BPA NEWS

Board on Physics and Astronomy • The National Academies • Washington, DC • 202-334-3520 • national-academies.org/bpa • Summer 2003

Major Research Equipment and Facilities Construction at the National Science Foundation

AT the request of the Senate Appropriations Committee, chaired by Christopher Bond, the National Academies recently established a committee to explore issues related to the Major Research Equipment and Facilities Construction account line at NSF. (The Major Research Equipment and Facilities Construction line in the NSF budget is often abbreviated MRE or MRE/FC.) The Board on Physics and Astronomy and the Committee on Science, Engineering, and Public Policy are jointly providing oversight and guidance on this project. The Committee on Setting Priorities for NSF-Sponsored Large Facility Research Projects is chaired by physicist William F. Brinkman of Princeton University. The committee has been charged to examine how the National Science Foundation sets priorities among multiple competing proposals for the construction and operation of large-scale research-facility projects across a diverse array of disciplines. The final report will make recommendations on how to make the priority-setting process as effective as possible, taking into account NSF's significant role in funding academic research in science and engineering in the United States. The committee has held public hearings and has met once to plan its work.

The first plenary meeting was held at the Keck Center of the National Academies in Washington, D.C., on May 19-20, 2003. The meeting consisted of closed-session discussions and extensive public presentations in open session. Over lunch on the first day, the committee talked with a panel of congressional staff, including Cheh Kim (Senior Staff, Senate Appropriations Subcommittee on VA, HUD, and Independent Agencies), Scott Giles (Deputy Chief of Staff, House Science Committee), David Goldston (Chief of Staff, House Science Committee), and Peter Rooney and Jim Wilson (House Science Subcommittee on Research). From this discussion, three issues were identified: (1) Congress is aware of an increased level of concern on the part of the science community about the process (in terms of both fairness and openness) by which NSF selects large facility projects for inclusion in the annual MRE/FC budget request, (2) Congress has a sincere interest in increasing the NSF budget and is interested in knowing "where" the additional funding might be spent (such as on other large facility projects), and (3) Congress wants to keep NSF "de-politi-

See "MRE" on page 4

In this issue:

The Impact of High Magnetic Fields on Nuclear Magnetic Resonance*

Robert Tycko, Laboratory of Chemical Physics, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health

Nuclear magnetic resonance (NMR) is one of the most important experimental techniques in modern science, with applications in physics, chemistry, materials science, biochemistry, biology, medicine, and essentially all other fields of research where the properties of macroscopic quantities of matter are of interest. The types of information available from NMR and the specificity of this information continue to grow as new techniques are invented and refined, as new applications are explored, and as NMR technology improves. High magnetic fields are a key component of NMR technology, and NMR applications have been an important driving force in the development of stable, homogeneous, high field magnets. Commercial superconducting magnets designed for NMR applications are currently capable of field strengths up to 21.1 tesla (T), with room-temperature bore diameters in the 4-9 cm range, field homogeneities of approximately 10 parts per billion over a 1 cm^3 volume, and drift rates less than 10 parts per billion per hour.

This article gives an overview of some of the capabilities of current NMR meth-

See "NMR" on page 6

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*This article summarizes a presentation made at the April 26th meeting of the Board on Physics and Astronomy. The National Science Foundation has commissioned an assessment of the science drivers for high magnetic fields science, and this presentation was requested to prepare the Board for oversight of the study, which is expected to begin later in the summer (see corresponding article on page 9).

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The Board on Physics and Astronomy is a continuing interdisciplinary body with expertise spanning the various subfields of physics, astronomy, and astrophysics. It serves as a focal point in the National Research Council for issues connected with these fields. The activities of the Board are supported by funds from the National Science Foundation, the Department of Energy, the Department of Defense, the National Aeronautics and Space Administration, the National Institute of Standards and Technology, and private and other sources, including the Keck Foundation.

Highlights of the Spring Meeting of the Board on Physics and Astronomy

The Board on Physics and Astronomy met at the Keck Center of the National Academies for its 20th anniversary meeting on April 25-26, 2003. Chair John Huchra and Vice Chair Bob Richardson led the meeting. On the first day, the Board heard from representatives of the federal funding agencies. Patricia Dehmer (Basic Energy Sciences), Robin Staffin (High-Energy and Nuclear Physics), and Anne Davies (Fusion Energy Sciences) presented status reports on these three offices at the Department of Energy's Office of Science. Dr. Dehmer reviewed several recent studies completed by the BES Advisory Committee, including the roadmapping contribution to the Office of Science's 20-year facilities strategic plan that Director Orbach has initiated. Dr. Staffin reported that the main foci of the HEP program are the Tevatron Run II at Fermilab, the SLAC B-factory, and the NuMI/MINOS experiment. The strategy is to maximize the science at these existing facilities while maintaining R&D efforts for new projects. The nuclear physics program is directed toward strengthening the research base, operating user facilities more effectively, and making investments for the future, he said. In a follow-up question about the potential for a national underground lab, Dr. Staffin indicated that DOE is looking to NSF for leadership in this effort. Dr. Davies discussed the broad plasma program in her office, but also focused on the negotiations for U.S. participation in ITER. She welcomed the December 2002 interim letter report from the BPA's Burning Plasma Assessment Committee and looked forward to that committee's forthcoming final report. All three representatives agreed that the administration is committed to maximizing the productivity of its capital investments, including its investments in the researchers themselves.

Over lunch, the Board resumed the fall meeting's discussion about women in physics. The conversation centered around how the BPA could (and should) respond in light of the many studies in progress on the issue of representation of women in science. It was agreed that the BPA will consider writing a letter to the President of the National Academies and/or the Committee on Women in Science and Engineering. The letter could express the Board's concern about the issue, support for continued study, and a list of recommendations (based on the International Union of Pure and Applied Physics resolution) that might ameliorate or at least further illuminate the problem. Based on some anecdotal evidence, the Board agreed that increasing the representation of women in physics requires addressing not only the mechanisms of academia but also the perceptions of young women entering the field. The second topic raised during lunch was support for theoretical physics research by the agencies and in the subfields. Many paper-and-pencil theorists—and their students—are being left behind as the emphasis on computing and simulation increases. A suggestion was made that grant records be searched to determine the trends of support for theoretical physics over the past few decades.

