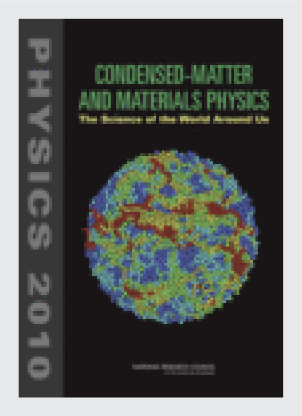

# Condensed-Matter and Materials Physics: The Science of the World Around Us

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# CONDENSED-MATTER AND MATERIALS PHYSICS

## The Science of the World Around Us

Committee on CMMP 2010

Solid State Sciences Committee

Board on Physics and Astronomy

Division on Engineering and Physical Sciences

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---

[1] Laura Garwin resigned from the committee in October 2006.
[2] Frances Hellman resigned from the committee in September 2006.

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# Preface

The National Research Council (NRC) of the National Academies convened the Committee on CMMP 2010 to study the opportunities and challenges in condensed-matter and materials physics (CMMP) in the next decade. The Solid State Sciences Committee (SSSC) of the NRC's Board on Physics and Astronomy developed the charge for this study in consultation with the study's sponsors at the Department of Energy and the National Science Foundation. The Committee on CMMP 2010 was charged to identify recent accomplishments, compelling scientific questions, and new opportunities in the field; to identify CMMP's potential future impact on other scientific fields; to consider how CMMP contributes to meeting national societal needs; to identify, discuss, and suggest priorities for the construction, purchase, and operation of tools and facilities; to examine the structure and level of the current research effort and funding for research; and to make recommendations on how to realize the full potential of CMMP research. The complete charge is presented in Appendix A. The report is part of the ongoing Physics 2010 survey, the latest decadal assessment of and future outlook for the field of physics conducted under the auspices of the Board on Physics and Astronomy.

In preparing for the decadal survey of CMMP, the SSSC called on the community for input on opportunities and challenges in the field. This input was compiled and presented to the Committee on CMMP 2010 at its first meeting, in February 2006. In addition, the committee received direct input from the community at five town meetings held at professional society meetings—the March (2006) meeting of the American Physical Society in Baltimore, Maryland; the spring meeting (March 2006) of the American Chemical Society in Atlanta, Georgia; the spring meeting

(April 2006) of the Materials Research Society in San Francisco, California; the fall meeting (November 2006) of the Materials Research Society in Boston, Massachusetts; and the March (2007) meeting of the American Physical Society in Denver, Colorado. The committee thanks the professional societies for their support and encouragement in helping to arrange these town meetings. The committee also solicited community input through nine focus groups at universities and national laboratories, each with an attendance of between 10 and 15 researchers. The committee thanks the hosts at these institutions for arranging these important sessions, at which the discussions were lively and enlightening. The committee also solicited input through a public Web site. The comments supplied by the CMMP community through these venues provided extremely valuable primary input to the committee.

The committee that prepared this report is composed of experts from many different areas of CMMP research, prominent scientists from outside the field, and leaders from industry (see Appendix D for biographical sketches of the committee members). The committee met in person four times (see Appendix B) to address its charge, forming subcommittees to study different aspects in greater depth. The committee thanks the speakers who made formal presentations at its meetings; those presentations and the ensuing discussions strongly informed the committee's deliberations.

The federal agencies that fund CMMP research in the United States also provided input to the committee, through their direct testimony at committee meetings and their written responses to requests for information on funding trends and other statistical data. These data are summarized in Chapter 10 of the report. The committee is also grateful to the staffs at the Office of Science and Technology Policy and the Office of Management and Budget for their input on connections between CMMP and national science policy.

In September 2006, the committee released a short interim report that summarized important opportunities and challenges for CMMP research in the coming decade.[1] That report was used as a basis for subsequent discussion with the CMMP community at town meetings and focus groups. This, the committee's final report, expands on these themes, discusses them in further detail, and provides recommendations for further advancement of the field.

To help address the charge to identify, discuss, and suggest priorities for the construction, purchase, and operation of tools and facilities, the committee convened a workshop in January 2007 to hear from members of the community and the federal agencies on future facility needs for CMMP researchers. Appendix C provides further details on this workshop. The committee expresses its apprecia-

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[1] National Research Council, *Condensed-Matter and Materials Physics: The Science of the World Around Us: An Interim Report*, Washington, D.C.: The National Academies Press, 2006.

tion for the input received from the 30 presenters and more than 70 participants in that workshop.

As co-chairs, we are grateful to the committee members for their wisdom, cooperation, and commitment to ensuring the development of a comprehensive report. The report reflects the committee's heartfelt enthusiasm for the field of CMMP and its future potential and past accomplishments. Finally, we also thank the NRC staff (Natalia Melcer, Donald Shapero, Phillip Long, and Caryn Knutsen) for their guidance and assistance throughout the development of this report.

Mildred S. Dresselhaus, *Co-Chair*
Committee on CMMP 2010

William J. Spencer, *Co-Chair*
Committee on CMMP 2010

# Acknowledgment of Reviewers

This report has been reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise, in accordance with procedures approved by the National Research Council's (NRC's) Report Review Committee. The purpose of this independent review is to provide candid and critical comments that will assist the institution in making its published report as sound as possible and to ensure that the report meets institutional standards for objectivity, evidence, and responsiveness to the study charge. The review comments and draft manuscript remain confidential to protect the integrity of the deliberative process. We wish to thank the following individuals for their review of this report:

Gordon A. Baym, University of Illinois at Urbana-Champaign,
Malcolm R. Beasley, Stanford University,
Paul M. Chaikin, New York University,
Elbio Dagotto, University of Tennessee and Oak Ridge National Laboratory,
Robert R. Doering, Texas Instruments, Inc.,
Martha A. Krebs, California Energy Commission,
James S. Langer, University of California at Santa Barbara,
Allan H. MacDonald, University of Texas at Austin,
Jose N. Onuchic, University of California at San Diego,
Julia M. Phillips, Sandia National Laboratories,
Sunil K. Sinha, University of California at San Diego,
Maury Tigner, Cornell University,
John Tranquada, Brookhaven National Laboratory,

Dale J. Van Harlingen, University of Illinois at Urbana-Champaign, and
Thomas A. Witten, University of Chicago.

We also wish to thank the following individuals for their review of the committee's interim report:

Elihu Abrahams, Rutgers University,
Frank S. Bates, University of Minnesota,
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J.C. Séamus Davis, Cornell University,
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Peter G. Wolynes, University of California at San Diego.

Although the reviewers listed above have provided many constructive comments and suggestions, they were not asked to endorse the conclusions or recommendations, nor did they see the final draft of the report before its release. The review of this report was overseen by Venkatesh Narayanamurti, Harvard University. Appointed by the NRC, he was responsible for making certain that an independent examination of this report was carried out in accordance with institutional procedures and that all review comments were carefully considered. Responsibility for the final content of this report rests entirely with the authoring committee and the institution.

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# Summary

Condensed-matter and materials physics (CMMP) is the science of the material world around us. Long ago, curiosity about the natural world led to questions about condensed-matter systems, such as water, snow, ice, and rocks, and how these respond to light, heat, and mechanical forces. This thirst for fundamental understanding has been inextricably tied to the desire to manipulate nature by harnessing its properties or creating new materials to serve human needs. The inherent intertwining of pure and applied research defines and enriches the CMMP enterprise to this day. This report surveys the field of CMMP during the past decade, including the state of federal and private support of CMMP within the United States, and looks ahead to the intellectual and technological challenges of the coming decade.

The 20th century was a period of remarkable fundamental and technological progress in CMMP. Continued federal and private investments led to considerable advances in the basic understanding of condensed-matter phenomena. Years and often decades later, these advances led in turn to the invention of devices that now form the basis of much of our technological society, including the transistor, the integrated circuit, the laser, magnetic resonance imaging, liquid-crystal displays, and, more recently, high-efficiency solid-state lighting. U.S. leadership in nurturing invention, from initial scientific discoveries to commercial technological products, has contributed significantly to this nation's economic strength. In particular, the industrial development of many of these technologies has led to current U.S. leadership in computing and global communications. Although the relationship is difficult to measure quantitatively, there is a consensus among economists that advances in technology have been the main driver of economic growth over the past 60 years.

In this report, the Committee on CMMP 2010 looks ahead to ask: What are the prospects for CMMP in the early part of the 21st century? One of the main findings of the report is the identification of six grand challenge areas in which CMMP research is poised to have a large and enduring impact in the next decade. These research areas reflect both fundamental intellectual challenges and societal challenges, in keeping with CMMP's dual pure and applied nature. While CMMP has been developing many of the key tools and is central to addressing many of these challenge areas, meeting all of the challenges successfully will require the combined efforts of researchers from many disciplines in order to succeed. The broad spectrum of research covered by CMMP includes many important problems beyond those identified in this report, and areas currently not foreseen are certain to arise from discoveries in the next decade. Nonetheless, as CMMP moves into the next decade, the intellectual vitality and breadth of the field are captured to a considerable extent in the following challenges:

- How do complex phenomena emerge from simple ingredients?
- How will the energy demands of future generations be met?
- What is the physics of life?
- What happens far from equilibrium and why?
- What new discoveries await us in the nanoworld?
- How will the information technology revolution be extended?

U.S. CMMP researchers will not be alone in tackling these challenges. The United States remains a leader in CMMP worldwide, but its premier position is in jeopardy. There are several contributing factors, which are detailed in Chapters 9 and 10 of this report:

- Other parts of the world are investing heavily in research and development (R&D) in CMMP.
- In the United States, industrial laboratories are now focused on much-shorter-term R&D goals, with little emphasis on fundamental, basic research.
- Federal research funding for CMMP has been approximately flat in the United States in inflation-adjusted dollars over the past decade.

The consequences of the decline of industrial involvement and nearly flat federal funding for CMMP are serious indeed:

- Many of the key technological innovations responsible for U.S. leadership in communications and computing were shepherded from fundamental research ideas to marketable products at the once-great industrial laboratories. The replacement of these industrial laboratories as sources of invention is a challenge.

- Many of today's leaders at the nation's universities, national laboratories, and other institutions came from industrial laboratories where they were able to conduct high-risk fundamental research with relatively little funding pressure. The opportunities for cooperation, leadership, and creativity experienced by researchers in these settings have greatly benefited the overall scientific enterprise. Currently, very few such research environments are available to young researchers to nurture their professional growth.
- At the National Science Foundation (NSF), a major supporter of university-based CMMP research, the chances of a grant application in CMMP being funded have dropped dramatically in the past 5 years, from 38 percent to 22 percent.[1] These low proposal-success rates greatly amplify the hidden "overhead" of writing and reviewing proposals and disrupt the continuity of scientific research. The corresponding numbers for new investigators show a drop from 28 percent to 12 percent; this lack of access to research funding severely impedes the establishment of viable research programs before tenure evaluation. These trends must be reversed.
- Strong support for principal investigators is particularly important for CMMP research, a field in which most investigators work in individual research groups or in small teams. Strong, healthy individual-investigator research programs are needed for effective, evolving collaborative efforts and for transitioning in and out of larger collective research activities.
- During the past 5 years, the size of grants increased only 15 percent, while the cost of supporting students increased by 25 percent, in as-spent dollars. Thus, the buying power of each dollar is also a concern.
- Over the past decade, the number of publications contributed by U.S. authors remained essentially flat in two major journals reporting CMMP research results worldwide (*Physical Review B* and *Physical Review E*), whereas foreign contributions nearly doubled in the same time frame.

## RECOMMENDATIONS

The Committee on CMMP 2010 bases the following recommendations on its assessment regarding the most efficient use of resources and projected growth in funding for the field of 7 percent per year over the next 10 years. This rate of growth reflects levels recommended in the President's American Competitiveness

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[1] These statistics are based on data gathered by the committee from the federal agencies and are discussed in further detail in Chapter 10.

Initiative, which seeks a doubling of the physical science research budget of the NSF, the Department of Energy (DOE), and the National Institute of Standards and Technology (NIST) in 10 years. In some cases, improved research quality and efficiency can be obtained through changes in the structure of funding. In other cases, additional funding is necessary in order to retain current expertise and to nurture emerging fields of science. Some new facilities are also required to advance science and to keep the U.S. research effort at the forefront. The committee's most important recommendations are presented below. More recommendations are found in Chapters 8 through 11 of the report.

**Recommendation 1:** Basic research in CMMP contributes to the economic strength and leadership of the United States. The following three recommendations to DOE and NSF (found in Chapter 10) are aimed at ensuring scientific progress toward meeting the challenges identified in this report and ensuring continued technological innovation to benefit the United States:

- Strong support should be maintained for individual and small groups of investigators, which are historically the primary source of innovation in CMMP. The ratio of support for individual and small groups of investigators relative to support for centers and facilities should not decline in the next decade.
- The average success rates for the funding of proposals should be increased to more than 30 percent over the next 5 years in order to give junior scientists the opportunity to obtain research results before the tenure decision and to enable currently funded researchers to maintain continuity in their research programs.
- The size of grants to individual and small groups of investigators should be increased to maintain the buying power of the average grant and to retain scientific talent in the United States.

**Recommendation 2** (from Chapter 8): Funding agencies should develop more-effective approaches to nurturing emerging interdisciplinary areas for which no established reviewer base now exists. The CMMP community should organize sessions at national meetings to engage funding agencies and the community in a dialogue on best practices for proposal review and for the support of nontraditional, rapidly evolving areas.

**Recommendation 3** (from Chapter 8): Outreach, K-12, and undergraduate science education initiatives should be supported through supplemental or stand-alone grants administered by separate NSF and DOE programs, instead of through individual research grant awards. In the present system, the quality of outreach programs is a criterion in the evaluation of NSF/Division of Materials Research grants. The present approach confuses two conceptually distinct goals to the point that neither is optimally served. The funding agencies and the research community both want outreach programs to succeed, and they should confer to determine how best to implement an effort to achieve that goal.

**Recommendation 4** (from Chapter 10): The CMMP community should work to improve the representation of women and underrepresented minorities in CMMP through mentoring; providing flexible working conditions, day-care opportunities, and viable career paths; and developing outreach programs targeted to students and the public and aimed at increasing the numbers of prospective researchers.

**Recommendation 5** (from Chapter 10): The Office of Science and Technology Policy (OSTP) should convene a study with participation from DOE, the Department of Defense, NSF, NIST, the physics community, and U.S. corporations to evaluate the performance of research and development activities that might replace the basic science previously done by the large industrial laboratories and the contributions that those laboratories made to the training of future scientific leaders and educators. This next decade will involve a series of new approaches to long-term R&D designed to recapture the ability to work on large difficult projects based on fundamental CMMP research. Such an evaluation should be an ongoing activity of OSTP since it may be several years before the performance of these activities can be adequately evaluated.

**Recommendation 6** (from Chapter 11): DOE and NSF should develop distributed national facilities in support of the design, discovery, and growth of new materials for both fundamental and applied CMMP research.[2]

**Recommendation 7:** State-of-the-art instrumentation and facilities are critical to CMMP and will be even more critical during the next decade. The committee's top-priority recommendations for instrumentation and facilities (all taken from Chapter 11) follow below. The committee also recommends action on the priorities for mid-scale instrumentation identified in a recent National Research Council (NRC) report.[3] Further recommendations on light sources, neutron sources, electron microscopy, magnetic field facilities, and nanocenters are offered in Chapter 11.

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[2] A current National Research Council study, "Assessment of and Outlook for New Materials Synthesis and Crystal Growth," will make detailed recommendations on how best to support this need. The report is expected to be released in the summer of 2008.

[3] National Research Council, *Midsize Facilities: The Infrastructure for Materials Research*, Washington, D.C.: The National Academies Press, 2006.

- DOE and NSF, partnering with the National Institutes of Health and NIST, should create a consortium[4] focused on research and development needs required for next-generation light sources. The consortium, with an independent chairperson, should include stakeholders from universities, industry, and government (both laboratories and agencies). The consortium should formulate a light source technology roadmap and make recommendations on the research and development needed to reach milestones on the roadmap for a new generation of light sources, such as seeded x-ray free-electron lasers, energy-recovery linear-accelerator-driven devices, and other promising concepts. The consortium should also take into account cost containment and the internationalization of research facilities. The sponsoring agencies of the consortium should fund the R&D needed to reach the milestones on the roadmap.
- DOE should complete the instrument suite for the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, together with provision of state-of-the-art ancillary equipment for these instruments, in order to gain the maximum benefit from the recent investment in the SNS.
- DOE and NSF should support the CMMP community's needs for electron microscopy instrumentation at universities on a competitive basis. Cutting-edge electron microscopy technique development (such as the DOE TEAM [Transmission Electron Aberration-corrected Microscope] project) should be continued in order to fully reestablish U.S. competitiveness in developing the next generation of electron microscopes.
- NSF should continue the support of the National High Magnetic Field Laboratory and high-magnetic-field instrumentation development following the priorities recommended by the NRC report *Opportunities in High Magnetic Field Science.*[5]

Without strong support for basic research, U.S. leadership in CMMP is unlikely to survive. Such a loss could cause the United States to miss critical opportunities in growing new markets and could significantly hamper U.S. economic innovation. The recommendations of the Committee on CMMP 2010 focus on ensuring U.S. leadership in this intellectually exciting field that is technologically and economically vital to the nation.

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[4] The committee used the term "consortium" in the sense of a partnership among the stakeholders described in the recommendation for developing a light source technology roadmap. The committee expects that the "consortium" will follow federal rules for providing advice to federal agencies.

[5] National Research Council, *Opportunities in High Magnetic Field Science*, Washington, D.C.: The National Academies Press, 2005.

# 1

# Overview

In the past decade, the field of condensed-matter and materials physics (CMMP) has enlarged its scope enormously, embracing a far wider range of problems than ever before. At the heart of CMMP is the quest to understand, through a combination of experimental, theoretical, and computational investigations, how unexpected phenomena emerge when large numbers of constituents interact with one another. These constituents, traditionally electrons, atoms, and molecules, have now been extended to a vast array, including complex biological molecules, nanoparticles, cells, and even grains of sand. In addition, researchers are now applying CMMP approaches and techniques to interacting systems of constituents such as Internet nodes, economic transactions, and entire organisms. This tremendous range of constituents leads to a spectacular diversity of emergent phenomena. By understanding these phenomena, CMMP researchers affect people's lives in countless ways, from improving our understanding of nature to developing new technologies.

Historically reliable drivers for the discovery of new emergent phenomena are new materials and devices. Examples of materials and phenomena first targeted by CMMP researchers can be found almost everywhere: semiconductor lasers are in DVD players, advanced magnetic materials store data on computer hard drives, liquid-crystal displays show us photographs and telephone numbers. But these technological marvels tell only half the story. Studies of new materials and phenomena have also led to significant advances in our understanding of the physical world. For example, the development of ultrapure layered semiconductors made possible not only the production of high-speed transistors for cellular telephones but also the discovery of completely unexpected new states of matter, such as the fractional quantum Hall state. Efforts to understand magnets, ferroelectrics, superconductors, polymers, and liquid crystals, exploited in innumerable applications, spurred the development of the elegant, unified conceptual framework of broken symmetry that not only explains how the characteristic behaviors of these materials are related, but also underlies much of modern physics. The pure and applied aspects of condensed-matter and materials physics are opposite sides of the same coin that define and enrich the CMMP field.

