as well as other Sub Committee members **Leon Balents, Phillip Bucksbaum, Jay Groves, Hemminger, Kohn, Tobin Marks and John Spence**, among others. Each member of the Sub-Committee consulted their colleagues so the report would represent a cross-section of the most important aspects to include in the Grand Challenges Report.

Fleming said properly posed Grand Challenges will provide the scientific foundation for transformative progress in BES. In addition, they will provide necessary instrumental theoretical framework and language for understanding what happens when previous Grand Challenges have led to the focus of our efforts:

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

For BRN workshops, Grand Challenge research is essential for and underpins all basic research need areas. Some of the specific goals of these reports were to:

- Create materials with new electrical, magnetic and strength characteristics based on emergent properties, strong correlations and complex systems
- Invent photosynthetic and photochemical energy systems based on the excited state dynamics of novel molecules and nanostructures
- Make higher Tc superconductors and make them a practical means of electrical transmission
- Make low cost, durable, and efficient solar cells
- Create new energy storage systems

Addressing the Grand Challenges is crucial for realizing these goals.

When discussing some of the connecting themes, **Fleming** provided a pictorial way of discussing the correlations and coherence and how they emerge from interactions. Four general areas – 1) Correlation, Coherence and Emergent Properties 2) Information and Energy Exchange 3) Self Assembly, Regulation and Repair 4) Systems Far From Equilibrium and Fluctuations. Each of these areas led the Sub-Committee membership to organize their thoughts into five science chapters.

Chapter One – "Control of Electrons in Atoms, Molecules and Materials: Creating a New Language for the Behavior of Electrons." The chapter essentially provides the challenge of manipulating and controlling material at the quantum level. (**Phillip Bucksbaum** and **Walter Kohn)**.

Chapter Two – "Basic Architecture of Matter: Directed Assembly, Structure and Properties." The challenge of creating robust soft matter and tailorable hard materials. (**Tobin Marks)**

Chapter Three – "Emergence, Complex Phenomena and Strongly Correlated Multi-particle Systems." The challenge of creating new correlated electron materials. (**Leon Balents** and **Julia Phillips)**

Chapter Four – "Nanoscale Communication – Energy and Information." The challenge of creating nanotechnology with functionalities that rival living systems. **(Jay Groves** and **Paul McEuen)**

Chapter Five – "Matter Far Beyond Equilibrium." The challenge of understanding and controlling systems that is far from equilibrium. (**Mark Ratner)**

Each chapter has sidebars, which provide background information and generalize such topics as molecular machines and molecular logic.

In Chapter One, the challenge of manipulating and controlling material at the quantum level can lead to revolutionary information technologies, nanoscale sensors for medical diagnostics and threat detection, unlocking the secrets of high-temperature superconductivity and can provide efficient ways to convert light energy into chemical energy or electrical power.

The needs are new light sources and theories and language beyond the Born-Oppenheimer Approximation.

Challenges

Understanding and control of conical intersections. Conical intersections (CIs) influence much chemistry. Calculating quantum evolution through CIs is a major theoretical challenge. For strong excitation and for conical intersections, theory beyond Born-Oppenheimer approximation is required.

Control correlated electronic states, which asks the question how does electronic qualitative coherence affect the properties of materials. Sophisticated magnetic materials are used widely (information storage, nanoscale sensors, and in the future for spintronics), yet these strongly correlated electronic states are not understood.

Experimental control over cold atoms can reveal many exotic properties, such as superfluidity, superconductivity and Bose-Einstein condensation. By tuning these interactions, it may be possible to simulate nuclear matter.

Directly observe Electron-electron Interactions asks how does matter behave on the timescale of the electron motion. Graphics were shown demonstrating the current state-of-the-art in the visible range; Moving the x-ray range would engage interactions of electrons to be directly visualized and the need to transform and limit ultrashort x-ray pulses.

In Chapter Two, “The Basic Architecture of Matter: Directed Assembly, Structure and Properties” present the challenge of creating robust soft matter and tailorable hard materials that can lead to low cost manufacturable photovoltaics, self-repairing regulating molecular devices, smart materials, integrated photonic devices for computing, communication and sensing, and nanoelectronic and nanoelectromechanical devices. The needs are crystal growth facilities, *in situ* monitoring of synthesis and especially catalysis, design rules for robust soft matter and theory capable of predicting properties and suggesting new synthetic approaches.

The challenge of constructing truly robust soft matter

- Enzymes which turn over reactive substrates degrade rapidly
- Excellent abiotic catalysts deactivate after minimal turnovers
- Polymeric materials degrade thermally, oxidatively, photochemically and mechanically

Can we devise revolutionary new design algorithms to create soft matter capable of?

- Built-in atomistic robustness
- Self-assembling into kinetically and/or thermodynamically most stable structure
- Self-passivating/self-protecting in hostile environments
- Self healing
- Disassembling/recycling
- Self-replicating

Another challenge is more durable and selective homogeneous catalysts.

- Enzymes, which turn over reactive substrates degrade rapidly
- Abiotic catalysts are expensive and frequently deactivate after minimal turnovers
- Selectivity of most homogeneous catalysts is very sub-state-specific and environment-sensitive

Can we devise revolutionary new algorithms to create heterogeneous catalyst?

- Built-in atomistic robustness
- Self-adjusting to substrate, environment for maximum selectivity, activity
- Self-passivating/self-protecting in hostile environments
- Self-repairing, self-replicating
- Straightforward, economical synthesis from abundant building blocks

An additional challenge was synthesizing hard matter with precisely predictable properties.

- Precise structural control over multiple length scales Å to μm
- Can we achieve the same level of control as nature exhibits, such as the elaborate, multiple length structures of silicate structures produced by diatoms?
- Multiple length scale ordering for heterogeneous catalysts, nanostructured photovoltaics, integrated photonic devices and nanoelectromechanical systems

With the emergence of complex phenomena – strongly correlated multi-particle systems, control of correlations and the science of strong correlations in systems without static order presents a challenge of creating new correlated electron materials which can lead to a new generation of materials that supersede present day semiconductors, with much smaller feature sizes, controllable and tunable magnetism and ferroelectricity for information technology, and highly efficient thermoelectric devices for generating electricity from thermal gradients. The needs include material synthesis, new theory, new light sources and multi-scale modeling.

In Chapter 3, **Fleming** noted that **Leon Balents** oversaw the challenge of understanding and controlling strongly correlated materials. The challenge was to understand and control correlations of d and f electron materials, which exhibit strong sensitivity to small chemical changes. This provides a payoff of new materials with tunable properties, devices combining them.

In controlling quantum correlations, the challenge was to manipulate atoms, electrons, spins or other particles into desired coherent many particle quantum states and/or engineered structures, potentials and interactions. The payoff was new quantum coherent tools (e.g. quantum simulators) and structures, exploring fundamental science of collective organization with unprecedented precision.

Another challenge briefly mentioned was observing correlations which develop in time from rich and novel electronic phenomema to branching off into unconventional superconductivity, multi-ferroics and colossal magnetoresistance. The ultrafast measurements separate correlated phenomena in the time domain and direct observations of the underlying correlations as they develop.

Fleming then began discussing Chapter 4, which concerned nanoscale communication – energy and information. The challenge of creating nanotechnology with functionalities that rival living systems can lead to new low energy computing systems, can enable two-way communication between a living system and solid state technology for profound advances in understanding cellular function, and can (using nanodevices which are inherently noisy, prone to defects and degrade with age) enable the design of reliable advanced computers. The needs are controlled 3D fabrication, linked chemical signaling with electrons and new imaging methods.

Next, **Fleming** discussed conceptual origins, how to link Maxwell's control randomness and Mendel's use randomness. He then began discussing the next challenge, which was interfacing biological and non-biological. (Learning the chemical language of cellular communication and developing very large integrated systems for producing and presenting biological signals.)

In Chapter 4, the Nano-Macro junctions and how to bridge the gap is one of the challenges. Carbon nanotubes have been used and the schematic of a nanometer-sized P-N junction created a carbon nanotube. Light omission as the P-N junction is moved along the length of the nanotube, demonstrates a tunable, nanometer-scale light source. The fabrication of flawless electronic devices at the nanoscale is an enormous challenge.

In addition, **Fleming** briefly discussed the use of stochastic fluctuations for definite outcomes, showing a graphic with dueling positive and negative feedback loops.

In Chapter 5, the challenge of understanding and controlling systems that are far from equilibrium can lead to nanomachines with optimized power and efficiency, powerful molecular electronics, new energy storage devices, new mitigation strategies for point sources of heat or pollution and greatly improved prediction methods for hurricanes, tidal behaviors and earthquakes. The needs are new theory, experimental techniques for the study of non-equilibrium systems (e.g. synthetic nanomachines).

In addition, creating a theory of organization and dynamics of matter beyond equilibrium has a confluence of factors, such as 1) including new tools for manipulating nanoscale systems 2) new theoretical insights and the urgent need for the design rules to guide the construction of future classical and quantum machines 3) make it essential and for the first time, plausible, to attempt to develop a thermodynamic formalism 4) valid for small systems that are not at equilibrium.

Extracting equilibrium information from non-equilibrium experiments was presented as another challenge, as well as developing a quantitative understanding on non-equilibrium dynamics, processes and configurations in terms of appropriate (drastically) reduced variables. In addition, linking up concepts for a broad range of length scales from the femtoseconds it takes to break a bond to the hours and years it takes a human body to mature. Characterizing and formally understanding pathways in equilibrium processes poses the last challenge listed in this group.

Fleming stated he would appreciate the BESAC's Committee members comments concerning infrastructure, facilities and human resources. He stated that pushing to the limits of one discipline generally leads to the interface of multiple fields of science where the boundaries between different disciplines cannot be resolved. Addressing challenges will require sustained efforts over long periods, new support and training structures, new probes of matter, new theoretical methods and new enabling facilities and capabilities.

In discussing the next generation's training and support of interdependent science, innovation in BES is critical to the nation and requires the engagement and support of our most creative scientists. Three ways to assist in this effort would be to 1) to provide sustained effort over long periods. (The DOE Energy Institute) 2) generate awareness of the technological, industrial and policy implications of their work (The Energy Sciences Study Group) and 3) ensure that scientists are firmly anchored in one or two areas and able to communicate effectively across physics, chemistry, engineering and biology, with new approaches to training. (The DOE Fellows Program).

Energy Science Senior Fellows need to have unrestricted, long-term support to allow the best minds to focus on Grand Challenge science and enhance the prestige and visibility of the DOE BES support. This will "enhance the prestige" and the selection of fellows will be made by a blue-ribbon panel committee of DOE, national laboratories and university leaders. Appointments in this program will provide (for five years) part, or all, of normal year funding.

