Minutes for the
Basic Energy Sciences Advisory Committee Meeting
February 23-24, 2004
Hamilton Crowne Plaza Hotel, Washington, D.C

BESAC members present:

Nora Berrah
Sue Clarke (Monday only)
Peter Cummings
Mostafa El-Sayed
George Flynn
Bruce Gates
Laura Greene
John Hemminger, Chairman
Eric Isaacs
Anthony Johnson
Kate Kirby
Walter Kohn
Gabrielle Long
William McCurdy, Jr.
Daniel Morse (Monday only)
Ward Plummer
John Richards
Richard Smalley
Kathleen Taylor
Mary Wirth

BESAC members absent:

Philip Bucksbaum
Martin Moskovits
Samuel Stupp
Stanley Williams

Also participating:

Paul Alivisatos, Director, Molecular Foundry, Lawrence Berkeley National Laboratory
Patricia Dehmer, Associate Director of Science for Basic Energy Sciences, USDOE
Doon Gibbs, Associate Laboratory Director, Brookhaven National Laboratory
Bruce Harmon, Deputy Director, Ames Laboratory
Richard Hilderbrandt, Program Manager, Basic Energy Sciences, USDOE
Linda Horton, Deputy Director, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory
Robert Q. Hwang, Director, Center for Functional Nanomaterials, Brookhaven National Laboratory
William H. Kirchhoff, Program Manager, Basic Energy Sciences, USDOE (Ret.)
Dale D. Koelling, Program Manager, Basic Energy Sciences, USDOE
Douglas Lowndes, Director, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory
Paul Maupin, Program Manager, Basic Energy Sciences, USDOE
Terry Michalske, Director, Center for Integrated Nanotechnologies, Sandia National Laboratories and Los Alamos National Laboratory
Frederick M. O'Hara, Jr., BESAC Recording Secretary
Raymond Orbach, Director, Office of Science, USDOE
Walter Stevens, Office of Basic Energy Sciences, USDOE

About 95 others were in attendance in the course of the meeting.

Monday, February 23, 2004
Morning Session

Chairman Hemminger called the meeting to order at 8:37 a.m. He welcomed the Committee members to Washington and had them introduce themselves. He then introduced **Patricia Dehmer**, Director of the Office of Basic Energy Sciences, to give an update on the activities and status of the Office. She welcomed the members to the 50th meeting of BESAC and said that her purpose was to review where the Committee and BES have come from and where they are going. The FY04 appropriation has just been made, and the FY05 budget has been submitted to Congress. That budget request responded to five investment drivers:

- Science that addresses the DOE mission
- Science that advances our understanding of the natural world
- Provision of enabling tools, the scientific user facilities and other unique instruments
- Stewardship of DOE-owned research institutions
- Workforce development and the nation's universities

In the area of mission challenges, the BESAC report "Basic Research Needs for a Secure Energy Future" was rolled out; it is a roadmap for many years to come. A follow-on report, "Basic Research Needs for the Hydrogen Economy," is the basis for a significant initiative in FY05 and for an upcoming solicitation.

Other high priorities include:

- Solar energy conversion, on which a workshop will be held later this year;
- Materials sciences for advanced energy systems; and
- Efficient, benign chemistry (green chemistry and processing) and materials synthesis and processing.

The fundamental science challenges needed to address the mission include:

- The ultrasmall: Science at the nanoscale;
- The ultrafast: Science at femtosecond and shorter time scales;
- Theory, modeling, and simulation, which is the subject of a BESAC subpanel that will report its progress at this meeting; and
- Complexity, which was the subject of a BESAC panel several years ago.

February is a busy time of the year for the BES staff. It is appearing before Congress defending the proposed budget and formulating the next year's budget request. House Report 108-212 added $8 million to the requested BES budget to increase operating time and enhance user support at Basic Energy Sciences user facilities. Senate Report 108-105 provided the President's budget request. The Conference Report, H.R. 108-357, included an increase of $8 million beyond the budget request. The additional $8 million for materials sciences and engineering research was to support additional nanoscience research at existing user facilities and the new nanoscale science research centers. The following investments were made with the $8 million:

- Postdoctoral research associates will be placed with national-laboratory scientists associated with the nanoscience research centers (NSRCs), and many of them will eventually be part of the NSRCs. These "pilot" user programs are being beta tested prior to the commissioning of the Centers.
- Instrumentation at the light sources will be increased.

All of these funds will be invested in FY05 with no "mortgage" of future funds.

BES did extremely well in the President's budget request, which was up about 5% over

FY04. The distribution of funds was similar to that of prior years, with 40% going to research (43% of that going to universities and 57% going to national laboratories), 27% to facility operations, 32% to construction, and 1% to the SBIR/STTR (Small Business Innovative Research/Small Business Technology Transfer) program.

All five NSRCs are under construction with a total funding of $217 million. The Linac Coherent Light Source (LCLS) x-ray free electron laser (XFEL) received increased funding for construction and engineering and design (a total of $99 million). And science in support of the President's hydrogen initiative totaled $50 million. Of that amount, $29 million is designated to go to BES and will (pending Congressional appropriation) fund many principal investigators (PIs). All of this funding is a direct result of BESAC's workshops and Millie Dresselhaus's follow-on activities.

The budget can be viewed at http://www.science.doe.gov/bes/budget.html. On the website, one will see the increases for basic research related to the President's hydrogen initiative and modest increases for facility operations. Those increases will allow the facilities to operate at current levels of service. The budget also provides full funding for construction of the Spallation Neutron Source (SNS), the preliminary engineering design (PED) and construction of the five NSRCs, and the PED and long-lead procurement (construction) for the LCLS.

The staff is just beginning its activities on the FY06 budget request. The Office of Science (SC) will be making its presentation to the Secretary this month. This is an important year for BES.

The BESAC report "Basic Research Needs to Assure a Secure Energy Future" was almost a seminal report. One area stood out: hydrogen (even before the President announced his hydrogen initiative). A follow-on workshop was held specifically on basic research for hydrogen production, storage, and use. It was closely coordinated with the Office of Energy Efficiency and Renewable Energy. This workshop was very important, and a number of activities have resulted from it.

The priority hydrogen research areas are

In production:
- Fossil-fuel reforming
- Solar photoelectrochemistry/photocatalysis
- Bio- and bio-inspired hydrogen production
- Nuclear and solar thermal hydrogen

In storage:
- Metal hydrides and complex hydrides
- Nanoscale/novel materials
- Theory and modeling

In fuel cells
- Electrocatalysts and membranes
- Low-temperature fuel cells
- Solid oxide fuel cells

Some useful references are included on the website http://www.eere.energy.gov/hydrogenandfuelcells/pdfs/national_h2_roadmap.pdf.

A solicitation will request preapplications for innovative basic research proposals to establish the scientific basis that underpins the physical, chemical, and biological processes governing the interaction of hydrogen with materials. We seek to support outstanding fundamental research programs to ensure that discoveries and related conceptual breakthroughs from basic research will provide a solid foundation for the innovative design of materials and processes to usher in hydrogen as the clean and sustainable fuel of the future. Proposals will be requested in

- Novel materials for hydrogen storage
- Membranes for separation, purification, and ion transport
- Design of catalysts at the nanoscale
- Solar hydrogen production
- Bio-inspired materials and processes

These five focus areas will be described in greater detail in the solicitation. Preapplications are required. No applications will be accepted without a preapplication followed by a BES response encouraging a full application. Preapplications must be submitted electronically, as specified in the call. Each Federally Funded R&D Center (FFRDC) is limited to the submission of six preapplications as the leading institution. For FFRDCs, BES reserves the right to encourage, in whole or in part, any, all, or none of the preapplications submitted, and BES may issue further guidance on the scope of full proposal submissions of those encouraged. Importantly, this solicitation will be silent on issues of project size, number of PIs, number of institutions, interdisciplinary or multidisciplinary nature of the work, etc. It is anticipated that up to $12 million annually will be available for multiple awards for each of the following: universities (typically 60%) and FFRDCs. Initial awards will be in Fiscal Year 2005, and applications may request project support for up to 3 years (may be extended to 4 years). All awards are contingent on the availability of funds and programmatic needs. BES will coordinate with all appropriate groups both inside and outside of DOE, particularly the Office of Energy Efficiency and Renewable Energy (EERE). The proposals will be peer reviewed with the help of others. DOE is committed to close coordination between basic science and applied science and technology. The proposed schedule is

February 23, 2004	Discussion at BESAC
May 15, 2004	Call for preapplications published
July 15, 2004	Preapplications due
September 1, 2004	Decisions on preapplications sent to PIs
January 1, 2005	Full proposals due
June – July 2005	Awards made

Some of the fundamental science that underpins the DOE mission was then discussed, specifically the National Nanoscience Initiative (NNI). An interagency working group formulated funding plans. The three major recipients were the National Science Foundation (NSF), Department of Defense (DoD), and DOE. BES now has about $200 million per year in nanoscale-science funding, which will be split roughly 50-50 between universities and national laboratories, a $150 million increase between FY01 and FY05 because of the NNI (all of BES's budget increase during the same time was $210 million). This result shows the impact of being ready with a science case when an opportunity arises.

Five NSRCs are under design or construction. They are a remarkable success story. The Secretary has taken a great interest in these centers. Secretary of Energy Spencer Abraham broke ground on the Center for Nanophase Materials Sciences (CNMS) on July 18, 2003, at the Oak Ridge National Laboratory (ORNL). Later that year, President Bush signed the 21st Century Nanotechnology Research and Development Act. The Secretary has now asked for a 1.5-day nanoscience summit. Another groundbreaking was held for the Molecular Foundry at Lawrence Berkeley National Laboratory (LBNL).