## SIX SCIENTIFIC CHALLENGES FOR THE NEXT DECADE

One of the main findings of this report is the identification of six grand challenge areas in which CMMP research is poised to have a large and enduring impact in the next decade. These research areas reflect both fundamental intellectual challenges and societal challenges, in keeping with the dual pure and applied nature inherent to CMMP. While CMMP has been developing many of the needed key tools and is central to many of these challenge areas, all of them will require the combined efforts of researchers from many disciplines in order to succeed. The broad spectrum of research covered by CMMP includes many important problems outside those identified in this report, and areas currently unforeseen are certain to arise from discoveries in the next decade. Nonetheless, the challenges identified here capture much of the intellectual vitality and range of the field as it moves into the next decade. These scientific challenges, discussed in turn below, are as follows:

- How do complex phenomena emerge from simple ingredients?
- How will the energy demands of future generations be met?
- What is the physics of life?
- What happens far from equilibrium and why?
- What new discoveries await us in the nanoworld?
- How will the information technology revolution be extended?

### How Do Complex Phenomena Emerge from Simple Ingredients?

The notably successful "reductionist" approach to physics focuses on the laws that govern the motion of ever-smaller fundamental constituents of matter. Indeed, in principle, all of CMMP, not to mention chemistry and biology, is believed to follow from the solution of one simple equation, the Schrödinger equation, governing the quantum dynamics of electrons and ions. Conversely, "emergence" refers to the fact that the behavior of large, complicated systems made of many diverse building blocks is often distinct from, and even relatively insensitive to, the detailed properties of the individual constituents. Reductionism stresses the understanding that comes from studying systems at a more and more microscopic level, while emergence finds conceptual clarity in the collective behavior of large systems.

A vivid example of emergence is the brain that you are using to read and understand this page. A human brain consists of roughly 100 billion neurons. Those neurons, which in one of the most notable advances of modern biology are now reasonably well understood individually, in some sense represent the building blocks of your consciousness. Yet no one would claim to understand how this most fascinating of all natural phenomena emerges from the behavior of the individual neuron. As a simpler example, metals exhibit very similar macroscopic properties, despite the fact that they might be made of copper atoms, or silver atoms, or even complicated organic molecules.

CMMP, more than any other scientific discipline, seeks to understand at a quantitative level the connection between the microscopic and the macroscopic in systems with many interacting constituents. Although all material systems consist, ultimately, of the same well-understood electrons, protons, and neutrons, their aggregate behaviors are stunningly diverse and often deeply mysterious. Superconductivity, the dramatic vanishing of all electrical resistance of certain materials below a critical temperature, is one of the best-known examples of emergence. In studying superconductivity, the goal is both to characterize the amazing macroscopic quantum behaviors of the superconducting state and to understand what aspects of their microscopic structure cause certain metals to become superconductors and other metals not to.

The discovery, understanding, and application of emergent phenomena are the core activities of CMMP. New materials inevitably exhibit new and often unanticipated behaviors. Existing materials, pushed to new regimes of high purity, low or high temperatures, high pressures, or high magnetic fields, have always yielded surprises, including wholly new phases of matter. Fresh theoretical perspectives frequently bring into focus hitherto perplexing or ignored features of existing observations that reflect previously overlooked organizing principles and suggest new avenues for further experimental inquiry. The ever-increasing precision with which the properties of materials can be measured permits new ideas concerning the underlying microscopic origins of emergent behaviors to be tested with unprecedented rigor.

Emergent phenomena are not merely academic curiosities; many result in technological advances of immense societal importance. The discovery of superconductivity in 1911 ultimately enabled, decades later, magnetic resonance imaging and thereby revolutionized modern medicine (see Figure 1.1). Liquid crystalline materials, in which large numbers of asymmetric molecules in solution exhibit a dizzying variety of emergent phases, are used in everyday electronics like cell phones and laptop computers.

The diversity of emergent phenomena ensures the beauty, excitement, and deep

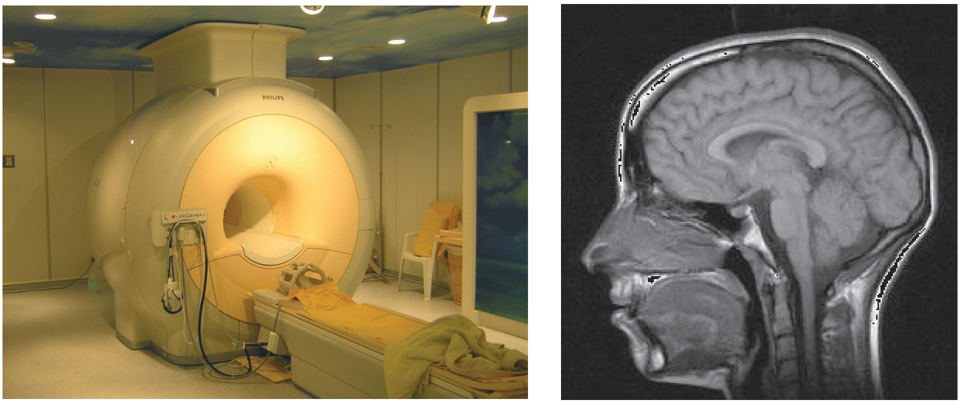

FIGURE 1.1 The emergent phenomenon of superconductivity plays a key role in magnetic resonance imaging (MRI), a technique that has revolutionized medicine. (Left) Modern high-field clinical MRI scanner. (Right) MRI scan of the brain. SOURCES: (Left) Photograph courtesy of Kasuga Huang. (Right) Image courtesy of Jon Dattorro, Stanford University.

practical utility of condensed-matter and materials physics as an inexhaustible resource. The challenge is to understand how such collective phenomena emerge, to discover new ones, and to determine which microscopic details are unimportant and which are essential.

### How Will the Energy Demands of Future Generations Be Met?

The availability of affordable and renewable energy sources represents one of the biggest challenges that will face humankind in the 21st century. The United States must develop affordable, renewable energy sources to reduce dependence on fossil fuels while minimizing carbon emissions and other sources of harm to the environment. Promising technologies for solar energy, hydrogen fuel cells, solid-state lighting, rechargeable batteries, and improved nuclear power will all play critical roles, but fundamentally new scientific approaches are also needed to address the magnitude of this challenge and its urgency effectively. CMMP is uniquely positioned to address these challenges, which require a better understanding of energy conversion and storage as well as the creation of new technologies for increasing end-use energy efficiency.

Basic scientific discoveries in these areas will provide the underpinnings for the creation of new advanced energy technologies. How can sunlight be converted to usable energy more efficiently? In what new ways can hydrogen be generated and stored? Can renewable, affordable, and benign fuels be developed? How can new approaches and new materials be used to create better light-emitting diodes and light conversion materials (see Figure 1.2)? Can new materials be developed to operate under extreme conditions, such as those found in nuclear and plasma fusion reactors and in receptacles for waste storage? Discovering and understanding new materials, especially nanostructured materials with novel materials properties, will be key to advancing the energy research frontiers. For example, new superconductors could dramatically reduce energy losses in power transmission, while new thermoelectric materials could enable the drawing of power from waste heat or geothermal energy.

No single strategy will provide all the answers, and some approaches may take decades to come to fruition, so research investment over a broad front is needed to meet this immense challenge. What is certainly clear, however, is that new materials, nanoscience, and new theoretical approaches will play a critical role in overcoming many of the technical barriers to achieving energy security.

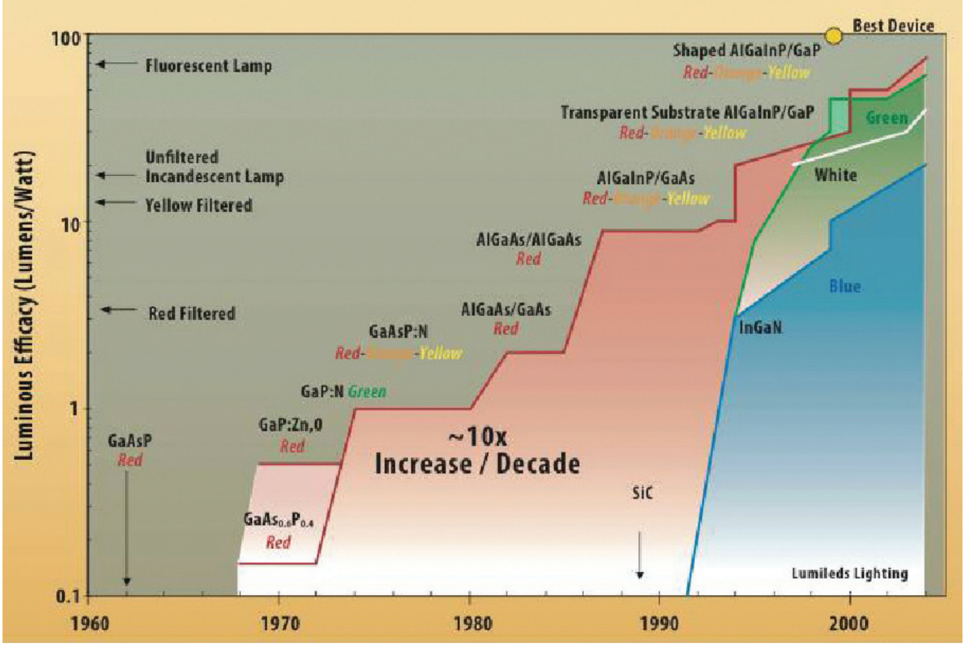

FIGURE 1.2 Comparison of the improvements in the luminous efficacy (lumens per watt) of light-emitting diodes (LEDs) with other lighting technologies (shown along the y-axis) since 1960, indicating the reality for this technology in future lighting applications. The theoretical maximum efficacy of white LEDs is about 300 lumens per watt. LED lighting has the potential to reduce overall electricity consumption in the United States by about 13 percent over the next 20 years. SOURCE: Lumileds Lighting.

## What Is the Physics of Life?

The phenomena of life offer some of the most profound challenges facing the physics community. How is it possible for functional behavior, recognized as characteristic of living systems, to emerge from inanimate matter? In the past decade, this grand but somewhat amorphous question has been sharpened into the appreciation of the physics problems that arise in thinking about specific biological systems. From bacteria to brains, from picosecond events in single molecules to evolutionary changes over millions of years, physicists are asking new questions about biological systems and providing new ways of studying them. New combinations of experimental techniques from physics and biology have uncovered a previously unimagined layer of richness and precision in the function of biological systems (see Figure 1.3). At the same time, theoretical approaches from physics have predicted new phenomena, provided solutions to classical puzzles, and generated new frameworks for the ever-expanding body of experimental data. With careful nurturing, the coming decade will see the continued emergence of biological physics as a branch of physics.

One of the central physics problems that organisms have to solve in order to survive is the problem of reliability in the presence of noise. This problem exists at many different levels of biological organization, from single molecules, to networks of molecules in single cells, to interactions among cells in complex organisms such as humans. Fundamental physical noise sources, such as the random motion of individual molecules and the random arrival of photons at the retina on a dark night, all have measurable effects on the function of biological systems. In some cases these random events provide a limit to the precision with which organisms can carry out their functions, while in other cases living systems exploit fluctuations to find their way more efficiently to a desirable state. New experimental methods are giving a direct image of these random events, sometimes literally. Theorists are trying to understand the strategies that organisms use to suppress or exploit different noise sources, and the next generation of experiments will test these ideas in their natural context. On the one hand, life is a phenomenon of extraordinary precision and intricacy, while on the other hand crucial mechanisms operate in a regime where noise is not negligible. The coming decade will bring a new understanding of this sometimes paradoxical interplay between functionality and randomness.

Physicists strive to situate the particular in terms of the general, and nowhere is this more apparent than in CMMP. Materials display a large diversity of behaviors, but over decades the CMMP community has struggled to classify these behaviors and to have general theories within which the behaviors of individual materials can be seen as examples. An important development in the physicists' attempts to understand the phenomena of life thus is the attempt to see biological phenomena as examples of a wider range of possible phenomena. Again, this idea cuts across

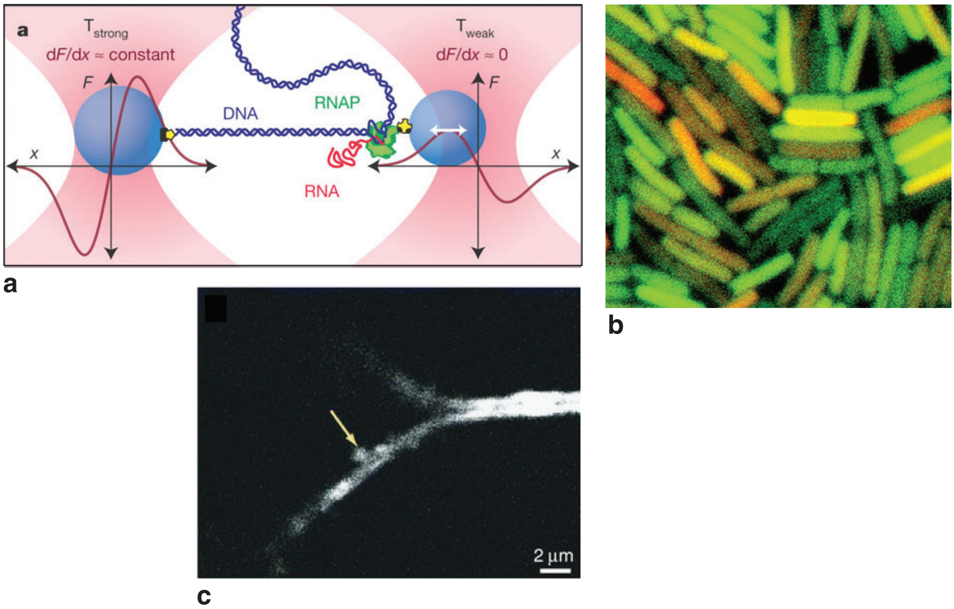

FIGURE 1.3 New questions and new methods for exploring the physics of life. (a) Optical trapping makes it possible to observe the "reading" of the genetic code by a single molecule of ribonucleic acid polymerase (RNAP), monitoring the steps from one base pair to the next along deoxyribonucleic acid (DNA). (b) Genetic engineering and fluorescence microscopy are combined to observe the intrinsic noise as cells regulate the expression of individual genes; here molecular noise is translated in changes in color. (c) Second harmonic generation from molecules dissolved in the cell membrane makes visible the dynamics of voltage changes in the submicron spine structures in the brain where cells make contact and change their properties as people learn. SOURCES: (a) E.A. Abbondanzieri, W.J. Greenleaf, J.W. Shaevitz, R. Landick, and S.M. Block, "Direct Observation of Base-Pair Stepping by RNA Polymerase," *Nature* **438**, 460-465 (2005). (b) M.B. Elowitz, A.J. Levine, E.D. Siggia, and P.S. Swain, "Stochastic Gene Expression in a Single Cell," *Science* **297**, 1183-1186 (2002). Reprinted with permission from the American Association for the Advancement of Science. (c) G.J. Stuart and L.M. Palmer, *Pflugers Archiv* **453**, 403 (2006).

many levels of biological organization. Progress is being made on understanding what makes proteins, essential molecular building blocks of life, special in the broad class of heteropolymers. Similarly, principles are being suggested that might single out what is unique about the networks of biochemical interactions in a cell as opposed to an arbitrary network. For many years physicists and biologists both have been interested in the way that molecular mechanisms of learning in the brain sculpt the dynamics of neural networks to perform particular functions, in effect selecting particular networks out of all possible ones. In the past decade, all of these problems have come into sharper focus through a combination of theory and experiment, often in vigorous collaboration. The essential tension is between the "fine tuning" of each mechanism for its particular function and the evident robustness of these functions to many variations, both in the life of one organism and over evolutionary history. The coming decade will see both practical and conceptual progress on this broad class of problems, shaping our view of how the many components of each biological system interact to achieve the functions recognized as life.

The study of biological systems has traditionally been organized around particular organisms and subsystems. Dramatic developments in biology itself have made it possible to break down some of these boundaries, so that the tools which allow researchers to explore the genetics of bacteria also can be used to explore the way in which neurons in the human brain acquire their identity and function. Physicists have gone farther, asking conceptual questions, such as those about noise and robustness described above, which cut across the classical layers of biological organization. While it remains to be seen if the physicists' questions will lead, as hoped, to a genuinely unified theoretical framework—in the same way that CMMP provides a theoretical framework for other macroscopic phenomena—the asking of these new questions has been remarkably productive and has had an impact on both the physics and biology communities. The challenge here is nothing less than to develop further a new branch of science that combines the theoretical depth and quantitative precision of physics with the beautiful and intricate phenomena of modern biology. These developments will have a profound influence on how people think about the world, on how they solve practical problems of human health, and on how they view themselves.

## What Happens Far from Equilibrium and Why?

Many of the most striking features of the world around us are far-from-equilibrium phenomena. The energy that continually strikes Earth from the Sun gives rise to far-from-equilibrium behavior ranging from chaotic weather patterns to the staggering diversity of life. If solar energy were no longer supplied, many systems on Earth would revert to the unchanging state that characterizes equilibrium. Much is understood about systems at equilibrium and near equilibrium, where systems respond as they do to naturally occurring fluctuations in the equilibrium state. However, scientists are just beginning to uncover some of the basic principles that govern a myriad of far-from-equilibrium phenomena, ranging from the molecular processes on the nanoscale that form the basis of life to the clustering of matter within the universe as a whole.

Far-from-equilibrium behavior is ubiquitous. It arises across the entire spectrum of condensed-matter and materials physics in a host of problems of fundamental interest and is intimately connected to cutting-edge materials processing.

Far-from-equilibrium behavior both benefits and plagues us in technology and in everyday life. Indeed, some of the most scientifically intriguing outcomes of behavior far from equilibrium emerge in situations familiar in everyday experience. For example, we can see turbulence in cloud patterns as well as in a bathtub; we take advantage of glassy behavior in nearly all plastics but suffer from it in traffic jams; we exploit the breaking up of a stream of fluid into droplets with fuel injection and ink-jet printing but also find it in every leaky faucet. The reach of far-from-equilibrium phenomena extends even farther, to many systems of profound societal importance. In the past decade, CMMP researchers have begun to tackle far-from-equilibrium behavior governing the workings of systems of critical national importance, including the economy, ecosystems, and the environment. As a result, breakthroughs in the area have potential for far-reaching impact across many scientific disciplines.

The microscopic origin of collective far-from-equilibrium behavior still remains largely uncharted territory. Most knowledge about how microscopic properties affect the ways in which systems with many constituent particles behave and evolve is based on a powerful formalism—statistical mechanics. However, this framework applies only to situations near equilibrium, in which a system is thermally and mechanically in balance with its surroundings, and thus it covers only a small subset of the phenomena observed around us and confronted in applications.

Within the past decade, CMMP research has set the stage for fresh approaches to long-standing problems concerning far-from-equilibrium behavior. Granular matter (Figure 1.4) has been established as a key prototype for a class of systems that exist far from equilibrium because they are trapped in configurations that structurally resemble a liquid (they are dense and highly disordered), but are unable to flow and thus they behave as solids. Systems of this type have prompted the introduction of the unifying paradigm of "jamming," which suggests that common physics underlies systems ranging from granular matter to the toughest plastics, strongest metallic alloys, concrete, paints, and foam. Ideas have flowered to describe the far-from-equilibrium aspects of living systems, ranging from mechanisms of transport within cells to the organizing principle of robustness, which suggests that living systems have been designed, through evolution and natural selection, to be robust to perturbations. This organizing principle has been connected with ideas from engineering to be applied as a mechanism of state selection in interacting networks ranging from transportation systems to the Internet to the human immune system.