The Energy Science study group is a two-year mentored program in energy policy, global energy needs and related R&D. Mentors and advisors would come from the energy industry, as well as energy and environmental policy. In addition, this program would create a group of young faculty and national laboratory scientists, while keeping pace with evolving technologies. Furthermore, it would convey understanding of the scientific and technical aspects of national energy security issues and an appreciation of the multidisciplinary nature of energy research. Lastly, the group would lead workshops to define science challenges, underpinning energy and environmental issues, in conjunction with the Energy Sciences Network.

Some of the new approaches to training with the Energy Sciences Network include expanding science training using the Nanoscience Centers as focal points (model: Cold Spring Harbor). In addition, a series of Grand Challenge-focused workshops would be conducted with two days of training in key issues for students followed by two-days of forefront Grand Challenge science. Lastly, in creating Grand Challenge Training Networks, collaborations will occurbetween teams of scientists with early stage scientists spending time in more than one team. Early stage scientists can customize their training, see multiple viewpoints and begin their own collaborations.

Fleming stated that "thinking about what would be possible if we meet these challenges will create some extraordinary opportunities," such as:

- Development of new energy technologies to transform national energy security and climate change mitigation
- Creation of successors to current semiconductors
- Design of robust, atom-efficient catalytic processes and materials
- Realization of the promise of nanoscience and creation of nanomachines and devices
- Increase of computing speed and capability with sustainable energy requirements
- Ability to learn to communicate with living systems at cellular level
- Harness of quantum mechanics for creation of new properties and capabilities
- Use of finite resources most effectively and creation of self-repairing and self-regulating materials

Fleming closed his presentation at 10:55 a.m., by offering a quote from **Mostafa El Sayed**, "The most important Grand Challenges are probably the ones we haven't thought of."

Hemminger requested we move forward without questions or comments and immediately introduced **Phillip Bucksbaum** to discuss Chapter 2 of the report, "Control of Electrons and Nuclei in Atoms, Molecules and Materials."

Bucksbaum began his presentation by stating the chapter describes the challenges of understanding and controlling coherence in new ways. The interaction is important between the two main concepts – coherence and control. Quantum coherence in materials control new phenoma, including quantum degeneracy and coherence, quantum coherence in photochemistry and quantum coherence in information science.

Coherence properties of novel light sources to control new materials include chemical composition and chemical bond control, laser-driven materials properties and imaging materials in important new ways.

We know there can be strong connections between materials and quantum coherence. Superconductivity is just one of a number of phases related to quantum coherence of electrons at low temperatures in certain materials. Sophisticated magnetic materials are widely used (information storage, nanoscale sensors and in the future spintronics).

The quantum state of matter at low temperatures presents quantum simulators. **Bucksbaum** provided several graphics included one showing vortex arrays in superfluids made of atoms, molecules and BCS pairs. One of the challenges is that quantum spin liquid at T → O: a triangular antiferromagnetic spin lattice. The future is simulating Quantum Chromodynamics.

The excited state chemistry requires a new description. Avoided crossings of "spaghetti" of the states of diatomics become a puff pastry of conical intersections in polyatomic molecules. **Bucksbaum** quoted **Walter Kohn** in stating "The Born-Oppenheimer approximation may be irrelevant. We don't yet have a language to describe the physics these experiments can probe."

Bucksbaum presented the question of why can't we calculate this information? Moore's original graph predicting Moore's Law in 1965, stated chip capacity will double every two years. This must fail soon, which is too bad for us because we need much more computing power.

According to **Kohn's** Nobel Prize Address in 1999, "traditional multiparticle wave-function methods when applied to systems of many particles encounter an exponential wall. The number of atoms *N* exceeds a critical value which currently is in the neighborhood of *N* ~10 (to within a factor of about two.)"

Quantum simulators, or some other new computing paradigm, are required. The analog logic is that 17 nm features on a crossbar circuit, shows atomic-scale bumpiness. Analog circuit elements, like memristors, may be able to use such circuits more effectively. For quantum computing, quantum entanglement is a resource.

Intense coherent sub-picosecond x-ray light sources will be able to track matter at extremes.

With coherent control, the control of quantum phenomena takes engineering control principles into the realm of quantum mechanics. Time cells are picoseconds to attoseconds, and the size of objects under direct control are angstroms to nanometers. The intellectual pay-off of this field is vast; essentially all dynamic events start with the atomic and molecular scale, including all of chemistry and much of materials science.

Coherent control in molecular systems includes pulse shaping and learning control. With pulse shaping, the optimal field, discovered by OCT, often has a broad bandwidth, with its phases adjusted to give a highly structured pulse. In learning control, the learning loop brings the same feedback used in the optimal control algorithms into the laboratory.

With the connections to nature, photosynthesis electron motion drives nuclear motion. The retinal molecule in the center of rhodopsin bends after absorbing light, to help move a proton across a membrane. Some molecules appear to utilize quantum coherence in the process of photosynthesis. The challenges are 1) to discover the general principles for control and 2) to obtain real-time feedback for quantum control.

New experiments are showing us attosecond electron dynamics for the first time.

As **Bucksbaum** closed, he stated the main questions that frame the challenges in Chapter 2:

A. Materials and coherence
  1. How does electronic quantum coherence affect the properties of materials?
  2. What is the role of quantum coherence in dynamics, especially photo-chemistry?

B. Coherence and control
  1. How can we control the quantum states of matter by applying coherent fields? (coherent control)
  2. How does matter behave on the timescale of electron motion (attoscience)
  3. How can we utilize new generations of coherent sources for materials science and chemical science?

At 11:12 a.m., **Hemminger** introduced **Tobin Marks** and requested an update on Chapter 3. The chapter, “Can We Control the Essential Architecture of Nature? Can We Build ‘Designer’ Materials?” offered Marks insight on how “a Grand Challenge is something scientifically very important that we yearn to do. The chapter looked at hard materials synthesis and soft materials synthesis.

When we think of soft materials, we think of exquisite control of atom-atom connectivity, processability and the direct connection to living systems and their properties. But, isn’t soft matter fragile and non-robust? When we think of hard materials, we think of thermally, mechanically robust, diverse electrical, magnetic, optical properties, traditional “heat-and-beat” syntheses. But, why can’t we achieve the atom-by-atom connectivity control, structural diversity of soft matter?

The statement of the Grand Challenges is that soft materials is a rational directed, atom-efficient syntheses of dramatically new types of soft matter having features of hard matter, coupled with incisive characterization over broad ranges of size, energy and time, and theory capable of accurately predicting properties and/or suggesting new synthesis directions. The hard materials states: rational, directed, soft matter-like materials synthesis for new types of hard matter exhibiting traditional soft matter characteristics, coupled with incisive characterization over broad ranges of size, energy and time scales, and theory capable of accurately predicting properties and/or suggesting new synthetic directions.

We know isolated examples of exceedingly robust soft matter – matter with extremely high thermal, chemical, mechanical, radiation stability. Phthalocyanine dyes, ultra-temperature resistant Nomex fibers and extremeophiles living in volcanoes and nuclear reactors and carbon nanotubes are examples. Nomex is a synthetic polyamide with a structure similar to amino acids displays remarkable mechanical flexibility and strength, along with flame resistance. But, we don't know the algorithm for truly durable soft matter.

One of the specifics in soft matter challenges is durability, with the goal of learning from nature and then going beyond. We achieve soft matter which is exceptionally durable with regard to thermal degradation, oxidative degradation, radiation damage, self-healing or self-protecting structures and recyclability via disassembly/reassembly or via selective biodegradation to other useful products.

An additional soft matter challenge specific is architecture. How do we synthesize soft materials organized or even self-organized in multiple dimensions over multiple length scales in:

- Connectivity of σ – and π bonds
- Cavities/protrusions of predetermined shapes, chiralities, functionalities and recognition (especially biorecognition) characteristics
- Surfaces of predetermined shapes, chiralities, functionalities and recognition (especially biorecognition) characteristics
- Controlled spatial organization of electron donor and acceptor groups, paired and unpaired electron spins
- Capture of essential structural and dynamic features of transition states of catalysis
- Surfaces which reorganize in response to environment to tune compatibility or incompatibility

Another soft matter challenge specific is homogeneous catalysis. Two questions were asked:

How do we create soft matter metal-ligand arrays capable of?

- Transforming saturated hydrocarbons into alcohols, olefins and other building blocks under mild conditions
- Creating conjugated carbon-rich structures such as Cn polyhedra, nanotubes, graphemes, diamonds at low temperatures
- Achieving >99% enantiomeric excess in any catalytic reaction with any substrate Catalyst structures self-adjust to optimize catalysis
- Reducing atmospheric N2 to NH 3 or organonitrogen compounds efficiently
- Copolymerizing polar and non-polar unsaturated substrates to produce unique polymeric materials
- Creating polymer chains with precisely tailored comonomer or branch incorporation points for unique mechanical and processing properties
- Creating copolymers combining biotic + abiotic monomers
- Dissolving/processing/functionalizing intractable substances, such as minerals, radioactive wastes or wood using reagents tailored to the surface of interest
- Using solar radiation to achieve selective, efficient splitting of H20, CO, CO2 or CH4

With electronic properties, how do we maintain soft matter properties of mechanical flexibility and processability, light weight and architectural diversity yet obtain?

- High carrier mobility selective for holes or electrons, with controllable carrier densities
- Tailorable band gaps, optical cross-sections, photoluminescence efficiencies and intersystem crossing rates
- Long-lived excitonic states with tunable emissive characteristics

- Structures that enhance exciton mobility or splitting into holes and electrons
- Tunable refractive index, dielectric constant, polarizing

With mechanical properties, the goal is to learn from nature and go beyond. How do we achieve soft matter with great strength yet formable into shapes or having mechanical properties "switchable" on or off in response to stimuli:

- Ultra-high modulus, yet processable into films, fibers, shaped objects
- Mechanical properties tunable with a stimulus (thermal, magnetic radiation, chemical)
- Exceptional impact resistance, yet processable
- Crosslinking reversible with external stimulus chain entanglement or density reversible with external stimulus

Next, **Marks** discussed the challenge of tailor-made hard matter with the finesse of soft matter synthesis. Hard matter encompasses the majority of elements of the Periodic Table. Only a small fraction of all possible compounds have been synthesized. Rather than "heat and beat" approaches, can we apply atomic level strategies of soft matter synthesis? The needs would be for expeditious characterization, new physical techniques and theoretical input.