Anne Kinney kicked off the afternoon discussions with a presentation about NASA's Office of Space Science. She discussed the budget, highlighted the new Beyond Einstein initiative, and emphasized the role that several NRC studies have played in shaping NASA's strategic plan, including that of the BPA's Committee on Physics of the Universe and the Astronomy and Astrophysics Survey Committee. When asked how the Board could help her office, Dr. Kinney replied that support and direction for the use of research and analysis monies was important. She also stressed the need for physicists to draw attention to their own successes in a way that is exciting and accessible to the public, pointing to several very successful NASA education and public outreach efforts. The National Science Foundation then took the stage, with Joseph Dehmer (physics), Lance Haworth (materials research), Wayne van Citters (astronomy), and Tomas Gergely (spectrum management) each presenting an update from his respective division. Dr. Dehmer emphasized the breadth of the physics division's programs and NSF's commitment to principal investigators. Dr. Haworth reviewed the variety of materials research being supported and reminded the BPA to “get the word out that materials research is one of the physical sciences.” Dr. van Citters outlined NSF’s broad support for astronomy, including its role as the major supporter of radio astronomy in the nation. He also said that thinking had begun about several of the priorities cited in the recent decadal survey.

The BPA’s Committee on Radio Frequencies works closely with the NSF Spectrum Manager, Tomas Gergely, who began his presentation by discussing the International Telecommunication Union’s World Radio Conferences (WRCs). The WRCs set the rules and provide advice for international management of the radio frequency spectrum. Dr. Gergely also noted the lack of representation by the scientific community. He cited a lack of recognition of the importance of the task on the part of observatory directors and others, insufficient resources to cover full-time spectrum managers or participants at WRCs, and the complexity of frequency regulation, which is dominated by powerful commercial interests.

Administration policy makers also spoke before the committee. J. Patrick Looney represented the White House’s Office of Science and Technology Policy with his remarks. After explaining the purpose and scope of OSTP, Dr. Looney discussed several of the interagency collaborations that his office is overseeing. In particular, he complimented the BPA on the Committee on Physics of the Universe report *Connecting Quarks with the Cosmos*, citing the intellectual framework, the synthesis and extension of existing reports, and the support expressed for current projects as key features of the report’s success. Finally, he commented on OSTP’s consideration of general policies concerning large facility research projects. Joel Parriott and David Radzanowski then presented remarks about the Office of Management and Budget, stressing that the federal budget for basic research is a scientific but ultimately political question. There are constraints on spending, and the discretionary portion of the budget is relatively small, they said. Dr. Radzanowski described aspects of the President’s Management Agenda and the administration’s interest in guiding the investment of federal monies into research by measuring results, relevance, and performance. After some general discussion, the Board adjourned for the day.

To commemorate the 20th anniversary of the Board on Physics and Astronomy, a reception was held in the atrium of the Academies’ new Keck Center. The reception was attended by past Board chairs, members of the Washington science and technology community, and representatives from the agencies. E. William Colglazier, Executive Officer of the National Research Council, addressed the guests and congratulated the Board on a meritorious and distinguished history. Dr. Colglazier cited several BPA reports as examples of the high quality and timely impact that other NRC reports strive to achieve.

The Saturday session of the Board meeting commemorated the 20th anniversary with retrospective summaries from each of the BPA’s standing committees by their respective chairs (see summaries of these presentations below). Robert Tycko and Greg Boebinger spoke on the science and application of high magnetic fields (see Dr. Tycko’s article elsewhere in this issue); Michael Turner discussed the implications of the recent WMAP cosmic microwave background measurements over lunch. The Board then turned its attention to current and new business with a proposal by member Jonathan Bagger (in collaboration with Dr. Turner) for a joint cosmology–particle-physics research briefing. The Board also spoke with the co-chair of the Burning Plasma Assessment Committee, Raymond Fonck, about the committee’s interim report and the endgame work plan. Finally, the Board discussed what roles it should assume as the next decadal assessment of and outlook for physics is launched. The meeting adjourned Saturday at 2:30 pm on a beautiful Washington afternoon.

CAA

The genesis of the Committee on Astronomy and Astrophysics (CAA) was a recommendation in *The Decade of Discovery in Astronomy and Astrophysics*, the 1991 Astronomy Decadal Survey chaired by John Bahcall. In its submission to the Survey Committee, the Policy Panel stated that “a standing committee of the National Academy of Sciences [should] be established to monitor the overall health of the field and to provide strategic, coordinated advice to all agencies that support research in ground-based and space astronomy.” The NRC acted on this recommendation, and the CAA was founded as a joint committee of the BPA and the Space Studies Board in 1992.

The CAA was initially chaired by Marc Davis of UC-Berkeley, and after his first term a co-chair arrangement was arrived at which one co-chair would sit on each of the overseeing Boards. During its exist-

See “BPA Meeting” on page 10

Committees of the Board on Physics and Astronomy

Committee on Astronomy and Astrophysics
Wendy L. Freedman, Carnegie Observatories, and
Roger D. Blandford, California Institute of Technology, *Co-chairs*

Committee on Atomic, Molecular, and Optical Sciences
Pierre Meystre, University of Arizona, *Chair*

Plasma Science Committee
Cary B. Forest, University of Wisconsin at Madison, *Chair*

Committee on Radio Frequencies
Donald Backer, University of California at Berkeley, *Chair*

Solid State Sciences Committee
Lee Magid, University of Tennessee at Knoxville, *Chair*

Committee on Smaller Facilities
Robert Sinclair, Stanford University, *Chair*

Burning Plasma Assessment Committee
John Ahearne, Sigma Xi and Duke University, and Raymond Fonck, University of Wisconsin, *Co-chairs*

Setting Priorities for NSF-Sponsored Large Research Facilities
William Brinkman, Princeton University, *Chair*

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More information on BPA committees may be found on the BPA Web site at <www.national-academies.org/bpa>.

MRE

(continued from page 1)

cized" and as earmark-free as possible. The representatives asked the committee to determine criteria and a process by which projects could be prioritized across all disciplines with a defensible and transparent rationale. A well-defined process would make everyone involved feel more comfortable and more confident, they concluded.

Two representatives from OMB then made some remarks and answered questions: David Radzanowski (Chief, Science and Space Programs Branch) and David Trinkle (Program Examiner, Science and Space Programs Branch). OMB emphasized that while NSF is increasing its investment in large facility projects, the OMB is still responsible for ensuring that the taxpayers' dollars are well spent. They discussed the review of NSF's "tools portfolio" in accordance with the President's Management Agenda and the NSF Strategic Plan. The program was rated as "effective," although the priority-setting process for large facility projects was identified as an area where more transparency was needed. As usual, they said, they are in a situation where there are more high-quality projects than can be funded. The OMB representatives concluded by saying that these types of large investment decisions are difficult and inherently political.