At the same time, BES is expanding research in ultrafast science and in complex systems, and a BESAC subcommittee is investigating needs in theory, modeling, and simulation.

BES has the largest collection of scientific user facilities in the world. Five NSRCs are under construction, each driven by science needs. The SNS is nearing completion and is starting to look like a real research facility. The SNS will begin operation in 2006 and will be the world's leading facility for neutron scattering. The Stanford Synchrotron Radiation Laboratory has undergone a major upgrade. It was rededicated on January 29, 2004, after being completely rebuilt from the floor up. This upgrade was achieved in 8 months and within budget. During the past decade, the number of light-source users has grown from hundreds to thousands; they were primarily physicists at first, and now biologists are the major users. The light sources transitioned from esoteric uses to a broad range of the sciences. Half of the light-source users come from academia; onsite users are a small portion. There is a large regional character to the user demographics, but all the user facilities have to serve all users from across the country. The facilities operate very reliably and close to the maximum number of hours (>95%). From the first-generation synchrotron sources in the mid-sixties to the third-generation machines of today, beam brilliance has increased by a factor of a trillion, and another increase by a factor of more than 10 billion is expected with the XFELs. A complication encountered is that this rate of increase is greater than the rate of increase in computer storage density. The LCLS just started construction. It was the top priority in the *Facilities for the Future* list. Its justification of mission need (CD-0) was approved in June 2001, its preliminary baseline range (CD-1) was approved in September 2002, its long-lead procurement baseline (CD-2a) was approved in July 2003, and its optimum schedule projects commissioning for FY 2008.

The organization chart was reviewed, new members of the Office were identified, and the need for personnel to fill several positions was noted. The Office will keep pushing for the future of funding research in cooperation with the technology offices of DOE.

Morse asked what the scale of awards was for the hydrogen initiative. Dehmer replied that it was $21 million in total, roughly $12 million to universities and about the same to the national laboratories.

Kohn sought to connect the hydrogen initiative with world food supply and renewable energy resources. The initiative promises to mitigate the U.S. contribution to global climate change. That is tied closely to global warming. A 1-degree increase in global temperature produces a 10% decrease in food productivity. He was concerned about the wording of the original proposition by the President and about the statement about the availability of fossil fuels. The fact is, natural gas supplies appear to have topped out. Supply has been flat, and the most recent data show a drop. He considered the estimate of 50 years of cheap fossil fuels to be overly optimistic; 100 years from now, there will not be an ample supply. It must be emphasized that hydrogen must be made from some energy source. He was worried that the general public does not appreciate that and asked what BES's perspective was on this situation. Dehmer commented that he had stated the situation well. Fossil fuels are only a short-term solution. Society needs to solve critical problems (e.g., storage) early and needs to get away from fossil fuels.

Hemminger introduced **Raymond Orbach**, Director of the Office of Science, to discuss the status of that office. Orbach focused on *Facilities for the Future of Science: A Twenty-Year Outlook*, the announcement of which report by the Secretary of Energy was an exciting event. The report has had a very positive reception at an international level. The dedication of BESAC and five other advisory committees has paid off. It has assured a future for some fields of science and technology. SC is undergoing a reorganization that will increase (1) the efficiency of the Office of Science and the national laboratories and (2) their ability to deliver science to the nation and the world.

SC facilities are used by more than 19,000 users worldwide. In the SC budget, there is funding to increase the running time of facilities from 92 to 95%. In some cases, the science has been increased rather than the facilities' productivity.

The report presents a list of 28 world-class facilities that would be established in the next 20 years; upgrades will ensure U.S. scientific pre-eminence for the next two decades. SC takes the continued operation of research facilities very seriously. Setting the priorities across disciplines and fields of research was very difficult to do, but the SC staff has succeeded where others have failed. All priorities were based on science. Finally, these efforts complement interests of other U.S. science agencies [e.g., the National Aeronautics and Space Administration (NASA), NSF, and in the National Institutes of Health (NIH)].

The time horizon of 20 years was selected because of the large number of major facilities under construction in SC. There is no outer-year funding for these projects; plans need to be developed for the future use of these facilities. Those plans are being built into the CD0s from now on.

The prioritization was accomplished by asking the associate directors to develop initial lists. The response resulted in a list of 46 facilities. To get additional guidance, the advisory committees were asked to add or subtract items and to assess all of the facilities according to two criteria: the importance of the science and the readiness for construction. The "Biggert" authorization bill (a four-year outlook) was used as an optimistic, arbitrary funding envelope. It presumed about a 60% increase in SC funding; then 4% per year beyond the initial 4-year planning horizon. The associate directors were asked to cost the research in future years; that amount was subtracted from the envelope, and then overhead costs were subtracted. What was left was considered to be what was available for construction and operation of facilities. This amount was apportioned among the offices of SC, and the associate directors were asked to phase in facilities over 20 years within that apportioned envelope. The advisory committees were asked to review these plans and to prioritize the facilities and to determine when they might be available. Twenty-eight of fifty-three facilities made the cut. These facilities then had to be prioritized across fields. Each proposed facility was categorized according to importance and time to completion. There are certain, secondary facilities for which major decisions still need to be made. Furthermore, in many cases, we do not have a clue as to how to assess scientific importance and the facilities' varying readiness for construction. Orbach himself prioritized these facilities and then went back to the associate directors. To the dollar, these facilities fit the projected 20-year budget. This is an important step for SC. There is now a response to the question, "If we gave you more money, what would you do with it?"

In the first epoch of construction, the International Thermonuclear Experiment Reactor (ITER) and the Ultrascale Scientific Computing Capability were the top-priority items. The ITER is a tough experiment. If it is successful, it will lead to a demonstration fusion plant. Siting of the ITER is now being negotiated. The Ultrascale Scientific Computing Capability has a direct importance to BESAC, especially in materials science, facility design, and systems analysis. $30 million has been budgeted in FY04, and a comparable amount is requested for FY05. DOE is now in consultation with NASA on the Dark Energy Mission, and $30 million is in the FY05 request for the LCLS. We also have the ability to align funds to provide $5 million in FY05 to support the Protein Production and Tags facility and $5 million for the Rare-Isotope Accelerator. CD0s have been issued for all four of these facilities. Also for the near term, CD0s are in process for the Characterization and Imaging of Molecular Machines facility and the upgrade to the

Continuous Electron Beam Accelerator Facility (CEBAF); CD0s are not required for the ESNet upgrade or the National Energy Research Scientific Computing Center (NERSC) upgrade. And a CD0 has been signed for the Transmission Electron Achromatic Microscope. A CD0 has also been signed for the lowest-priority facility in this epoch, the BTeV ("B physics at the TeVatron").

In the second epoch of construction, projects that will be addressed in the midterm, the priority facilities are the (offshore) Linear Collider, Cellular Systems Analysis and Modeling, SNS Upgrade, SNS Second Target Station, Whole Proteome Analysis, Double Beta Decay Underground Detector, Next-Step Spherical Tokamak, and Relativistic Heavy Ion Collider (RHIC) II.

In the third epoch of construction, which covers the far term and reflects higher uncertainty, the priority facilities are the National Synchrotron Light Source (NSLS) upgrade, Super Neutrino Beam, Advanced Light Source upgrade, Advanced Photon Source upgrade, eRHIC, Fusion Energy Contingency, High-Flux Isotope Reactor Guide Hall II, and Integrated Beam Experiment.

This schema will have to be revisited, but the prioritization is robust. The president's FY05 budget is a good one for SC. Everyone recognizes the discipline and success that DOE has had in project management and construction. We have taken the responsibility very seriously for planning out-year spending. This was the right process to go through; it has been well received by the scientific community.

Smalley commented that Orbach had made a terrific presentation and commended his role in the preparation of the strategic plan. During the next 20 years, the world will critically rely on science research for meeting energy needs. He believed a larger percentage of funding should go for energy research. Serendipitous advances have largely come from the funding of PI research. More of the nation's wealth needs to be put into scientific research that holds promise for improving the lot of mankind. Orbach thanked him for stating the situation so eloquently. Hydrogen storage is a question of binding versus release. All kinds of substances and configurations have to be looked at. Catalysis will be a major contributor to advances here. Balance between research and facilities must be maintained. The research numbers used in the presentation came from the associate directors of SC. He did not change those numbers after he received them.

Berrah agreed that funding for research must be increased. The core research program's funding has been flat for many years. She asked whether BES could increase that core research funding. Orbach responded that the President's budget must be supported. The core-research funding's flatness is worrisome. The research community has a diversity of funding sources available to it. Those opportunities have diminished with time. He worries about a single-agency dominance of science funding, making the system subject to fads. Also, research must be long term; the system is messy and uncertain. He is concerned about the magnitude and balance of research funding. We now know how additional funds would be spent. That is the way to improve SC's budget: to be able to show the country what can be done for it in terms of science.

Johnson asked how workforce issues influenced his decisions. Orbach said that more than half of the graduate students at U.S. universities are foreign and asked where the Americans have gone. DOE used to have an Education Program. That was zeroed out by Congress. Last year about $1 million was budgeted for teacher laboratory experiences. This year has $0.5 million for a minority sabbatical program. Minority researchers must be introduced into the research enterprise. The salaries in minority institutions are low, and colleges and universities provide only half that amount for faculty on sabbatical. DOE will supplement that pared-down salary to encourage faculty to work at laboratories and to write a funding proposal for their institutions. DOE does not want to duplicate NSF, but it has the national laboratories that can provide a meaningful work experience and encouragement to participate in science to the students of this nation.

A break was declared at 10:48 a.m. The Committee was reconvened at 11:07 a.m. **Douglas Lowndes**, Director of the Center for Nanophase Materials Sciences (CNMS) at ORNL, was introduced to give an update on that center.