The goal of taming hard matter surface reactivity depends on real-time images of processes with atom-scale precision, femtosec time resolution; selective conversion of "impossible feedstock; "single-site" heterogeneous catalysts and hybrid enzyme-abiotic catalysts, among others.

The hard matter challenge specific of nanoscience is selecting in nanocrystal synthesis. First, with monodispersity, can we achieve a "mole" of nanocrystals? How many atoms constitute a surface? What tools are necessary to characterize these surfaces? Secondly, alloy, line phases and multi-functional nanocrystals, at nm length scales, when atoms tend to phase-segregate and intended nanostructures are strained. Can "perfect" alloys or discrete compounds be achieved in nanocrystals? Third, perfecting nanocrystals for assembly means understanding/controlling forces for assembly of 1-100 nm size structures. Can we control driving forces for assembly and use external stimulus? **Marks** questioned "How do you make a nanomolecule?"

With harnessing synthetic power of biology, nature is expert in assembling certain hard matter structures. How far can we extend/enhance to tailor-make structures on precise length scales? What are the design rules? Our ability to control size of pure single crystals to Si, GaAs, diamond, zeolites, etc., is limited. Can biological apparatus be reprogrammed to grow very large crystals of predetermined shapes?

With materials with contra-indicated properties, what are design rules and techniques to prepare materials, combining:

- Ferroelectricity and ferromagnetism coexisting at room temperature (e.g. multiferroics). What are the limits?
- High thermoelectric power and electrical conductivity (thermoelectrics). What are the limits?
- High (tunable) optical transparency, electrical conductivity, mechanical flexibility (TCOs). What are the limits?
- High temperature superconductivity, perhaps with optical transparency. What are the limits?

With materials discovery by combinational computation, the question was asked if it is possible to propose a desired band structure and 1) search for combination of atoms and crystal structures that yields this band structure? 2) Compute thermodynamics of target phases? 3) Compute thermodynamically most plausible synthetic route?

In concluding, **Marks** questioned how to address Grand Challenges in materials design and synthesis. In synthesis-driven research, it is labor-intensive and most productive when strongly coupled to world-class characterization and theory. When research mode is required, the challenges include sustained focused funding at meaningful levels: team environment leveraging multiple capabilities; interface soft and hard matter scientists; leverage strengths of multiple universities, national laboratories and countries; and fellowships, exchange of personnel, real and virtual meetings, workshops and tutorials.

At the end of his presentation, **Hemminger** asked if there were any comments from the Committee. **Moskovits** said he was surprised at the challenges. “It appears you are looking at the big picture, challenges and goals. Did you find anything that you didn’t anticipate while conducting the workshop?“

Marks replied that he had tried to provide glimpses and that the goal was to “bring diverse disciplines together, the physical tools and theory.”

Ward Plummer said that with discovery-based research, “none of us are wise enough.” He suggested focusing on things about which we do not have knowledge.

Marks responded by saying we are “investigators with capabilities.”

Frank DiSalvo said it is clear that “we went back decades and what we have implemented has come with a lot of progress, but we have a long way to go. With that being said, scientists seem to be the only ones who relate on how to get from here-to-there. We need to find out how to get great ideas implemented and must communicate.” He added that we should consider two versions of the Grand Challenges – one for scientists and one for staffers and then we should provide constructive feedback.

Ratner responded by stating “we spend the majority of time to make a substantial, time-tracking message comprehensible. If not, we do not have the science and it becomes nothing but buffer.”

Hemminger called for a lunch break at 11:50 a.m. and asked everyone to reconvene at 1:00 p.m.

Hemminger called the afternoon session back to order at 1:10 p.m. and introduced **Leon Balents** to discuss Chapter 4 of the report, “Emergence of Collective Phenomena: Strongly Correlated Multi-Particle Systems.”

Balents began his presentation by thanking Julia Phillips, Walter Kohn and many others for their assistance in writing the report.

With correlations and emergence, there is 1 cm^3 of matter = 10^{23} atoms, electrons. The motion of one influences another and controls the correlation to achieve positive results. **Balents** showed two graphics, one showing traffic congestion (correlations jammed) and a lesser congested area (controlled correlations, which is fast and efficient).

In a scientific setting, the emergence and correlations are everywhere, such as every solid and molecule. In a single crystal, two atoms’ relative positions are determined within small fraction of an Angstrom even when micros or mm’s apart. Other types of correlations are more subtle and still waiting to be uncovered. Correlated particles include electrons, atoms, molecules, grains, biological structures and cars.

To understand and harness the mechanisms to utilize them, you must have electronics correlations →unique materials and device properties, such as superconductivity, all magnetism, spin-charge coupling, such as multiferroics, large thermopower and controlled many-electron coherence in nanostructures. With atomic correlations, we must understand Quantum: ultra-cold atoms and Classical: amorphous solids, glasses, self-assembly, non-equilibrium processes. Lastly, we need to have a better understanding of biological correlations.

It is impossible to discuss this chapter without knowing the importance of electronic materials. Semiconductors are a success story, being a multi-billion dollar industry. The science has had a Hall effect, nanostructures and at least four Nobel prizes. There is an accurate understanding and modeling and the major energy applications, photovoltaic solar cells (clean, unlimited energy) and light emitting diodes (efficient, durable lighting). The major challenges that relate to electronic materials are 1) Going beyond semiconductors, such as achieve semi-conductor-level fabrication with correlated electron materials? 2) Gaining of new multifunctional materials and devices, which do more and do it better than semiconductors 3) Understanding phenomena, controlling materials and interfaces.

In comparing semiconductors and correlated electron materials:

Semiconductors

- Large overlap of s+p orbitals gives very extended wavelengths
- High quality and flexible fabrication (Advantage)
- Sensitivity due to weak donor/acceptor binding
- No intrinsic magnetism or other correlations (Disadvantage)
- Intrinsic length scale = large effective Bohr radius a_0 (Disadvantage)
- Weak correlation and large a_0 enable simple and accurate modeling

Correlated Electron Materials

- Localization of d+f orbitals enhances Coulomb interactions
- Materials chemistry challenging (Disadvantage)
- Sensitivity due to competing ordered states
- Diverse magnetic and other correlations (Advantage)
- Intrinsic length scales as short as atomic size (Advantage)
- Strong correlations very challenging to existing theoretical tools (Disadvantage)

Balents discussed “The beyond and what could we do.” He suggested combining magnetic and electric functionality, build dissipationless wires and devices from high temperature superconductors, make better thermoelectrics and make smaller, faster and more efficient electronics.

The most obvious challenge of correlated interfaces is to produce quality materials and interfaces needed for heterostructures, which has shown some exciting progress and metallic interfaces have been observed with mobility of 10^5 $cm^2V^{-1}s^{-1}$ comparable to high quality GaAs.

With strong correlations, there is a possibility of new emergent phenomena at the interface itself.

In harnessing competing orders, frustrated materials have competing interactions, exhibit tunable ordered states.

In correlated quantum liquids, the liquids are described as superconductors. What are the mechanisms? We need to understand the normal state first. In nanoscale quantum correlations, electrons confined to small structures experience enhanced Coulomb forces, such as nanowires, nanotubes and quantum dots. We want to control the full quantum state.

With atomic/molecular correlations, the correlations between atoms and molecules are usually strong in solids or dense liquids, but can be described classically. One illustration shown was stress fields of compressed amorphous “solid” mixtures of photoelastic polymer disks. The obvious strong correlations in the stress must be understood to fathom the limits of strength and failure mechanisms of amorphous materials and glasses.

It would be difficult to find biological systems that do not involve correlations. Biological systems involve correlations of large numbers of designed, active elements operating highly out of equilibrium, on many length scales simultaneously, such as the human heart, which is developmentally programmed to occur in the same position over and over again.

In summarizing the needs on a broad scale to meet the challenges of correlation, he must look at experiment, material synthesis and theory.

- Experiment: New and improved tools must be developed to probe "hidden" correlations
- Materials synthesis: High quality, single crystal samples are needed for many experiments
- Theory: a combination of first-principles and phenomenological approaches is needed to encompass the broad range of length scales in strongly correlated systems.

Balents concluded his presentation at 1:38 p.m.

Hemminger once again requested holding all questions until the designated time later in the afternoon. He introduced **Jay Groves,** who provided a Grand Challenge Report on "Nanoscale Communications: Energy and Information."

Groves said that we must tap the existing world of biological nanotechnology by constructing molecular level, functional interfaces between living systems and synthetic technology, (domesticate life at the molecular and cellular level). In addition, we posed the question if we could develop design and fabrication principles that enable the construction of synthetic devices, with capabilities that rival those of living systems (bottom-up design and construction)

There have been two nanoscale revolutions – technology and biology. With technology you have:

- Technology, by human design
- Nanoscale dimensions beginning to be achieved
- Nanoscale properties harnessed in isolated examples, which are unique and need to be observed
- Very limited capabilities compared to the things we see in the living systems

With biology, it is:

- Self-evolving
- Understanding scientifically by discovery how Biology works
- Intrinsically nanoscale
- Innumerable unique properties, which poses the problem that we can not get to them to control them
- Capabilities generally can not be harnessed

All aspects of life are naturally emergent physical properties, which tell us what the physical bounds are. We are a long way from having a complete understanding of what the technology is when relating it to living systems that enable them to perform. Can the functionalities be harnessed and can similar levels of functionality be engineered into synthetic systems? Can living and nonliving be integrated?

In the first part of the chapter - integrating living and non-living barrier

Actively communicating with and direct cellular behavior:

- Establish two-way communication as in living organisms at the molecular level
- Decode biological communication principles
- Establish synthetic (molecular-level) communication with loving cells

Develop minimal self-sustaining (living or non-living) organism

- Bottom-up synthetic cell
- Top-down minimal cell

We need to connect electronic logic with biological logic.

Building synthetic surfaces harvested from solid state electronics and then using synthetic cell membrane, synthetic receptor protein and living receptor protein are needed to produce a living cell.

In nano-macro junctions, photonic (plasmonics and subwavelength light control), electrical/magnetic (molecular wirebonds), mechanical (chemomechanical motor drive) and combining different approaches were examined, with **Groves** stating "we have a long way to go to make photon/electron transduction connections.

In the next part of the chapter, **Groves** looked at energy transduction at the nanoscale.

Photonic, electronic and chemical transitions

- Photon – electron/ion coupling
- Photon – chemical coupling

Groves added, "These can be controlled, but can we get to that stage? We could then make tangible products."

Stochastic processes, signals and noise

- Biological signal transduction and information processing
- Molecular motors

Groves moved to a graphic of a molecular motor, stating ions run through to cause rotation and movement. Another graphic showed how the open state (ATP weakly bound), the displacement and the closed state (ATP tightly bound).