The NSF Director and Deputy Director, Rita Colwell and Joe Bordogna, made a presentation discussing the NSF process for setting priorities for large facility projects. To summarize, Dr. Colwell identified four stages of project selection and award: concept and proposal formulation, proposal review and recommendation, priority setting, and the award and postaward management. She focused on the priority-setting stage, although a careful distinction was drawn between eligibility for MRE/FC funding and priority-setting criteria for MRE/FC-approved projects. Dr. Colwell also described the role of the NSF internal MRE/FC panel: the panel reviews candidate projects and selects those worthy of support and later places them in priority order, interspersed with discussions and decisions by the National Science Board. She emphasized that briefings and community involvement are used to move projects forward and that the priority setting depends on the expert judgment of many highly trained people. During the question-and-answer follow-up, Dr. Bordogna pointed out that there were consequences of having a very open and transparent process that needed to be considered. Both Dr. Bordogna and Dr. Colwell agreed that the negotiations with OMB about the NSF budget were confidential. They reiterated that MRE/FC projects were treated with nearly identical standards of quality, process, and merit-review as single-investigator awards. When asked to identify the explicit stages of community input, Dr. Colwell pointed to the astronomy and astrophysics decadal survey, the directorate advisory committees, and the National Science Board. Dr. Colwell also introduced Mark Coles, the new Large Facility Projects Deputy. (He began work with NSF on June 9, 2003.) NSF concluded by saying that they were eager to hear the wisdom of the committee, and any guidance that could be provided in its final report would be appreciated and useful.

The committee then heard from a panel of experts in the various disciplines on large facility projects—Barry Barish (Caltech), Martha Haynes (Cornell), Ted Moore (Michigan), and James Tiedje (Michigan State). Dr. Barish discussed the need for large facility projects in physics and described four MRE projects at different stages: CESR/CLEO/Cornell, LIGO, IceCube, and RSVP. He identified preconstruction support as a weak point in the current model, stated that the science community needs to play a major role in making the hard priority choices, and concluded that—from his perspective—it was not the precise timing or phasing of MRE projects that mattered as much as picking the right projects and doing them well. Dr. Haynes described the role of the astronomy and astrophysics decadal survey in determining community priorities in a manner that is considered inclusive, fair, and effective. She suggested that the current system does not respond well to projects that evolve in scope or partnership during development. Dr. Moore described the voluntary science advisory structure that the oceans research community uses to guide its future as well as the reliance on NSF as one of its largest sources of funding. Strategic planning and periodic program reviews involve the entire community and have helped make the oceans program one of the most successful geoscience programs at NSF. Finally, Dr. Tiedje discussed the likely role that large facilities will play in biology. He presented some conditions he felt large facility projects

Committee on Setting Priorities for NSF-Sponsored Large Facility Research Projects

William Brinkman, *Chair*
Princeton University

David H. Auston
Kavli Foundation

Persis Drell
Stanford Linear Accelerator Center

Alan Dressler
Observatories of the Carnegie Institution

William Friend
Bechtel Group (retired)

David Galas
Keck Graduate Institute of Applied Life Science

Bruce Hevly
University of Washington

Wesley T. Huntress
Carnegie Institution of Washington

Chris Llewellyn-Smith
University of Oxford

Linda J. (Lee) Magid
University of Tennessee at Knoxville

Marc Y.E. Pelaez
Newport News Shipbuilding

Robert H. Rutford
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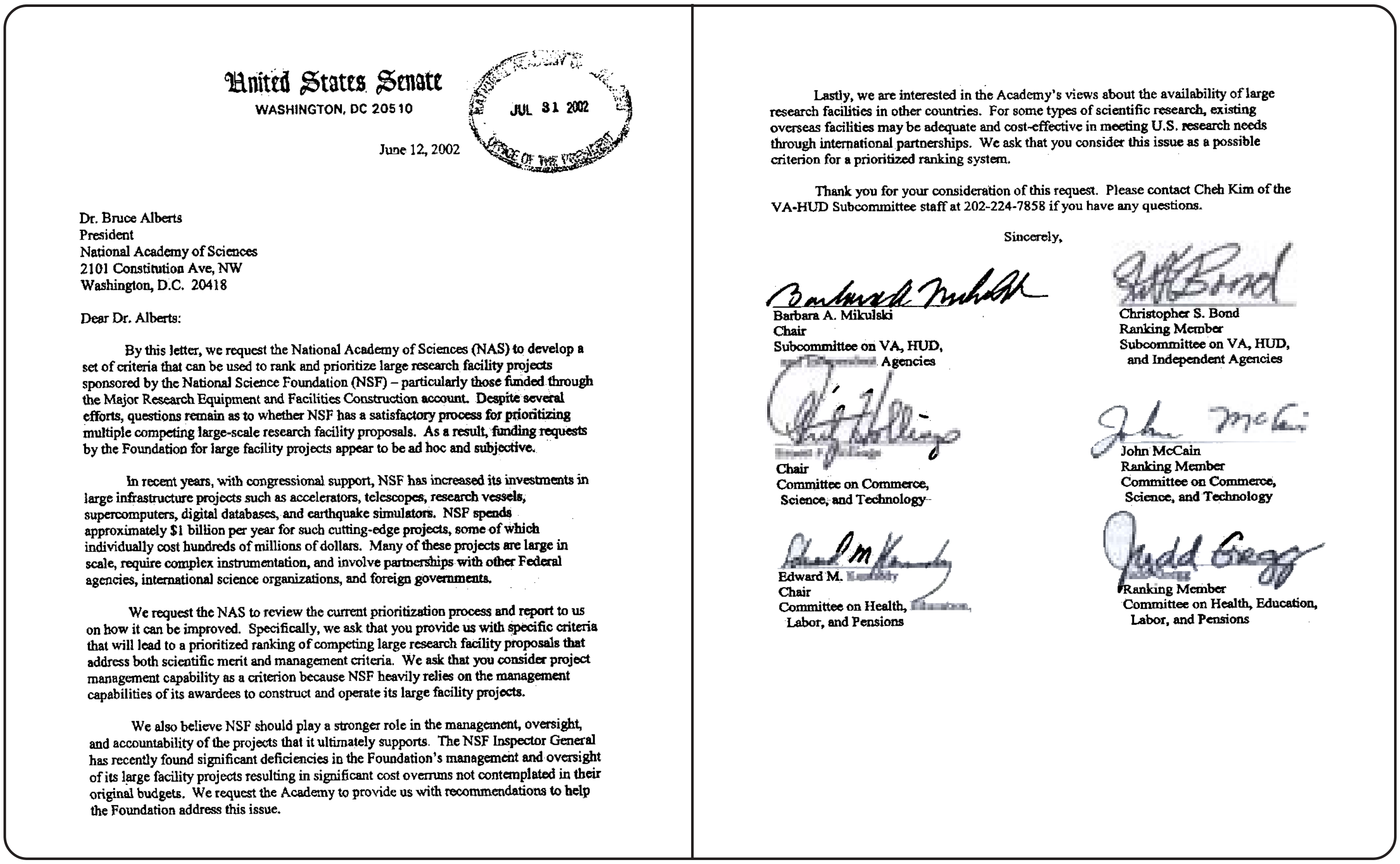
Dr. Timothy I. Meyer, BPA, *Program Associate*



United States Senate
WASHINGTON, DC 20510

JUL 31 2002

June 12, 2002

Dr. Bruce Alberts
President
National Academy of Sciences
2101 Constitution Ave, NW
Washington, D.C. 20418

Dear Dr. Alberts:

By this letter, we request the National Academy of Sciences (NAS) to develop a set of criteria that can be used to rank and prioritize large research facility projects sponsored by the National Science Foundation (NSF) – particularly those funded through the Major Research Equipment and Facilities Construction account. Despite several efforts, questions remain as to whether NSF has a satisfactory process for prioritizing multiple competing large-scale research facility proposals. As a result, funding requests by the Foundation for large facility projects appear to be ad hoc and subjective.