These examples illustrate that CMMP researchers are tackling ever-bigger and -broader problems in far-from-equilibrium phenomena. This expansion drives critical needs. Currently, research on far-from-equilibrium phenomena is fragmented into small subfields. These are typically divided along the types of materials

FIGURE 1.4 Granular materials consist of individual solid grains interacting only at contact, yet large assemblies of such grains exhibit a rich set of complex behaviors. (Left) Ripples in a sand dune. (Right) While fluids mix when stirred, granular materials size-separate; this magnetic resonance image of the interior of a layered granular system shows the upward motion of a large particle (dotted circle) in a bed of smaller ones. SOURCES: (Left) Photo courtesy of http://philip.greenspun.com. (Right) Matthias Möbius and Heinrich Jaeger, University of Chicago.

or specific phenomena studied—for example, fracture in solids or turbulence in fluids. The field of far-from-equilibrium physics is vast, and it is unlikely that any one organizing principle will work for all far-from-equilibrium systems. Nonetheless, there is great value in identifying *classes* of systems that might have common underlying physics or that might be tackled by common methods. There have been few incentives to adopt such broader approaches. Despite this, CMMP researchers are finding important connections to a wide range of other fields, both within and outside physics. Over the next decade, it will be critical to find ways to stimulate new links and to nurture crosscutting approaches in order to realize the vast potential of this research.

### What New Discoveries Await Us in the Nanoworld?

Nanoscale materials straddle the border between the molecular and the macroscopic. They are small enough to exhibit characteristics reminiscent of molecules but large enough for their properties to be designed and controlled to meet human needs. The first human nanotechnology, the integrated circuit (Figure 1.5), gave birth to the information age. The goal of nanoscience is to plant the seeds needed to grow even more nanotechnologies, ones capable of manipulating matter, energy,

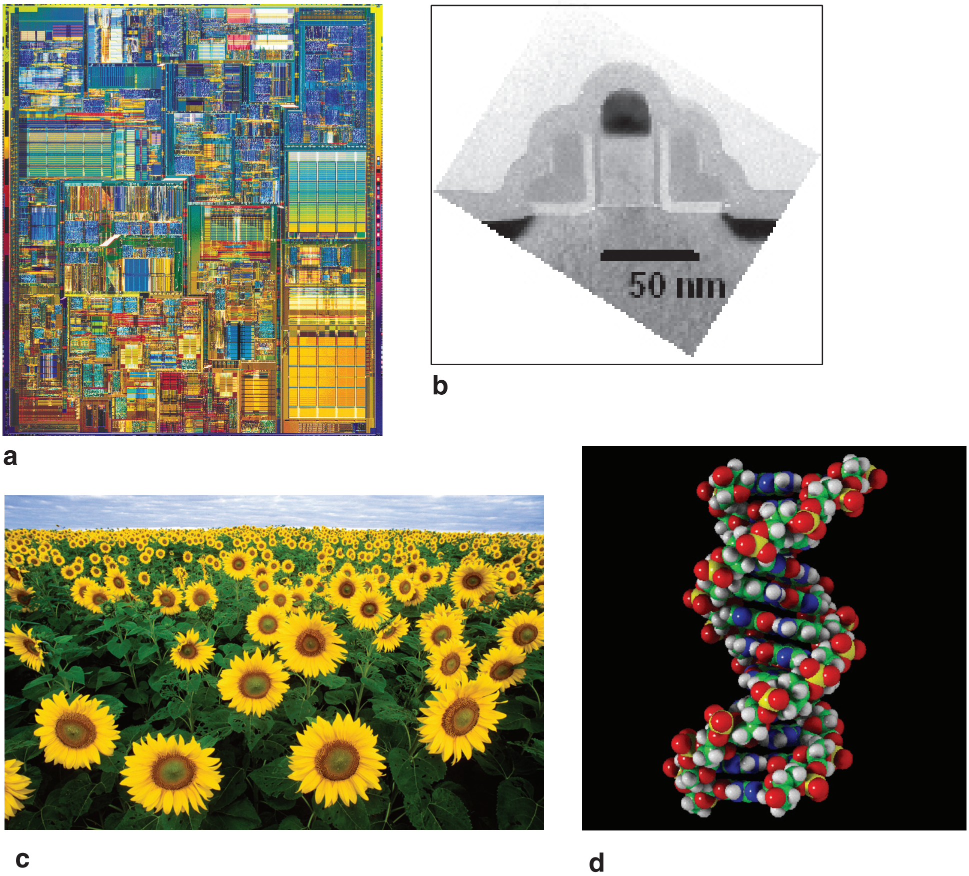

FIGURE 1.5 The first human nanotechnology—the modern integrated circuit (a), constructed from billions of individual transistors, such as the one shown (b). An example of nature's nanotechnology—a field of sunflowers (c), constructed from nanoscale building blocks like deoxyribonucleic acid (DNA) (d). SOURCES: (a) Intel Corporation. (b) Texas Instruments. (c) Bruce Fritz, Agricultural Research Service, U.S. Department of Agriculture. (d) Joseph W. Lauher, State University of New York at Stony Brook.

and light the way that integrated circuits manipulate electrons. Nature shows what is possible: life assembles self-replicating complex structures out of carbon-based building blocks that can harvest energy, store information, and control matter from the atomic to the macroscale. Will we someday be able to duplicate, and improve upon, the incredible abilities of life? Will we someday be able to build complex, functional (and beautiful) structures from nothing but a patch of dirt and a splash of sunlight?

The field of nanoscience occurs at the intersection of three great trends: Moore's law and the shrinking of electronic devices into the quantum realm, rapid advances in molecular biology that reveal the operation of nature's nanotechnology, and the evolution of chemistry toward the construction of large molecules and supramolecular complexes. These trends lead to a scientific "perfect storm," in which new nanotechnologies could be created if scientists can first overcome a series of fundamental challenges:

- How can nanoscale building blocks be both precisely and reproducibly constructed?
- What are the rules for assembling these nanoscale objects into complex systems?
- How can the emergent properties of these systems be predicted and probed?

Nanoscience is a core discipline whose advances will affect all of the other challenges, from emergent phenomena (Chapter 2) to information technology (Chapter 7). It encompasses an enormously wide range of topics, including ones in condensed-matter physics; atomic, molecular, and optical physics; materials science; engineering; chemistry; and biology. This breadth of influence and impact poses significant organizational and funding challenges, and special effort must be made to support the integration of knowledge from different disciplines. The stakes are high: the U.S. ability to address key social, environmental, and economic problems in the future will be dramatically affected by the investments made in fundamental nanoscience now.

### How Will the Information Technology Revolution Be Extended?

The phenomenal growth of information technology in recent decades has been enabled by fundamental discoveries in condensed-matter and materials physics that stretch back to the 1930s and 1940s, particularly the invention of the transistor. Now, after more than five decades of continuous progress based largely on improving and repeatedly miniaturizing the transistor, opportunities for further gains appear limited. Industry leaders are beginning to ask themselves what new devices can carry the "smaller, faster, cheaper" banner of information technology in coming decades. The answer to this question is of strategic economic interest to the United States. To maintain the flow of new products and services, the economic growth, and the dynamism of the industry, new devices to store, process, and communicate information will be needed—devices that can eventually be shrunk to the scale of molecules and atoms. Figure 1.6 illustrates how far information technology has come and how far it can go in the future. What will replace the silicon transistor? What new materials and phenomena will be incorporated into the logic gates of the future? CMMP researchers have ideas, but not answers. There are many physically promising approaches, and each approach presents deep intellectual challenges. The new approaches go by names such as spintronics, plasmonics, and molecular electronics. The possibility of communicating information via spin currents or subwavelength pulses of light, instead of traditional electrical charge currents, opens new vistas for research. And there is the grand quest to harness individual quantum states for computation—quantum computing—with the promise of exponentially accelerated computational speed and potentially unbreakable encryption schemes. As experimentalists study model systems such as Josephson junction-based quantum bits (qubits), theorists are developing new conceptual models such as topological quantum computing. The future looks exciting, and the

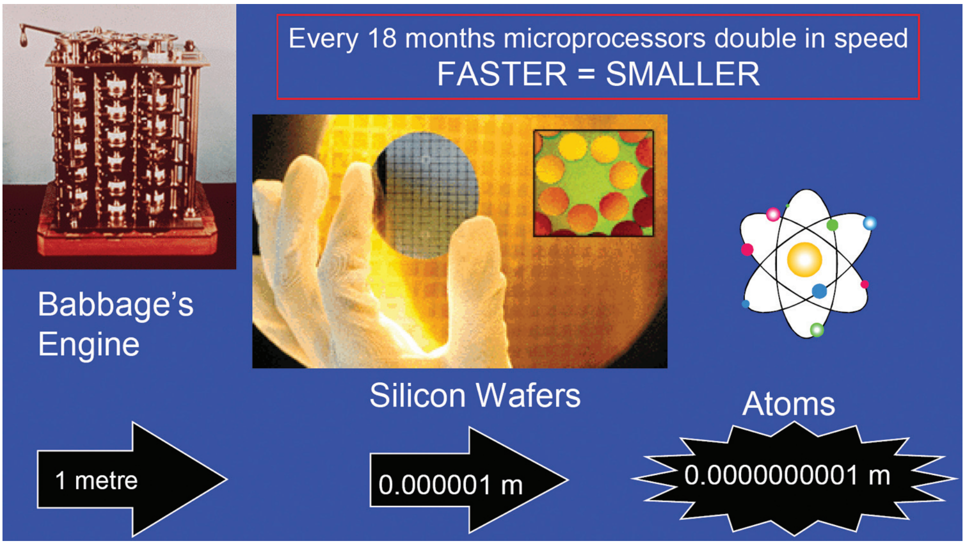

FIGURE 1.6 The past, present, and future of information technology, from Babbage's mechanical computer, to the silicon era, to perhaps atomic- and molecular-level systems in the future. SOURCES: Courtesy of Artur Ekert, University of Cambridge, and Tim Spiller, Hewlett-Packard Laboratories, Bristol, United Kingdom.

stakes are high. CMMP researchers can play a key role in extending the information technology revolution, but the CMMP community must be prepared to lower the barriers between basic and applied research and between experiment and theory. The entire scientific and technological community has a unique opportunity to join together to meet this grand challenge.

## SOCIETAL AND SCIENTIFIC IMPACT OF CMMP RESEARCH

CMMP is remarkable for the breadth and depth of its impact on society as well as on other scientific disciplines. While CMMP research formed the cornerstone of the electronics revolution of the 20th century, it is now poised to make vital contributions to addressing problems of the 21st century, such as the global renewable energy challenge and the revolution occurring in the biomedical health care arena.

Along with the six scientific challenges for CMMP that are identified here and discussed in greater detail in Chapters 2 through 7 of this report, the challenge to educate the next generation of scientists and citizens is given equal importance by the Committee on CMMP 2010, although the nature of the challenge is admittedly different in character. Further refinement of this challenge identified three key issues: how to educate the next generation of CMMP researchers, how to attract talented people to the field, and how to increase the scientific literacy of the general public and school-age children. Limited public awareness and understanding of science are an increasing danger to U.S. economic security. The CMMP community must now extend educational efforts not only to improve the scientific literacy of the public at large and of the student populations at all levels, but also to increase the pool of students interested in in-depth study of science and engineering. It is critical to infuse a new generation of scientists with the knowledge, skills, creativity, versatility, and sense of wonder needed to meet the challenges to society in the 21st century. The next generation of CMMP scientists should therefore be exposed to many opportunities for hands-on research experience—for example, through undergraduate research involvement—to stimulate interest and excitement in recent discoveries in CMMP, and they should be exposed to a more interdisciplinary educational experience to allow them to work at the newly emerging research frontiers of science and to utilize CMMP research for societal benefit.

CMMP is responsible for technological innovations that are leading contributors to national economic development and that enhance the quality of life. The electronics industry today is about a $1.5 trillion industry worldwide, based principally on technology arising from CMMP research, some done more than 50 years ago. This CMMP research has been recognized by Nobel Prizes and many other accolades. Most economically developed regions of the world have large and growing efforts in research over a broad range of scientific fields, including

CMMP, with the belief that this effort will enhance economic growth. For continued growth in the world's economy, research in the fundamental aspects of CMMP, both experimental and theoretical, is considered by the committee to be essential. It is therefore important to the future of the United States to maintain a leadership position in this basic research field.

The energy challenge is an area of great societal concern in which the CMMP community has an exciting opportunity to make major contributions based on the developments of new materials, new systems, and advanced computation and modeling. To succeed in making the transition to renewable energy sources within the first half of the century, a broad research investment strategy is required, based on multiple energy technologies. In addition, given that the energy challenge is clearly a global problem, basic energy-related research also presents an exciting opportunity for international collaboration on basic science and on the new technologies emanating from this research.

Condensed-matter and materials physics has a long history of seeding not only developments in fundamental biology, such as the use of x-ray diffraction to study biological structure, but also developments in the practice of medicine. The past decade has been rich with examples in which CMMP has had major societal impact, from the widespread adoption of reliable home pregnancy tests based on gold nanoparticles, to routine magnetic resonance imaging using ever-improving superconducting magnets, to using nanoparticle-based contrast enhancement to image everything from tumors to brain function, to the development of new materials for the increased lifespan of surgical implants. It is expected that CMMP researchers will continue to develop tools that revolutionize the biological and medical fields.

CMMP also plays a vital role in other disciplines of science, in two ways. First, CMMP technologies such as materials and devices, ranging from nonlinear organic materials to charge-coupled-device detectors, are ubiquitous in laboratories throughout the scientific enterprise. Second, as science expands and the disciplinary boundaries blur, concepts originating in CMMP find increasing relevance to other physics subfields and other science disciplines, often forming entirely new research subfields (see Chapter 8).

Scientific and technological connections between CMMP and atomic, molecular, and optical (AMO) physics are historically strong, principally because of similarities between the energy and length scales of the two fields. Laser and optical technology, developed primarily within the AMO community, has wide application in CMMP research for a variety of materials characterization and processing purposes. While lasers and optics have been the most prominent and wide-reaching connection so far, the recent development of methods to trap and cool atoms in the nano-kelvin regime also has the potential to profoundly affect CMMP by enabling the realization of some of the most fundamental models of condensed-matter physics. Conversely, emergent phenomena in interacting electronic and atomic systems from CMMP inspire new directions in AMO physics.

Condensed-matter physics has significantly impacted nuclear and particle physics over the years, from studies of laboratory nuclei, to the study of neutron stars, to models of elementary particles. Such connections are not unexpected, since nuclei, as complex many-body systems, present intellectual challenges with many similarities to condensed-matter physics. The discovery of the Bardeen-Cooper-Schrieffer theory of superconductivity had an immediate impact on nuclear physics with Cooper pairing of neutrons and protons, thereby explaining many features of actual nuclear excitation levels. Further, the neutron matter that comprises neutron stars is expected to be superfluid, and the proton matter superconducting. The connections between CMMP and astrophysics instrumentation are also strong. Virtually every modern telescope has a sophisticated solid-state detector at its focus. At optical wavelengths, silicon charge-coupled-device arrays long ago supplanted photographic plates, as they have done recently in ordinary photography. Advances in solid-state devices are also having an immediate impact on increasing the resolution and the accessible space (time) range of astronomical observations.

Advances in a number of areas of CMMP have had an important impact on developments in chemistry, especially in the areas of materials chemistry and physical chemistry. In the area of computation, density functional theory is now used extensively by chemists to calculate the electronic structures of materials and by polymer physicists to calculate the structure of polymer molecules in solutions and melts. CMMP has also had a huge impact through the development of advanced characterization tools, such as synchrotron light sources, neutron probes, scanning probes for studying the nanoworld of new materials, and nuclear magnetic resonance, which has become one of the most powerful characterization tools in chemistry and polymer science. The symbiotic nature of the relationship between CMMP and chemistry is reflected in the fact that synthetic chemists have enabled some of the most exciting advances in CMMP in recent years, such as the remarkable advances in conducting polymers, buckminsterfullerene ($C_{60}$) and carbon nanotubes, lanthanum cuprate high-temperature superconductors, and $MgB_2$, now being developed for use in advanced superconducting magnets for magnetic resonance imaging.

The experimental methods of CMMP have also had an enormous impact on biology and medicine and have ushered in a new era of quantitative approaches to biological measurements and prediction. Biomolecular structures are now being catalogued through the use of technologies such as synchrotron radiation and x-ray crystallography developed in the CMMP community. Fundamental studies of energy transfer between two spins have allowed measurement of the distance between atoms in proteins even as the protein tumbles freely in solution. Magnetic resonance studies of proton relaxation in water have enabled detailed studies of neural activity and blood flow. Lasers in confocal microscopy systems, near-field optics, and scanning multiphoton fluorescence microscopies have made it possible to reach deep into tissues at the single cell level to study brain function and observe the dynamics of biological motion at the nanometer scale.

In computer science, CMMP has also contributed enormously not only to the development of the hardware devices that implement information technology but also to the theory of computation and algorithms as well. First used in nuclear physics and further developed in CMMP, Monte Carlo methods, which compute properties by the judicious sampling of possibly favorable configurations, led to a new class of optimization and search algorithms in computer science. Correlation and scaling laws from statistical mechanics are used to describe and understand the structure and emergent behaviors of large computer networks. Concepts of self-organized collective behavior from CMMP are now at the frontier of computer science and robotics. The role of CMMP in quantum computing is even more central. The theory of the transmission and processing of intact quantum states has significantly altered the assessment of the kind and quantity of physical resources needed to solve various computational problems, with applications to cryptography and potential quantum computation. Moreover, CMMP research is contending to be the provider of the physical qubits for the hardware implementation of this new kind of computing.

## INDUSTRIAL RESEARCH

In the United States, the once-great industrial laboratories, where much pioneering work was accomplished on semiconductors, computers, memories, and communications, have undergone major changes. The research funding from companies that had a de facto monopoly has significantly declined and in some cases disappeared. Many of the laboratories have been redirected, sold, or closed, and much of the fundamental work has ceased. With the remaining U.S. industrial laboratories often focused on much shorter-term goals, there is concern that the next great revolution in technology will be triggered by research developments elsewhere in the world.

The industrial laboratories also served as incubators for scientific and technological leadership. Many of today's leaders at the nation's leading universities, national laboratories, and other institutions originated from the industrial laboratories, where they were able to establish their careers working on fundamental, high-risk problems with relatively little funding pressure. In spite of the differences between corporate and academic culture, the overall impact of these scientists on academia has been positive, and the source of such researchers is now drying up.

As pointed out in this report, the rebuilding of industrial laboratories with the ability to do long-range research does not seem feasible on the timescale of the next decade. Global competition and the disappearance of industrial monopolies have changed the environment for industrial research. The replacement of the great industrial laboratories as sources of invention and leadership is a major challenge to the United States. The physics community, the federal government, and interested private-sector parties, such as investors in new technology, individual companies, foundations, and industrial consortia, must work together to create organizational and funding mechanisms that work well to create future technical breakthroughs and to provide the United States with a pathway for future scientific and technological leadership. A number of new approaches to long-term research are being explored to establish viable routes from fundamental CMMP discoveries to technological inventions to industrial leadership (as discussed further in Chapter 9). Based on the analysis of the quantitative data, the trends now occurring, and the various approaches now in progress, the committee sees the next decade as a period of great opportunity for developing new ways to increase economic growth through technological innovation and to improve the quality of life.

## STRUCTURE AND LEVEL OF THE CURRENT RESEARCH EFFORT

To address its charge to examine the structure and level of the current research effort, the Committee on CMMP 2010 provides an overview of recent trends in CMMP regarding funding, demographics, and publications. The research funding for CMMP over the past 10 years shows a net increase of about 10 percent in inflation-adjusted dollars, using the Office of Management and Budget (OMB) deflators. But when analyzed using the average cost increase of about 5 percent per year per graduate student, the committee estimates that the buying power of research grants has decreased by about 15 percent over the past decade. As a result, most grants now allow support of one graduate student.