The first Science Advisory Committee (SAC) meeting was held June 19-20, 2003, and groundbreaking was held July 18. On July 22, the call for proposals was issued for the “jump start” user-initiated nanoscience research program using existing ORNL facilities and expertise. Construction started in August, and a BES Operations Budget Review was held February 19. The completion of construction is expected on April 2005, and the center’s management will take beneficial occupancy in April of that year. The first full-year operating budget will start in October 2005, and user operations in all scientific-theme areas will be started. The CNMS Project completion should occur in September 2006, when the initial technical equipment set will have been installed and accepted.

The Center is joined to the main building of the SNS with access to machine rooms, cafeteria, etc. of the SNS building so duplication is not needed. The CNMS will have 80,000 sq ft on four levels; have 32 wet dry synthesis and characterization laboratories; have office space for 190 staff and visitors designed to maximize collaborative, multidisciplinary, and educational interactions; have offices and laboratories to access terascale computing facilities at the ORNL Center for Computational Sciences (CCS); and rooms for high-resolution scanning probes.

The Nanofabrication Research Laboratory will have class 100, 1000, and 100,000 clean areas; an electromagnetic, vibration, and acoustical (EVA) controlled area; diffusion and low-pressure chemical vapor deposition (LPCVD); soft–hard materials integration laboratory, physical-vapor-deposition (PVD) and chemical-vapor-deposition (CVD) film facilities; dry and wet processing; photolithography; e-beam lithography; and scanning and focused electron-beam microscopes.

The Center will be collocated with the SNS and the Joint Institute for Neutron Sciences (JINS) on ORNL’s “new campus.” JINS will have meeting rooms, classrooms, and support facilities for research visitors and students. SNS will provide access to unique neutron-scattering capabilities for nanoscience. The Center will provide urgently needed capabilities for materials synthesis and characterization, nanofabrication, theory and modeling, and nanomaterial design.

The vision and plan for the CNMS is to create an environment to accelerate discovery and drive technological advances. Nanoscale science is highly integrative; it brings together the best ideas and the best instruments along with a highly interactive and multidisciplinary user research community. The Center is being developed in partnership with the national scientific community.

This environment will be created by exploiting synergies with two rapidly emerging ORNL strengths (neutron scattering and leadership computing) and by addressing the need for a new generation of nanoscience instruments that combine nanoscale imaging with simultaneous sample-characterization and -manipulation capabilities. The intent is to operate the Center reliably to deliver these unique capabilities to the national user community.

There is a high level of demand for such a facility. The CNMS supports a focused research agenda with this high level of demand.

The Second CNMS Planning Workshop asked participants to define candidate research focus areas and equipment needs and to identify the desired CNMS mode(s) of operation.

Seven scientific themes were identified for the CNMS:

$ Macromolecular complex systems;
$ Functional nanomaterials;
$ Nanoscale magnetism and transport;
$ Catalysis and nano building blocks;
$ Theory, modeling, and simulation at the Nanomaterials Theory Institute;
$ Developing methods for controlled synthesis and directed assembly; linking nanoscale phenomena to the macroscale, and developing methods for the functional integration of soft and hard materials; and
$ Nanoscale imaging, characterization, and manipulation.

The seven themes are scientifically and operationally connected.

Two classes of instruments for NSRCs are needed that are critical to support the scientific research agenda. The first class is often expensive, but not unique (e.g., high-resolution scanning electron microscope, e-beam writer, and nanomaterials synthesis). These instruments can be purchased together with a maintenance contract. The second class is truly unique, offering new research capabilities. They are currently

unavailable to the national community, but they are critical to the advance of nanoscience (e.g., for imaging, properties measurements, sample manipulation, assembly, and environmental control). These instruments are critical but not normally available to user nanoscience and scientists. The Center will make these instruments available to the user community.

The first SAC meeting recommended that the Center (1) begin immediately to highlight and develop new capabilities that will be world-class and (2) engage the external community in the development of new capabilities.

Nanoscale imaging, characterization, and manipulation techniques include neutron and X-ray scattering (as specialized scattering techniques and environments for nanoscience), ultrahigh-vacuum (UHV) scanning probes (for magnetic and quantum-transport properties in nanostructured materials), and electron microscopy and spectroscopy with special sample environments for soft materials. The Center will also provide technicians, staff, and budget to make these unique instruments reliably available to the national user community.

Neutron techniques are exquisitely suited for soft materials. Some of the challenges are to understand how morphology, symmetry, structure, and phase behavior relate to function and to develop new approaches for the rational design and fabrication of soft and hybrid materials. Some of the neutron-scattering opportunities are (1) SANS (small-angle neutron scattering) for investigating shape, location, and evolution at the nanometer scale; (2) reflectometry for studying molecular-scale structure near surfaces and material interfaces; and (3) hydrogen/deuterium contrast for component-by-component imaging on all nanometer-length scales. There are some exciting new possibilities here.

Some unique and state-of-the-art measurement capabilities that are under development are (1) atomically resolved imaging, manipulation, and spectroscopy and (2) in situ diagnostics of nanomaterial synthesis. The first is a high-resolution scanning electron microscope for spin-polarized analysis (SEMPA). It will have an initial resolution of 15 nm and will be upgraded to a higher resolution as the technology advances. The second includes

$ The “ultimate STM” (scanning tunneling microscope) with a temperature range between 300mK and 150K, a B_{max} of about 9.0 Tesla, the ability to exchange samples from room temperature, and cryogenic ultra-high-vacuum sample cleavage and a

$ Four-point-probe STM with SEM to carry out the electrical transport of nanoscale objects on surfaces and the fabrication and characterization of nanoscale devices with four probes operating independently with a tip separation of less than 100 nm and the ability to perform chemical vapor deposition.

Acquisition of this equipment has begun. Orders have been placed for the e-beam lithography system and for the SEMPA. Bids are under review for the four-probe STM/SEM. And two other pieces of clean-room equipment have been ordered. The ultimate STM is in collaborative development.

Another capability under development is the "Computational Multiscope." The current capability of computational nanoscience gives excellent clarity for some systems at specific levels of description, but moving from one scale to another requires changing out the lens (switching to a fundamentally different technique). The Nanomaterials Theory Institute (NTI) of CNMS will develop scale-spanning methods and combine with leadership-class computing at ORNL's CCS to create a "computational multiscope" that creates seamless clarity at length and time scales from electronic to macroscopic. This vision will be enabled at the NTI by using the expertise of about 40 theorists and computational chemists, physicists, and materials scientists at ORNL and by users working with NTI and CCS staff, guest scientists, postdocs, and graduate students.

An outstanding user program has been jump-started at ORNL this past year with an initial user program and call for proposals. Research areas were selected at CNMS planning workshops. The major strengths of current ORNL and BES research programs are able to provide support for controlled synthesis research; for a broad range of imaging and characterization; and for theory, modeling, and simulation.

User research has been initiated in five of seven CNMS scientific themes. The first area addressed was the design, synthesis, and characterization of macromolecular materials. The second was the controlled synthesis and assembly of functional nanomaterials (nanotubes and related composite materials).

The Center initiated several workshops in 2003. In 2004, the NTI will support the User Research Focus Laboratories Program. That program will (1) allow the development and application by users of selected, powerful computational nanoscience techniques together with world leaders; (2) address key problems and issues of users' choice in understanding nanoscale materials and phenomena; and (3) allow users to run their applications "hands on" with supercomputers at ORNL's CCS.

An interim nanofabrication laboratory for users will provide training and supervision for new users, skilled technicians for some tasks and users, and communication and enforcement of safe-use and clean-use policies. The Center will also offer Nanoscale Imaging and Characterization, providing nanoscience user access to high-resolution electron microscopy analytical instruments, scanning-probe instruments, and SEMPA in ORNL's Shared Research Equipment (ShaRE) collaborative, High Temperature Materials Laboratory (HTML), and Materials Analysis User Center and at the Max Plank Institute–Halle in Germany.

The Center has memoranda of agreement (MOAs) with selected ORNL user facilities that allow CNMS to internally coordinate requests to use other ORNL nanoscience research capabilities. The CNMS Proposal Application Form includes appendices for access to other user facilities. The goal is timely, one-stop shopping for all needed resources. These MOAs and appendices are already in use for the

jump-start operations. In the future, the CCS, SNS, High-Flux Isotope Reactor (HFIR), and HTML will be included in this one-stop shopping.
There was an enthusiastic response to the call for proposals with 71 proposals received, representing 18 states, 50 universities, 6 industries, 10 ORNL, and 5 foreign. Of these, 41 proposals were selected for support, based on external review (10 on a proof-of-concept basis).

The scientific and operational management of the Center and its advisory groups ensure safe, reliable operations of the Center. The Scientific Leadership Team has been put in place. The Center is led by a director. The SAC recommends research focus areas and priorities. The Users Executive Committee represents the user community regarding CNMS operations and needs. The Proposal Review Committee (PRC) peer reviews and ranks user proposals. The Management Integration Team ensures integration with other ORNL facilities and programs. The seven scientific themes are

- Macromolecular complex systems
- Functional nanomaterials
- Nanoscale magnetism and transport
- Catalysis and nano-building blocks
- Nanomaterials Theory Institute
- Nanofabrication Research Laboratory
- Nanoscale imaging, characterization, and manipulation

The members of the SAC and the PRC were identified.

Looking to the future, the Center expects to

- Operate laboratories and offices with high reliability and safety and in compliance with all regulations;
- Manage a world-class and highly collaborative nanoscience user research program of approximately 250 users and 7500 user-days in FY08;
- Provide a concentration of unique and state-of-the-art instruments and operational expertise, so that users have access to both;
- Continually improve operation of instruments and capabilities;
- Together with the national user community, carry out R&D and make investments needed to keep CNMS at the instrumental and computational frontiers that define the nanoscience state-of-the-art; and
- Together with the SAC, periodically redirect CNMS's effort to stay focused on the most important scientific challenges and technological opportunities.