In recent years, with congressional support, NSF has increased its investments in large infrastructure projects such as accelerators, telescopes, research vessels, supercomputers, digital databases, and earthquake simulators. NSF spends approximately $1 billion per year for such cutting-edge projects, some of which individually cost hundreds of millions of dollars. Many of these projects are large in scale, require complex instrumentation, and involve partnerships with other Federal agencies, international science organizations, and foreign governments.

We request the NAS to review the current prioritization process and report to us on how it can be improved. Specifically, we ask that you provide us with specific criteria that will lead to a prioritized ranking of competing large research facility proposals that address both scientific merit and management criteria. We ask that you consider project management capability as a criterion because NSF heavily relies on the management capabilities of its awardees to construct and operate its large facility projects.

We also believe NSF should play a stronger role in the management, oversight, and accountability of the projects that it ultimately supports. The NSF Inspector General has recently found significant deficiencies in the Foundation's management and oversight of its large facility projects resulting in significant cost overruns not contemplated in their original budgets. We request the Academy to provide us with recommendations to help the Foundation address this issue.

Lastly, we are interested in the Academy's views about the availability of large research facilities in other countries. For some types of scientific research, existing overseas facilities may be adequate and cost-effective in meeting U.S. research needs through international partnerships. We ask that you consider this issue as a possible criterion for a prioritized ranking system.

Thank you for your consideration of this request. Please contact Cheh Kim of the VA-HUD Subcommittee staff at 202-224-7858 if you have any questions.

Sincerely,

Barbara A. Mikulski
Chair
Subcommittee on VA, HUD,
and Independent Agencies

Kit Bond
Christopher S. Bond
Ranking Member
Subcommittee on VA, HUD,
and Independent Agencies

Fritz Hollings
Ernest F. Hollings
Chair
Committee on Commerce,
Science, and Technology

John McCain
John McCain
Ranking Member
Committee on Commerce,
Science, and Technology

Edward M Kennedy
Edward M. Kennedy
Chair
Committee on Health, Education,
Labor, and Pensions

Judd Gregg
Judd Gregg
Ranking Member
Committee on Health, Education,
Labor, and Pensions

must meet. Dr. Tiedje's closing observations were that biologists are not an integrated community (and are therefore at a disadvantage when establishing community priorities) and that biologists are not experienced in large facility projects and their management. During question-and-answer follow-up, the four community representatives agreed that they were not unhappy with the history of MRE/FC projects, but that they were uncertain about how the projects had been selected, approved, and prioritized. The role of explicit nurturing of project concepts before translating them into MRE/FC proposals was also discussed.

John Marburger, Science Advisor to the President and Director of the Office of Science and Technology Policy, joined the committee for dinner and made some general remarks on his thinking about the importance of, and the organization of, the prioritization of large facility research projects. In particular, he suggested five organizing principles when considering priorities: service to multiple fields of science, exploitation of major opportunities, cost-sharing with other nations in light of the potential for spin-off, support for and empowerment of large communities of scientists, and addressing major national needs.

The second day was dedicated to committee deliberations and development of the work plan. In closed session, committee member Chris Llewellyn-Smith presented an in-depth analysis of several models from other countries that addressed large facility project selection, approval, and prioritization. An hour-long public comment session in the morning allowed representatives from the community to make short remarks. Michael Lubell (American Physical Society), Kevin Marvel (American Astronomical Society), Adrienne Froehlich (American Institute of Biological Sciences), and Eric Nagy (Organization of Biological Field Stations) presented personal comments. Dr. Lubell suggested the establishment of a large facility projects directorate, urged the committee to consider the role of advisory committees, and outlined a detailed procedure for strategic planning and roadmap development. Dr. Marvel described the need for large facility projects by astronomers, challenged other communities to follow the highly successful model of astronomy and astrophysics priority-setting through the decadal survey, and argued for a more explicit strategic planning process, akin to that of NASA's Office of Space Science. Dr. Froehlich explained that while AIBS does not have a long history of MRE/FC projects, the growing field of regional- and continental-scale biology will require vast networks. She recommended several strategies for prioritizing projects and concluded by saying that a transparent process won't make the bitter pill any easier to swallow for the winners and losers. Dr. Nagy presented the case for biological field stations and described the large variety of scale, support, and management of these essential research laboratories.

The committee plans to meet again on July 21-22, 2003, in Menlo Park, California. The final report is scheduled to be released this winter. ■

NMR

(continued from page 1)

odology and some of the reasons why high fields are important. Applications of NMR in structural biology, especially issues related to studies of protein structures, are emphasized. Several other areas of application that benefit from high fields are mentioned briefly in the final section.

Basics of NMR

In a typical NMR measurement, one places the sample of interest in a coil that is part of an LC circuit tuned approximately to the NMR frequency, which is typically 10-1000 MHz. With the coil inside the magnet, one then applies pulses of radio-frequency (rf) voltage, producing rf fields at the sample of about 1 mT for periods of about 10^{-6}-10^{-2} s, and subsequently detects the rf voltages induced in the circuit by the precession of bulk nuclear spin magnetization within the coil. Fourier transformation of the time-dependent NMR signals yields an NMR spectrum.

In general, the NMR spectrum reflects the interactions of nuclear spins with one another and with their chemical and structural environment. Important interactions include:

(1) Zeeman interaction with the static magnetic field, typically 10-1000 MHz. Shielding of the external field by the electronic structure of diamagnetic molecules produces small shifts of the NMR frequencies, typically of order 1-100 parts per million, called "chemical shifts." The phenomenon of chemical shifts is the basis for the power of NMR as an analytical tool, allowing chemists to determine or confirm the chemical structure of a newly synthesized organic molecule by taking its ^{1}H or ^{13}C NMR spectrum. Chemical shifts are also the primary source of spectral resolution in biomolecular NMR. In magnetic resonance imaging (MRI), the Zeeman interaction is deliberately made position-dependent by the application of controlled magnetic field gradients. The NMR spectrum then becomes a spatial image of the nuclear spin polarization density.