In addition, there has been a dramatic decrease in the past 5 years in the chances of a grant application in CMMP being funded at the National Science Foundation's (NSF's) Division of Materials Research, from 38 percent in 2000 to 22 percent in 2005. For investigators who have not had NSF funding for the past 5 years, including new investigators, the situation is even bleaker, with a drop from 28 percent in 2000 to 12 percent in 2005. These low success rates speak to the hidden "overhead" of writing and reviewing proposals, lowering the efficiency of the scientific community and lowering the morale of new investigators.

From these data, one can understand why many CMMP research groups in the United States are having a hard time participating in the exciting research opportunities (such as those described in Chapters 2 through 7 of this report). At the same time, China, Korea, Taiwan, and other countries show rapid growth in funding. Although CMMP remains the most popular subfield in physics, there has been a decline in the number of U.S. CMMP Ph.D. degree awards by 25 percent over the past decade. The extent to which this decline has been correlated with funding trends needs to be better understood. In fact, the whole physics community have suffered a corresponding percentage drop in their Ph.D. awards over this period. This is a matter of concern at a time when national policy makers have verbally encouraged increases in the training of science and engineering personnel.

There has also been a decline in the fraction of U.S. publications compared with total publications in two major journals of CMMP worldwide (*Physical Review B* and *Physical Review E*), from 31 percent to 24 percent over this decade (see Figure 1.7). The major increase in the number of publications during this period has come from Western Europe, with strong increases from Asia and the rest of the world. These data show that CMMP is in general flourishing, with the overall number of publications doubling since 1993. The data, however, show that the United States has not been able to participate in the growth of the field.

Further investigation of publication citation data shows that the United States continues to rank at about the same level that it was at 5 years ago in terms of the fraction of the top 100 most-cited papers per year. However, if other parts of the

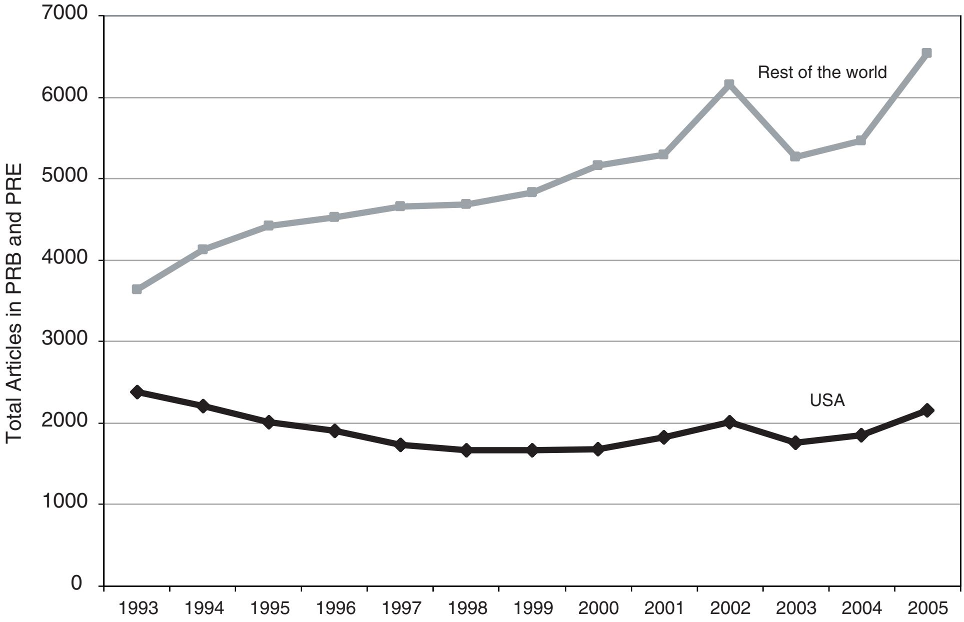

FIGURE 1.7 U.S. leadership in number of CMMP articles published in two leading journals, *Physical Review B* (PRB) and *Physical Review E* (PRE), is eroding. SOURCE: Publication data supplied to the Committee on CMMP 2010.

world continue to outpace the United States in support for CMMP research, it will be difficult to recruit and retain top scientific talent in the United States.

For the United States to remain competitive with the rest of the world in CMMP research, the committee believes that the present number of CMMP investigators should increase modestly for core CMMP activities and growth in new areas, and that the *buying power* of grants should be restored to their fiscal year 2000 levels at a minimum. An increase in funding (for example, 20 percent above inflation over the next decade) is also needed to allow for the nurturing of newly spawned frontier interdisciplinary areas connecting CMMP with other physics subfields (such as AMO physics), and with other science disciplines that are now merging strongly with CMMP at its boundaries, such as biology and chemistry.

## TOOLS, INSTRUMENTATION, AND FACILITIES FOR CMMP RESEARCH

CMMP researchers have developed remarkable tools to uncover the microscopic origins of emergent phenomena. These tools were designed to observe, predict, and control the arrangements and motions of the constituents that comprise condensed-matter systems. The constituent particles span an enormous range of sizes—from electrons and atoms in semiconductor devices, to polymers in plastics, to bubbles in foams—and their motions span a correspondingly immense range of timescales. As a result, the experimental, computational, and theoretical tools required to study them are extremely diverse. Many of these tools are developed by individual research groups; other tools, such as synchrotron x-ray and neutron sources, are developed at large-scale national laboratory facilities.

Measurement techniques designed to probe the properties of matter at smaller length, time, or energy scales, or with greater quantitative resolution and sensitivity, advance the forefront of CMMP research. Likewise, techniques designed to synthesize high-quality materials with precisely controlled structures underpin many great CMMP discoveries. By pushing the boundaries of materials fabrication and measurement forward, experimental CMMP researchers have uncovered new phenomena that were often unanticipated.

These discoveries have not only transformed CMMP, but they have led in turn to new ways to manipulate and image matter, crucial to many new technological advances with a broad range of applications. As a result, the benefits of new techniques often stretch far beyond condensed-matter and materials physics. For example, the CMMP technique of x-ray diffraction, applied to DNA, led to the founding of molecular biology, and scanning probe microscopes have now evolved into universal tools at the nanoscale for the physical and life sciences. Experimental condensed-matter tools underlie many noninvasive medical diagnostics, while theoretical and computational tools from CMMP, such as local electron density approximations and numerical simulation methods, are now used to develop new pharmaceuticals. As CMMP researchers seek to answer fundamental questions about materials, they will continue to design tools that will benefit CMMP, other scientific disciplines, and also society.

The discovery and synthesis of new materials are central to CMMP and to each of the six challenges identified in this report. The United States is no longer a leader in the creation of new materials and must recapture its lost status. The consequences of delay and neglect are long-term erosion of the U.S. international competitive edge and a loss of intellectual property. A National Research Council (NRC) study is now under way to determine how best to address the new materials synthesis challenge.

The Committee on CMMP 2010 was specifically charged to look at facility and instrumentation needs for the future. To help address this charge, the committee convened a workshop in January 2007 to obtain broad input from the community. The resulting recommendations are focused on priorities for the next decade but with an eye toward further evolution of the facilities programs for the following decade because of the long time lines necessary for planning purposes. The workshop participants gave the committee a clear message that investment should also be spread across all the areas identified in this report and not concentrated on any one kind of facility. Balance is also needed between the support of facilities and instrumentation relative to the research programs of the individual research groups or small teams of investigators, remembering that CMMP is driven by the individual research groups.

The U.S. light sources represent a large capital investment by the federal government to support advances in basic research. Light sources allow the extension of the power of the optical microscope to obtain images of condensed matter at much smaller distances in real space, as well as in the space spanned by momentum and energy, and in what is becoming increasingly important, a mixture of the two. The committee was impressed by the technological advances that had taken place in the past few years, and focused its recommendations on capturing the tremendous research opportunities seen for the coming decades.

The U.S. capabilities in neutron scattering, including diffraction, reflectivity, time-of-flight, and small-angle scattering probes, are being greatly enhanced with the construction and commissioning of the Spallation Neutron Source. The committee's recommendations are based on strategies to build on these investments and to exploit the capabilities of these new tools to understand properties at the nanoscale and to meet CMMP grand challenges.

Electron microscopy, a basic tool for the characterization of materials, is utilized at the local level through central facilities that normally provide standard and high-end scanning and transmission electron microscopes, along with some support staff to facilitate their usage. Forefront instruments are available at Department of Energy national laboratories for sophisticated users through peer review evaluation of proposed research. Recently, great strides have been made with the development of aberration-free electron optics, thereby providing images with atomic resolution and putting the United States for the first time in many years in a competitive position in this research field. Recommendations aimed at strengthening the competitive position of the United States in electron microscopy techniques while supporting the needs of the CMMP research community are presented.

High magnetic fields of 15 to 20 tesla are now available in many local laboratories through superconducting magnets. For higher magnetic fields, use of the National High Magnetic Field Laboratory is necessary. Not only does this laboratory provide a wide range of best-in-class static and pulsed magnets, but it is also the center for the development of the next generation of advanced materials (such as $MgB_2$) for superconducting magnets and instrumentation for the entire suite of high-field magnets and associated facilities. The next decade is poised to see continuing gains in static and pulsed magnetic field capabilities as well as the utilization of high magnetic fields in conjunction with synchrotron and neutron-based probes to study selected frontiers of CMMP, as discussed in a recent NRC study.[1]

Computation has become an indispensable tool in all aspects of condensed-matter and materials physics theory and experiment. Maintaining and developing high-performance computing resources for condensed-matter and materials physics should continue to be a high priority. Computer time and scientific programming support should be available at a variety of levels, from centralized national supercomputer facilities to the state, local, university, and individual-research-group levels. The diversity of facilities and their distributed character make it difficult to track exactly what resources are available, and it is clear that lack of computational resources represents a significant bottleneck for some researchers, particularly junior university faculty members; attention to the improved distribution of resources could have a significant impact.

## CONCLUDING COMMENTS

Moving into the 21st century, CMMP faces exciting scientific and technological opportunities, summarized in the six grand challenges identified in this report. These and other challenges will drive the continued vitality and growth of CMMP, as well as its continuing impact on the U.S. economy and society. The fundamental scientific questions, the close interplay between theoretical and experimental research, and the technological applications that will contribute to solving important societal problems all drive enthusiasm for the field. Attracted by such compelling research opportunities, more starting graduate students in U.S. programs choose

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[1] National Research Council, *Opportunities in High Magnetic Field Science*, Washington, D.C.: The National Academies Press, 2005.

CMMP than any other single subfield of physics. These young minds are the future of CMMP and of its role in society.

However, the Committee on CMMP 2010 also concluded that there are danger signs on the horizon. U.S. leadership in fundamental CMMP research is seriously threatened by the low success rates in proposals submitted for government funding of research, the precipitous decline of involvement of industrial laboratories in fundamental CMMP research, and the increasing competition from other countries for the best scientists. Due to tremendous momentum in the research establishment, the ill effects of these structural problems are only just starting to manifest themselves in measurable terms, such as publication rates, and in the ability to attract the best young scientists to research positions in the United States. The Committee on CMMP 2010 therefore urges that action be taken now. Prompt attention to these structural problems is needed to ensure U.S. leadership in CMMP research and technological innovation now and for the future.

# 2

# How Do Complex Phenomena Emerge from Simple Ingredients?

Most materials are made of simple, well-understood constituents, and yet the aggregate behaviors of materials are stunningly diverse and often deeply mysterious—a direct result of the complexity of large systems. Just as a crowd can act in ways uncharacteristic of any individual within it, surprising emergent phenomena are also seen in collections of electrons, molecules, and even familiar objects such as grains of sand. For example, sand can be poured like water from a bucket, but unlike any liquid, it also supports the weight of a person walking on the beach. In the fractional quantum Hall state, a bizarre liquid state of electrons, an added electron will break up into new particles, each of which carries a precise fraction of the charge of the original electron. In a superconductor, an electrical current can flow indefinitely without decaying. These are impossible feats for individual grains of sand or individual electrons. The relationship between the properties of the individual and the behavior of the whole is very subtle and difficult to uncover and lies at the heart of condensed-matter and materials physics (CMMP). The challenge is to understand how collective phenomena emerge, to discover new ones, and to determine which microscopic details are unimportant and which are essential.

## EMERGENT PHENOMENA: BEAUTIFUL AND USEFUL

Twentieth-century physicists created a spectacularly successful understanding of the structure of atoms and molecules, the interaction of subatomic particles with light, and a unified description of all fundamental forces in nature but gravity. Quantum mechanics and quantum electrodynamics, the most successful quantitative theories developed by humankind, allow for extraordinarily accurate calculations of the properties of individual and small collections of particles.

Nature, however, confronts us with materials consisting of unimaginably large numbers of particles. For example, there are many more electrons in a copper penny than there are stars in the known universe. It is therefore not surprising that condensed-matter and materials physicists regularly discover phenomena that neither were foreseen nor are easily understood. These phenomena *emerge* as collective aspects of the material at hand. *Emergent phenomena* are properties of a system of many interacting parts that are not properties of the individual microscopic constituents. It is often not readily possible to understand such collective properties in terms of the motion of individual constituent particles. Emergent phenomena occur at all scales, from the microscopic to the everyday to the astronomical, and from the precincts of quantum mechanics to the world known to Newton and Maxwell. The infinite diversity of emergent phenomena ensures that the beauty, excitement, and deep practical utility of condensed-matter and materials physics comprise an inexhaustible resource.

Emergent phenomena are not merely academic curiosities. Some, like the emergence of life from biomolecules, define our very existence. Others, like the regular arrangements of atoms in crystals, are simply so familiar that we rarely even pause to wonder at them anymore. There are countless examples of this kind. At the same time, the discovery and study of emergent phenomena often lead to immensely important practical applications. Superconductivity, discovered almost 100 years ago, is a good example. While Dutch physicist Kamerlingh Onnes did envision producing magnetic fields using solenoids wound from superconducting wire, he could never have foreseen superconducting magnets big enough to surround a human, nor that such a magnet would be the heart of a technological marvel (magnetic resonance imaging; see Figure 1.1 in Chapter 1) that would revolutionize medicine. Looking ahead, one can imagine that the recently discovered high-temperature superconductors, which have so far seen limited application, might ultimately play a major role in reducing world energy consumption by allowing lossless transmission of electrical power over long distances. Unlike superconductors, which took many decades to see large-scale application, there is the very recent dramatic example of giant magnetoresistive materials, which came to dominate hard disk data storage in just a few years. Liquid crystalline materials, in which large numbers of asymmetric molecules in solution exhibit a dizzying variety of emergent phases, are used in everyday electronics like cellular telephones and laptop computers. Jamming of granular materials (discussed below), perhaps unfamiliar to the average citizen, is an emergent phenomenon with real economic consequences in the mining, pharmaceutical, and other industries. And the list goes on.

Emergent phenomena are so widespread that a comprehensive review is both impossible and inappropriate. The Committee on CMMP 2010 fully expects that much of the most significant research in the coming decade, as was true of past decades, will be triggered by the discovery of new emergent phenomena that are unlikely to be anticipated in any present list of "most important" problems. Here, a few examples are discussed to illustrate the quest, which underlies much of CMMP, to understand the relation between the properties of the "microscopic" constituents of matter and the macroscopic behavior of the whole.

Superconductivity, a century-old phenomenon, is discussed first because it is both an extraordinarily dramatic example of emergence and one of the most active fields of research in CMMP today. That example is followed by more general discussions of current trends in research on Fermi and non-Fermi liquids, on quantum Hall effect systems, and on critical phenomena and universality in classical and quantum-phase transitions. Emergence in ultracold atomic gases and in granular matter round out the list of case studies. (Further discussion of important emergent phenomena in CMMP can be found elsewhere in this report, especially in Chapter 4 on the physics of life and Chapter 5 on systems far from equilibrium.) Following the examples are some brief remarks on how to realize the full potential of emergence.

## SUPERCONDUCTIVITY: AN ILLUSTRATIVE EXAMPLE AND A FRONTIER OF RESEARCH

In many materials, exotic and unexpected phenomena emerge from strong interactions between the constituent particles at the microscopic level. Quantum mechanics often plays a key role and renders the phenomena particularly puzzling and counterintuitive. *Superconductivity*, the property of certain materials to carry electrical currents without any dissipation of energy, is the quintessential example of such a quantum emergent phenomenon. First discovered in mercury in 1911 by Kamerlingh Onnes and his graduate student Holst in their pioneering experiments on the properties of matter near the absolute zero of temperature, superconductivity was utterly unheralded and resisted explanation for nearly 50 years. Nowadays, CMMP researchers have a good understanding of the phenomenon in mercury and other similar metals where the transition to the superconducting state occurs at very low temperature. But nature is much more resourceful, and this comfortable situation was radically upset just 20 years ago with the discovery of a new class of superconductors having much higher transition temperatures. No accepted theory of high-temperature superconductivity has yet been developed, in spite of immense effort and the application of the most sophisticated tools of theoretical physics by large numbers of researchers across the globe. Unlike the low-temperature metallic superconductors, these new materials are not completely understood even in their normal, non-superconducting, states. Indeed, high-temperature superconductors highlight one of the broadest and most important current problems in all physics, the strongly interacting quantum many-body problem.

All materials conduct electric current to some extent, but the amount of force that must be applied to maintain a current varies greatly from material to material. The resistance of a material quantifies how large a voltage must be applied to obtain a given amount of current flow. Put another way, to maintain a given amount of current consumes power in proportion to the resistance. In a superconductor, the resistance is precisely zero, so a persistent current can flow, forever, around a superconducting ring without need of a battery or a generator!

In an attempt to be quantitative about the meaning of "forever," measurements have been carried out to try to detect the rate of decay of persistent currents in superconducting rings. In these experiments, the current in a ring is measured very accurately at an initial time and then again a long time later. Despite the extreme accuracy of these measurements, no decrease in the current is detected. Even if the current were decaying at the fastest rate possible consistent with the accuracy of the measurement, the current would not decay within the age of the universe.

Superconductivity appears when the temperature is reduced below a critical value. What this means is that the resistance of a metal, such as the mercury studied by Kamerlingh Onnes, has a non-zero value at a temperature just a fraction of a degree above the critical temperature. However, at any temperature below the critical temperature, the resistance is zero. It is the same piece of metal both above and below the critical temperature, and the same electrons are carrying the current. At the critical temperature, something subtle but spectacular happens in the organization of the vast number of electrons in the metal that causes them to form a superconducting state.

Normally, scientists think of quantum mechanics as the set of physical principles that govern the motion of small numbers of microscopic particles—atoms and electrons and nuclear matter. Quantum mechanics is usually only indirectly seen in the properties of macroscopic matter—objects large enough to hold in one's hand. However, superconductors have many counterintuitive properties that reflect their underlying quantum nature. The existence of a persistent current is a concrete demonstration of quantum mechanics at a macroscopic scale. Since currents produce magnetic fields, it is perhaps not surprising that the magnetic properties of superconductors are likewise unprecedented. Indeed, in 1933 Meissner and Oschenfeld discovered that superconductors entirely expel (small) magnetic fields from their interior. In fact, in a superconducting quantum interference device (SQUID), a relation exists between the frequency of current oscillations and an applied voltage that only involves the charge of the electron and the fundamental constant of quantum mechanics, Planck's constant. This relation has been found experimentally to be universal to a precision of better than 3 parts in $10^{19}$, which means that clocks based on two independent Josephson junctions kept at the same voltage would differ from each other by no more than one-tenth of a second over a time interval equal to the age of the universe! It is inconceivable that any of the founders of quantum mechanics could have foreseen that a measurement of macroscopic quantities would depend directly, and with such precision, on the laws of quantum mechanics. Finally, macroscopic quantum phenomena are certainly not limited to superconductors. The ordinary magnet holding up a note on a kitchen refrigerator offers a dramatic everyday example: A steady magnetic field is present without any battery to keep currents flowing. This macroscopic quantum phenomenon is just as spectacular as the persistent currents in a superconductor.