Kohn noted that, for fission and fusion energy, material-science problems loom large and asked if the nanoscience institutes can contribute to the solution of these problems. Lowndes responded that his center was in the process of finding that out. It is looking particularly at energy challenges. Kohn went on to ask if nanoscience will be able to counter the tremendously destructive environments of fission and fusion devices. Lowndes replied that that is clearly a research objective, looking at defect effects and degradation processes.

El-Sayed asked about the distribution of the proposals that the center received. Lowndes said that many of the proposals related to multiple themes. Also, no proposals were solicited in theory, modeling, and simulation (TMS). When all was said and done, 39 proposals were received in the macromolecular area, 35 in nanotubes and other functional nanomaterials, 24 in imaging, 34 in nanofabrication, and 4 in theory.

Hemminger asked what the problems and challenges were at this juncture. Lowndes answered that the principal challenge is gaining experience with researchers and providing support to each with instruments from a variety of research themes. This diversity of experience that needs to be provided is a challenge. He added that this is a qualitative difference between the CNMS and other user facilities.

Hemminger asked how many of the jump-start PIs had never been to Oak Ridge before. Lowndes replied that he did not know but would estimate at least half.

Gates asked how they got user feedback. Lowndes said they got feedback from a user questionnaire and through BES.

Berrah asked how users are selected. Lowndes answered that all potential users have to submit a proposal that then goes through the PRC. That committee evaluates proposals according to the criteria of the International Union of Pure and Applied Physics (IUPAP): scientific merit, technical feasibility, impact on field, and capabilities of investigators. This evaluation process produces a numerical score; to this is added a subjective evaluation and justification.

McCurdy noted that the construction design considered collaboration between experimentalists and theorists and asked what the long-term vision for the support of such collaboration is. Lowndes responded that the Center would like to support more computational nanoscience and is working with the SAC to review the operational budget documents. The SAC agreed that this is something needing long-term support. It is hoped that top researchers can be brought in for an academic quarter apiece to present tutorials, to work with small groups of researchers, and to operate a computational nanoscience laboratory. The Center's staff is working on a definition of a computational nanoscientist. McCurdy followed up by asking how experimentalists will find theorists to collaborate with. Lowndes said that TMS has been integrated into each theme. The Center holds workshops to get experimentalists and theorists together. It also integrates the two in each theme and would like to commit more resources to that process.

A break for lunch was declared at 12:01 p.m.

Afternoon Session

The meeting was called back into session at 1:16 p.m. with the introduction of **Paul Alivisatos**, Director of the Molecular Foundry at LBNL, to give an update on the progress of that NSRC. The purpose of the Molecular Foundry is to provide a national facility to enable interdisciplinary nanoscale science and engineering by fostering, developing, and disseminating methods and knowledge for the patterning and control of matter on the nanometer scale. Its focus is on the creation of materials. The artificial materials that can be made are on the order of magnitude with proteins, bringing together soft and hard matter. The Microlab at LBNL was looked to for inspiration. That laboratory operates at more than the cottage-industry mode. It makes things modularly and makes them available to many users.

A wide range of building blocks is available to work with: nanocrystals, nanorods, nanotubes, patterned surfaces, cells, and proteins. The main question is, "How do we organize ourselves so people can work efficiently?" The Foundry's goals for 2003 were to set the stage for construction to begin, initiate the jump-start phase, engage in public outreach, and conduct advance planning for operations. Those goals have been accomplished. The Molecular Foundry has been integrated into the scientific community of the Bay Area. The building has been fully designed, and construction has started.

Outreach successes include a successful second workshop with more than 300 attendees, groundbreaking, the Nano High School, interactions with the community, and outreach within the Laboratory. One reason the Molecular Foundry has captured the interest of the economic community is a large number of companies that have been spun off by LBNL; they have a capitalization of more than $1 billion. DOE research is having a tremendous input on the economy of the Bay Area. Nano High is held one Saturday each month for 350 local high school students, filling the auditorium and an overflow room. The enthusiastic student response has garnered prominent press coverage.

The total Molecular Foundry project cost will be $85.0 million. The CD3 was approved Nov. 12, 2003, and the contractor notice-to-proceed was given Dec. 24. Construction is expected to take 24 months with occupancy and startup in 2006. Excavation, shoring, and underground utility work has begun. Bids for all remaining work are within 5% of the bid contingency carried.

A jump-start pilot program has been started before the project construction has been completed. Six facilities have been established; these are laboratories ready or being remodeled with general plant project/non-capital asset project funding; 350 applications have been received; 8 postdocs/scientists have been hired for the facilities; and 11 proposals have been approved. These staffers have to learn a method of fabrication and a high level of sophistication. A lot of junior faculty have applied to conduct research at the Molecular Foundry. There was a wide geographic range to the initial responses. During the jumpstart program said core capabilities will be provided to users out of the resident expertise. There will be six facilities within the Molecular Foundry: Inorganic Nanostructures; Biological Nanostructures; Nanofabrication; Organic Nanostructures; Theory; and Imaging/Manipulation. Each will have its own director and a typical staffing plan that includes a foundry scientists, two fellows, a one-third time secretary, a staff scientist, two technicians, and a postdoc.

The key capabilities of the Nanofabrication Facility will be advanced lithography with a nanowrite and a nanoimprinter and process integration (taking structures constructed by other means and replicating them with photolithography). This work will be equipment-intensive, and renewal issues will need to be dealt with.

The key capabilities of the Organic Nanostructures Facility will be nanotube synthesis, nanowire synthesis, and colloidal nanocrystal growth.

The key capabilities of the Biological Nanostructures Facility will be mammalian cell culture, RNA preparation, bioconjugation chemistry, and cell immortalization via telomerase expression. At full operation, additional capabilities will include molecular cloning, protein expression, and purification. Laboratory management has been working with the community, dealing with issues of biological nanoscience; many are supportive, but there are some of that are unhappy with this technology and its potential environmental and health effects. Management would like to bring in a staff scientist in 2006 to study these questions of fate and toxicity.

The key capabilities of the Organic Nanostructures Facility will be synthesis and preparation of building blocks, small libraries, functional assemblies, device components, electroactive oligomers and polymers, light-harvesting materials, reactive surfaces, and porous organic materials; surface modification and growth from surfaces; and characterization of organic and macromolecular materials.

The key capabilities of the Imaging and Manipulation Facility currently are scanning probes (atomic-force microscopy, AFM) for studies of nanomaterials in air and controlled atmospheres; AFM characterization of liquid films and nanodroplets; and force spectroscopy (using AFM) of surfaces, polymers, and macromolecular films, including biomaterials. Additional capabilities at full operation will include electron microscopes with in situ manipulators and electrical probes, ion- and electron-beam-assisted fabrication of nanostructures, and optical systems for imaging and fluorescence studies at the single-molecule level.

Demand in the areas of imaging and theory was not as great as expected.

The local community has also stepped forward, offering individual capabilities to be used in cooperation with the Molecular Foundry; these community members are the 21 affiliated laboratories.

Gates asked how the Molecular Foundry will validate or characterize something new. Alivisatos answered that nanoscale materials still pose great challenges in characterization, but to the extent that those questions are answerable, the Molecular Foundry will have the capabilities to find those answers. Many of the techniques available at the Molecular Foundry will be available elsewhere, but the path of learning will be greatly enhanced at the Molecular Foundry.

Berrah asked if the Molecular Foundry had a Science Advisory Committee. Alivisatos answered, yes; they have made a lot of great recommendations that have been adopted. The Proposal Study Panel is currently made up of staff members. Eventually, external people are expected to be brought in to staff that committee.

McCurdy commented that the BESAC Theory and Modeling Subcommittee is struggling with the integration of theory and experiment. He asked how one brings together experimentalists and theorists across the broad range of topics the Molecular Foundry is engaging in. Alivisatos responded that the long term outlook is good. The scales of experiment and theory are now the same, aiding comparison. Also, time resolutions are matching. The tougher issues are what discrete capabilities will be needed. The Molecular Foundry is struggling with that in the staffing plans for the six facilities within the Molecular Foundry.

Kohn noted that the Theory Group that provided support for this type of facility at Bell Labs 50 years ago numbered a dozen, and they served 3000 practitioners (although a large number of theorists were also scattered throughout the research groups). He cautioned that (1) there will be an enormous variety of issues, so the Molecular Foundry will want people with breadth and flexibility, and (2) management must make sure that there is interaction and that the theorists will be expected to pursue their own interests even if those interests are not related to what is going on at the laboratory. The best people do not want to be service people; plus, the independent exploration that they do will eventually feed into the laboratory’s interests. Alivisatos responded that the major question before the Molecular Foundry is whether it can attract the best people. They should recognize that they are at the cutting edge and should draw inspiration from that. Kohn added that the opposite experience is to have a distinguished leader who lets the workers do whatever they want and give no guidance. In cases where that has occurred, the workers began to quit.

Long asked what the relation between creating and characterizing materials was. Alivisatos said that there has been a great investment in tools for characterizing materials. The material-creation portion of the chain needs more effort because its organization has not reached a mature state. There will be a good synergistic relationship with the characterization facilities. Some of the NSRCs are building beamlines, but the Molecular Foundry is not doing that at this time. It should not duplicate what is already there.

Richards asked if care had been taken to avoid duplication from NSRC to NSRC. Alivisatos responded, yes. The Molecular Foundry is not going to have certain activities (e.g., beam epitaxy facitities) that will exist at another NSRC. The synchrotrons evolved into different uses, and that type of evolution will happen to the NSRCs, too. They will serve regional roles and respond to other influences. To ensure that needless duplication does not occur, the leaders and staffs of the different NSRCs are talking to each other frequently. Each NSRC will have its own suite of specialities.