(2) Nuclear magnetic dipole-dipole couplings, typically 1-20 kHz. The strengths of these interactions depend on internuclear distances R as R^{-3}. In isotropic liquids, rapid molecular tumbling averages the dipole-dipole couplings to zero, but the fluctuating couplings drive nuclear spin relaxation processes. In particular, fluctuating dipole-dipole couplings drive two-spin flip-flop transitions, called cross-relaxation or the nuclear Overhauser effect (NOE), at rates that depend on a distance R as R^{-6}. Measurements of NOEs provide the most important structural constraints in determinations of biomolecular structures in liquids by NMR.

(3) Scalar or indirect spin-spin couplings, typically 1-100 Hz. These are interactions between pairs of nuclear spins that are mediated by electron spins in orbitals that encompass both nuclei. Scalar couplings are often called "through-bond" couplings, to distinguish them from the "through-space" dipole-dipole couplings. Scalar couplings permit the transfer of nuclear-spin polarization among nuclei that are connected by one or more chemical bonds within a macromolecule. Such polarization transfers, effected by appropriate rf pulse sequences, are essential for the assignment of NMR lines to specific atomic sites in studies of complex molecules.

(4) Electric quadrupole couplings, typically 0.1-10 MHz. These interactions occur only for nuclei with spins greater than ½. Quadrupole couplings are of limited importance in NMR studies of liquids, where they are averaged to zero by molecular tumbling, but are quite important in structural and dynamical studies of solids, especially inorganic materials.

(5) Hyperfine couplings, typically 0.01-10 MHz. These interactions between electron and nuclear spins give rise to the Knight shifts, Korringa relaxation, and related phenomena that make NMR a sensitive local probe of the electronic properties of solids. In proteins or other biological macromolecules, hyperfine couplings to artificially introduced electron spin labels or to naturally occurring paramagnetic centers can be used as sources of long-range distance constraints.

(6) Interaction with rf fields, typically 10-100 kHz. The effect of an rf pulse is to rotate the spin angular momenta of nuclei with NMR frequencies close to the rf carrier frequency. When the rf fields are strong enough to dominate internal couplings and chemical shifts, as is commonly the case, one can design sequences of rf pulses that produce a certain desired time evolution of a system of coupled nuclear spins, such as a specific pathway of nuclear spin polarization transfer or evolution that reflects only a subset of multiple competing internal interactions.

The concept of two-dimensional (2D) spectroscopy, first formulated by Jean Jeener in 1971, implemented by Richard Ernst's group several years later, is an essential ingredient of modern NMR. In a 2D NMR measurement, one applies a sequence of rf pulses that generally consists of a fixed "preparation" period in which a nonequilibrium nuclear spin state is initially excited, an incremented "evolution" period t_1 in which the spin system is allowed to evolve under Hamiltonian H_1, a fixed "mixing" period in which nuclear spin polarization transfers or other processes take place, and a "detection" period t_2 in which NMR signals are detected while the spin system evolves under Hamiltonian H_2. Fourier transformation with respect to t_1 and t_2 results in a 2D spectrum that is a function of the two frequencies n_1 and n_2. Intensity maxima in the 2D spectrum, called "cross peaks," reveal the correlations between NMR frequencies in spectra corresponding to H_1 and H_2 brought about by the mixing processes. In the simplest case, the cross peaks connect the NMR frequencies of nuclei that are coupled to one another or cross-relax with one another during the mixing period. Since the introduction of this flexible and powerful concept, numerous types of 2D spectroscopy have been developed for structural and dynamical studies of biological, chemical, and physical systems. Extensions to 3D and 4D spectroscopy, involving multiple evolution and multiple mixing periods, have become common.

Determination of biomolecular structure

One of the triumphs of modern NMR has been the development of methods for determining complete molecular structures of biological macromolecules, especially proteins, that are soluble in an aqueous environment. These methods depend on isotopic enrichment of all carbon and nitrogen sites in a protein with ^{13}C and ^{15}N (spin-½ isotopes), usually by producing the protein with genetically engineered bacteria that are grown on isotopically enriched nutrients, and on the use of 3D and 4D NMR spectroscopy to resolve the chemically shifted NMR lines of nearly all carbon, nitrogen, and hydrogen sites in the protein, to assign these lines to individual sites, and to measure enough structural parameters to determine the structure uniquely and precisely. With current methods and technology, full structures can be determined for proteins with molecular weights up to approximately 45 kilodaltons (kDa), corresponding to approximately 400 amino acid units and approximately 4,500 carbon, nitrogen, and hydrogen atoms.

In the most common approach to protein structure determination, two distinct types of multidimensional spectroscopy are employed. In the first type, used primarily for assignment of NMR lines to specific atomic sites, polarization transfers during the mixing periods are driven by scalar couplings. Thus, cross peaks appear at positions that connect the NMR frequencies of scalar-coupled (i.e., chemically bonded) nuclei. By comparing experimental cross peak connectivity patterns with the known amino acid sequence of the protein and making use of the known chemical shift ranges of the various carbon, nitrogen, and hydrogen sites of each amino acid, one can obtain nearly complete resonance assignments. In the second type of multidimensional spectrum, used primarily to obtain structural constraints, polarization transfers during one of the mixing periods are driven by NOEs. Cross peaks then appear at positions that connect the NMR frequencies of nuclei with sufficiently short internuclear distances (typically less than 0.5 nm). Several thousand NOEs are measured in large proteins. Distance measurements from NOEs are supplemented by several other types of structural constraints, including empirically calibrated dependences of scalar couplings and chemical shifts themselves on molecular structure, in order to derive structures with better than 0.1 nm precision in atomic positions.

According to Protein Data Bank statistics as of June 2003, roughly 2,600 protein structures have been determined by multidimensional NMR methods to date, while roughly 19,000 protein structures have been determined by x-ray crystallography (although a substantial fraction of these structures may be largely redundant). Although x-ray crystallography can currently be applied to much larger proteins than can NMR, certain classes of systems are generally more amenable to NMR methods than to crystallographic methods, including weakly interacting protein/protein complexes, protein/nucleic acid complexes, and partially structured states of proteins that are of relevance to the protein folding problem. NMR methods are also better suited to studies of protein dynamics, as the amplitude and time scale of molecular motions at a site-specific level can be extracted from nuclear-spin relaxation rate and NMR lineshape measurements. Most importantly, when one examines any specific multicomponent biological system, one is likely to find that neither crystallography alone nor NMR alone can answer all pertinent structural questions. For example, of the 15 proteins encoded by the HIV-1 genome, structures of three proteins (protease, reverse transcriptase, and gp120 envelope glycoprotein) were determined first by crystallography, while structures of three proteins (nucleocapsid, matrix protein, and Nef) were determined first by NMR. Structures of various fragments of three other proteins (capsid, integrase, gp41 envelope glycoprotein) have been determined by either NMR or crystallography. Partial structural information for four HIV-1 proteins (Vpu, Vpr, Tat, and Rev) was obtained by NMR methods, with no contribution from crystallography in these cases.