One of the great triumphs of 20th-century CMMP is the microscopic theory of superconductivity in ordinary metals, the Bardeen-Cooper-Schrieffer (BCS) theory. Not surprisingly, since superconductivity involves only a subtle, low-temperature change in the properties of the electrons in the metal, the BCS theory is based on the equally successful Fermi liquid theory of the properties of normal metals. (Fermi liquid theory and its breakdown are discussed below.) Moreover, hundreds of different metals that are BCS superconductors have been identified, although mostly with superconducting transition temperatures less than 10 K. While the theory has rarely led to the prediction of new superconductors, it has provided qualitative guidance for the search for new, low-temperature superconductors.

Starting with the 1986 discovery of superconductivity at 30 K in $La_{2-x}Ba_xCuO_4$ by Bednorz and Mueller, a new class of materials, now known as high-temperature superconductors, became the focus of intensive research. The highest superconducting transition temperature found to date in these materials is approximately 150 K in $HgBa_2Ca_2Cu_3O_{8+x}$ under pressure—roughly 10 times higher than any previously known superconductor. The microscopic interactions responsible for the transition to the superconducting state are different from those in BCS superconductors. Moreover, the so-called normal state observed at temperatures above the superconducting transition is very different from that of a normal metal and is not well understood.

The high-temperature superconductors belong to a large class of synthetic materials (i.e., they do not appear in nature) known as highly correlated electronic materials (see Figure 2.1). Research in this area in the past two decades has been rich in discovery and in producing challenges to the entire quantum theory of solids. These new materials exhibit a startling array of emergent phenomena: ferromagnetism and antiferromagnetism, orbital ordering and long-period charge ordering, giant and colossal magnetoresistance, new types of superconductivity with new forms of broken symmetry, and all sorts of fluctuation phenomena over unprecedentedly wide ranges of temperature and material parameters. Obtaining a well-founded qualitative understanding of the normal state, at the level of the Fermi liquid theory of simple metals, is among the most challenging and most profound problems facing CMMP. Clearly, understanding the mechanism of high-

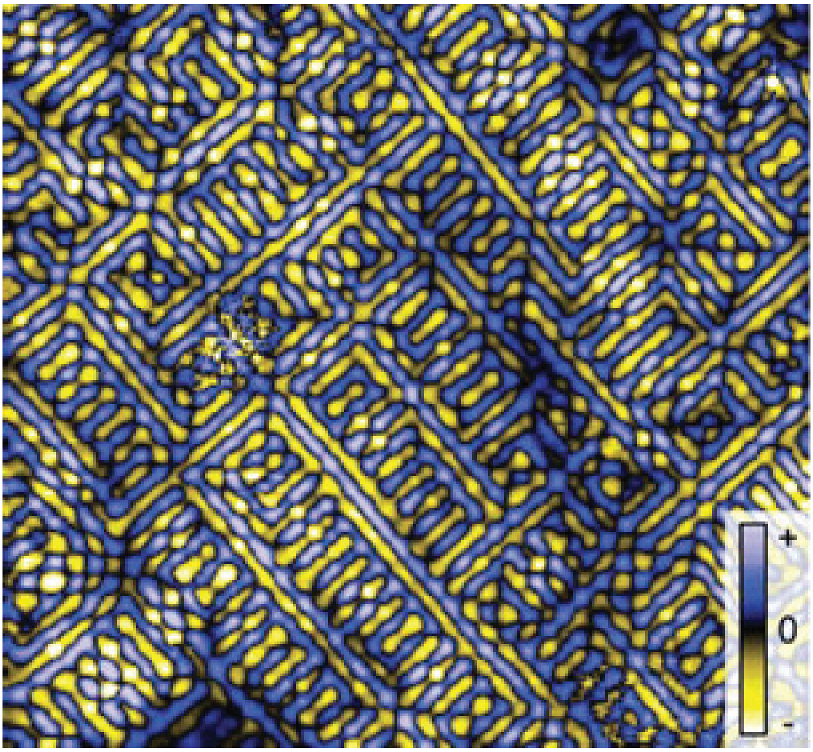

FIGURE 2.1 Local electronic structure of a highly correlated electronic solid visualized with sub-atomic-scale resolution using a scanning tunneling microscope. This is not an Abstract Impressionist painting. It is a self-organized structure "seen" on the smooth, cleaved surface of a crystal of the high-temperature superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$. The patterns represent changes in the electronic structure that are pinned in a highly organized but ultimately random ("glassy") pattern. The detailed information concerning the organized structures of electrons in solids that this kind of experiment provides has opened unprecedented opportunities to explore the ultimate connections between microscopic physics and the emergent properties of materials. SOURCE: Y. Kohsaka, C. Taylor, K. Fujita, A. Schmidt, C. Lupien, T. Hanaguri, M. Azuma, M. Takano, H. Eisaki, H. Takagi, S. Uchida, and J.C. Davis, "An Intrinsic Bond-Centered Electronic Glass with Unidirectional Domains in Underdoped Cuprates," *Science* **315**, 1380-1385 (2007). Reprinted with permission from the American Association for the Advancement of Science.

temperature superconductivity at a level that can provide qualitative guidance for the search for other, possibly even higher-temperature superconductors is a problem of enormous importance. It is surely not an accident that so many other sorts of emergent states (ordered phases) occur in this class of materials—understanding the relation between the various types of ordered phases of these materials and understanding how they relate to the properties of the non-Fermi liquid normal phase are problems that will occupy much of the focus of CMMP in the coming decade.

## FERMI LIQUIDS AND NON-FERMI LIQUIDS

If one could ignore the interactions between electrons in a solid, the properties of the material could be derived from a theory that treats only one electron at a time. While this might seem to be an absurd assumption, since electrons are charged and repel one another strongly, such single-electron theories often work remarkably well. Quantum mechanics is essential for understanding why this is so. All electrons are intrinsically identical to one another, just as are all protons, all neutrons, and so forth. Quantum mechanics sets very stringent rules for the behavior of systems containing many identical particles. If the positions of two identical particles are interchanged, quantum mechanics naturally insists that there be no observable consequence. Except in certain rare cases to be described below, there are only two ways in which the quantum wave function of the material can satisfy this requirement: either (1) nothing at all happens to the wave function upon interchange of two particles, or (2) it changes its sign. Particles for which the wave function changes sign are called fermions, while those for which the sign is preserved upon interchange are known as bosons.

Electrons are fermions, and thus a many-electron wave function changes sign when two are interchanged. This property underlies the Pauli exclusion principle, which high school chemistry students are usually told means that no two electrons can be in the same place at the same time. More precisely, two electrons are forbidden from occupying the same quantum state. Despite their vagueness, these statements make it easy to see why the Pauli principle has such vast significance for the theory of materials. If no two electrons can be in the same place at the same time, they rarely get so close together that their mutual repulsion is extremely strong. If no two can occupy the same quantum state, then at low temperatures the many electrons in a material are forced to sequentially occupy higher and higher energy levels, forming a "Fermi sea." In some circumstances, interactions between electrons are not strong enough to disturb any but the relatively few levels that are near the surface of this sea. In effect, the Pauli principle converts what at first appears to be a hopelessly strongly interacting system into a more weakly interacting one. In a nutshell, this is why scientists understand the properties of simple metals as well as they do.

Remarkably, a more sophisticated version of the "Fermi liquid" picture just described often works very well even when the repulsive interactions between electrons are fairly strong (compared to the average kinetic energy of electrons). In these cases, the properties of the material can be described in terms of new entities, known as quasi-particles, which behave in much the same way as the original particles—that is, electrons—except that they do not interact strongly with one another (see Figure 2.2). One can think of these quasi-particles as consisting of an electron plus a disturbance among the other electrons around it. In some cases, the quasi-particles behave so similarly to the original electrons that it is hard to remember that they are distinct objects. In other cases, the quasi-particle behaves like an electron with strongly modified properties—for instance, in the "heavy fermion materials," metal alloys containing heavy elements such as uranium and cerium, the quasi-particle can be as much as a thousand times heavier than an electron. A system in which the properties of a dense electron fluid can be related to those of a gas of weakly interacting quasi-particles is called a Fermi liquid. The very successful theory of normal metals, as well as the equally successful theory of simple semiconductors, is based on Fermi liquid theory.

However, in many electronically interesting solids, over a wide range of temperatures, pressures, and compositions, the Fermi liquid description fails badly. This class includes many of the most interesting materials that have been discovered

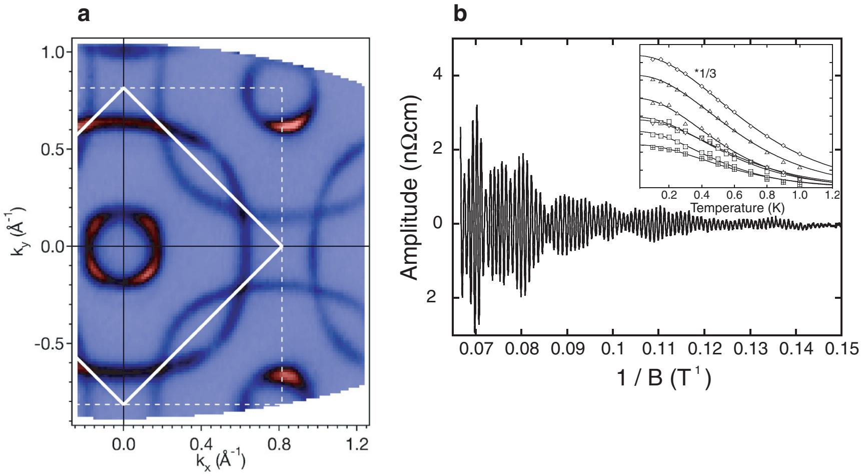

FIGURE 2.2 Signatures of the Fermi liquid state in $Sr_2RhO_4$, a strongly correlated material. (Left) A map of the Fermi surface (constant energy surface at the Fermi level) in reciprocal space revealed by high-resolution angle-resolved photoemission experiments. (Right) The resistance as a function of magnetic field at temperatures close to absolute zero; these "quantum oscillations" reflect the shape of the Fermi surface. Despite the fact that this material is structurally extremely similar to cuprate high-temperature superconductors (such as $La_2CuO_{4+\delta}$), these experiments unambiguously demonstrate that at low-enough energies, the electronic properties of $Sr_2RhO_4$ are perfectly represented by a gas of essentially non-interacting, electron-like "quasi-particles." SOURCE: Reprinted with permission from F. Baumberger, N.J.C. Ingle, W. Meevasana, K.M. Shen, D.H. Lu, R.S. Perry, A.P. Mackenzie, Z. Hussain, D.J. Singh, and Z.-X. Shen, "Fermi Surface and Quasiparticle Excitations of $Sr_2RhO_4$," *Phys. Rev. Lett.* **96**, 246402 (2006). Copyright 2006 by the American Physical Society.

and studied in the past two decades, among them the high-temperature superconductors and quantum Hall effect systems. There are many well-understood qualitative reasons why Fermi liquid theory is less successful in these new materials. More importantly, the experimental evidence that the behavior of these systems is incompatible with Fermi liquid theory is clear and incontrovertible. This evidence ranges from direct tests of the quasi-particle hypothesis, such as angle-resolved photoemission measurements that can directly "see" a quasi-particle if it exists, to indirect tests, such as a measured metallic resistivity that exceeds the maximum that is consistent with the quantum motion of independent quasi-particles. Lacking today is a conceptually clear and computationally tractable framework for understanding the properties of a "non-Fermi liquid" of electrons.

Some of the essential ingredients in an understanding of a non-Fermi liquid are clear. The basic objects that move are no longer electrons, but more likely large clusters of electrons moving in concert. The building blocks of a theory of such a state are thus very different from the quasi-particles of Fermi liquid theory. A better intuitive picture may come from envisaging a fluid made up of pieces of melted electron crystals, or magnets, or superconductors, not just individual quasi-particles. Correspondingly, the properties of such a system are not readily inferred from the properties of individual electrons. For instance, a fluid of partially ordered magnets can have magnetic properties intermediate between those of a magnet and a normal metal (see Figure 2.3). Such behavior is most readily addressed in the proximity of a "quantum critical point" separating two distinct phases, as discussed below.

However, this is just the tip of the iceberg. The broad occurrence of non-Fermi liquid phenomena suggests that it is related to new quantum phases, or at least to extremely new regimes of matter. Correlated motion of many particles is difficult to characterize and still more difficult to understand. However, the non-Fermi liquid character exhibited by a rapidly increasing number of interesting materials imbues the problem with an immediacy and focus that is compelling. Moreover, various new theoretical ideas, new experimental discoveries, and methodological advances in theory and experiment (some of which are discussed in Chapter 11) give hope that substantial advances in understanding are occurring.

One set of new ideas involves the existence of broken-symmetry quantum phases possessing "hidden" (i.e., hard to detect) types of order. For example, interest has recently focused on a class of states with complex patterns of spontaneously generated persistent currents. No such state has yet been unambiguously identified in a real material; conversely, even if such a state occurs, it would be very difficult to detect by most conventional measurements.

Another interesting class of states with hidden order is electronic analogues of the classical liquid crystalline states that occur in complex fluids. In a simple liquid, the particles can flow from one point to another, all points in space are

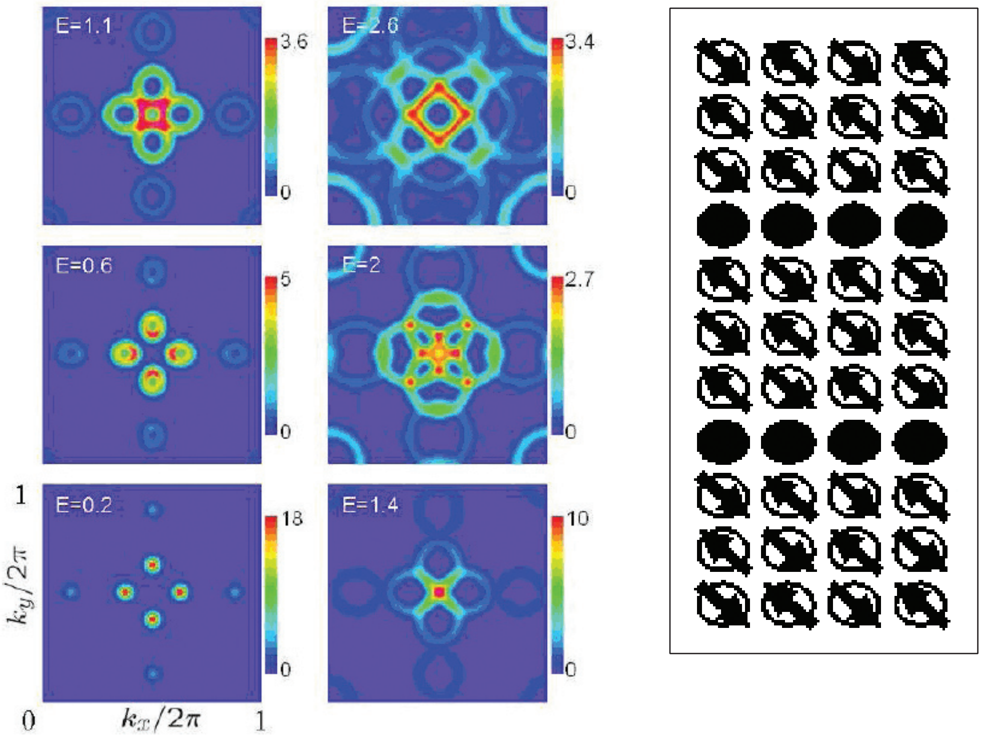

FIGURE 2.3 Calculated magnetic structure factor for a "stripe-ordered" antiferromagnet. Strong interactions between electrons can lead to complex ordered states with particle-like excitations that look nothing like those of an electron. One such state, which has been directly identified in neutron scattering experiments on a number of transition metal oxides, including some high-temperature superconductors (such as $La_2CuO_{4+\delta}$), is a unidirectional incommensurate antiferromagnet, or "striped phase," shown schematically (right panel). The emergent particle-like excitations that occur in such a state are charge-neutral "spin-waves," whose spectrum is calculated here (left panels) and which are valid deep in the ordered phase. SOURCE: (Left) Reprinted with permission from D.X. Yao, E.W. Carlson, and D.K. Campbell, "Magnetic Excitations of Stripes and Checkerboards in the Cuprates," *Phys. Rev. B* **73**, 224525 (2006). Copyright 2006 by the American Physical Society. (Right) Steven A. Kivelson, Stanford University.

equivalent, and all directions are the same. In a crystal, there is a lattice on which the atoms or molecules are localized in a pattern that repeats periodically through space, so that different points within the unit cell are different from each other, and different directions, relative to the axes of symmetry defined by the crystalline order, are distinct from each other. Liquid crystalline states exhibit patterns of symmetry breaking intermediate between those of a simple liquid and a crystal.

For instance, a “nematic” is a uniform fluid state in which one spatial direction is distinguished from the other two. Traditionally, a nematic is described as consisting of a fluid of cigar-shaped molecules, in which the molecules can flow, but they are preferentially oriented along one direction. At first sight, a nematic electron fluid seems improbable, since electrons are point-like, not cigar-shaped. However, in some circumstances it is legitimate to think of a highly correlated electron fluid as consisting of melted fragments of an appropriate electron crystal; these fragments, in turn, can play the role of the cigar-shaped molecules in the classical nematic. An electron nematic phase is also difficult to detect for various technical reasons, including the fact that crystalline imperfections can mask its occurrence on macroscopic scales and that it can be hard to distinguish from a more conventional strain-driven change in the crystal structure of the host material. However, as discussed below, strong evidence for an electronic nematic phase has recently been found in extremely high mobility quantum Hall devices. Moreover, evidence of the existence of such phases has recently been found in a number of interesting highly correlated materials, including $Sr_3Ru_2O_7$ and certain of the high-temperature superconductors (e.g., $La_{2-x}Ba_xCuO_4$).

A still more revolutionary circle of ideas, built around the notion of “fractionalized” phases, has been the focus of increasing attention in recent years. The key idea here is that sharp distinctions can exist between distinct quantum phases of matter that have nothing to do with distinct patterns of symmetry breaking. Rather, these phases are characterized by an abstract form of order—so-called topological order. Because the order is so subtle, it is difficult to establish experimentally where such phases occur in nature. The most directly experimentally accessible characteristic of these phases is the existence of new types of quasi-particles that behave like a “fraction” of an electron. For instance, in one of the best theoretically characterized of these phases, there are no quasi-particles that carry both the charge and spin of ordinary electrons. Instead, two new and very strange kinds of particles appear, one of which carries only spin and another of which carries only charge. In other systems, the quasi-particles carry a specific fraction—for example, one-third—of the electron charge. Under some circumstances, these quasi-particles are also believed to possess “fractional” quantum statistics. In other words, the wave function of two such identical particles neither preserves nor changes its sign when the particles are interchanged but instead is multiplied by a complex number (e.g., the cube root of $-1$!). Such particles are neither bosons nor fermions; they are called anyons.