Terry Michalske, Director of the Sandia–Los Alamos National Laboratory (LANL) Center for Integrated Nanotechnologies (CINT), was introduced to review the progress of that NSRC. That center is unique in that it is a joint effort between a scientific community and a manufacturing community. Connecting scientific disciplines and multiple length scales is key to success in addressing problems in energy and the environment. The SNL–LANL team has developed a core-and-gateway structure. The CINT Core Facility brings experimentalists and theorists together. The Gateway to LANL makes facilities, expertise, and computational tools available. And the Gateway to SNL makes microfabrication and computational tools available. The Core Facility is being constructed in Albuquerque outside the Air Force Base for accessibility. It is anticipated that the buildings will be complete in November 2005, that operations will begin in March 2006, and that construction will be completed in June 2007.

The Core Facility's design is complete, site utilities are under way, a construction contract is out for bid, and the contract is expected to be awarded in May. The design-build bidding for the Gateway to LANL is complete, the award is expected in March, and a site-preparation design has been begun.

The Core Facility has three wings for integration [with e-beam lithography, photolithography, thin-film deposition, reactive-ion etching (REI), and plasma etch], synthesis [with molecular beam epitaxy, pulsed-laser deposition (PLD), and P-CVD], and characterization [with transmission electron microscopy (TEM), scanning electron microscopy (SEM), field-emission scanning electron microscopy (FESEM), AFM, Fourier transform, nano-indenter, low-temperature mobility, ultrafast laser spectroscopy, and Raman spectroscopy]. The Gateway to SNL will have the special capabilities of atom-tracking STM, interfacial force microscopy, chem prep oxide, Langmuir-Blodgett film, and microfluidics. The Gateway to LANL will have the special capabilities of near-field scanning optical microscopy (NSOM), AFM, SEM, nano-indenter, ultrafast laser, and a computer cluster.

The CINT thrust areas provide a broad base of expertise to the users, and several areas have been identified that use several of these capabilities. One is nonlinear response, which offers new behaviors for switching and sensing. Teams have been formed from both laboratories to pursue these types of opportunities. One has pursued quantum-dot nanocomposite materials for nonlinear optics and lasing. Another challenge is to combine top-down and bottom-up assembly to produce new functions from complex and hierarchical materials and devices. Still another challenge is the interfacing of biological and synthetic systems to produce active assembly, healing, repair, reconfiguration, and adaptation. SNL and LANL are teaming together to produce the assembly of nanocomposite materials through the use of biomolecules.

Many jump-start user projects have been initiated. The first call produced 78 proposals, of which 36 were approved. These proposals came from 16 states and the United Kingdom., representing 24 universities. There is a wide geographic distribution of the researchers seeking this expertise. In the call for proposals, researchers were asked to address the integration of top-down fabrication with bottom-up assembly, energy and charge transport across multiple length scales, coupling of mechanical and fluid forces across multiple length scales, and integration of biological and synthetic materials.

At full operation, the program is expected to deliver

$ A management team to support a user-friendly, open, and peer-reviewed international user program that meets the safety and security needs of DOE and the laboratories;
$ Foundations staff to operate, maintain, and continually upgrade experimental and

computational capability in support of the user community and CINT's integrated science directions;

- $ Leading laboratory scientists and visitors to advance the state of the art for CINT's scientific thrust areas and integrated science directions;
- $ Funding and technical support for maintenance, upkeep, and recapitalization of CINT's specialized scientific equipment; and
- $ Access to capabilities and expertise at both laboratories.

At full operation, staffing would be divided between the Foundations Staff (funded by the NSRC) and the Science Leadership staff. About 75% of the Foundations Staff would reside at the Core Facility and Gateway to SNL, and 25% at the Gateway to LANL. The Foundations Staff would include 18 technician FTEs, 14 postdoc FTEs, and 8 junior staff FTEs. The Science Leadership staff would include 10 senior scientist FTEs, 4 junior scientist FTEs, 6 postdoc FTEs, 4 faculty sabbatical FTEs, and 6 graduate student FTEs.

The management structure is keyed to the plurality of laboratories. A memorandum of understanding (MOU) spells out how this operation is to be conducted. Leadership consists of a director, an associate director, a chief scientist, and an outreach coordinator. The executive management has convened a Governance Board, a Science Advisory Committee, a Laboratory Management Council, a Proposal Review Committee, a User Committee (in the near future), and the Foundations Staff and Science Leadership.

At this point, the center needs to build community. It needs to identify and address grand-challenge science and discovery platforms for working at the nano/microscale transition. It may offer a CINT Prize for solving specific problems. It needs to bring in visiting scholars who are the best and the brightest. Workshops and summer institutes are an important part of pulling the nanoresearch community together.

Flynn asked if there were any plans for developing new characterization tools. Michalske said that CINT sees that as a critical function of the foundation staff. Examples of what we have now are atom-tracking machines at Sandia. These staff push the frontier to provide what is needed.

Wirth asked how they planned to integrate people into the laboratories. Michalske responded that the CINT has thrust leaders; they meet semimonthly to discuss these kinds of issues. Site visits are now being run at the two laboratories to build those connections. Oftentimes, the ability of researchers' being able to work together is hindered by incompatibility among systems. The CINT is going to try to build in compatibility from instrument to instrument.

Hemminger asked what challenges they were facing because of having a National Nuclear Security Administration (NNSA) laboratory working with a DOE laboratory. Michalske replied that great cooperation had been seen between the two. The administration at NNSA has exhibited a great support of the concept and facility.

El-Sayed asked where the patent rights will reside. Michalske said that the CINT was using the processes that each of the laboratories currently has in place. There is a joint agreement between the laboratories. A user intellectual-property (IP) agreement is not yet in place. It is hoped that a uniform policy will be developed among the NSRCs. El-Sayed suggested that, to encourage researchers to participate, one must be up front about the IP rights and spell that agreement out on the Web page and in calls for proposals.

Kohn asked if there were any security issues at these two laboratories, which, after all, do classified work. Michalske answered that the CINT does have a big issue with how DOE handles foreign-national access. The policy has to be spelled out ahead of time. It is driven by DOE policy. It is a process that requires adequate lead time.

Gates asked what activities Michalske and the other leaders had responsibility for besides CINT. Michalske replied that the management team is solely dedicated to CINT.

Eric Isaacs, Director of the Center for Nanoscale Materials (CNM) at Argonne National Laboratory (ANL), was introduced to present an overview of that center.

The CNM is a partnership between DOE and the State of Illinois. It is to be a world-class research facility for tackling the grand challenges of nanoscience:

$ To explore novel phenomena associated with the interplay between spatial, physical, and chemical length scales and proximity effects;
$ To develop the equipment and techniques needed to transform the art of nanomaterial and nanodevice fabrication into a science;
$ To characterize the 3-D structural, electronic, magnetic, and chemical properties of a single nanoparticle; and
$ To lay foundations for new information, medical, and other technologies based on the principles of nanoscience.

The CNM's scientific themes are built on current ANL capabilities to address the research interests in bioinorganic interface, nanocarbon, nanomagnetism, complex oxides, nanophotonics, Virtual Fab Lab, and X-ray imaging. The goal is to produce

$ A world-class research facility for tackling the grand challenges of nanoscience;
$ Open access for all users;
$ New science and capabilities for ANL, the region, and the nation;
$ A leveraging of the strengths of ANL and the region;
$ One-stop access to BES facilities at Argonne (such as the Advanced Photon Source, Intense Pulsed Neutron Source, and Electron Microscopy Center); and
$ A complement to the four other NSRCs.

The purpose of the Center is to enable science through technical capabilities. The CNM experimental themes share common technical activities in synthesis, sculpting (with nanolithography and milling and etching), characterization, and theory and simulation (leveraging resources from ANL's petaflop initiatives and the DOE/SC computing infrastructure investment).

A central question is how to get more functionality out of self-assembly. The first stage in doing this is to prepare a substrate with lithographically prepared trenches; this is the standard top-down approach. The second stage is to prepare a self-assembled diblock copolymer aligning within the trenches; again this is a standard procedure. The third stage is to prepare a 1-D nanomagnetic array that selectively adsorbs on hydrophobic polymer stripes, "decorating" the arrays to get beyond giant magnetoresistance (GMR; > 5MB/cm^2). This process cross-cuts many themes in nanoscience and the CNM.

The key fabrication and characterization tools include e-beam lithography, focused ion-beam SEM for milling away material, plasma-enhanced CVD systems for producing carbon diamonds, and combined SEM and scanning-probe microscopy (SPM).

One special instrument is the hard X-ray nanoprobe, a unique, versatile instrument to study individual nanostructures with a 30-nm resolution. It is capable of quantitative measurement of atomic-scale structure, strain, and orientation and of imaging. It can be used for sensitive trace-element and chemical-state analysis and operates in both scanning-probe and full-field modes.

Some of the grand challenges for nanoscience with X-rays are

$ X-ray-wavelength resolution (with a resolution of ½ or 1/4 the wavelength of the X-rays);

$ 3-D structural, chemical, electronic, and magnetic properties at the nanoscale;
$ Determining the structure of a single macromolecule (a protein);
$ Dynamics of single nanoparticle;
$ Coherent manipulation of nanoparticles (this is appropriate for the LCLS);
$ Nonlinear x-ray processes (this is appropriate for the LCLS).

Today, hard X-ray imaging is being used at the nanoscale to show antiferromagnetic domains in materials and to invert the image derived from coherent-diffraction data to produce an absolute X-ray density map (e.g., of *E. coli* bacteria).