A separate set of NMR techniques that are under active development and exploration in a relatively small number of research groups, collectively called biomolecular solid state NMR methods, are capable of probing the structures of proteins that are not soluble in water or other isotropic liquid phases. Solid-state NMR measurements are often performed with magic-angle spinning (MAS), i.e., rotation of the sample about an axis at an angle of $\cos^{-1}\sqrt{1/3}$ with respect to the static field direction. In high fields, rapid MAS of a solid (at rotation frequencies up to 50 kHz) has the effect of averaging magnetic dipole-dipole couplings, and the anisotropy of chemical shifts to zero, thereby mimicking the effects of rapid molecular tumbling in liquids and producing high-resolution NMR spectra of polycrystalline and noncrystalline solids. Solid-state NMR methods can be applied to proteins and protein complexes that are considerably larger than 50 kDa, although the structural information obtained with these methods is generally less complete. One current target for biomolecular solid-state NMR is the structural characterization of amyloid fibrils, which are filamentous aggregates of various proteins associated with Alzheimer's disease, prion diseases, and other so-called amyloid diseases.[1] Proteins that embed in biological membranes, including proteins that act as ion channels and hormone receptors, are a second important target of solid-state NMR.[2] Amyloid fibrils are inherently noncrystalline, while membrane proteins are notoriously difficult to crystallize. In such cases, solid state NMR may be the only experimental method for obtaining site-specific, atomic-level structural constraints.

Why are high fields important?

High magnetic fields affect the feasibility and quality of NMR measurements in several ways, most simply by improving sensitivity and resolution. The signal-to-noise ratio (S/N) of an NMR measurement ideally varies with field H_0, NMR linewidth Δ, and temperature T according to the relation $S/N \propto H_0^{3/2}\Delta^{-1/2}T^{-3/2}$. The 3/2 dependence on H_0 results from linear dependences of spin polarization (high-temperature limit of a Boltzmann factor) and induced voltage (Faraday's law) on the NMR frequency and a square-root dependence of Johnson noise on the NMR frequency, assuming a fixed *Q* factor for the NMR detection circuit. In practice, the lower efficiency of the detection circuits at higher frequencies typically produces an approximately linear dependence of S/N on H_0, corresponding to an inverse quadratic dependence of experimental signal averaging time on H_0. The number of NMR lines that can be resolved in an N-dimensional spectrum varies as H_0^N, assuming a field-independent Δ and an NMR frequency range proportional to H_0. Higher fields, therefore, allow NMR experiments to be carried out on systems of greater complexity, both because the number of NMR lines (i.e., number of inequivalent atomic sites) increases with increasing complexity and because the available quantity of material generally decreases with increasing complexity.

In addition to the rather obvious improvements in sensitivity and resolution described above, higher fields result in less obvious but equally important advantages that arise from the field dependences of spin interactions and spin relaxation processes. For example, in NMR spectroscopy of proteins in aqueous solution, an anomalous reduction in certain ^{13}C and ^{15}N NMR linewidths has been observed at fields in the 17-21 T range.[3] This linewidth reduction is due to destructive interference between two sources of coherence dephasing (or transverse spin relaxation)—namely, dephasing due to fluctuating dipole-dipole couplings, which are independent of H_0, and dephasing due to fluctuating chemical shifts, which depend linearly on H_0. Not only does this effect (referred to by the acronym TROSY, for “transverse relaxation optimized spectroscopy”) produce improvements in spectral resolution, but it also results in significant improvements in sensitivity in multidimensional NMR experiments on large proteins and protein complexes. In such experiments, the sensitivity is limited by signal losses from transverse spin relaxation during polarization transfers in the mixing periods. Reductions in transverse relaxation rates due to the TROSY effect therefore result in greater signal intensities.

The combined effects of higher sensitivity, higher resolution, and TROSY at high fields have recently allowed several groups to obtain high-quality multidimensional NMR data of surprisingly large proteins and protein complexes. For example, 3D and 4D NMR methods have been used to resolve and assign nearly all ^{1}H, ^{13}C, and ^{15}N NMR signals from backbone atoms of an 81.4 kDa protein, the enzyme malate synthase G.[4] High-quality 2D NMR spectra correlating the chemical shifts of backbone ^{15}N and directly bonded ^{1}H sites have been obtained for the 10 kDa bacterial protein GroES in a multimeric complex with the bacterial protein GroEL with a total molecular weight of approximately 900 kDa.[5] Although determination of full molecular structures of proteins of this size by NMR has not yet been achieved, it is almost certain that significant progress in this direction will be made over the next several years.

Additional advantages associated with higher fields can arise from field dependences of the physical properties of the samples themselves. In the case of soluble proteins, very high fields can induce a small but measurable departure from the purely isotropic molecular tumbling that occurs in zero field. Under anisotropic tumbling, nuclear magnetic dipole-dipole interactions no longer average to zero. Measurements of residual dipole-dipole couplings in high fields can then be used as new sources of structural constraints, providing information about the direction of individual chemical bonds relative to a common molecule-fixed axis system.[6]

High magnetic fields in other areas of NMR

Of course, high fields also have a significant impact on applications of NMR to nonbiological problems. In addition to the improvements in sensitivity and resolution expected on general grounds as described above, specific field-dependent factors amplify the importance of high fields in certain classes of systems. For example, the structural and dynamical properties of inorganic materials containing nuclei such as ^{27}Al and ^{17}O, both of which are quadrupolar, spin-5/2 nuclei, can be studied by solid-state NMR methods. Under MAS, first-order quadrupole couplings are averaged to zero, but orientation-dependent second-order quadrupole shifts still produce significant broadening of the NMR lines, masking the chemical shift differences that are most useful as structural signatures. Because second-order quadrupole effects vary inversely with H_0 and chemical shifts vary linearly with H_0, ^{27}Al and ^{17}O NMR spectra of disordered solids (and spectra of other quadrupolar nuclei) have considerably better resolution and higher information content at the highest available fields than at lower fields. High fields are therefore essential for NMR studies of systems such as industrial zeolite catalysts, inorganic glasses, and minerals of geological interest.[7]