At present, fractionalization is an established experimental fact only in the fractional quantum Hall state, as explained in the next section. Evidence suggestive of the existence of fractionalized phases has been reported in the past few years in a number of strongly correlated materials that exhibit particularly unusual properties. Moreover, the search for fractionalized states has gained added impetus from the realization, discussed in Chapter 7, that such phases might produce uniquely favorable structures for the construction of a quantum computer. However, it is an issue for the coming decade to discover which of these phases actually exist in nature, and where (i.e., in what materials).

## QUANTUM HALL SYSTEMS AND THE DISCOVERY OF NEW QUANTUM STATES OF MATTER

The concepts of fractionalization and non-Fermi liquids have roots in electronic materials that are less than three-dimensional. For example, it has been known since the 1960s that a disorder-free, one-dimensional electron system cannot be a Fermi liquid. Unlike electrons in two and three dimensions, the distribution in momentum space of one-dimensional electrons does not have a discontinuity at the Fermi momentum, even at zero temperature. Experimental evidence for such "Luttinger" liquids has accumulated in recent years from studies of electrical conduction in carbon nanotubes and along the edges of two-dimensional electron systems in a high magnetic field, as well as from more complex experiments (such as angle-resolved photoemission and optical conductivity) performed on various other "quasi-one-dimensional" materials in which electrons can move readily only in one direction.

Fractionalization is already well known in two-dimensional electron systems (see Figure 2.4). A large magnetic field perpendicular to the two-dimensional plane breaks up the otherwise-continuous distribution of electron energies into a ladder of discrete states known as Landau levels. Since the energy of an electron in a circular cyclotron orbit does not depend on where the orbit is located, each Landau level can hold many electrons, the total number being proportional to the magnetic field. Consequently, at sufficiently high magnetic fields, all two-dimensional electrons in a given sample can fit into the lowest Landau level and have precisely the same kinetic energy. With no variation in the kinetic energy, the Coulomb interaction between electrons completely dominates the physics in clean samples. In a real sense this is the most strongly interacting quantum system imaginable. It is in this regime that Tsui, Stormer, and Gossard discovered the famous fractional quantum Hall effect (FQHE) in 1982.[1] They observed that when the lowest Landau level is one-third filled, a wholly unexpected quantized plateau in the Hall resistance appears, signaling the opening of an energy gap. Shortly thereafter, Laughlin explained the effect as the emergence of a new state of matter, one driven entirely by strong Coulomb correlations among the electrons.[2] Laughlin's theory was the

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[1] D.C. Tsui, H.L. Stormer, and A.C. Gossard, "Two-Dimensional Magnetotransport in the Extreme Quantum Limit," *Phys. Rev. Lett.* **48**, 1559 (1982).

[2] R.B. Laughlin, "Anomalous Quantum Hall Effect: An Incompressible Quantum Fluid with Fractionally Charged Excitations," *Phys. Rev. Lett.* **50**, 1395 (1983).

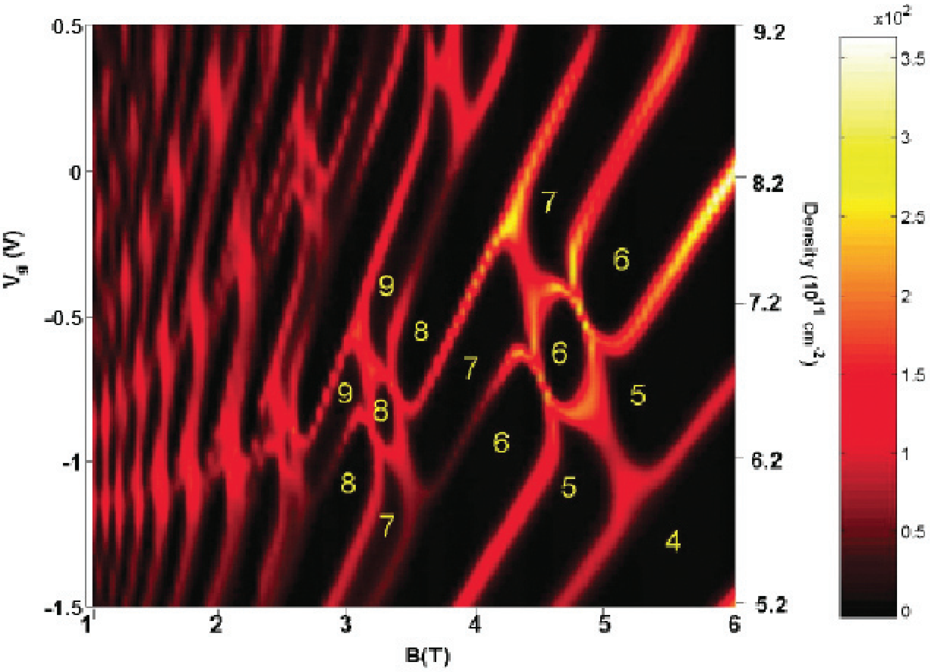

FIGURE 2.4 Quantum phases and phase transitions in a two-subband quantum Hall device. Shown here is a contour map of the resistivity of a two-dimensional electron gas that has been trapped at the interface between two semiconductors. The y-axis is the gate voltage applied across the sample (which changes the density of electrons), and the x-axis is the strength of an applied magnetic field. The dark regions, where the resistivity becomes vanishingly small as the temperature tends toward absolute zero, are various quantum Hall effect states, where the integers label the value of the quantized Hall conductance in units of the quantum of conductance. The bright regions mark the points at which quantum phase transitions occur between the different phases. The fact that the resistance neither vanishes nor diverges as the temperature tends to zero along the quantum critical lines is a tangible reflection of the existence of quantum fluctuations at all length scales. SOURCE: Reprinted with permission from X.C. Zhang, D.R. Faulhaber, and H.W. Jiang, "Multiple Phases with the Same Quantized Hall Conductance in a Two-Subband System," *Phys. Rev. Lett.* **95**, 216801 (2005). Copyright 2005 by the American Physical Society.

first to imply the existence of fractionalized elementary particles within a strongly correlated electron system. These new particles, which carry precisely one-third the charge of an ordinary electron, are neither bosons nor fermions, possessing instead the bizarre anyonic exchange statistics mentioned above. Very strong experimental evidence for the fractional charge of these particles now exists, and experimental proof of fractional statistics is currently being hotly pursued.

The FQHE at one-third filling of the lowest Landau level turned out to be only one member of a large family of similar correlated phases of two-dimensional electrons. Over the past 25 years, many dramatic experimental observations have been made, and a sophisticated and unified theoretical understanding of much of FQHE phenomenology has been developed. The field remains vibrant, with the pace of new discoveries paralleling the steadily increasing quality of the semiconductor heterostructure samples grown by molecular beam epitaxy. Most recently, interest has focused on an FQHE that appears at one-half filling of the first excited Landau level (the so-called 5/2-state). This fragile state is expected to possess an even stranger form of exchange statistics in which the outcome of multiple interchanges of pairs of particles depends on the order in which the interchanges occur. Observation of such "non-Abelian" statistics would have deep fundamental significance for physics and possible impact on schemes for quantum computation, since non-Abelian systems are anticipated to be especially insensitive to the kinds of disturbances that ordinarily disrupt quantum coherence.

The steady increase in sample quality has also led to the recent discovery of new electronic phases outside the FQHE paradigm. At modest magnetic fields, where several Landau levels are occupied, collective states emerge that are reminiscent of both classical liquid crystals and pinned charge density waves. For example, near one-half filling of highly excited Landau levels, electrical conduction in the two-dimensional system spontaneously becomes extremely anisotropic at very low temperature (below about 150 mK). Strikingly, this anisotropy disappears on moving slightly away from one-half filling and is absent altogether at both very low and very high magnetic fields. The effect is widely believed to reflect a stripe-like pattern of charge density modulation in the two-dimensional system. While quantum and thermal fluctuations destroy the long-range order of the stripes, local order persists. In effect, the two-dimensional electron system is broken up into a collection of striped domains. Above about 150 mK, these domains are apparently randomly oriented, and the net resistivity of the system is isotropic. At lower temperatures, orientational order sets in and the resistivity rapidly becomes anisotropic. As discussed above, this situation is highly analogous to the isotropic-to-nematic phase transition in classical liquid crystals (see Figure 2.5). In this case, the local stripe domains of electrons play the role of the funny-shaped molecules in the liquid crystal. That a system of point-like electrons would emulate a liquid crystal is one of the most dramatic examples of emergence in recent years.

Excitingly, the quantum Hall effect has recently been observed in graphene (single atomic layers of graphite). This is especially interesting since graphene is a semimetal whose low-energy band structure precisely mimics the dynamics of massless relativistic particles, the so-called Dirac fermions familiar to high-energy physicists. In other words, the kinetic energy of electrons (or holes) in graphene is directly proportional to their momentum, rather than its square. This aspect (and others) of the graphene band structure creates a spectrum of quantum Hall states that is distinct from that found in conventional two-dimensional electronic

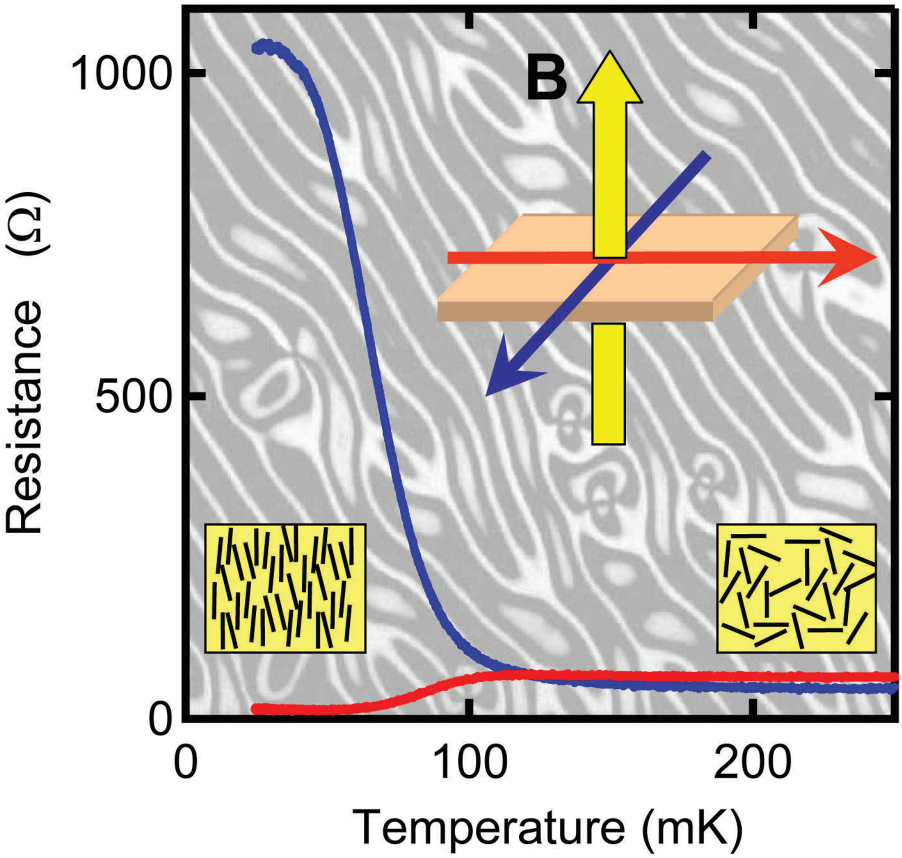

FIGURE 2.5 Quantum and classical nematic liquid crystals. The background image is a polarization microscope image of a classical nematic liquid crystal, similar to those found in cellular telephones, computer displays, or wristwatches. The graph and the insets describe the development of *quantum* liquid crystalline behavior in a collection of electrons moving on a plane surface of a nematic liquid crystal in the presence of a perpendicular magnetic field. The red and blue traces show how the electrical resistance of the system, measured in two mutually perpendicular directions, becomes extremely anisotropic at temperatures close to absolute zero. This anisotropy is believed to arise from the spontaneous orientational ordering of small elongated clumps of electrons, as suggested by the black rods in the lower insets. SOURCES: (Graph) J.P. Eisenstein, "Two-Dimensional Electrons in Excited Landau Levels: Evidence for New Collective States," *Solid State Commun.* **117**, 123-131 (2001). (Background image) Photograph by Oleg D. Lavrentovich, Liquid Crystal Institute, Kent State University.

materials (e.g., in silicon inversion layers or gallium arsenide quantum wells). To date, only integer, as opposed to fractional, quantized Hall states have been detected in graphene. This suggests that the quality of the current samples is not high enough for the subtle, many-particle correlations of the FQHE to hold sway over the disordering effects of impurities. The intensity of research on graphene is now enormous. There is every reason to believe that significant advances, including the discovery of new emergent phenomena and the development of more effective means for creating, manipulating, and employing clean graphene films, will occur in the coming decade.

Clearly, the nature of correlated motion of strongly interacting particles is a conceptually deep problem with broad implications in areas of condensed-matter and materials physics and in other areas of physics as well. The quest to understand the emergent behaviors produced by these correlations is one of the central issues in physics today. Moreover, with the spirit of the past as a prologue, there is every reason to believe that some of these new emergent phenomena will be the basis of future technologies of profound importance.

## CRITICAL PHENOMENA AND UNIVERSALITY

Generally, the phases of matter are well defined in the sense that many of the properties of a given material depend primarily on the material's state (for example, solid, liquid, or gas), and not so much on the substance itself. All liquids behave in many familiar ways; as elementary school students learn, a liquid has a fixed volume but takes the shape of its container; it flows; sound can propagate through it; and so forth. These and many other features are common to liquid water, gasoline, alcohol, and liquid helium. A metal—be it copper or silver or an organic metal made largely of carbon and hydrogen—is shiny and conducts electricity readily. Indeed, an organic metal and an organic insulator, even though they may be made of essentially the same constituent elements, have physical properties that share many fewer features than do an organic metal and copper. This universal character of the phases of matter generally holds all the way from the nanometer to the centimeter scale and beyond.

Phase transitions can occur as a function of temperature, or pressure, or magnetic field, or composition, and so forth. When water freezes, the water at temperatures just below the freezing point is a solid (ice), which behaves pretty much in the same way as ice that is far colder. The water just above the freezing point is a liquid, and similar to liquid water at higher temperatures. The change in the behavior is highly discontinuous across the freezing point. This is an example of a first-order transition.

Some other transitions, such as the transition from a paramagnetic to a ferromagnetic phase, occur in a much more mysterious manner, by a "continuous transition." Close to the critical temperature, it becomes increasingly difficult to tell which side of the transition the system is on. On length scales that get increasingly large in proximity to the transition, the system cannot decide which phase behavior to exhibit, and so it exhibits a new, intermediate behavior—critical behavior—that is different from the behavior of either of the phases themselves. At a critical point, there are fluctuations on all length scales from the microscopic to the macroscopic.

The broad distribution of length scales at a critical point—or technically, the scale invariance—is a spectacular phenomenon. Most phenomena in nature have a characteristic size. Atoms are all (within a factor of two) a couple of angstroms in diameter, and people are typically 5 to 6 feet tall. In a piece of ice, when atoms rearrange (i.e., flow on a microscopic scale), typically only a few atoms move at a time. However, near a ferromagnetic critical point, collective motions occur involving reorientation of the magnetic dipoles of small groups of a few electrons and enormous patches of millions or billions of electrons.

The "renormalization group" theory of critical phenomena in classical systems undergoing a continuous phase transition, which was developed throughout the last three decades of the 20th century, is one of the most significant contributions of CMMP to science. It provides an understanding of how scale invariance at a critical point arises from simple microscopic interactions. Because physics near a critical point occurs on such a broad range of length scales, much of the detailed information about the microscopic constituents of the material is averaged out. In a quantifiable sense, the behavior of systems near a critical point is "universal"—that is, precisely the same for different systems. Not only does the magnetization grow with decreasing temperature in precisely the same way in ferromagnets made of pure iron or of neodymium alloys, but it grows in exactly the same way that the concentration difference grows near the critical point for phase separation of a mixture of water and oil.

Indeed, renormalization group theory offers a top-down perspective for understanding condensed matter that is opposite to the usual bottom-up reductionist approach, which focuses on the identification of a small number of elementary building blocks. Since the behavior of the system is independent of what material is being studied, there is not a unique route from the microscopic understanding of the laws of quantum mechanics to the macroscopic properties of a system near its critical point. Rather, the "answer" is largely independent of the "question." So powerful is the notion of universality that the solution of even a vastly simplified abstract mathematical model problem, so long as it respects certain symmetries and constraints of the real world, can be used to obtain a precise and quantitative understanding of experimental observations in the complex real world! This is the most precisely understood realization of the more general notion of emergence.

As with any revolutionary change, the full implications of the renormalization group approach continue to reverberate. When continuous phase transitions occur at zero temperature, quantum mechanics on a macroscopic scale becomes important. Here, quantum mechanics intertwines dynamics and thermodynamics in a way that they never are in finite temperature ("classical") phase transitions. The naïve extension of the successful theory of classical phase transitions has already been shown to produce results that are in conflict with experiment for quantum phase transitions. It remains unclear whether minor modifications of the classical approach or much more fundamental changes are needed to address these difficulties. Transitions occur, as well, in non-equilibrium, "driven" dynamical systems, of which the best known is the transition from laminar flow to turbulence. Many driven dynamical systems exhibit phenomena on a broad range of scales—exhibiting an approximate form of scale invariance. Much beautiful work has already been done applying renormalization group ideas to this broad class of systems, but it is clearly just the tip of the iceberg, as discussed in Chapter 5. Another vast area in which many related open problems exist is systems with quenched disorder—in which there are degrees of freedom, such as the locations of impurity atoms, which are not in thermal equilibrium. Phase transitions—even classical phase transitions—in the presence of quenched disorder are not fully understood, and where quenched disorder and quantum phase transitions intersect, there is a growing understanding that entirely new conceptual tools are needed.

## EMERGENCE IN ULTRACOLD ATOMIC GASES

The rapidly dissolving boundary between conventional atomic physics and CMMP has focused yet another spotlight on the phenomenon of emergence.[3] The convergence of these two fields began about 10 years ago when, upon cooling dilute gases of atoms (e.g., $^{87}$Rb) trapped in magnetic bottles into the nano-kelvin temperature range, atomic physicists succeeded in directly witnessing the phenomenon of Bose-Einstein condensation (BEC). In a BEC, quantum uncertainty obscures the identity of the individual atoms and instead endows the entire ensemble with a single coherent wave function. While Bose-Einstein condensation had been long known to CMMP physicists to be responsible for the phenomenon of superfluidity in liquid helium, its unambiguous observation in a wide variety of highly controllable atomic systems was a watershed event in physics.

Since the initial observations of BEC, the field of ultracold atomic gases has expanded dynamically in both experiment and theory. Particularly dramatic among many exciting developments has been the observation of Cooper pairing in cold fermionic systems and the detection of the superfluid-to-insulator transition among cold bosonic atoms held in an optical lattice potential. These two examples illustrate the power of the ultracold atom field to study classic condensed-matter phenomena in an extremely controllable way. Moreover, ultracold atoms in specially tailored optical lattices, as described in Chapter 8, may be used to simulate

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[3] National Research Council, *Controlling the Quantum World: The Science of Atoms, Molecules, and Photons*, Washington, D.C.: The National Academies Press, 2007.

models of some of the most significant outstanding problems in condensed-matter physics, including high-temperature superconductivity and related strong correlation phenomena. These optical lattice-based systems, acting as "analog quantum computers," may provide solutions to problems that have been found to be essentially unsolvable using conventional digital computers. Most importantly, ultracold atoms offer the prospect of discovery of wholly new and highly exotic states of condensed matter that have no roots in traditional material systems.