Facilities beyond CNM that will be available to Center users include the Advanced Photon Source (APS), Intense Pulsed Neutron Source, and Electron Microscopy Center. The Center will provide the user one-stop access to all four of these facilities. The CNM building will be adjacent to the APS, be integrated with the APS site design, and use APS site utilities. The building will have 85,000 gross sq ft, including 13,000 sq ft of laboratories, 11,000 sq ft of cleanroom facilities, and 33,000 sq ft of offices and public spaces.

A balance will need to be maintained between user support and CNM science. Construction will start this spring; completion is expected in 2006, with the servicing of users with an e-beam tool at that time.

Staffing will be split approximately 50-50 between technical support and scientific staff. The goal is to achieve full staffing by FY08. At that time, about 200 user visits per month are projected (including multiple visits by most users). This estimate is based on current nanolithography user activity projected into the future, which gives a rough idea of user throughput.

Building community is an important task. Universities will play a critical role in the CNM. Center staff are conducting workshops at various universities (e.g., Northwestern, Notre Dame, and the University of Michigan). The first CNM user meeting will be held in May 2004, and a workshop will be conducted on developing a vision for the ultimate X-ray microscope.

The Center received $1.5 million in FY03 for a jump-start program. It has hired six postdocs. This postdoc program is very strong, cross-pollinating among disciplines and engaging external users. A high-resolution e-beam lithography facility has been started up jointly with Bell Laboratories. A user coordinator has been hired. A nanoscience summer school was held last year and was tremendously successful.

In terms of nanoscience and health, a person has been hired to do risk assessment, address environmental and worker-health concerns, perform public relations (with community forums), pursue joint opportunities with other NSRCs and workers at other agencies, and support research.

The CNM has a SAC that reviews and addresses scientific themes and technical-equipment plans. It reports to the Director and Project Manager, as does the Project Advisory Committee of ANL. The director and project manager supervise five groups:

$ Nanoprobe;
$ Nanolithography and Processing;
$ Nanosynthesis and Characterization;
$ Project Management, Integration, and Infrastructure; and
$ Conventional Facilities.

Taylor noted that the beamline brought industry into the light sources and asked what provisions were being made to draw in industry and allow them to create a product of real use. Isaacs replied that Cabot and others will be an important part of the user base, using a fast-access proposal process. The issue of IP came up. If the work is publishable in the scientific literature, access will be free; proprietary work will be allowed on a cost-recovery basis.

Hemminger asked how the big range of people who might be both industrial and academic would be dealt with. Isaacs had no good answer to that. This situation gets into very complicated legal issues. Discussions are being held with the University of Chicago and DOE.

Kohn noted that, in the 3-D properties of nanoparticles, theory has the potential to play a very useful role. Depending on the atomic weight of the atoms involved, geometry (interatomic distances) in these nanoparticles up to several hundred atoms may be calculated very accurately. Once one has that, one is a long way toward characterization with the help of theory. There are many cases with close energy minima where theory cannot distinguish among structures. With heavy atoms, once one gets into the tens of atoms, one gets hybridization of shells, which is a different problem, and the nanoscale may open a way into that problem. Isaacs replied that that problem had been encountered with TiO_2. With Center-provided software, one can use theory to resolve such experimental results.

Greene reiterated that one does not want to have overlap among NSRCs and pointed out that the NSRCs also fill a critical role between industry and universities. They must have IP policies in place to deal with the problem posed by that role. Isaacs replied that the Center knows how to do it with the tools. The issue is more problematic with materials. Greene added that, when the Center staff talk about moving materials from one place to another for characterization, they are not taking into consideration the great reactivity (and other properties) of these nanomaterials.

A break was declared at 3:41 p.m. The Committee was called back into session at 3:55 p.m. to hear **Robert Hwang** review the status of the Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory (BNL). The Center's user program will be developed from the science program, producing a coordinated, laboratory-wide infrastructure. Strong science programs will be developed through interactions with users and core programs. A key emphasis will be the integration of theory and modeling to the experimental programs. Technique development will emphasize quantitative measurement to support interdisciplinary research. Some users will want to collaborate, and some will come to conduct specific measurements. A very interdisciplinary environment is being envisioned for nanoscience research, incorporating theory and modeling, synthesis, and characterization.

The Center will have a series of laboratories for nanopatterning, electron microscopy, proximal probes, materials synthesis, ultrafast optical sources, theory and computation, and use of the National Synchrotron Light Source (NSLS). It will integrate the other divisions of BNL and various scientific disciplines and will foster collaboration. One of the foci of the Center will be Nanostructured Catalysts to address the problems of local electronic and atomic structure of size-selected clusters, stability of supported nanoparticles, reactive trajectory calculations, and wet-chemical synthesis of nanoparticles. This is an area that will produce significant commercial applications. The Center will tap into the strong catalysis initiative at BNL, leading to the rational design of catalysts.

BNL researchers are currently looking at electronic nanomaterials, probing organic nanomaterials and interfaces, and investigating organic molecular self-assembly and wetting. Their use of quantitative microscopy provides a very robust test of theory with experimental results. This technique is an important contribution of all the NSRCs. The individual spatial, temporal, fabrication, functional, and energy (composition) variables have been pushed to high levels. What is needed now is to look at phase space with the simultaneous variation of several variables.

In the science of synthesis enabled by in situ imaging, one can look at the process of self-assembly of templates for catalysts with atomic-force spectroscopy (AFS). These measurements allow one to understand (and then control) the intermediate steps.

TEAM, the transmission electron aberration-corrected microscope, is a collaborative development project to design, build, and operate next-generation electron microscopes.

The CFN outreach effort has made contact with universities and industries from Pennsylvania to Maine.

The Center started its jump-start program last fall. In response to the first call, 71 proposals were received from 26 universities, 3 national laboratories, 4 industrial institutions, and 3 foreign institutions; 42 were accepted. In full operation, the Center expects about 300 users per year. The real interest is not in single measurements but in conducting several activities.

The total project will cost $81 million for construction and capital equipment. The building will have 94,100 ft^2, of which 23,000 ft^2 will be for laboratories, 5,000 ft^2 will be for clean rooms, and 37,000 ft^2 will be for office and circulation. It will have instruments for submicron diffraction, small-angle x-ray scattering (SAXS), wet chemistry, molecular beam epitaxy, PLD, e-beam deposition, e-beam patterning, resist process and development, deep reactive ion etch, ion-beam patterning, sum-frequency generation (SFG), difference-frequency generation (DFG), extreme ultraviolet/soft X-ray (XUV/SXR) terahertz microscopy, Laser-Electron Accelerator Facility (LEAF), high-resolution TEM, scanning auger, scanning electron microscopy, electron holography, scanning transmission electron microscopy, electron energy-loss spectroscopy (EELS), ultrahigh vacuum-SPM, NSOM, infrared microscopy, Env. SPM, low-energy electron microscopy (LEEM), photo-emission electron microscopy (PEEM), spin-polarized low-energy electron microscopy (SPLEEM), linearized augmented plane wave (LAPW), plane-wave pseudopotential, quantum chemistry, quantum Monte Carlo, molecular dynamics, and symmetric multiprocessors computing. It will be located adjacent to the NSLS. Design includes areas for materials synthesis, electron microscopy, nanopatterning, clean rooms, proximal probes, and ultrafast sources.

The CD0 was signed on June 12, 2002. The CD2 is expected to be approved on May 14, 2004. The CD3 construction is expected to start at the end of this year. Initial operations are expected to start at the beginning of May 2007 with full operations a year later.

A CFN organizational structure will have a director, CFN/NSLS coordinator, SAC, User Executive Committee, and PRC. It will have five facilities: Electron Microscopy Facility, Nanomaterials Synthesis and Characterization Facility, Proximal Probes Facility, Nanoscale Theory and Modeling Facility, and Nanopatterning Facility. It will also have four science-theme areas: Organic Nanomaterials and Interfaces, Nanostructured Catalysts, Electronic Nanomaterials, and Synthesis Science. Users will be able to access the Center through a facility or through a science-theme area.

El-Sayed asked what BNL would be able to do in 2008 when the center was in full operation that it could not do now. Hwang answered that all the capabilities listed in the slide describing the facility and its costs would be new. El-Sayed asked if the people who were there now were limited in tools. Hwang replied, yes.

Berrah asked if they would have some formal method to use facilities at the other NRSCs. Hwang replied that the center directors had not worked that out yet but that it is a wonderful idea. That is what cooperation among the clusters should be about.

Taylor noted that all the centers were planning on employing a lot of postdocs. But postdocs do not get tenure, and they want to improve their employment prospects. Hwang acknowledged that the centers need to nurture them and help them in their career development. The centers have to be careful how they integrate and assign the postdocs. He went on to point out that these centers offer a way for researchers to get a lot of expertise for free.

Richards asked if it were harder for noncitizens to get into the DOE labs after the events of September 11, 2001. Hwang said that, at BNL it is more difficult, requiring more planning. However, it has not hindered operations at the light source. Morse commented that, at another center at LLNL, a Canadian student of his was not allowed to touch computers or instruments, making it necessary for a researcher to be there to do what she could have done on her own. Greene added that it *is* difficult to get into the DOE laboratories. DOE must work with the Department of State on this. The policies also affect conference attendance because students are concerned that they might not get back into the country after attending a foreign meeting.

Hemminger opened the floor to open discussion.

Plummer said that the core programs at the national laboratories are hemorrhaging. If the core programs take a hit to fund the NRSCs, it may be fatal.

El-Sayed raised the question of how much money should be devoted to facilities. He pointed out that the scientists themselves have to be funded to use them. Also, the position of the postdocs at these centers should be limited to 2 or 3 years, or they should be accorded tenure at the institutions where they are working.

Gates asserted that the Committee and the programs need to get feedback from the users. Dehmer responded that, at the previous week's review of the NRSCs, the most important topic was the metrics for the success of these centers. Metrics exist for other facilities, but these centers are different. We may hold a workshop with the centers to discuss this topic.