In condensed matter physics, the availability of high magnetic fields with the stability and homogeneity required for NMR spectroscopy permits NMR studies of phenomena that occur intrinsically at high field. Examples include studies of the properties of 2D electron systems in the quantum Hall effect and fractional quantum Hall effect regimes[8] and studies of field-induced magnetic ordering in quasi-2D transition metal oxides.[9]

Finally, the quality of anatomical images obtained with MRI has been found to increase substantially as the fields used for whole-body imaging have increased from 1 T to the current maximum value of 8 T.[10] In MRI, higher sensitivity permits higher spatial resolution. The relatively recent and revolutionary development of functional MRI[11] (fMRI) as a means of measuring the spatial localization of brain activity in response to motor tasks, sensory input, and even cogitation on moral dilemmas[12] also stands to benefit from the higher sensitivity that accompanies higher fields, especially because fMRI studies depend on the detection of subtle differences in MRI image intensities observed with and without an external stimulus. ■

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New Study on Opportunities in High Magnetic Field Science

The National Science Foundation has agreed to support a proposal from the BPA and its Solid State Sciences Committee for an assessment of high magnetic field (HMF) science. The study, which will be carried out by the NRC's Committee on High Magnetic Field Science (COHMAG), will inform the future planning of the field by NSF and other federal agencies. The report will also highlight the compelling nature of the science in this dynamic field. In recent years this field—like others centered around state-of-the-art physics-based instrumentation—has become increasingly important to other disciplines, including biology. The last major report in this field was published in 1988 following an NSF panel study. That study recommended the establishment of a National High Magnetic Field Laboratory, which was created by NSF in 1990. The original science drivers identified 13 years ago now need to be reconsidered. The instrumentation has evolved considerably, and new possibilities have opened up. Consequently, an assessment of future opportunities and initiatives is timely. The new study will assess the current state of and future prospects for high magnetic field science and instrumentation in the United States.

The number of research articles based on NMR and MRI techniques published each year has grown significantly over the last decade, particularly in medicine and biology, but also in chemistry and physics. The most rapidly growing applications are the use of MRI in medicine and the use of NMR in structural genomics and biology. Protein structure determinations using NMR require very high fields to obtain the needed spectral resolution. Advanced MRI requires high magnetic fields in large volumes. These requirements are driving magnet technology development.

In the last decade, the annual number of protein and nucleic acid structure determinations by NMR grew by a factor of 10. Even stronger growth occurred in x-ray structure determination, and within that growth, the role of synchrotron light sources in this work has increased dramatically. In addition to structure determinations, NMR sheds light on other aspects of large, complex biomolecules, including molecular recognition, catalysis, protein folding, and conformational equilibria. These aspects give insight into the *function* of biomolecules as well as their structure, a key part of the program of biology over the next decade. Time-resolved studies of changes in tissue are possible. Chemical and physical processes such as diffusion and the action of enzymes can be studied in living tissues.

High magnetic fields play an important role in research in chemistry and physics as well as biology. In physics, low-dimensional electron systems can be prepared and studied through the use of high fields, probing possible new phases of matter in semiconductors and shedding light on how disorder arises at the microscopic level. Likewise, new magnetic materials that can operate in tesla-scale magnetic fields will be required to advance electronic storage media technology.

The challenge of creating next-generation HMF instruments is considerable. In particular, a major challenge is developing the magnetic system for a 1.2-GHz NMR machine. This study will outline the science drivers that make such a system desirable and will also consider the feasibility of developing the required magnets. Similar challenges exist for other instruments that use high magnetic fields. The assessment will be carried out in the context of the science outlook for other materials characterization techniques, including neutron scattering, x-ray studies, and ultrasound.

The purpose of this study is

(1) To assess the current state and future prospects of HMF science and technology in the United States.

(2) To assess the current status of U.S. high-field efforts in the international arena. What are the trends in the this arena?

(3) To identify particularly promising multidisciplinary areas for research and development with respect to high magnetic fields.

(4) To discuss and prioritize any major new initiatives in the construction of high-field magnets for the coming decade.

A committee of approximately 15 members with a diversity of expertise is currently being assembled and is expected to hold its first meeting by mid-autumn of 2003. The first meetings will concentrate on data gathering on the key HMF science opportunities as well as considering the challenges involved in realizing those opportunities. The later meetings will focus on writing the report. The committee will solicit community input through a town meeting at an appropriate research conference and through a general solicitation via e-mail. In addition, the committee will consider conducting a small number of site visits as appropriate. The committee will produce a report of up to 100 pages. ■

BPA Meeting (continued from page 3)

ence the committee has taken on a number of tasks, ranging from advice to the agencies in the form of letter reports on various missions (AXAF, SIRTF, and SIM, among others) to policy studies (*Federal Funding of Astronomy Research* and *U.S. Astronomy and Astrophysics: Managing an Integrated Program*), as well as scientific reports on a number of topics (cosmology, space astronomy). In addition, the CAA oversaw the successful initiation of the most recent Astronomy and Astrophysics Survey. Currently, the CAA is contemplating three new tasks—a solar system formation research briefing, a gravity research briefing, and a new study on the complementary nature of ground and space observatories—and is keeping tabs on a number of issues in the astronomy community, including the progress of the James Webb Space Telescope and the activities of the National Astronomy and Astrophysics Advisory Committee (NAAAC).

CAMOS

The Committee on Atomic, Molecular, and Optical Sciences (CAMOS), which has its origins in the Committee on Atomic and Molecular Science, predates the Board on Physics and Astronomy. Today, CAMOS strives to provide a means by which federal agencies can obtain technical information and assistance from the NRC through the initiation and oversight of studies concerning AMO science and its multidisciplinary connections with other fields of science and technology. In addition, the committee provides a forum for discussion among AMO scientists and between the AMO community and the program staff of federal agencies, thereby providing a unifying force for this diverse and varied field. The committee is currently chaired by Professor Pierre Meystre from the University of Arizona in Tucson.

Reports from studies initiated by CAMOS have included research briefings entitled *Ion Storage Rings for Atomic Physics Research* (1988); *The State of Theoretical Atomic, Molecular, and Optical Sciences in the United States* (1987); and the science fact sheets *Using Light to Cool, Confine, and Position Atoms,; Carbon Fullerenes;* and *Atomic Clocks*. The committee also jointly oversaw *Database Needs for Modeling and Simulation of Plasma Processing* in 1996 with the Plasma Science Committee. The committee is currently considering the next field assessment and outlook to follow up on the 1994 report *Atomic, Molecular, and Optical Science: An Investment in the Future* (FAMOS Report). This fieldwide assessment and outlook will also follow up on the successful CAMOS report *Atoms, Molecules, and Light—AMO Science Enabling the Future,* which was published in 2002 as an accessible text on the cutting edge of AMO science.