Lastly, Groves looked at the functional systems and colonies. We need to "learn a lot more and work together on building nanoscale assemblies, self-regulating adaptive interactive systems (Metabolism, information replication, and self-replicating life) and ad-hoc networking among nanoscale devices. We need to take advantage of conceptual origins from Maxwell (control randomness) and Mendel (use randomness, by use of random selection). Random biological evolution has developed technology that controls randomness, which is a good process that Biology has executed and proven that it is possible and that is a Grand Challenge.

At 2:03 p.m. **Hemminger** asked **Mark Ratner** to provide an overview on Chapter 6, "Matter far from Equilibrium."

Fifty years ago, these issues of behaviors would not have existed. He spoke of setting a challenge that an "intelligent high school student" could understand.

He showed how with an array of windmills in Washington state, we want to stay close to equilibrium. He showed how it has an effect on global weather patterns and problems relating to earth science.

Ratner stated there were 15 things listed as "points at issue" and "targets for progress" for which we would like to have answers. The fundamental challenges are complicated including:

- Appropriate (drastically) reduced variables ($10^{23} \rightarrow$ few)
- Linked up concepts for a broad range of length scales

- Nonlinear structures and behaviors
- Emergent properties (which makes something go from small to large scale)
- Inputs of new fluxes (changing behaviors of equilibrium system)
- Emergence, amplification, selection, combinatorics, complexity, feedback and eventually-consciousness and like itself

Ratner discussed a sidebar in the report regarding a glass sculpture being one of many forms of art that relies on non-equilibrium. The glass is a super-cooled liquid, relaxing on many differing timescales, approaching equilibrium, but never attaining it.

Beluzhov/Zhabotinsky oscillating chemical reaction was also observed. These spatial patterns are observed when the initially-mixed chemical reagents diffuse to form patterns (without stirring). Other similar patterns (in space and in time) are observed in many systems whose dynamical equations are nonlinear.

DySA is nature's preferred way of building its animate creations on various length scales. Three graphics were discussed including fluorescently labeled microtubules in a cell confined to a 40 μm triangle on a SAM-patterned surface of gold; a fractal bacterial colony and a school of fish. With magnetohydrodynamic DySA, two magnetic particles rotate at the interface due to a rotating magnet. They reach a non-equilibrium steady state at which the magnetic force is balanced by the pairwise hydrodynamic repulsion between vortices created by the particles. This simple system combines a conservative confining potential with dissipative, hydrodynamic interactions, which asks the question is there an extremum principle that describes this "contained" non-equilibrium steady state? Scale bars are 2 mm.

When looking at equilibrium and non-equilibrium, it depends on "how much energy you put in and how much heat you take out." At equilibrium, a collection of millimeter-sized magnetic particles float on a liquid-air interface in a "clump." If one supplies energy by rotating a magnet below, the particles assemble spontaneously into an ordered array. Hydrogel particles doped with camphor floating at a water-air interface mimic chemotactic bacteria, responding to chemical gradients, which they also emit. At high densities, particles organize into a lattice due to repulsive interactions.

In quorum sensing, colonies of the bacterium Panibacillus dendriteiformis organize themselves into extravagant formations to maximize their food intake in a given environment.

An Icelandic poppy rose is an example of circadian rhythms – systems that use external energy inputs (sunlight) to drive them through cyclic behaviors, as the rose closes at night and opens in the sunlight.

Football players are a highly non-equilibrium system that uses energy inputs to perform useful work by processing whose efficiency is difficult to characterize, and whose functioning depends on non-equilibrium at many levels. Such self-organizing complexity is perhaps the ultimate challenge for our understanding of non-equilibrium systems.

A simple example is the molecular transport junction. **Ratner** reviewed sketches and images of junctions in which single molecules act as conductors in a highly, non-equilibrium situation. One graphic discussed was a sketch of molecular junction and an organic pi system suspended between two metallic electrodes and an image of a fabricated junction, with the invisible molecule in the invisible crack between two blue metal tips. The image also shows sketches of more complex molecules, which include a metal atom. The observations show characteristic phenomena due to strong correlations of the electronic system: the so-called Kondo resonance, where the conductance through the junction can become very large at low temperatures, and the so-called Coulomb blockade, in which there can be a long flat area around zero source voltage, when the electron simply cannot be forced onto the molecule, so no current is observed.

When looking at "The Science of Life," **Ratner** said there had been some specifics and some accomplishments. He discussed a look at some of the sidebars in the report, calling attention to nanothermodynamics of molecular machines. Equilibrium thermodynamics describes how energy is exchanged in systems: liquids, magnets, superconductors and ven black holes, blindly comply with its law. The observed behaviors of macroscopic systems, such as steam engines are reproductible and fluctuations are small. However, virtually all approaches now being considered in the energy sciences involve small systems that are not fully described by conventional bulk thermodynamics.

Next, Ratner looked at recent developments toward a unified treatment of fluctuations in small systems which are embodied in fluctuation theorems (FT). FT relate the probabilities for a system to exchange certain amounts of energy with the thermal bath. Experimental techniques, such as optical tweezers and atomic force microscopy, have recently allowed scientists to directly test the validity of several fluctuation theorems.

There are several FTs, each applicable to slightly different thermodynamic systems. The Crooks fluctuation theorem and the closely related Jarzynski equality are directly applicable to mechanically perturbed small systems, such as RNA hairpins or single proteins. The Jarzynski equality (JE) asserts something remarkable. The JE has been tested by mechanically stretching a single molecule of RNA.

Many of the processes that characterize energy flow, capture, production, storage and transduction occur far from equilibrium; so do most significant biological behaviors and important processes in molecules, solids, oceans and atmospheres.

Since most current understanding of physical and biological systems is based on equilibrium concepts, far-from-equilibrium behaviors are intrinsically and crucially significant. The combination of significance and energy relevance, of intrinsic scientific knowledge and its application, characterize the Grand Challenge of systems far from equilibrium. Progress in understanding and quantifying these behaviors must be made, to deal effectively with the energy, climate, materials, biological and security issues facing humankind.

A break was declared at 2:25 p.m. The Committee was called back into session at 3:03 p.m. **Hemminger** reminded everyone that there would also be a couple of hours to discuss topics and issues the next morning. He stated that with more speakers scheduled before the end of the day, he would like to stay as close to the agenda as possible.

At 3:05 p.m., he opened the floor to Committee members for discussion. **Hemminger** requested more information from **Dehmer** on the audience of the report. He also stated the Committee and all of the people associated with the report have done "a tremendous job and a tremendous amount of work." He asked the Committee members if they believed all Grand Challenges had been identified. He said he knows that there are a lot of issues that people want to talk about. Lastly, he suggested that BESAC members should self-select with chapter leads to discuss the respected chapters for further discussion.

Dehmer said the audience for the report should be accessible to upper-level college students, graduate students, policy makers, administrative staffs, among others. All sections will not be accessible to all members to policy makers and scientists in the field. She encouraged all staff in BES to address different audiences. **Dehmer** will look at the challenges of this situation.

Hemminger asked if there was anything that someone thinks should not be in the report and the Committee answered unanimously "no." He then opened the floor for discussion.

Moskovitz stated he "was delighted while reading the report." He learned a great deal from the cohesion section, but felt it was not clear why it was written and questioned what the motivation for writing it was? He asked if we need special instruments that we do not have. He also wanted to know if we are in crisis concerning the number of people we have to fill vacant positions.

Moskovitz also stated he had discussed with **Dehmer** that science has a “punctuation evaluation of new theories” and we graze on these ideas and then come up with new things. Most people do not want to figure out theories. We have been at a plateau for a number of years and believe that we will see new technologies and theories coming about.

McCurdy, Jr. spoke more critically of the report and broke down the Executive Summary and each of the chapters for comment. His first impression was the Executive Summary has the same phrases repeated numerous times. He did not believe the introduction was interesting or stimulating. In Chapter Two, he saw a group of notions and good ideas, but the message was obscure. He thought the details drew one’s attention, but did not deliver an end result and was not easy to understand. In Chapter Three, there were too many questions, bullets and lists, and he saw the chapter as redundant. In Chapter Four, he saw several good headings, but it did not capture the relevance and it reiterated the same information. Chapter Five, He thought was a very good chapter and got to the point of what was trying to be said. Chapter 6, He thought was an intellectually difficult subject, but the opening is attractive. He concluded by saying he saw 136 pages of good ideas and the discussion at the BESAC meeting has been more stimulating than the actual book/chapters. He also stated the sidebars were not actually sidebars because some of them were as long as two pages. He believes there are enough examples and they need to be more thoroughly explained.

Mark Ratner reminded **McCurdy, Jr.** that this project is still in the draft stage, but this is the type of feedback he wants to receive. “Comments of this kind are appreciated.”

Frank DiSalvo believed the chapters and discussions focus too much on long-term things and did not believe the material stated what was actually the “new” information.

Nora Berrah complimented the Committee and thought everyone had done “more than an excellent job.” She thought **McCurdy** was too severe in his criticisms and believes the report shows a lot of credibility. She believed the Executive Summary should be written more upbeat and convey some excitement that we are ready for the next breakthrough in science. This report should trickle down through each chapter to convey the excitement. It should be inclusive to appeal to everyone from students to staffers.

Bruce Gates also complimented the work and discussed the clarity of the presentations. In the Executive Summary and the Introduction, he believed “the notion of themes overlap and should be developed more effectively, because along the way, something is not articulated. The element of what guides the way we are moving into the future is missing.” He said there was too much discussion and it is difficult for the readers (audience) “to distinguish between data and cartoon.”

John Richards said the information about biology was a great general theme. He said that facts must be thoroughly checked and must be correct. He liked all of the ideas, but the reports needs to teach us enough for those who may not know the background of the subject to understand and appreciate the information.

Kohn has heard some interesting remarks, but said in the section about Maxwell vs. Mendel, he heard a lot about evolution, but not technology. It included a lot about Maxwell, but not Mendel. The evolutionary aspect is clearly essential; most important concept in Biology is evolution. We have to be careful about excluding that in the report.

Peter Cummings has not read the complete report, but his initial thoughts were that Mendel might not be the best person to compare work to. He was disappointed that theory was not highlighted in the Grand Challenges.

Eric Isaacs said "there is a lot of great information and new material." He said a number of Committee members said it needs to be more readable. At one point, Isaacs said he went through 16 pages of text with no images. "Images need to be arresting and attention getting." He stated there needs to be more sidebars and take the best images and bring them to the front of the report.

Leon Balents said more information could and would be added to sections, with **Jay Groves** agreeing.