Berrah noted that these centers should not compete but should cooperate heavily, and cross-center use should be promoted and facilitated. Dehmer asserted that one first has to figure out what behavior is desirable to enhance and what unintended results may be produced by any action. This concern does not just affect the NRSCs but all user facilities.

Hemminger opened the floor to public comment. There being none, he adjourned the meeting for the day at 4:44 p.m.

Tuesday Morning, February 24, 2004

Hemminger called the Committee back into session at 8:34 a.m. and discussed the date for the next meeting in early August. He then introduce a series of presentations on TMS. The first speaker was **Richard Hilderbrandt**, who reviewed the use of TMS in the Chemical Sciences, Geosciences, and Biosciences Division of BES. He began by reviewing the activities and opportunities of each group in that division related to theory, modeling, and simulation. In Chemical Physics, about 30% of the program is in computational chemistry. It studies how to address open states, turbulent flow, barriers, etc. with precision. Atomic, Molecular, and Optical Science team studies intense laser fields, molecular breakups, and many-body physics of quantum condensates and fermionic condensates. Catalysis and Chemical Transformations has a small theoretical component to design new catalytic systems and nanocatalysts. Heavy Element Chemistry investigates complications related to relativistic pseudopotential treatments to understand the participation of 5f electrons in the chemistry of actinides. In Photochemistry and Radiation Research, 11% of the portfolio is computational chemistry. Some of the challenges faced there are the factors controlling photoinduced long-range electron transfer, charge injection at the semiconductor/electrolyte interface, and photoconversion in biomimetic assemblies for solar photocatalytic water splitting. Chemical Energy and Chemical Engineering is almost fully theoretical, studying complex fluids (polymers and glasses), electron transport, and aqueous solutions.

One of the challenges being addressed by theory and simulation is the problem of time scales. New simulation techniques are being developed for treating rare events (e.g., the dissociation of water molecules). Others are the treatment of quantum effects for chemical reactions in condensed phases and the reconciliation of scale boundaries from the atomistic/molecular scale to the nanoscale to the mesoscale to the continuum. In addition, new approaches with guaranteed precision and speed are promising to treat chemically relevant systems.

Computational challenges include the need for computational algorithms that scale linearly to large terascale or ultrascale computers while achieving a high percentage of peak performance. Many codes scale to tens of processors, but only a handful will scale to thousands of processors. Many algorithms achieve only a small percentage of theoretical peak performance on terascale computing architectures. Today, software development requires multidisciplinary teams with close interaction among computational scientists, computer scientists, and applied mathematicians. Emphasis has been placed on reusable code, good software engineering practices, and the use of optimized libraries.

SciDAC (Scientific Discovery through Advanced Computing) is a good example of the application of TMS to chemical problems. BES SciDAC Awards were made in three areas. In the area of chemically reacting flows, four projects were funded. In the area of unstable species and large molecules, six projects were funded. And in the area of actinide chemistry, one small group project was funded to develop relativistic pseudopotentials for determining the chemical properties of the actinide elements.

A $6.0 million program on theory, modeling, and simulation in the nanosciences that is a joint venture between BES and the Office of Advanced Scientific Computing Research (ASCR) funded four new projects this year:

$ Computational Nanophotonics
$ Predicting the Electronic Properties of 3D, Million-Atom Semiconductor Nanostructure Architectures
$ Scalable Methods of Electronic Excitations and Optical Responses of Nanostructures
$ Integrated Multiscale Modeling of Molecular Computing Devices

Three of these projects are associated with NSRC activities, and all of them involve very large teams and the usage of terascale resources. About 25 PIs used 5,350,780 hours on Seaborg at NERSC, and three SciDAC PIs used 784,638 hours. The demand for resources exceeds supply by quite a bit. The SCaLeS Workshop identified need for increased investments in both hardware and software infrastructure to take full advantage of opportunities for scientific discovery. This shortage of computing capabilities may be alleviated this year by access to resources at ORNL.

A new competitive program, entitled Innovative and Novel Computational Impact on Theory and Experiment (INCITE), was initiated by Ray Orbach. In its first year, 52 proposals were submitted for the use on supercomputer processor time. Three awards amount to 10% of the total computing time available this year on NERSC’s current IBM supercomputer. One of these projects, Quantum Monte Carlo Study of Photoprotection via Carotenoids in Photosynthetic Centers, led by William A. Lester, Jr., of LBNL and the University of California at Berkeley, was awarded 1,000,000 processor hours.

Kohn asked if they had any density function theory (DFT) work. Hilderbrandt replied, definitely. It is an important research method. Kohn noted that Hilderbrandt had cited a value of 10^7 for chemical accuracy and scaling and that such a value could not have come from DFT calculations. It gives a very different picture. These are the traditional wave-function-based methods. At least for the lighter elements, the work that has been done gets what chemists call chemical accuracy to within a factor of <2 but can deal with vastly larger systems. Even the Gaussian program has incorporated DFT. It limits one's predictive power somewhat, but one gains the ability to deal with hundreds of atoms. He asked if that had penetrated the Division. Hilderbrandt answered in the affirmative, but an error of just a few percent can rapidly propagate in such systems as combustion. But then one eliminates most of the interesting chemistry going on, objected Kohn.

Cummings asked how much money was being spent buying computers. Maupin answered that DOE does not track small-scale computing resources that are bought with project funds. Often a PI will request equipment or support for computer resources, and they are given money that is matched by their institutions. A small number of researchers ask for funds with which to upgrade their systems.

Dale Koelling then gave an overview of TMS in the Materials Science and Engineering Division. That Division is split into two teams, which are organized differently, and they address and use theory to different degrees. He began with a sampling of core research activities in the teams of the division, mostly atomistic modeling with centroids. The Structure and Composition of Materials Team includes an effort on the constrained local moment model for spin dynamics. The Engineering Physics Team is a sleeping giant and has a lot of topics amenable to computational approaches. An INCITE award was given to one of the research projects sponsored by this group. That project is investigating the dynamics of spins (ab initio electrodynamics for magnetism), which follows the dynamics of a collection of spins. This is a major step toward understanding magnetic materials. This theory extends DFT and uses it in regimes where numerous aspects are still not well understood. Consequently, applying this theory will simultaneously enhance our understanding of magnetic materials and of the basic theory. It is also a nontrivial computational effort.

As mentioned by Hilderbrandt, the INCITE program garnered 52 proposals. Three awards amount to 10% of the total computing time available this year on NERSC's current IBM SP3. One of these was in Engineering Physics: Fluid Turbulence and Mixing at High Reynolds Number, led by P. K. Yeung of Georgia Tech. This project was awarded 1,200,000 processor hours.

In the other team, Condensed Matter Physics and Materials Chemistry, theory is primarily concentrated in the Theoretical Condensed Matter Physics activity, although it is not exclusively so. There is a need for multidisciplinary efforts. Materials Chemistry has a lot of its own theoretical work.

The Computational Materials Science Network pulls together laboratory research teams and builds on other funding from DOE, industry, and other government agencies. The criteria for cooperative research team proposals call for

$ A focus on a critical scientific issue,
$ Having a clear path to relevance,
$ Being of the type best pursued through broad cooperative efforts,
$ Build on existing BES funded programs, and
$ Defining some short-term deliverables combined with long-term objectives.

In FY04, there are five active collaborative-research teams.

The program on Theory, Modeling and Simulation in Nanosciences issued a solicitation in February 2003, which yielded 34 applications, of which 4 were funded. The program was funded at a level of $6 million jointly by BES and the Office of Advanced Scientific Computing Research. The applications were evaluated jointly on science and then separated into appropriate BES divisions. All the funded projects were listed by Hilderbrandt. Koelling focused on the project, Predicting the Electronic Properties of 3D, Million-Atom Semiconductor Nanostructure Architectures. Here, the full electronic structure (but not the full DFT) is needed; this project is trying to look at what one has to do each step of the way.

Computing is important. Last year, more than 3.35×10^6 processor hours were used on the IBM SP3 at the NERSC, and about 1.6×10^6 IBM SP3 and SP4 processor hours helping evaluate computers at ORNL. At 45 repositories, Materials Science is the program with the largest population of users. This past year, requests for time ran roughly 3 times the resources available even before the new, large special requests were factored in. The same will be true this year.

El-Sayed asked what kind of nanostructure it represented when he referred to a million atoms in the calculation of nanostructure. Koelling said that the National Renewable Energy Laboratory (NREL), which was driving this research, was focused at the optical properties of semiconductors. If one wants to do some of the terrestrial thermophotovoltaics, one has to achieve a very small bandgap to keep the systems from wiping out. If one tries to do that with standard materials, it does not happen; one has to use nanostructures.

Kohn called attention to the million-atom calculation that had been referred to and commented that one of the easiest many-body systems to deal with is one with an infinite number of atoms. There is a crossover point in nanostructures. It is useful to keep each of those perspectives in mind. He also had a comment on semantics. We characterize a physical situation by length scales, the nanoscale. Anthony Leggett of the University of Illinois, while speaking at the University of California at Santa Barbara, called it macroscopic superfluidity. As scientists, we should know that length alone is not relevant. The size of an atom and the number of atoms is important. As one goes to more and more atoms, one loses the atomic length scale and moves into another scale. The physically relevant scale changes. Koelling noted that, if one has 10^6 atoms in a cube, one has 100 atoms (20 nm)on a side; that can be a semiconductor. One does not get away from surface as one goes into bulk.

McCurdy said that it is easy to get a distorted picture of the BES portfolio. A large portion of the PIs in chemistry are using DFT. He asked what the balance was elsewhere in the portfolio. Kirkoff answered that the answer is “yes.” There is a heavier emphasis on methods development than on application in chemical physics.