CAMOS is also actively working with the Committee on Astronomy and Astrophysics on a proposal for a study on Laboratory Astrophysics as well as forging new links to the other BPA standing committees, starting with the Solid State Science Committee.

PLSC

The Plasma Science Committee (PLSC) was created by the National Research Council in 1989, upon recommendation of the executive committee of the Division of Plasma Physics (chaired at that time by Charles Kennel) of the American Physical Society. Initially funded by NSF, DOE, NASA, and ONR, the PLSC became a standing committee of the NRC under the Board on Physics and Astronomy. The original terms of reference were to appraise the development of plasma science as a whole, to foster a sense of unity and commonality in the field, to promote the teaching of plasma science, to assess the need for new facilities, to encourage interagency cooperation, and to oversee the interfaces of plasma science with other sciences. The first committee was chaired by Dr. Kennel (then at UCLA) and vice-chaired by Francis Perkins (then at Princeton University).

Since its inception, the PLSC has undertaken several significant projects. First, it cosponsored, with the Office of Naval Research, a workshop on non-neutral plasmas that brought together many of the loosely affiliated practioners. Next, it sponsored a study on plasma processing of materials that recommended a concerted focus of funding, computer-aided design, and cooperation on the rapidly growing field of plasma processing; the report *Plasma Processing of Materials: Scientific Opportunities and Technological Challenges* was released in 1991. The 1995 Panel on Opportunities in Plasma Science and Technology released the decadal assessment *Plasma Science: From Fundamental Research to Technological Applications* and was chaired by Clifford Surko and John Ahearne. It helped lead to the reorganization of the Office of Fusion Energy Sciences in DOE to accommodate a stronger science focus and played a role in developing the DOE/NSF partnership fund for basic plasma science. The plasma processing community received another boost from the PLSC in 1996 with the release of *Database Needs for Modeling and Simulation of Plasma Processing*, chaired by David Graves and Mark Kushner, which resulted in additional federal and industry funding and the launching of many new careers in the field. The Kennel panel's report in 2001, *An Assessment of the Department of Energy's Office of Fusion Energy Sciences Program*, brought new vision and vigor to the field, developing the Snowmass and FESAC consensus-building processes and drawing attention to the issue of workforce development. Just this past year, the PLSC oversaw the completion of a report on high-energy-density physics, *Frontiers in High Energy Density Physics: The X-Games of Contemporary Science*, under chair Ron Davidson, which is building new bridges between astrophysics, stockpile stewardship, and plasma physics. John Ahearne and Raymond Fonck are currently leading the Burning Plasma Assessment Committee in an effort to assess the need (and the readiness) for a burning plasma experiment; its interim report in December 2002 was instrumental in reopening negotiations for U.S. participation in ITER.

SSSC

The Solid State Sciences Committee (SSSC) is a continuing interdisciplinary body with expertise in solid-state physics, solid-state chemistry, electronic materials, metallurgy, polymers, and the basic materials science aspects of ceramics. The committee is convened to monitor the nature of the needs of the materials physics research, development, and applications community, particularly in connection with research opportunities and support, and to provide guidance to federal agencies regarding their materials sciences research programs.

Since its inception, the SSSC has produced assessments of the field such as *Condensed-Matter and Materials Physics: Basic Research for Tomorrow's Technology* (1999) and *Biomolecular Self-Assembling Materials: Scientific and Technological Frontiers* (1996). The committee has also established the need for national synchrotron, neutron, and other user facilities through reports such as *Letter Report on Spallation Neutron Source* (2000) and *Current Status of Neutron-Scattering Research and Facilities in the United States* (1984). The SSSC also promoted dialogue and communication with the scientific community, government, and the general public through the release of the popular booklet *The Physics of Materials: How Science Improves Our Lives* (1997).

The SSSC has organized a series of workshops called "The Materials Forum"—more recently in cooperation with the National Materials Advisory Board—to promote dialogue and interaction between and among the key players in materials science and engineering—namely, representatives from government, academia, and industry. Recent forums were *Materials and Society: From Research to Manufacturing* (2003) and *Materials in the New Millennium: Responding to Society's Needs* (2001). The SSSC's current projects include a study on smaller facilities, planned studies on biomolecular materials and high magnetic field science, and the convening of the Materials Roundtable.

Reflecting the increasingly interdisciplinary nature of condensed matter and materials physics research, the SSSC is forging new links and strengthening current relationships with other NRC boards and committees such as the National Materials Advisory Board, the Board on Life Sciences, the Board on Chemical Sciences and Technology, and the BPA's Committee on Atomic, Molecular, and Optical Sciences. Finally, the SSSC is considering the next assessment and outlook for condensed matter and materials physics. This forward-looking study will identify new opportunities while reviewing the current status of the field. Among the issues the report would address are the compelling science at the frontiers of nano-research, the opportunities for theory and advanced computation, the promise of quantum phenomena and lower-dimensional structures, the connections to other fields, including AMO physics, biology, and chemistry; meeting national needs through innovations in science and technology; and identifying paths to strengthen the U.S. materials research portfolio and the national suite of facilities. ■

BPA's New Home Gets a New Name

ON April 15, 2003, the National Academies and the W.M. Keck Foundation of Los Angeles announced a 15-year, $40 million grant from the foundation to underwrite the National Academies Keck Futures Initiative, a new program designed to realize the untapped potential of interdisciplinary research.

Photo credit T.I.Meyer

The Keck Futures Initiative will stimulate new modes of inquiry and help to break down conceptual and institutional barriers to interdisciplinary research. Specifically, the program will engage scientists, engineers, and health professionals in identifying new questions that can guide cutting-edge avenues of interdisciplinary research and will encourage and reward outstanding communication between disciplines as well as between the scientific, engineering, and health communities and the public. (The Keck Foundation helped support several BPA projects in the past, including the recent astronomy and astrophysics decadal survey.) Many people throughout the Academies played a role in bringing the grant and the Futures Initiative to fruition, and the BPA is deeply grateful for their work and creativity.

In recognition of the Keck Foundation's foresight and strong support, the 500 Fifth Street building has been named the Keck Center of the National Academies. The Keck Center was formally dedicated on May 13, 2003, in a ceremony in the new Center's atrium. (Please note, however, that the our mailing address has not changed.) We welcome your visit to the new building! ■

THE BPA Web site at **www.national-academies.org/bpa** provides news on recently released reports and other developments as well as a link to this newsletter in PDF format. Reports may be ordered at **www.nap.edu**.

Recent Reports:

Frontiers in High Energy Density Physics: The X-Games of Contemporary Science

Neutrinos and Beyond: New Windows on Nature

Burning Plasma Assessment Committee Letter Report

Coming Soon:

Final Report of the Burning Plasma Assessment Committee

Report of the Committee on Setting Priorities for NSF-Sponsored Large Research Facility Projects

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