## EMERGENCE IN CLASSICAL CONDENSED-MATTER SYSTEMS

A number of examples of emergence in classical condensed-matter systems illustrate the scope and unity of the concepts underlying the study of emergence, where neither quantum mechanics nor even conventional thermal physics plays any direct role in determining the emergent behavior (see Figure 2.6). A few examples are described below.

Granular matter, like other forms of condensed matter, is made up of an enormously large number of simple constituents—the individual grains, for instance, of sand or wheat. The difference is, however, that the grains themselves are very large compared with the atoms and small molecules that make them up. Since the

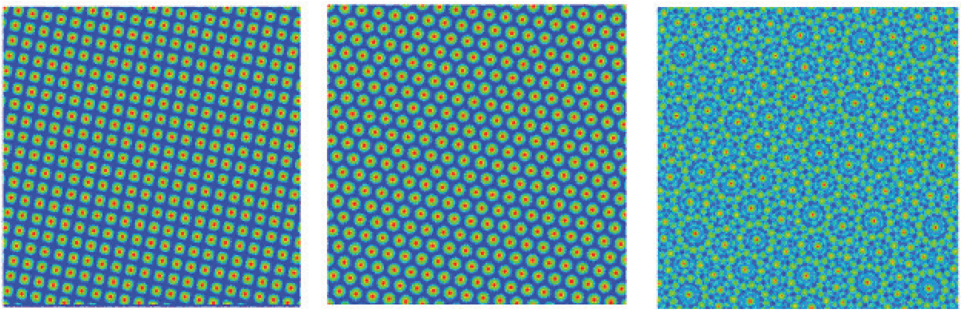

FIGURE 2.6 A wide variety of regular patterns spontaneously emerge in many systems driven away from equilibrium. There is a growing understanding of the variety and complexity of the patterns in terms of the nonlinear interaction and competition between spatial modes that become unstable owing to the drive away from equilibrium. The three panels in this figure show results of simulations of a simple partial differential equation that captures these effects—the different patterns are given by changing parameters. Patterns remarkably similar to these are seen in experimental systems such as boiling water, vertically shaken fluids, and granular flows. SOURCE: Ron Lifshitz, Tel Aviv University. Based on R. Lifshitz and D.M. Petrich, "Theoretical Model for Faraday Waves with Multiple-Frequency Forcing," *Phys. Rev. Lett.* **79**, 1261-1264 (1997).

characteristic energy scale that characterizes the quantum motion of a collection of particles decreases rapidly with the increasing size of the particle, even at the lowest accessible temperatures quantum effects in granular systems are negligible. Conversely, even at room temperature or above, thermal effects are also negligible: the interaction energy between pairs of grains increases with size (roughly in proportion to the surface area) and so is always large compared with the temperature. Put another way, the ratio of the entropic and interaction contributions to the free energy at any fixed temperature decreases rapidly with the size of the grains. Thus, granular matter effectively presents scientists with a problem in which temperature can also be ignored, so the collective phenomena typically involve nonequilibrium physics, as discussed in Chapter 5. Nevertheless, emergent phenomena occur in granular matter in much the same manner that they occur in conventional fluids and solids, although often with new and fascinating wrinkles.

When a granular material is fluidized, by shaking it vigorously or by blowing gas through it, the resulting non-equilibrium state has many features in common with a simple gas—for example, the individual grains exhibit a distribution of speeds that is very similar to that of molecules in a gas at an "effective temperature," which depends on how violently the granular matter is shaken. A dense granular material, like sand on a beach, shares many properties with a solid, including its ability to support a person. However, unlike a simple solid, where the strain is fairly smoothly distributed throughout the material, in a compressed granular system the strains can be highly irregularly distributed along lines of force (Figure 2.7). The principles that govern the distribution of strain in dense granular matter, and which features are universal (i.e., do not depend on the nature [size, shape, hardness] of the individual grains), are at present an area of active research. It is similarly not fully understood to what extent the motion of broader classes of driven granular systems can be related to properties of a related equilibrium system at an effective temperature.

*Jamming* is a phenomenon in granular materials that, when better understood, may shed light on a broad class of phenomena in condensed-matter systems. At low density, it is clearly easy for granular matter to flow—each grain simply moves in the general direction of the flow and is occasionally scattered when it collides with another grain. This is a classical analogue of the motion of quasi-particles in a Fermi liquid. However, when hard grains, such as grains of sand, reach a critical density, there is simply no room for the grains to flow. Every grain is jammed in a cage of other grains from which it cannot escape. Here, the strong correlations between grains entirely quench the free motion of the individual grains. Since there is no balance of quantum and classical energies, no competing tendencies of energy and entropy, this jamming transition may be, in some sense, the simplest model problem in the physics of strong correlations. Jamming is, in a sense, a purely geometric phenomenon.

FIGURE 2.7 A collapsing grain silo provides a dramatic example of the unexpected behavior of granular materials. If the grains are flowing in some regions and jammed in others within the silo, there can be large variations of the stress on the silo walls, leading to disaster. SOURCE: J.M.Rotter, University of Edinburgh, and J.W. Carson, Jenike and Johanson, Inc.

## REALIZING THE FULL POTENTIAL OF EMERGENCE

Emergent phenomena in condensed matter are often discovered serendipitously. The discovery of superconductivity by Kamerlingh Onnes in 1911 was certainly accidental. The discovery of the fractional quantum Hall effect by Tsui, Stormer, and Gossard in 1982 was similarly unanticipated. These two great discoveries, decades apart in time, have some important similarities that offer insights into how to increase the odds for the discovery of emergent phenomena. For example, both experiments were part of a program of curiosity-driven, "blue-sky" research, and both fundamentally altered the landscape of CMMP. At the same time, both discoveries are intimately connected to the technological side of CMMP. With superconductivity, that connection lay in the future applications of the phenomenon itself. Conversely, the discovery of the fractional quantum Hall effect was enabled by technical advances in semiconductor crystal growth critical to the development of high-speed transistors for telecommunications. These two discoveries beautifully illustrate the inseparability of the applied and fundamental sides of CMMP. They also illustrate the need to maintain a robust funding base for the pursuit of curiosity-driven CMMP research and the ready availability of the exotic materials that enable such great discoveries. Both of these issues figure prominently in the recommendations of this report.

Superconductivity and the fractional quantum Hall effect were discovered by investigating the properties of matter under extreme conditions. Kamerlingh Onnes, having recently succeeded in liquefying helium, was studying the resistivity of metals cooled to near absolute zero. Tsui, Stormer, and Gossard, also examining electrical conduction, were subjecting their ultrapure semiconductor samples to the highest-available magnetic fields. The fruitfulness of high magnetic fields and low temperatures of course remains fully appreciated, with the National High Magnetic Field Laboratory in Tallahassee, Florida, the most visible evidence. Beyond high magnetic fields and low temperatures, CMMP researchers regularly subject their samples to high pressures, intense electromagnetic fields, dimensional confinement, and other extreme conditions in search of understanding and, best of all, surprises.

Discoveries of emergent phenomena sometimes have the appearance of mere lucky breaks in an otherwise random walk. This is no truer of superconductivity or the fractional quantum Hall effect than it is of Edison's discovery of the correct filament material for incandescent light bulbs. Kamerlingh Onnes was naturally trying to understand the conduction of electricity in metals in the context of the Drude theory advanced just a few years before. Similarly, Tsui, Stormer, and Gossard were guided in part by theoretical predictions that electron gases would freeze directly into a crystalline solid at high enough magnetic field. Both examples illustrate the close interaction between theory and experiment that characterizes CMMP; each informs and guides the other.

## CONCLUSIONS

Emergent phenomena in condensed-matter and materials physics are those that cannot be understood with models that treat the motions of the individual particles within the material independently. Instead, the essence of emergent phenomena lies in the complex interactions between many particles that result in the diverse behavior and often unpredictable collective motion of many particles. It is wonderful and exciting that the well of such phenomena is infinitely deep; CMMP researchers will never run short of mysteries to solve and phenomena to exploit—they are out there for the inquisitive to find.

Emergent phenomena beautifully illustrate the inseparability of the fundamental and applied research in CMMP. In some cases, the application of an emergent phenomenon is nearly immediate; in other cases it takes decades to occur; and in still others it may never occur. At the same time, technical advances in one area of CMMP can enable the discovery of an exotic phenomenon in a seemingly remote area of the field.

The nation's CMMP community has historically been extraordinarily successful at discovering, understanding, and applying emergent phenomena. In terms of opportunity, the future is extremely bright. Ever-more-complex materials are being synthesized and ever-more-sophisticated tools are being developed for their study. The explosion of research on nanoscale systems and the rapidly dissolving boundaries between CMMP and other scientific disciplines will surely lead to new vistas in emergent phenomena. The challenge is to make sure that U.S. researchers have access to the best new materials and tools and the time and resources to make the most of them.

The paths between discovery, understanding, and applications of scientific research are obscure and unpredictable. They are full of sharp turns, dead ends, and unexpected forks in the road. But they also can lead to beautiful places that no one knew existed. Robert Frost had it right: It is important to take the road less traveled, for that will make all the difference.

# 3

# How Will the Energy Demands of Future Generations Be Met?

The availability of affordable and renewable energy sources represents one of the greatest challenges that will face humankind in the 21st century. In the United States, there is a pressing need to develop energy sources in order to reduce dependency on fossil fuels while minimizing carbon emissions and other sources of harm to the environment. Promising technologies for solar energy, hydrogen fuel cells, solid-state lighting, supercapacitors, rechargeable batteries, and improved nuclear power will play critical roles, but fundamentally new scientific approaches are also needed. To meet U.S. needs, many profound scientific challenges must be addressed with urgency. Condensed-matter and materials physics (CMMP) is uniquely positioned to address these challenges, which require better understanding of energy conversion and storage as well as new technologies for increasing end-use energy efficiency. How can sunlight be converted to usable energy more efficiently? In what new ways can hydrogen be generated and stored? Can renewable, affordable, and benign fuels be developed? How can new approaches and new materials be used to create better light-emitting diodes (LEDs) and light-conversion materials? Discovering and understanding new materials will be key. No single strategy will provide all the answers, and some approaches may take decades to come to fruition, so research investment over a broad front is needed to meet this immense challenge. What is certainly clear, however, is that new materials, nanoscience, and new theoretical approaches will play a critical role in overcoming many of the technical barriers to achieving energy security.

## SETTING THE CONTEXT

For the past half century, U.S. economic growth has been based partly on the availability of plentiful and cheap energy. The United States, with only 5 percent of the world's population, is now consuming 25 percent of the world's oil production.[1] However, with oil production in many countries now in decline and demand predicted to double during the next two or three decades, the era of cheap oil is over. The same is true of natural gas. Coal could provide a solution, since the United States has 25 percent of the world's proven supplies, but increasing U.S. dependence on coal for electricity generation could have unfavorable environmental consequences unless it is accompanied by carbon capture and storage. Indeed, there is compelling evidence that increasing emissions of anthropogenic greenhouse gases are leading to global warming and concomitant stress on the environment. As a consequence, whereas science in the second half of the 20th century focused its attention on launching the information age and in employing the revolution in molecular biology to design new classes of medical therapeutics and to solve the human genome, it is expected that during the first half of the 21st century, science will be called on to help address the massive task of transforming the global energy supply from fossil fuels to renewable sources. Many of the issues are political and/or economic in nature and therefore lie outside the scope of this report, but for the transition to renewable energy sources to occur on the required timescale, many scientific and technological breakthroughs will be necessary. These are global challenges, of course, but as the world's most prolific energy consumer, the United States bears a responsibility to demonstrate leadership. Furthermore, with a growing energy deficit (Figure 3.1), the U.S. economy and quality of life are highly vulnerable to these inexorable trends.

The role of CMMP scientists in the energy challenge is to create more technical options for lawmakers to consider for the U.S. energy portfolio. The CMMP community is already contributing strongly to the technologies surrounding the energy sector, and it is well positioned to do so even more in the future. For example, CMMP will be able to exploit some of the exciting developments in nanotechnology in order to solve some of the most pressing problems (see Chapter 6). This can only happen, however, if there is a national commitment to meeting this energy challenge and if sufficient funding is made available. Both the urgent need to address this challenge in the coming decade and the scientific opportunity for CMMP to contribute to the solution motivate the choice of energy as a grand challenge by the Committee on CMMP 2010. Further, energy research offers an opportunity for answering basic questions about materials and advancing a fun-

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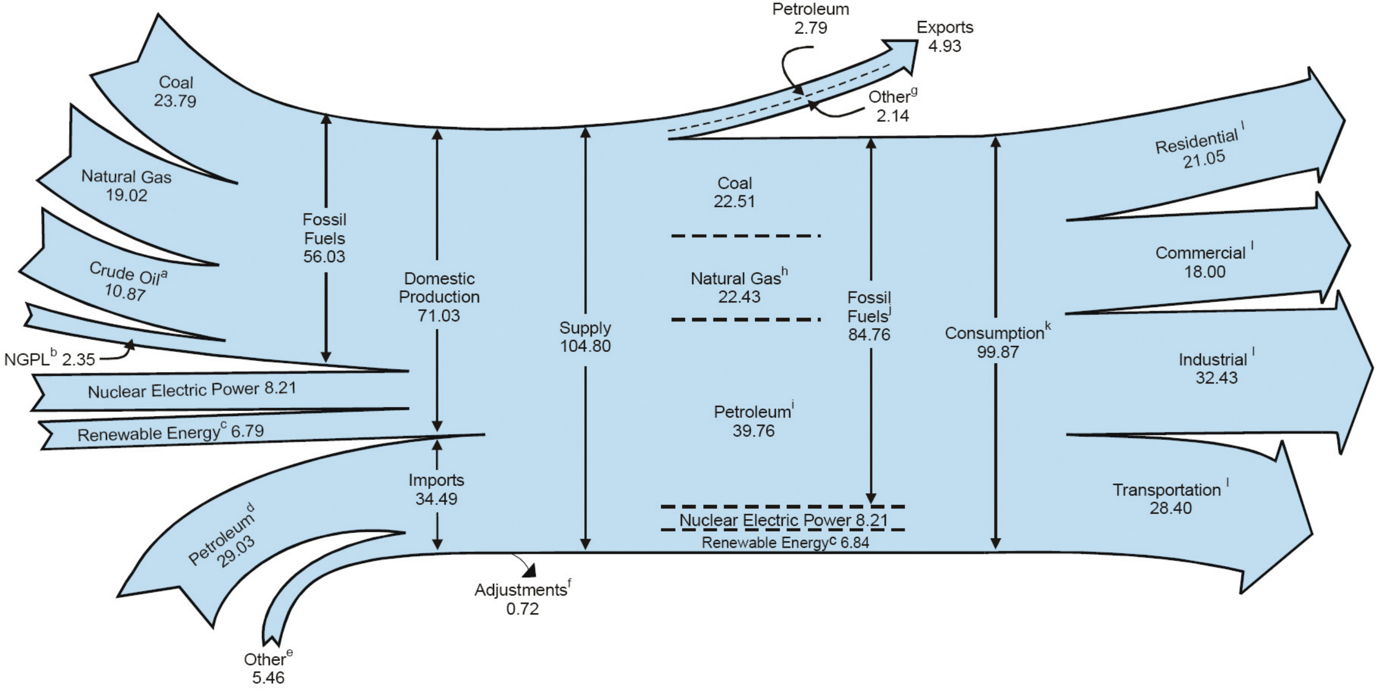
[1] For more information on international petroleum (oil) consumption, see http://www.eia.doe.gov/emeu/international/oilconsumption.html; last accessed September 17, 2007.



[a] Includes lease condensate.

[b] Natural gas plant liquids.

[c] Conventional hydroelectric power, biomass, geothermal, solar/PV, and wind.

[d] Crude oil and petroleum products. Includes imports into the Strategic Petroleum Reserve.

[e] Natural gas, coal, coal coke, fuel ethanol, and electricity.

[f] Stock changes, losses, gains, miscellaneous blending components, and unaccounted-for supply.

[g] Coal, natural gas, coal coke, and electricity.

[h] Natural gas only; excludes supplemental gaseous fuels.

[i] Petroleum products, including natural gas plant liquids, and crude oil burned as fuel.

[j] Includes 0.06 quadrillion Btu of coal coke net imports.

[k] Includes 0.06 quadrillion Btu of electricity net imports.

[l] Primary consumption, electricity retail sales, and electrical system energy losses, which are allocated to the end-use sectors in proportion to each sector's share of total electricity retail sales. See Note, "Electrical Systems Energy Losses," at end of Section 2.

Notes: • Data are preliminary. • Values are derived from source data prior to rounding for publication. • Totals may not equal sum of components due to independent rounding.

Sources: Tables 1.1, 1.2, 1.3, 1.4, and 2.1a.

FIGURE 3.1 Total U.S. energy flow, 2006 (quadrillion British thermal units [Btu]), showing input energy sources (production) at left (including imports at lower left) and output (end-use) sectors at right. SOURCE: Energy Information Administration, *Annual Energy Review 2006*, available at http://www.eia.doe.gov/emeu/aer/pdf/aer.pdf.

damental understanding of solids. Two examples of crosscutting opportunities for the coming decade include the development of new materials by design: (1) the promotion of specific energy-related technologies such as photonic crystals to enhance photovoltaic efficiency and broaden the photosensitive response range and (2) the endowment of nanomaterials with properties not found in their bulk counterparts through the use of theoretical modeling, experimental synthesis, materials characterization, and properties measurements. The latter, for example, could address the need for independent control of increased hydrogen adsorption and faster kinetics for hydrogen release in the hydrogen storage needs of a hydrogen economy. In the sections below, the committee highlights some of the ways in which the CMMP community can develop cutting-edge science that will strongly influence future developments in energy conversion, energy storage, and end-use energy efficiency.

## ENERGY CONVERSION

For the foreseeable future, electricity will play a central role in the U.S. energy strategy on account of the extensiveness of the existing distribution network and the fact that electricity can be produced from a variety of sources, including gas, coal, oil, hydropower, and nuclear energy. The coming decades will see a greater emphasis on localized electricity generation from solar energy, biomass, thermoelectric devices, and fuel cells for both automotive and stationary use. In addition, there is already clear evidence that hybrid power systems, such as those now used increasingly in automotive applications, will become much more prevalent. In the subsections that follow, the vital role that CMMP is expected to play in energy conversion is discussed. There are several relevant energy-conversion technologies, including sunlight to electricity (photovoltaic cells), sunlight to chemical energy (the photocatalytic splitting of water to make hydrogen or the photochemical production of other chemical fuels), chemical energy to electricity (fuel cells), heat to electricity (thermoelectric devices), biomass to chemical energy (biofuels), and nuclear energy to electricity (nuclear fission and fusion).

### Solar Cells

The ultimate source of all energy is the Sun: there are 120,000 terawatts (TW) of solar energy potential globally, in comparison with the total global energy consumption of 12.8 TW in 1998.[2] To capitalize on this important renewable resource, many researchers are working toward cheaper, more efficient solar cells

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[2] Department of Energy, *Basic Research Needs for Solar Energy Utilization*, Washington, D.C., 2005. Available at http://www.sc.doe.gov/bes/reports/files/SEU_rpt.pdf; last accessed September 17, 2007.

that are manufacturable at large scale. There is now a hierarchy of solar cells with different costs and efficiencies, ranging from very expensive triple-junction cells, with efficiencies approaching 40 percent, to the low-cost flexible systems based on conducting polymers, with power efficiencies of up to 5 percent. All of the different solar technologies pose difficult materials and design challenges. Triple-junction systems, for example, could be further improved by incorporating narrower band gap semiconductor materials that can harvest solar energy in the infrared range. Polymer-based cells are typically based on polythiophene derivatives, which act as the hole carriers, and fullerenes, which provide the electron transport. Charge separation can be achieved quite efficiently in the polymer cells, but charge transport is relatively slow, especially for the electrons, and carrier recombination prior to reaching the electrodes is a problem. Device architectures that use nanomaterials in order to reduce the likelihood of recombination are being explored, and new polymers with greater carrier mobility are being sought. An additional challenge is that many conducting polymers are unstable in the presence of light and oxygen owing to the formation of reactive oxygen radicals, so strategies for minimizing this problem are urgently needed, especially through the design of new materials.