Ward Plummer suggested to the Committee that BES hire a science writer to make the book more consistent.

Graham Fleming said this has been a difficult job and welcomed suggestions on how to make it better. He said he liked all of the ideas and would consider all of them in making revisions.

Eric Isaacs agreed the report looked like it had been written by numerous people and the writing styles were not consistent.

Graham Fleming reiterated the report was still in the draft stage and wanted to wait to get comments before turning it over to a writer for proofreading and editing.

Tobin Marks said we "have stumbled on some great information and ideas while looking at our current challenges."

Hemminger said "these were not accidental discoveries, it has happened because it has been there and we are simply putting the right people in the right places to find the information."

Martin Moskovitz disagreed with **Hemminger,** saying the questions outstrip the technology and that possibilities are not always available. "With these possibilities, we do not have the means to materialize them."

At 4:03 p.m., **Hemminger** requested closing the discussion and moving into the additional presentations. He also suggested Sub-Committee members meet with Leaders during the evening to brainstorm additional ideas.

At 4:06 p.m., **Hemminger** thanked **Andrew McIlroy** for giving up a portion of his vacation to attend. **McIlRoy** was asked to discuss the "Basic Research Needs for Clean and Efficient Combustion of 21st Century Transportation Fuels." He began his presentation with stating the transportation combustion challenges include efficiency and cleanliness being difficult to achieve. Diesels are efficient, but difficult to keep clean because of no throttling losses, high compression ratios, continuum of rich to lean and soot and NOx often are anti-correlated. Spark ignited engines are 'clean,' but less efficient due to stoichiometric burning, little soot, three-way catalyst eliminates NOx, throttle losses and low compression ratios.

The motivation was the transportation sector is the key to energy use.

- Transportation accounts for ~1/3 of energy use
- When electricity generation is factored out, transportation dominates.
- Demand is projected to increase
- Ninety-seven percent of transportation energy comes from petroleum
- Relatively small number of technologies employed
- Transportation sector energy use can impact national security and environmental impacts

The changing world of fuels and engines was cited as another motivation for the challenge. Fuel streams are rapidly evolving, such as heavy hydrocarbons and new renewable fuel sources and new engine technologies, such as direct injection (DI), homogeneous charge compression ignition (HCCI) and low temperature combustion. New engine technologies are beating the competition with efficiency.

The charge to the workshop is that “we were looking at non-traditional fuels, instead of an alternative fuel.” The Sub-Committee wanted to explore basic research needs in the areas of gas-phase chemistry, combustion diagnostics and combustion simulation that will enable the use of transportation fuels derived from non-traditional sources in a manner that optimizes engine efficiency and minimizes pollutant formation.

- Non-traditional fuels are defined as those derived from carbon-neutral, renewable resources, such as biodiesel or ethanol and those derived from non-traditional fossil fuel reserves, such as heavy crude oil, tar sands, oil shale and coal
- The output of the workshop will seek to define a set of basic, primary research directions (PRDs) that would employ and expand the current broad expertise base in gas-phase chemistry and combustion research into the realm of non-traditional fuels

The workshop panels were divided into three groups – novel combustion, fuel utilization and crosscut science. The co-chairs of the organizing committee were McIlroy and Greg McRae. The panel leads for novel combustion were Dennis Siebers and Volker Sick. The panel leads for fuel utilization were Phil Smith and Charlie Westbrook. The crosscut science panel leads were Craig Taatjes, Anaud Trouve and Al Wagner. The DOE/BES representatives and sponsors were Eric Rohlfing, Frank Tully and Dick Hilderbrandt.

The participants consisted of 95 university and laboratory employees, with less than 20% coming from government and industry (Forty-two percent came from universities, 39% laboratories, 12% government, 7% industry). The plenary speakers were James Eberhardt, Charlie Westbrook, Hukam Mongia and David Greene. Afterwards, there was a meeting of the core writing group. The final report preparation followed the workshop, with the draft report delivered February 21, 2007.

The priority research directions identified:

1) Combustion under extreme pressure
2) Surface chemistry in transportation systems
3) Breakthrough discovery tools focused in need of new diagnostics
4) Multi-scale modeling
5) Basic research needs for smart engines
6) Physical and chemical properties for combustion of 21st century transportation fuels
7) Automated discovery of fuel chemistry kinetics
8) Spray dynamics and chemistry for new fuels

The Grand Challenge from the workshop is predictive modeling of combustion in an evolving fuel environment. Predictive modeling is the key to combustion optimization in a non-linear parameter space. The challenges are:

- Nine orders of magnitude in space and time
- Complex chemistry, varying with fuel evolution
- Work needed in:
    - Chemical mechanism development
    - Turbulence-chemistry interaction
    - Algorithm development
    - Large dataset analysis

Additional challenges are new engines demand high pressure chemistry and physics, novel fuel/engine cycle combinations require the understanding of interfacial and condensed phase phenomena and the evolving fuels increase chemical complexity.

Hemminger asked if there was a lot of discussion concerning evolving fuels increasing chemical complexity as a predictive modeling of combustion.

Kohn said **McIlroy** should contact a friend of his as a source on the subject. He also commented that Detroit will build what consumers want to buy.

Hemminger introduced **Donald DePaolo** at 4:35 p.m., to discuss "Basic Research Needs in Geosciences: Facilitating 21st Century Energy Systems." The meeting was held February 20-24, with 127 participants and 84 panelists. Depaolo and Lynn Orr served as co-chairs. DePaolo thanked BES shepherds Nick Woodward and John Miller for keeping the group organized, on-schedule and for excellent advice throughout the process. The report was published July 10.

The outline included identifying the technical challenges (CO_2, sequestration and nuclear waste disposal), the workshop organization and summary of results. The two driving objectives in meeting the technical challenges were meeting energy demand in the coming century and drastically reducing CO_2 emissions. We need to keep CO_2 from going into the atmosphere.

The basic research needs for the hydrogen economy report was "because both gas and coal reforming processes generate CO_2 (coal generates approximately twice as much per unit H_2.), their value in meeting the fundamental goals of a hydrogen economy depends on developing safe, effective and economical methods for CO_2 sequestration."

In addition, the "reliance on coal as a sole source of energy for generating hydrogen for Freedom Car transportation needs would require doubling of current domestic coal production and consumption.

For nuclear power to have a significant impact on energy production and at the same time reduce greenhouse gas emissions, the estimated needs for nuclear power production are as high as 300 EJ/year by the year 2050. This represents nearly an order-of-magnitude increase over the ~440 nuclear reactors that are presently in operation.

Advanced waste forms will have to be designed to ensure safe performance for periods ranging from hundreds to hundreds of thousands of years... in the complex, highly coupled natural environment of the near field in a geologic repository.

Looking at "the underground" as a long-term container, the advantages are enormous volume (as required). Distance from the surface environment keeps nuclear wastes away and having a pre-made container. The challenges were that it was designed by nature, only approximately fits the design criteria for containment, complex materials => complex processes, it is difficult to see and monitor and the uncertainty about the long-term performance.

CO_2 must be trapped underground. The geology needs to be in place. For CO_2 plume, two primary forces act on the injected CO_2. Buoyancy drives injected CO_2 upward, and the pressure differential between the injection zone and the rest of the formation forces CO_2 outward. These two forces form a CO_2 plume in the shape of an inverted cone, with mobile CO_2 migrating laterally below the impermeable "cap" rock.

The scale of CO_2 sequestration is a large footprint, large number of wells, multiple subsurface processes and rates. The global target is 10,000 MT CO_2/year.

The workshop structure had five panels – multiphase fluid transport, chemical migration processes, characterization, modeling and simulation and cross-cutting and Grand Challenge science themes. The Grand Challenges were computational thermodynamics of complex fluids and solids (material properties and chemical interactions); the integrated characterization, modeling and monitoring of geologic systems (seeing into the Earth); and simulation of multi-scale systems for ultra-long times (predicting performance). The cross-cutting issues were the microscopic basis of macroscopic complexity, the highly reactive subsurface materials and environments and thermodynamics of the solute-to-solid continuum.

To summarize the workshop, **DePaolo** said he was “extremely pleased with the report, where we are in the process and where we need to go.” The workshop provided an up-to-date assessment of geoscience research needs for the coming decades. The participants are excited by the research possibilities, committed to the technical objectives and enthusiastic about the goals of the workshop. The research described involves and depends on continued advances in theory, material analysis and modeling, and hence aligns with fundamental aims of DOE Office of Science. Lastly, the report conclusions are complimentary to those of recent reports on the hydrogen economy, advanced nuclear energy systems, advanced computing, alternative fuels, and with the capabilities of major BES research facilities.

Bruce Gates asked **DePaolo** about the costs of CO_2 in the ground. **DePaolo** responded by saying if done at the commercial scale, there is significant cost involved.

George Flynn said the reaction rates are high and CO_2 must be bought in large volumes. Sites must be selected that have low probability to deal with problems as they develop.

Gates asked what is the density of CO_2? **DePaolo** stated 500-700 KG**.** When CO_2, is dissolved, the driving force is small.

At 4:55 p.m., **Hemminger** introduced **Michelle Buchanan** to discuss “Basic Research Needs for Electrical Energy Storage.” Buchanan stated “we need to look at a portfolio to take us into the future without foreign oil and the omission of carbon monoxide into the environment.

Moving to electrical energy sources and use requires electrical energy storage. The problem is two-fold, energy storage is critical to expandable use of renewable energy sources (solar and turbine) and plug-in and all-electric vehicles place greater demands on energy storage.

She discussed the Tesla car and revealed if it used computer batteries, it would take approximately 7,000 batteries to drive 200 miles.

Electrical energy storage enables a broad range of energy technologies, including energy management, bridging power and power quality.

The workshop was held April 2-4, with **John Goodenough** serving as chair, and **Hector Abruna** and **Michelle Buchanan** serving as co-chairs. More than 135 attended, with the majority being from foreign countries. The charge was to identify basic research needs and opportunities underlying batteries, capacitors and related technologies, with a focus on new or emerging science challenges with potential for significant long-term impact on the efficient storage and release of electrical energy. Highlighted areas include coupled ionic and charge transport, electrolyte physics, theory and modeling, and novel materials and approaches.

Batteries, to the end user, appear to be simple; however, they are dynamic systems that change with every charge/discharge cycle over their lifetime. What would appear to be a simple interface between the battery electrodes and electrolyte is in fact a complex set of phases that change with time.

The fundamental challenges in chemical storage science is that there is a knowledge gap, a need for basic understanding of the mechanisms and kinetics of the elementary steps involved in chemical storage. In addition, how to correlate interface structure with reactivity? How do structural defects, such as dislocations, change during cycling? To what extent are the thermodynamics and kinetics of ion reactions different between nano and bulk?