El-Sayed asked how much effort is going into surface states and their instability. Koelling replied that that topic is an important concern, and a lot of people are working on it [e.g., at Lawrence Livermore National Laboratory (LLNL) on bucky diamonds].

Hemminger expressed a concern about the small ratio of projects that are funded (4 funded out of 34 proposals). He asked how many co-PIs were represented in those 34 proposals. Koelling responded, about 300. Hemminger characterized that as “dramatically disturbing.” The amount of work going into proposals is greater than the work going into science. McCurdy pursued the question by asking, of those 300 PIs, how much money they were bidding on. Koelling replied, up to $6 million, $3 million from BES and $3 million from the Mathematical, Information, and Computational Sciences (MICs) Division of ASCR (of which $2 million was spent). This comes to about $280,000 for each team of about 40 members. Cummings pointed out that there were 300 distinct PIs; one could not be on more than one proposal.

Flynn brought up two issues: The community is healthy enough to produce this level of competition; but if the rewards are so sparse, young researchers will be discouraged . Preproposals should be used to limit the waste of time and effort on the part of the proposal submitters. Dehmer noted that government agencies can have a call for preproposals and BES will use that mechanism for the hydrogen solicitation.

Flynn asked how many preproposals had been submitted. Kirchhoff replied, 78. So, Flynn concluded, there were many more than 300 interested PIs.

Hemminger declared a break at 9:45 a.m. The meeting was reconvened at 10:16 a.m., and **William McCurdy** presented a report from the Subcommittee on Theory and Computation. That Subcommittee had been charged by Orbach. The charge to the Subcommittee was to identify current and emerging challenges and opportunities for theoretical research within the scientific mission of Basic Energy Sciences, with particular attention paid to how computing will be employed to enable that research. A primary purpose of the subcommittee is to identify those investments that are necessary to ensure that theoretical research will have maximum impact in the areas of importance to Basic Energy Sciences, and to guarantee that BES researchers will be able to exploit the entire spectrum of computational tools, including the leadership-class facilities contemplated by the Office of Science. This charge was fairly broad and clear; the breadth is what the Subcommittee is struggling with.

By May, the preliminary, substantive ideas will be needed from the Subcommittee members. If the Subcommittee's findings are compelling, BES may set a very high priority for a significant budget increase in this area in FY06. To be useful for FY06, a report is needed by August, prior to the Office of Management and Budget (OMB) budget briefing that occurs the first week in September. The final report is to be issued in December or January.

The Subcommittee is not doing a review of existing BES theory programs. Preferably, the report will not describe the details of scientific opportunities in many subspecialties. Rather, it will provide a high-level discussion, a roadmap of investments, and a focused theme. The challenge is finding the focus of the Subcommittee's work.

The Subcommittee is populated by people with breadth and talent.

Telephone conferences have led to a strategy:

$ Holding no workshops,
$ Broadly soliciting testimony from the community,
$ Developing a short series of specific questions that will posted on the Web,
$ Issuing an e-mail solicitation via appropriate American Physical Society and American Chemical Society divisions that seeks experts for key contributions,
$ Collecting written testimony on a website, and
$ Having in-person presentations in Chicago in April.

The first Subcommittee meeting was held February 22 in Washington, D.C. The second meeting will be the Chicago meeting in April, where initial recommendations and ideas will be gathered and the first writing assignments will be made. The Subcommittee will incorporate relevant data and observations of previous reports: "SCaLeS," "Theory and Modeling in Nanoscience," "Complexity," etc. A preliminary letter report will be prepared for BESAC and BES in early May.

The Subcommittee must make a case not only why greater support for theory and modeling is needed but also, "Why now?" Five nanoscience facilities, the SNS, and the LCLS are under construction, and basic research for the hydrogen economy is urgently needed. All of these activities need to couple experiment with theory.

The proposed principal components of the report are expected to be (1) identifying the major research opportunities and challenges for theory and computation in BES; (2) coupling of the theory program with existing and future BES facilities; and (3) dealing with issues of infrastructure, resources and support necessary for a successful BES theory and computation program.

The task of the Subcommittee is to identify a small number of major themes to describe the new opportunities for BES theory and to distill a complex array of new problems into overarching ideas; the compelling argument for addressing these issues now; and the simple, exciting story.

A number of ideas present themselves. The "new conventional view" of pursuing fundamental questions (e.g., electronically excited states of molecules, large molecules, and solids) and complex systems (bridging length and time scales) is already stale. This is a way of looking at the truth, but it is conventional and lacks insight. But there is a rich palette of ideas from which to work. Interesting problems that are durable (will be meaningful for five or more years) come from condensed matter, from materials physics and engineering, from the chemical sciences, and from advancing the understanding of complex systems.

Some interesting questions have already emerged naturally. Is quantum information viable? All the tools that will answer this question are in the BES portfolio, but quantitative information is not in that portfolio. Can nanoscience be transformed to nanotechnology? Are self-assembly and rare events (e.g., protein folding) predictable and controllable? These themes should be added to the BES research portfolio.

The Subcommittee has talked about the connection of the theory program with the BES facilities. The traditional strategy for coupling theory to experimental programs at the BES facilities is the "Blanche Dubois" plan, to "… rely on the kindness of strangers." Users must find theoretical collaborators who are willing and already funded to work on their problems. A mechanism is needed to make this happen more easily. The nanoscience centers recognize the need for theory programs, but their theory programs are currently being designed independently. Should not they be coordinated? An SNS theory program seems to be under development.

The in-house theory efforts at the facilities are necessary, but designing them is a challenge. An in-house effort probably cannot provide coverage for the broad spectrum of experiments at each facility, and it may not be possible to engage the best talent for a service role. In-house theory programs should be complemented by distributed theory efforts in support of specific facilities.

Traditionally, theory has been a cottage industry. Today, a hierarchy of computational resources is necessary to express modern theory: leadership-scale capability; high-performance, massively parallel, large-scale capacity; and local computing resources. But building those facilities must be coupled with funding the BES theory community to exploit them. A new style of support is needed for software projects that encompasses several generations of graduate students and postdocs. Examples of such a style are NorthwestChem and the Air Force's GAMES. European programs that existed over generations have set an example, producing large libraries and user-adaptable codes. Perhaps what is needed is a renewal and expansion of the SciDAC style of large-scale-project support in BES. (However, only Chemical Sciences participated in SciDAC and only for $2 million per year.)

Isaacs, speaking as an experimentalist, said that the Blanche DuBois model is very powerful and asked why DOE did not just fund more theorists so they are "down the hall." McCurdy agreed; discussions between experimentalists and theorists prompt creative insights. But one needs to go to several theorists to find the right one. The Subcommittee is not suggesting that theorists be mapped onto projects. Perhaps more theorists are needed.

Berrah commented that theorists are not funded well enough; core funding for experimentalists *and* theorists should be increased. And those theorists should be at both national laboratories and at universities.

Cummings stated that this is an opportunity for DOE to distinguish itself. It could provide long-term investments in theory at the national laboratories. The European computer codes have shown that the codes evolve to the point that they can be used without the help from theorists. These codes that work on big machines will never be ported to commercial machines.

El-Sayed stated that the funding of theorists should be included in proposals (e.g, those to the NSRCs).

Kohn referred to the reports that the subcommittee will consider and asked if the Committee members could get copies of those reports. McCurdy replied, yes; the scales, nanoscience, and complexity reports all came from DOE. He went on to point out that the fields represented in the BES portfolio are the ones that can best benefit from the new computational capabilities, but the number of cycles that are used do not reflect that. This imbalance needs to be corrected.

Gates stated that the theorists need to work with the experimentalists to select samples, determine what experiments can be run, etc. The fact that the NSRCs recognize the need for theorists is in stark contrast to the light sources that use photons, not intellect. McCurdy said that that is the frustration the Subcommittee feels. BES concentrates experimentalists in a few places. Those are ripe fields for the theorist.

Kirby pointed out that it is the PI who trains the future practitioners. The PI should be rewarded for that service. McCurdy commented that, often, large teams are necessary, but they are not the only way to use large facilities.

Dehmer said that she did not believe that the Subcommittee should put any artificial boundaries on subjects that are currently outside the BES portfolio but that could logically fit into that portfolio.

Hemminger opened the meeting to discussion. Smalley pointed out an article in the *New York Times*, "Forecast of Rising Oil Demand Challenges Tired Saudi Fields" by Jeff Gerth [*NewYork Times*, Feb. 24, 2004, p. 1], as a fascinating article. It says that Saudi Arabia may not be able to sustain its current production of 10 million barrels of oil per day. If Saudi Arabia peaks, the world peaks. What will come after petroleum needs to be considered. He noted that Matt Simmons, an investment banker in oil in Houston, is preparing a book on the same topic and has come to the same conclusion. The NSRCs need to focus on the DOE mission. Each one needs to be a nanoscience-for-energy miracle garden.

Hemminger said that meeting energy demand will require fundamental science, and BES must make people aware that we will not reach the future without breakthroughs in fundamental science.

Hemminger opened the floor for public comment.

Doon Gibbs, said that the European light sources also use the Blanche DuBois method, and it has been effective.

Bruce Harmon rhetorically asked, "Why now?" Because the number of Blanche DuBois experimentalists knocking on his door has increased tremendously. The number of neutrons and photons has increased this demand. The number of theorists needs to increase, also.

Linda Horton suggested that the Subcommittee also look at the energy report because it points to the need for theory in cross-cutting areas. Theory efforts should be integrated with

experimental efforts, not "distributed," as stated in the Subcommittee report.
Hemminger adjourned the meeting at 11:07 a.m.

Respectfully submitted
Frederick M. O'Hara, Jr.
Recording Secretary
March 8, 2004

Revised