The fundamental challenge in capacitive storage science is the need for a basic understanding of key issues in capacitive storage involving interfaces, dynamics and charging.

It is very important to understand the rational materials design through theory and modeling. The objectives were combined, electrical and transport modeling of electrode and fully predictive performance and stability modeling of active component. How do we get there?:

- Predictive kinetics of phase changes
- Electrochemistry at the nano-scale
- Charge transport in mixed conductors
- Computational materials design
- Transport and evolution in electrode microstructures
- Structures and role of reaction interfaces (SEI)

This enables the modeling of performance, lifetime and safety, accelerated innovation in new materials and new designs to higher energy and power at lower cost.

Buchanan closed her presentation by addressing four cross-cutting areas of electrical energy storage – advances in characterization, nanostructured materials, innovations in electrolytes to get optimal behavior and theory, modeling and simulation.

At 5:25 p.m., **Hemminger** opened the floor for discussion.

Greg Exarhos from Pacific Northwest National Laboratory was impressed with Chapter 7, stating college students are receptive to what is going on at laboratories and that more discussions are needed at the college – undergraduate, graduate and post doctoral level.

Hemminger made a list of lead chapter writers and requested they meet with Sub-Committee members concerning issues from today's discussion and bring some solutions to Tuesday's meeting

With there being no other public comment, **Hemminger** adjourned the meeting for the day at 5:30 p.m.

Wednesday, August 1, 2007

Hemminger called the meeting to order at 8:47 a.m. and told the Committee members he hoped last night's meetings with Sub-Committee members were successful. Afterwards, he introduced **Richard (Rick) Osgood** and requested a report on the Committee of Visitors (COV) for the BES Scientific User Facilities Division.

Osgood began his presentation by stating that the purpose of the report was to "review the reviewers." He wanted to examine the way people reviewed facilities and determine whether the process was going in the right direction. "I believe this is a very important exercise because BESAC has to formally accept this report."

The Sub-Committee met April 11-13 at BES/DOE Germantown. This was the second COV review of the facilities division. The present panel assessed operations of Division's programs during FY04, FY05 and FY06. During this period, the Sub-Committee examined all files to see what feedback they were receiving. The Division components for review were the following:

- Synchroton-Light and Electron-Beam Sources
- Neutron Sources
- Electron-Microscopy Sources (new division)
- Nanoscale Science Research Centers (relatively new division)

- Accelerator and Detector Research (just evolving into the program, but not yet a part of the division)
- New projects

After the report is accepted by the BESAC committee, the COV report will be presented to the Director of Office of Science.

During the first COV meeting, the following recommendations were made concerning the Jacket format:

- Timelines of the review history for each facility or center. Each timeline should take the form:
    - Review→Recommendations→Results (including written response to COV/BESAC); Re-review and its results if deemed necessary
    - History should be in front of jacket of most recent review for each facility and a brief overall review history for the facility. Cross-references to the full jacket for previous reviews are also useful.

- Several elements should be contained in the report and file of every BES facility review; these were noted in the report

The review process found the following:

- Evaluation of the success of facilities should be done on the basis of quantifiable metrics – these may vary with type of facility
- Revision of the review process, e.g. more executive sessions, more time to hear about related lab issues
- Broad users' input strongly recommended at all stages of construction of five centers, since they are designated as national user facilities
- Clear and current definition of a user
- Consensus report may be best

The Facilities Division Operation recommended:

- Careful attention to coordination between the two major science program divisions and the Scientific User Facilities Division; strongly recommend that science program managers participate in facility reviews
- Careful thought of integration of nanocenter science across centers and with core programs
- Strong coordination with two scientific divisions urged

Next, **Osgood** recapped the members of the DOE/BES COV review panel, including four panelists attending the Neutron review; four attending the nanoscience review; five attending x-rays/machines and three attending the microscopy. BESAC Committee Members **Gabrielle Long** and **Hemminger** also attended.

The charge of the Committee was that the panel will consider and provide evaluation of the following four major elements.

1) Assess efficacy and quality of processes used to:
    a. Solicit, review, recommend and document proposal actions (how were proposals done, was monitoring done correctly and what were the consequences of the evaluations)
    b. Monitor active projects, programs and facilities
2) How has the award process affected:
    a. Breadth and depth of portfolio elements
    b. National and international standing of portfolio elements

3) Provide input for OMB evaluation of BES progress toward long-term goals. Each of the components of the Scientific User Facilities Division should be evaluated against each of the four-part long-term goals. If not applicable, please indicate so.
4) Note OMB guideline ratings of (1) excellent, (2) good, (3) fair, (4) poor, (5) not applicable. Also, comment on observed strengths or deficiencies in any component or sub-component of the Division's portfolio, and suggestions for improvement.

The report included the introduction, charge, committee composition, review process used, response to prior review, the actual review (including the COV review process, facility review process and reports on specific classes of facilities), comments on the emerging facilities, metrics, general comments and conclusions.

The summary stated that COV concludes that the newly constituted Scientific User Facilities Division is well-launched and is operating extremely well. The facility reviews were fair and even-handed and had significant and clear beneficial impact on several facilities, even though many of the facilities are just now reaching the point of operational review. (Some facilities are just now receiving their first review.) The COV found the review process has served existing facilities well. In some cases, reviews have prompted changes in management and operations and improved the scientific impact of these facilities. The reviews have added clarity and focus to a wide spectrum of concerns from user community, facility personnel and the BES. The COV made specific recommendations for improvements and changes in review process, both in general and in terms of specific facility types.

In addition, the Committee was satisfied the Division is operating well and expects further definition and refining of the review process as SUFD matures. The Committee continued to urge very careful attention to the coordination of the two major science-program divisions (Materials Sciences and Engineering and Chemical Sciences, Geosciences and Biosciences) with the Scientific User Facilities Division; healthy growth of the BES organization will necessitate balance between these two organizational units.

The committee was PART ratings of excellent for materials research, chemistry and instrumentation and not applicable for energy research.

The COV Review recommendations are BES should adopt a practice of having a separate document summarizing the reviewers' comments (Executive Summary) and a letter detailing actions requested by BES following the review. In addition, a timeline of actions and reviews of each facility should be attached to the cover of each review jacket. Lastly, the previous COV report and BES response should be distributed to the next COV prior to the meeting.

With Facilities-Division review recommendation came feedback that the overall basic review system works exceptionally well and there should not be any changes (although it was discussed that it may need to be "tweaked.")

The Facilities Division staff should begin to plan for an improved strategy for the review process of the largest facilities.

To the extent possible the results of the review should be provided in a timely fashion. In addition, the comments of the reviewers should be summarized separately from the letter containing requested actions by the SUF Division Director.

The Committee recommended that the planned increase by five in the SUFD staff proceed promptly; it is needed for a well-managed facilities program. In addition, allowance for increased travel, i.e. funds and time, to facilitate to encourage informal evaluation of facilities should be made. **Osgood** stated this was a "huge program with very few people to manage it. We must have funds and time to encourage informal evaluations."

The Committee recommends that each SUFD review explicitly discuss collaborations between core-research programs and SUFD operations.

Some of the general recommendations included:

- Institute a uniform, integrated and transparent proposal system for all five NSRCs
- Include explicit time for facility research and instrumentation review in each SUFD review
- The Committee does not recommend the adoption of a single cost metric; such a metric would not be an effective management tool and its use would leap to poor management behavior
- SUFD should plan to discuss in more detail its strategy for developing theory at the full complement of BES facilities during the next COV

Osgood provided several facility-specific comments concerning the nanocenters. He said there was a dynamic tension between having good science and not having proper centers and questioned how and what is the balance. In closing, he thanked the COV members for generously giving their time and thanked **Dehmer** and **Pedro Montano** and the staff for providing assistance.

Montano addressed that some centers need more focus than others and that some were excellent. “The centers will eventually find their niche and the goal is for them to excel. The reviewers were very tough in some cases concerning the nanocenters. The group did not expect to receive excellent feedback in all areas. We must continue to have evaluations from users.”

Hemminger agreed that it is important that these centers excel. He questioned the comments about the Spallation Neutron Source (SNS).

Osgood said that a standard committee will look at operational and user science. “It is a lot of work in a short period of time. There were some problems. The SNS review was overwhelming and needs to be better thought-out.”

Walter Kohn asked if the Sub-committee looked at cost effective measures.

Osgood said “this is not a happy thought. The federal government wants to see if things are being run at its most cost effective. If you are trying to do something very sophisticated, people want it without a great deal of cost involved.”

Kohn questioned why the report was a “not-applicable” concerning Energy Research. He made a comment that “Al Gore had to straighten people out about global warming and the impact on nuclear energy does not impact global warming. Coal produces global warming in the worst way.” He asked **Osgood** to discuss global warming and the effect of coal on energy research.

Osgood said the Sub-Committee “did not have the time or resources to answer every question concerning global warming in the report. It was a complicated process and in the end, it was simply not a part of the exercise.”

Bruce Gates asked if generalizations at one facility were considered at another one.

Osgood said is a difficult question because several centers are very strong and that nanocenters are just now launching and very formidable. “We did not have a database to compare each facility. The threshold expertise was very important to have experts, which is complicated. It is just not a simple question to answer.”

Osgood added that the Sub-Committee would like to see the theory idea be fleshed out more and the following questions needed to be answered: Would it be part of the review? Would it be the same for every center? How would it help BES?

Anthony Johnson asked if there was an issue to access. Do training programs have equal access?

Osgood said that people are “very interested from all points of view. Surprisingly, as long as you have a good idea, there will always be an interest.”

Hemminger asked for a show of hands if the Committee would accept the report. The report was unanimously accepted. He thanked Osgood and the Sub-Committee for their hard work and asked that the meeting move forward to hear from **George Crabtree**, who provided a report on the BES Workshop on “Basic Research Needs for Materials Under Extreme Environments.”

Crabtree (Workshop Co-Chair) reported the workshop was held June 11-14, with himself, **Jeff Wadsworth (Workshop Chair)** and **Russell Hemley** (Associate Chair) overseeing the meeting. He also acknowledged **Michelle Buchanan** for her assistance. There were 150 participants from the academia, industry, national laboratories, Basic and Applied DOE Energy Offices.

There were four panel leads and a cross cutting science lead. The charge was to identify basic research needs and opportunities in materials under extreme environments encountered in energy generation, conversion and utilization processes, with a focus on new, emerging and scientifically challenging areas that have the potential to significantly impact science and technology.

When looking at energetic photon/particle damage, he said we can not put a lot of energy through polished glass. The technology drivers are the next generation nuclear reactors, megawatt lasers for fusion, microelectronic sensors for active environments. For research directions, capturing in situ, real time, atomic scale damage characterization, capture multi-scale damage dynamics and detect free or detect tolerant materials to withstand these fluxes.

In flux extremes, **Crabtree** examined the synthesis of new materials and stated “Black Si (silicon)” is laser-generated chalcogen-rich plasma and solar cells.

In chemically reactive extremes, high efficiency steam plants, next generation turbines, all types of fuel cells, nuclear power conversion and thermochemical production of hydrogen were examined.

Controlling reactive environments by having a protective oxide layer, which includes the following:

- Strongly bonded to substrate
- Chemically inert to environment
- Thermodynamically stable at all temperatures
- Atomic scale defects trigger damage growth
    - Local chemical reactions
    - Internal stress
- Defects form at exposed surface and buried interface
- Complex damage trajectory
    - Many interacting degrees of chemical and mechanical freedom
    - Linked across many length and time scales

The research directions included atomic scale, real time, in situ measurements, capture of multiscale damage evolution, multifunctional protective coatings and transformation of empirical data to predictive science.

Thermomechanical extremes have technology drivers that include high temperature/strength materials for coal gasification, ultra-supercritical boilers and turbines, next generation manufacturing technologies.

Some of the thermomechanical challenges are:

- Characterization of high static and dynamic pressure phases
    - In situ experiments at BES x-ray, neutron, and electron scattering and NNSA high energy facilities
    - Time evolution of structural phase transitions and role of defects
- Chemical reaction dynamics of high energy materials
- High pressure response of disordered materials
- Limits of high pressure static and dynamic generation need to be raised

With electric field extremes, research directions are ultra-fast in situ characterization, theoretical framework, and new dielectric materials. Dielectric breakdown has performance limits for power cables (run at higher voltage), high energy capacitors, motors and generators microelectronics (electric fields are remarkably high).

In magnetic field extremes, higher fields →higher performance motors/generators. The research directions are higher magnetic fields and in situ field experiments at scattering surfaces.

The Crosscutting Challenges indicate needs to:
1) Experiment on the scale of the fundamental interactions (atomic scale, in situ, real-time characterization at user facilities)
2) Develop theoretical and simulation framework for predicting and extrapolating performance (beyond current capacity of measure for capturing complex multi-scale phenomena and predictions beyond accessible regimes.)
3) Design and synthesis of transformational materials (to understand these extreme environments control atomic structure and complex damage evolution) and
4) Create extreme environments for materials design and synthesis (used to make materials otherwise; photon/particle flux, chemical reactivity, thermomechanical, electromagnetic fields.

The priority research directions:

- Control and synthesize materials with new properties using photon and particle beams
- Design materials with revolutionary tolerance to extreme photon and particle fluxes
- Work toward ideal surface stability
- Control reaction dynamics at extremes
- Design novel materials – beyond what we know
- Use chemical and materials dynamics in complex systems
- Discover disordered materials in the extreme
- Determine fundamental processes of dielectric breakdown at the atomic level
- Achieve the quantum limit of extreme magnetic field

Lastly, the Grand Challenge is the Extreme Materials, which “summarizes the entire workshop.” To achieve the fundamental performance limit, orders of magnitude improvement and realization of the potential of unexplored extremes are key.

At 9:45 a.m., **Hemminger** asked **Raul Miranda** to provide a Workshop Update on “BES Basic Research Needs for Catalysis for Energy,” which is scheduled for August 5-10 in Bethesda, Md. The workshop included Co-chairs Alexis Bell, Bruce gates and Douglas Ray.

Miranda began his presentation by showing a slide that was a representation of P450 with bound camphor. The enlarged active site region shows the camphor substrate, heme moiety and cysteine residue, which forms the dital heme ligand. In the representation of the full enzyme, the protein backbone was shown in green, the heme moiety in blue and the substrate is colored according to atomic species. Oxygen atoms, carbon, nitrogen, sulfur and iron were also shown.

Three Basic Research Needs workshops with the catalysis: a cost cutting discipline have taken place since February 2003.

The charge to 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. The workshop should uncover the principal technological barriers and the underlying scientific limitations associated with efficient processing of energy resources. Highlighted areas must include 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. A report will be published by November 2007.

The Basic Research Needs in catalysis for Energy Panels include:

Panel 1: Grand Challenges in Catalysis as a multi-disciplinary science and technology

Panels Leads: Mark Barteau and Dan Nocera

Identify the most innovative recent advances in catalysis science and the persistent challenges for the future. Focus on identifying the potential breakthroughs that may emerge at the interfaces of established sciences, such as chemistry, materials, science, physics and biology. Identify opportunities for creating applications of engineering science to enable the processing of energy carriers in an energy-efficient manner through the use of novel separating agents (e.g., ionic liquids and ceramic membranes) and technologies.

Panel 2: Advanced Catalysts for the conversion of biologically derived feedstocks

Panel Leads: Johannes Lercher and Marvin Johnson

Identify the scientific requirements underpinning the development of innovative catalytic processes for fossil energy applications. Focus on the fundamental chemistry advances that may emerge in response to the need to efficiently convert fossil hydrocarbons into energy, energy carriers or materials during the next 25 years. Project such requirements even farther into the future, to an era of deleting fossil resources. Identify strategies for producing liquid and gaseous energy carriers from low-hydrogen content feedstocks, while minimizing the production of carbon dioxide.

Panel 3: Advanced Catalysts for conversion of biologically derived feedstocks

Panel Leads: Harvey Blanch and George Huber

Identify the novel advances most recently attained in the catalytic processing of biomass into energy, energy carriers or materials. Focus on the fundamental breakthroughs that are needed in the area of bioinspired catalysis in the next 10 years. Determine opportunities for single-pot processing of complex mixtures. Identify what catalytic technologies will be needed in the future, when crops will be specially bred for energy production.

Panel 4: Advanced Catalysts for the non-thermal conversion of water and carbon dioxide

Panel Leads: Michael Henderson and Peter Stair

Determine the scientific needs to better understand and utilize catalyst for the efficient photochemical and electrochemical conversion of water and carbon dioxide into storable and transportable energy carriers. Focus on the fundamental breakthroughs needed to achieve high energy efficiency and the application of abundant catalytic materials. Project the requirements into the future when solar radiation may become the primary source energy for the production of energy carriers.

Crosscutting Themes: Theory-Modeling-Simulation, Materials, Advanced Instrumental Methods

Identify the new understanding of catalysis derived from the use or development of new materials and new theoretical and advanced instrumental methods. Identify the synergistic interactions among the classical disciplines of homogeneous, heterogeneous and enzymatic catalysis and identify pathways leading to an increasing integration among those disciplines.

The meeting will take place August 6-9 at the Bethesda North Marriott Hotel.

Hemminger said that since the workshop has not happened yet, all questions on this topic should be deferred to a future meeting.

Linda Blevins was introduced by **Hemminger** at 10:05 a.m., to provide the Committee members a summary of "Chemistry and Physics Gender Equity Workshops and Planning for a Related Workshop." The meeting took place August 1. Thus far, there has been two workshops, the first being in 2006.

Blevins provided a snapshot of Chemistry in 2005, with statistics stating 10,000 Bachelor Degrees were given out; 50% to women. There were 2,000 Ph.D.'s in Chemistry the same year, with only 35% being received by women. She also added that women are only 13% of faculty at the top 50 universities in the country.

In the first workshop, the goal was to bring the top 50 department chairs to meet with Social Sciences and Federal Agencies. **Blevins** stated it was an excellent workshop and all of the time and efforts of all of those involved was greatly appreciated.

The goals were to develop and implement strategies to significantly increase the number of women chemists in tenured academic positions in our research universities and to eliminate the gender biases that negatively impact their career progress.

The workshop was carefully planned with various leaders, 56 Department Chairs, ~30 University Leaders, funding agency leaders and speakers and panelists. The data-driven presentations by social scientists and academic leaders were an opportunity to share antidotes, looking at data in a scientific, non-judgmental way to work toward a common goal. There were interactive skits, panels and break-out sessions to develop action items and assessment plans for institutions, departments and funding agencies. The Chairs committed to action items at the workshop and answered pre- and post-survey questions. Afterwards, the Chairs returned to their departments, armed with knowledge of the practices necessary to change the cultures of their chemistry departments and to move rapidly toward gender equity, aided by federal programs and policies.

The action items developed for departments included:

- Double the percentage of women applicants in applicant pool in the next year
- Establish effective mechanisms for assisting career development of young faculty, especially women
- Consider personal obligations in academic scheduling and planning
- Develop and implement programs that educate all faculty members and students in your department regarding the accumulated disadvantage of women

The action items developed for institutions included:

- Make diversity an academic priority and develop programs that enhance recruitment and retention of faculty
- Develop policies to facilitate the hiring of women, including facilitating spousal hiring

- Assure that mid- and senior-level faculty, especially women, are participating in leadership roles
- Recognize the importance of and advocate for institutional support of child care
- Ensure that promotion and tenure policies are compatible with the needs of candidates who have families
- Ensure that the spirit and letter of Title IX are followed in your university

The action items developed for funding agencies included:

- Institute procedures for training of reviewers and grantees on diversity issues
- Modify peer review processes where necessary to ensure gender equity
- Secure Title IX compliance by accumulating data and tracking, as in NSF's ADVANCE programs, including surveys of lab space and resources
- Foster gender equity in highly visible Federal programs, such as national labs, large research centers and prestigious awards

As a follow-up, each Chair was asked to select two action items on an interactive Web site and report progress. Forty-five out of fifty-six gave positive feedback for follow-through. Action items included in feedback reports included establish effective mechanisms for assisting career development of young faculty, especially women; double the percentage of women in the applicants in the pool; assure that mid- and senior-level women faculty are in leadership roles and develop policies to facilitate the hiring of women, including spousal hiring.

The Chemistry gender equity workshop produced measurable attitude shifts. Before the workshop, principle factors limiting Chairs' ability to hire women were beyond their control, e.g., too few applicants, losing candidates to other departments and spousal hires. After the workshop, the Chairs were more likely to report limiting factors were within their control, e.g., departmental faculty not committed to or opposed to hiring women and did not have enough financing. There was a significant difference in attitude after the workshop, especially with things that were within their control.

On May 6-8, the "Gender Equity: Straightening the Physics Enterprise in Universities and National Laboratories" workshop was held with the goal to examine the underlying causes for the scarcity of women in physics and to formulate specific recommendations for action to improve the recruitment, retention and promotion of women in physics. **Nora Berrah** and **Arthur Bienenstock** were the Chairs for the workshop.

The Physics Gender Equity Workshop followed the Chemistry workshop model with a few changes, such as:

- Involved social scientists and physical scientists focusing on data
- CRLT players interactive skit, speakers, panels and breakout sessions
- Attendees
    - 50 Physics Department Chairs from major universities
    - 14 national laboratory managers or laboratory scientists
        - One each from 10 SC labs; one each from three NNSA labs
        - BES-, NP-, HEP-, FES-, ASCR-, BER-, and NNSA-funded lab managers present
    - Speakers, panelists, funding agency representatives and physics opinion shapers
- Topics included American Competitiveness Initiative, *Beyond Bias and Barriers*, Title IX, National Labs
- Unique components (relative to Chemistry workshop)
    - Inclusion of national labs in the target audience
    - Session on improving the climate for students in the pipeline

- More structured breakout groups
- Engaged top physics leaders in identifying ways to increase, retain and promote women in physics

The initial feedback of the workshop has generated an enormous amount of press coverage and has received positive reviews. It exposed a new audience to the social science of gender equity; possibly created agents of change to disseminate results; drafted recommendations for universities, national labs and for funding agencies; attendees committed to implement two action items; pre- and post-surveys were administered by COACH, with the results currently under analysis. The press coverage included *National Public Radio, Nature, Nature Physics, Physics Today and APS News*. A final report is currently being written and is expected Fall, 2007.

Some report elements are still being defined. However, the draft recommendations and some examples from breakout reports for departments and institutions include:

- Make hiring, retaining and promoting women a priority
- Decide on hiring criteria ahead of time
- Celebrate successes uniformly
- Provide primary care-giver accommodations for graduate students and post-docs
- Be aware of subtle biases
- Take advantage of two-body opportunities
- Consider sick child acre/emergency care
- Teach Chairs how to facilitate meetings
- Protect junior faculty members from politics

Preliminary recommendations for funding agencies include:

- Embed diversity in all direction-making levels
- Collect demographic data
- Sponsor grant-writing workshops for early career faculty
- Train reviewers on diversity – e.g., how to handle a career interruption in a C.V.
- Involve women in the review process
- Increase postdoctoral awards with mentoring opportunities
- Allow grant extensions for parenting pay off
- Encourage the availability of child care during conferences

There will be another workshop September 24-26, *Excellence Empowered by a Diverse Academic Workforce: Achieving Racial and Ethnic Equity in Chemistry*." The charge is to promote the development of a cadre of academic leaders who create, implement and promote programs and strategies for increasing to equitable proportions the number of racial and ethnic minorities on the faculties of departments throughout the academic chemistry community.

At 10:22 a.m., **Hemminger** called for a break.

At 10:36 a.m. he requested all Committee members reconvene and continue with the meeting. **Hemminger** stated "we still have a lot of ground to cover. We are currently a half-hour behind on the agenda. We need to discuss in detail the recommendation chapter of the Graham's report and need to discuss the things the Sub-Committees talked about last night at dinner." He also requested rapid turn-around for changes over the next few weeks so there can be discussion at the September BESAC meeting.

Graham Fleming stated that Chapter 7 is a task that is still ahead of the Committee and that it has had the least intellectual input. He wants the Committee to tell the implementation strategies.

Hemminger called for suggestions.

Ward Plummer said one of the greatest challenges is imaging functionality. He said seeing is the beginning of understanding and what we see is what we can control. We are still combining techniques to get the desired functionality. He added that he went through the report and there are several images that do not reflect the balance of Chapter 7.

John Spence said he strongly agreed with Plummer's comments. In the future, if we do not see what we can control, there is little hope.

Tobin Marks believes more images need to be included in Chapter 3.

Graham Fleming said he thanked everyone for their feedback and to please send more suggestions to him and for incorporation into the report.

Hemminger asked for comments concerning human resources development.

Bruce Gates said scientists are "scurrying and thinking short-term and not looking at the Grand Challenges." He questioned whether we are going to discuss mechanisms to make sure scientists deserve the resources they are given. "Unfortunately, today scientists do not have a lot of time. Everyone is looking for fast results and immediate satisfaction."

Hemminger said it was important to identify the people who are the most deserving and to make sure they receive the resources and backing they deserve.

Gates added people need to be "sustained long enough to make things (projects) successful."

Hemminger said that "programs are not forever and that there are a lot of renewable programs."

Gates asked what it takes to get renewals.

Fleming said there is a set of requirements and criteria that must be met.

Plummer questioned how we attract the best young scientific minds and nurture them?

Daniel Nocera said "there are a huge number of kids in biological research. We need to start them off in areas where they are most comfortable. The key is to start them early and that investment in young students is essential for the future.

Peter Cummings asked "How do we recruit these young people? At this moment, there is a group of young people to be captured. Chemical Engineering numbers are up this year. There are a lot of people just now entering college that are concerned about the energy crisis. This is the generation that needs to be captured at the earliest stage."

Mary Wirth said that students need to see that there is a career in this and that it takes a long-term commitment.

William McCurdy Jr., said from the strategic side, "DOE grants have not been seen as prestigious. We need to support academic community to ensure we get the best out there."

Frank DiSalvo said "Personally, I would like to have long-term funding, but every time I write a proposal, I think differently." He likes the idea of giving young people the opportunity to develop their passion."

Gates said what is challenging the landscaping of research are the universities think that funding can change things in a substantial way. We need to have 'monies' to fund long-term research."

Teri Odom said that getting building loyalty and investing in a project or student in the beginning is key. Regarding DOE-funding, when she talks to someone about it, they believe that it is very hard to receive. This perspective is what she has heard for years.

Plummer asked if it was possible to model career awards. “We have a tremendous opportunity to interest young people as young as the high school level.”

Hemminger said there is not a lot concerning graduate students and that it is very important for them to receive cross-training and encouragement to work in different areas of science. He questioned what is the best way to train these students to be successful?

Gates said cross-disciplines get students learning about a discipline, but the reality is that grants do not get renewed. DOE must begin offering something other than short-term funding to sustain the research effort.

Nora Berrah said that summer school programs would be effective. “We need to organize workshops, increase funding for PIs, (which are terribly expensive) and pay for tuition.” She added “We turn down students due to lack of funding. We must be able to subsidize these students.”

Walter Kohn asked if there was an existing document that serves as a career guide for young people that assists them with seeing opportunities available to them.

Pat Dehmer said the basic research needs to “lay out ideas for the next 15 years. If it is listed, then ask to find their niche. Students are finding workshop reports very useful and such reports should be given to all interested young people.”

John Richards said there are long-term grants that do not have to renew every 10 years.

Eric Isaacs said that Chapters 2-4 are excellent and that Chapter 7 says that “we want everything.” He said that he sees a laundry list of needs, but it needs to be written in a way that reflects the need for research money. He also added that to have a jumpstart early in your career, someone has to give you a lot of help. DOE has the potential to give investigators this opportunity.”

John Spence said some projects could not be funded because of high risks.

Anthony Johnson said we see demographics dropping for those going into science. Some of his early experiences happened during the summer, (agreeing with Nora Berrah’s comments). He believes it is critical to get undergraduate students excited about the sciences.

Hemminger said that a tremendous number of students are excited about working with science issues, challenges and problems. “I think these issues have captured the consciousness of a lot of people.”

Phillip Bucksbaum said one of the main purposes of going through this exercise was to interest not only scientists, but students.

Hemminger said that we have spent a significant amount of time discussing HR issues. He would now like to hear about the infrastructure needs, things that were presented and hear some comments and suggestions.

Frank DiSalvo said “We do not look at only what we need, but if there is any wisdom here it is the need for balance of the portfolio.

Graham Fleming said he agrees and needs an examination from BES and a lot of reflection on the current needs.

DiSalvo said he did not think it could be done by the September meeting.

Hemminger said that we have a charge to go back to Basic Research Reports and look at the needs and develop implementation strategies. The community is clamoring for answers, which will be on-going. He is concerned that Chapter 7 has a lot of things that need to be answered. He believes there has not been a lot of attention to this chapter and there are things missing. He also questioned if things are included that should not be there.

Peter Cummings said when we started this process, we were trying to find the Grand Challenges and how and what impact they will have on DOE.

Hemminger said the Grand Challenges were set up for BES.

Pat Dehmer said "The Committee has responded. There is no confusion. When you look at Chapter 7, these need to be challenges for BES. One of the things that may need to happen is that the group takes a leadership role to define for BES community." She thinks "the report will admirably do that."

Nora Berrah said one of her concerns is that we forget about light sources. There is not enough information about this in Chapter 7, and we need to keep updating the information.

Hemminger said that he thinks it would be appropriate and asks Nora to give suggestions to **Graham Fleming**.

Walter Kohn suggested more information on theory. "Theory is an essential part of BES and should be an essential part of the Grand Challenges."

McCurdy Jr. said that he agrees that some of the challenges may not be clear, but "we understand what the problems are relating to the Grand Challenges."

Bruce Gates said the report does not give a sharp discussion and needs to be more specific about Facilities.

Graham Fleming again thanked everyone for all of their input.

Mark Ratner said that he and Graham have a little over a month to make updates to include the suggestions and it will be reviewed again at the September meeting.

Hemminger asks Committee members to review each chapter. "You need to buy into this report. In September, it will be in its final form. We do not want this to go on and on."

McCurdy Jr. said "we will assist with rapid turn-around, but that can be slightly dangerous. We need to make sure this is a 'crown jewel'. We have given a lot of advice to incorporate into this report. We want to make sure that everyone is happy with the way it is written because things can be written many different ways."

Hemminger said it is important that we do not make mistakes. If someone is an expert, ask them to make sure that everything is factual. We must receive critical feedback. He then asked for members of the Committee to provide feedback on respective chapters:

Chapter 1 – Executive Summary - John Hemminger, Jack Roberts
Chapter 2 – Nora Berrah and William McCurdy Jr.
Chapter 3 – Tobin Marks, Gabrielle Long, Frank DiSalvo,

Chapter 4 – Leon Balents, Eric Isaacs, Laura Greene
Chapter 5 – Jay Groves, Graham Fleming, Jack Roberts
Chapter 6 – Peter Cummings
Chapter 7 – Peter Cummings and Ward Plummer

At 12:10 p.m., **Hemminger** opened the floor to public discussion. **Greg Exarhas** commented he was impressed with Chapter 7. College students are receptive to information of what is going on at laboratories and said more discussion is needed at the college level.

There being no other public input, **Hemminger** adjourned the meeting at 12:13 p.m.