One approach for improving the cost-effectiveness of the more expensive solar cells is to use them in combination with concentrators that can harvest the sunlight from a large area and focus the incident energy onto a small area of active cells. This approach has the potential to double the efficiency of flat panel photovoltaic cells and to reduce the cost of producing solar electricity by over 50 percent. Solar concentrators normally have to be used in combination with a tracking system, however, which is not required with conventional flat panels. An even more dramatic enhancement in efficiency may emerge from a recent CMMP-related scientific breakthrough based on the production of multiple electron-hole pairs from a single solar photon within nanoparticles of PbSe.

### Hydrogen Generation by Photocatalysis

The energy required to split water into hydrogen and oxygen is too high to be supplied by simple heating. Hydrogen can be extracted by electrolysis, although this is expensive and certainly less attractive than the direct splitting of water to generate $H_2$ and $O_2$, which could then be used in a fuel cell, as described below. Sunlight, however, can be harnessed to split water into hydrogen and oxygen by means of photocatalysis. Photocatalysts are typically based on semiconductors with band gaps in excess of ~1.7 electronvolts (eV); this is sufficient to drive the chemical reaction and to overcome the energy loss at the electrodes. In this context, $TiO_2$ has been widely studied, especially as a photocatalyst for decomposing organic molecules, but it has poor efficiency for direct water splitting (<0.5 percent), in part because less than 2 percent of the solar photon flux has an energy greater than the band gap of 3.0 eV. Even the best materials at the present time, which include mixed oxides based on $Bi_2O_3$ and $WO_3$ with band gaps of about 2.6 eV, have efficiencies of only about 2 percent. Further effort is urgently needed to develop new materials and nanoscale structures that meet the technical requirements for good photocatalysts; these requirements include excellent chemical stability, resistance to photocorrosion in the presence of light and water, and low electron-hole recombination rates. As with the solar cell developments, the use of nanomaterials may offer significant advantages in addressing some of these issues, with CMMP providing modeling and design tools for the development of advanced photocatalysts.

An alternative strategy, based on the production of hydrogen and oxygen from water by using biocatalysts such as hydrogenase enzymes, is under development at the pilot-plant scale and may make its mark in the longer term. This exciting biotechnology approach will be especially attractive in the event that the hydrogen economy becomes a reality. One of the major obstacles in this area is the fact that the natural enzymes that catalyze the dissociation of water are destroyed by the very oxygen that they produce. However, progress is being made to address this problem using a combination of molecular biology approaches and computer modeling of protein/protein interactions, structure-function relationships, intramolecular gas diffusion, and metallocluster electronic structure.

## Fuel Cells

Fuel cells, which are an integral part of the concept of renewable chemical fuels, already have an advantage over the internal combustion engine in terms of their efficiency, but to make this technology viable, substantial further increases in fuel cell efficiency are needed, as well as dramatic improvements in hydrogen generation and storage capabilities. Fuel cells present a number of difficult technical challenges to the CMMP community. There are several fuel cell formats, the most common ones being the high-temperature (>800°C) solid oxide fuel cell (SOFC) and the low-temperature (~75°C) polymer electrolyte membrane (PEM) fuel cell. SOFCs are ideally suited for large-scale electricity generation in the megawatt range, whereas the PEM systems are appropriate for 1 kilowatt (kW) to 100 kW applications, such as in automotive power. Both types of fuel cell present challenges, including mechanical breakdown of SOFCs under extended high-temperature operation and the durability of the electrolytes in PEM cells. Nafion, a sulfonated tetrafluoroethylene copolymer, is widely used as the proton conductor, but its proton transport kinetics is impaired at higher operating temperatures owing to dehydration. A recently developed photochemically cured PEM coming out of CMMP basic research, however, appears to offer greatly enhanced performance at higher temperatures (Figure 3.2).

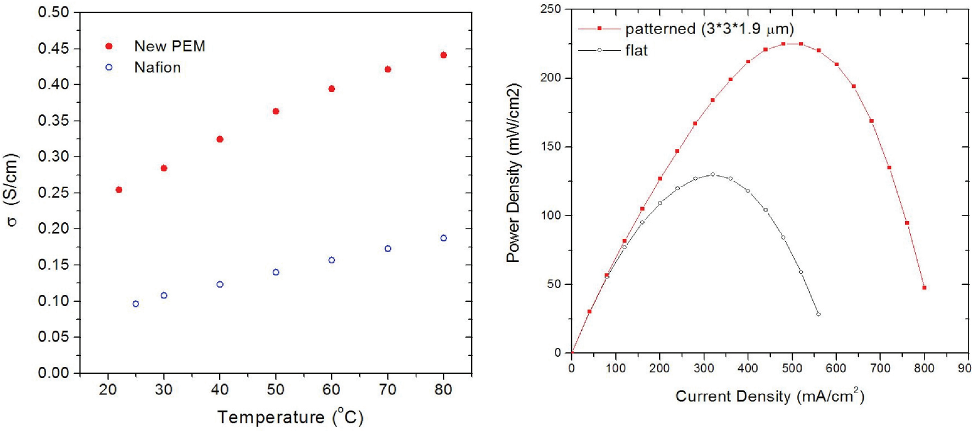

FIGURE 3.2 (Left) New photochemically cured liquid polymer electrolyte membrane (PEM) having higher acid content and therefore higher electrical conductivity (σ) and greater power output. (Right) Lithographically patterned "liquid PEMs" lead to higher surface area of the membrane and the catalyst and therefore to higher power output. SOURCE: Joseph M. DeSimone, University of North Carolina at Chapel Hill.

Further advances in membrane materials development could be expected from CMMP efforts. One of the cost barriers stemming from low operating temperatures arises from the need to use platinum coatings at the electrodes in order to help dissociate hydrogen or to reform hydrocarbons to produce hydrogen in situ. The development of inexpensive catalysts to replace platinum would have a significant impact, and further CMMP research is needed in this area. Theoretical models have recently shown that catalysts made from Pt-Ni alloys, for example, require less platinum and achieve improved performance.

## Thermoelectrics

The physics behind thermoelectricity is the basis for the interconversion between thermal and electrical energy and for the controlled cooling and heating of materials. Several fundamental breakthroughs in this field starting in the early 1990s led to the development of bulk materials with nanostructured constituents, as well as to an intellectual framework for the control of the nanostructures themselves to enhance their thermoelectric performance. Achievements using these two different approaches led to a doubling of the thermoelectric performance over the next decade, as the two approaches came together. Bulk thermoelectric materials have now been made using Si and Ge nanoparticles, which may be compacted into centimeter-size nanocomposites whose properties may be controlled by the processing parameters and guided by theoretical modeling considerations. The introduction of size as another system parameter facilitates the enhancement of thermoelectric performance through a simultaneous decrease in the thermal conductivity, which is phonon- and interface-dominated, and an increase in the power factor, which is dominated by electrons and holes and their interaction with phonons in the interconversion process of thermal and electrical energy. A significant remaining challenge is to develop a suite of nanothermoelectric materials that can operate efficiently over the wide temperature ranges desired for power conversion for energy-related industries, cooling (and heating) for the optoelectronics industry, power generation applications for space vehicle propulsion, energy harvesting from the waste heat in cars, and the utilization of geothermal energy.

### Biofuels

The production of so-called biofuels from renewable biomaterials, such as palm oil and sugar, is attractive from many perspectives. There are two important strategies in this area. In the first, vegetable oils that are based on the triglyceride esters of long-chain fatty acids can be transesterified to yield the corresponding methanol esters and glycerol. These methanol esters are sufficiently similar to conventional diesel fuel that they can be mixed with oil-derived diesel in virtually any ratio and burned in a conventional diesel engine. This biodiesel approach is becoming popular in Europe, where many countries have no oil or gas reserves and diesel is already widely used as an automotive fuel. Countries such as Indonesia and Malaysia, producers of vegetable oils for use in foods and personal care products, are gearing up to increase their output, while several oil companies are constructing plants for biodiesel production.

The second strategy involves the production of ethanol from sugarcane or other agricultural products. The fermentation technology for converting sugar into ethanol has been extensively exploited in Brazil, where ethanol accounts for about 40 percent of automotive fuel, and where many automobiles have flexible engines that can run on gasoline-ethanol mixtures in any ratio.[3] In the United States, ethanol is used as a fuel additive at the 10 to 15 percent level, and its use is likely to increase sharply in the near future. Most of the ethanol in the United States is made from corn rather than sugar, which has directly impacted the price of animal feed.

Many of the issues in the biofuels area (such as the evaluation of alternative crops, the impact of biofuels on food prices, and the question of land use and its

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[3] The Aspen Institute, *A High Growth Strategy for Ethanol*, Washington, D.C., 2006.

environmental ramifications) lie outside the domain of this report. In terms of the technologies that are required for the development of biofuels, however, CMMP researchers can play an important role in a number of materials issues. These include the development of improved processes for converting less-expensive cellulosic biomass into ethanol or another liquid fuel, the development of better catalysts for the remediation of emissions from diesel engines (thus enabling the wider use of biodiesel fuels), and the structural characterization with synchrotron x-rays of the enzymes that are used for enzymatic hydrogen production. Furthermore, the development of biofuels presents many excellent opportunities for collaborations between CMMP and the biosciences.

### Nuclear Energy Conversion

Concerns over energy resource availability, climate change, air quality, and energy security suggest that nuclear power technologies may play an important role in the future. The CMMP community has an opportunity to contribute to the development of advanced materials for use in the extreme environments found in fission and fusion reactors. Although the technology for electricity production from nuclear energy is already well developed, the United States has joined a multinational initiative aimed at designing the next generation of power reactors, the so-called Generation IV systems. The technology roadmap for this initiative is aimed at designing systems that address a number of societal concerns, including sustainability, economics, safety, and reliability, as well as issues relating to security and proliferation.

The materials-related challenges associated with the various reactor designs under consideration are discussed in *A Technology Roadmap for Generation IV Nuclear Energy Systems.*[4] Research areas of great opportunity include the transmutation of intermediate-lived actinides into shorter-lived or stable nuclides by means of irradiation, the development of materials with good temperature stability combined with superior resistance to fast neutron fluxes and fluences, the design of novel refractory fuel concepts with enhanced fission product retention capability, and the development of advanced glassy materials for nuclear waste disposal applications. Some of the proposed designs are able to produce either electricity or chemical fuels such as hydrogen or both. The projected limitations on the availability of uranium ores are a consideration that will stimulate CMMP research in the area of partially or fully closed fuel-cycle systems that are enabled by the recovery

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[4] U.S. Department of Energy Nuclear Energy Research Advisory Committee and the Generation IV International Forum, 2002. Available at http://nuclear.energy.gov/genIV/documents/gen_iv_roadmap.pdf; last accessed September 17, 2007.

of the heavy, long-lived radioactive elements. The closed-fuel-cycle approach also reduces the problem of radioactive waste disposal.

Energy from nuclear fusion is also an important technology option for the future, and the international ITER project will provide a number of important challenges in the CMMP area. In particular, materials in the vicinity of the plasma will be subjected to extreme conditions of temperature and neutron irradiation that can lead to mechanical degradation and activation. Tritium contamination could also be a problem. Materials that minimize these challenges will have to be developed, and there is a likely need for a dedicated materials-testing facility to assist with the development of such advanced materials.

## ENERGY STORAGE

In addition to energy generation, energy storage represents an important and challenging element of the overall energy strategy. The principal means of storing energy at the present time include the use of batteries; chemical storage in high-energy-density synfuels such as hydrogen, ethanol, and methane, ideally produced in a renewable manner as discussed in the previous subsections; and the use of supercapacitors.

### Batteries

Rechargeable lithium batteries have had a major impact on consumer electronics, such as cellular telephones and laptop computers. They typically employ oxide cathodes (such as $LiCoO_2$), carbon-based anodes, and electrolytes that afford efficient lithium transport. Energy density is a critical parameter, since it determines both the storage capacity and the weight of a battery. The output voltage is another critical parameter. Rechargeable lithium batteries typically deliver about 3.7 V, compared with ~1.2 V for conventional nickel-based batteries. Among the many materials challenges is the need to develop superior cathodes with a combination of good thermodynamic properties, which give high energy densities and sufficiently fast kinetics at the desired temperature. Such materials must exhibit good electronic and high ionic conductivities in combination with a sufficiently high redox couple. A variety of electrolytes have been developed, including liquids, solid polymers, and solid inorganic materials that are suited for various purposes. Recent work has shown, rather surprisingly, that crystalline polymer electrolytes can be superior to non-crystalline ones in certain instances. Major improvements in kinetics, however, are most likely to be achieved through nanostructuring. For example, the resiliency of nanostructured, multiwalled carbon nanotubes, when used as a filler, prevents the structural degradation of graphitic crystallites during the expansion/contraction processes that occur in the graphitic electrodes during the charging/discharging cycles. The high electrical conductivity, resilient elastic properties, and high surface-to-volume ratios improve the battery performance and significantly increase battery lifetimes. Here CMMP scientists can play a major role in both the modeling and the materials design of advanced battery systems, especially through collaborative efforts with materials chemists.

## Hydrogen Storage

The efficient storage of hydrogen for fuel cell applications represents one of the major challenges for the hydrogen economy. The goal of the Department of Energy for the year 2015 is to achieve 9.0 percent (by weight) hydrogen storage at reasonable pressures and ambient temperatures.[5] The ideal medium for automotive applications would be a storage material, probably a solid or a liquid, that could reversibly adsorb and desorb hydrogen without the physical removal of the storage medium from the vehicle. The most common storage media are porous solids that adsorb hydrogen through a physisorption mechanism and metal hydrides or chemical hydrides that bind hydrogen through a chemisorption mechanism. Porous materials that store hydrogen by physisorption include inexpensive activated carbons, aluminosilicate zeolites, and hybrid metal-organic framework materials. Physisorptive host-hydrogen interactions, however, are intrinsically weak (~5 kilojoules per mole [kJ/mol]), so these materials will only store significant amounts of hydrogen at cryogenic temperatures. The hydrides, by contrast, will bind hydrogen strongly but in some cases have too high a mass density for automotive applications or suffer from poor release kinetics at ambient temperatures. CMMP researchers who have recently entered this field are already impacting the modeling and design of new materials and the development of advanced measurement techniques to study and control hydrogen adsorption and desorption mechanisms.

There is much current interest in chemical hydrides, such as borohydrides (e.g., $NaBH_4$); these have excellent gravimetric and volumetric storage capacities, but many chemical hydrides suffer from poor reversibility. It is very expensive to regenerate borohydride from its oxidation products, so fuel cells using liquid storage media may be good alternatives to rechargeable lithium batteries for portable applications, but they are unlikely to be economical for large-scale applications such as automotive use.

A series of recent developments have stimulated considerable interest in storage media that can bind hydrogen more strongly by chemisorbing dihydrogen, without dissociation, at under-coordinated metal sites in porous inorganic or hybrid metal-

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[5] Department of Energy, *Basic Research Needs for the Hydrogen Economy*, Washington, D.C., 2003. Available at http://www.sc.doe.gov/bes/reports/files/NHE_rpt.pdf; last accessed September 17, 2007.

organic framework materials. These materials have heats of adsorption of ~10 kJ/mol, approximately double those associated with conventional physisorption, and can therefore retain hydrogen at much higher temperatures. Further work is needed in order to create new materials that contain large numbers of such binding sites and that can operate in the desirable temperature range for specific applications. CMMP researchers are collaborating strongly with materials chemists and materials scientists in the modeling and design of new metal-organic framework materials suitable for hydrogen storage.

Many other gas storage and separation technologies are closely related to the hydrogen storage problem. Important examples include methane storage for fuel applications and carbon dioxide disposal in the context of carbon sequestration and storage. The latter will become extremely important as increasing amounts of coal are used to produce electricity.

### Supercapacitors

In the past decade, supercapacitors in the form of electric double layer capacitors (EDLCs) with high charge-storage capacity have been actively studied as an attractive energy storage device to replace batteries for some applications. In particular, EDLCs are able to store and deliver energy rapidly and efficiently. The EDLCs have a long life cycle because of their simple charge separation mechanism, which uses highly porous carbons as the electrode material. Their widely scalable storage capabilities make it possible to hybridize EDLCs with other energy storage devices, such as batteries and fuel cells. Even though EDLCs are now being used in various types of electronic device applications, such as for memory backup in vehicle computers, their intrinsically low energy density limits their impact on the energy storage market. The present challenge is to increase energy storage density and to lower fabrication costs through the optimization of the cell design and the development of improved electrode materials. CMMP has the opportunity to make key contributions to the development of advanced nanocarbon materials for model systems and for specific applications to fuel cells, hybrid electrical vehicles, and portable electronics. It is expected that the market for supercapacitors with enhanced performance will expand rapidly in the next decade.

## END-USE ENERGY EFFICIENCY

In addition to recognizing the role of energy conversion and storage, it is important not to underestimate the role of conservation in the global energy challenge. As discussed in Chapter 8, the per capita consumption of energy in the United States is approximately double that in most other advanced countries. While there are good reasons why consumption in the United States may be somewhat higher than that in, say, Europe, this fact also points to the largely untapped potential of conservation in meeting the nation's energy needs. The following subsections address some of the specific CMMP-related technology areas where this might be achieved.

## Solid-State Lighting

Among the newly emerging end-use energy-efficiency technologies, solid-state lighting deserves special attention because it was in its infancy at the time of the last decadal review of CMMP and remarkable progress has been made since then. The discovery of blue light-emitting diodes in 1994 facilitated a large number of developments in the lighting and displays area. White lighting systems based on blue InGaN LEDs operating at about 460 nanometers (nm) in combination with yellow phosphors using $Ce^{3+}$-garnets give a reasonable quality of white light that is good enough for off-grid lighting applications, flashlights, traffic lights, and automotive lighting (Figure 3.3). CMMP has played an important role in establishing the science base for LEDs from their discovery until the present time.

FIGURE 3.3 Emerging applications of solid-state lighting: (a) landscape lighting, (b) roadway lighting, and (c) traffic signals. SOURCE: Philips Lighting.

The efficiency of the blue LEDs has improved to the point that solid-state lighting is comparable to fluorescent lighting and has the potential to be two to three times superior in converting electrical power (watts, W) into light (lumens, lm) (see Figure 1.2 in Chapter 1). The theoretical maximum for solid-state lighting is about 300 lm/W, but 200 lm/W represents a more realistic goal for practical applications. Lighting consumes approximately 22 percent of the electricity that is generated in the United States, and solid-state lighting has the potential to reduce energy consumption for lighting requirements by about 60 percent by 2025.[6] Success in this area would therefore reduce electricity consumption in the United States overall by around 13 percent over the next 20 years, making it a very important element of the nation's energy strategy and virtually guaranteeing that solid-state lighting will emerge as a multibillion-dollar industry worldwide. In addition, when combined with solar panels, the solid-state lighting approach can provide lighting for homes and villages in remote, off-grid locations in developing countries (Figure 3.4).

Among the technical challenges for CMMP, improvement in LED efficiency is, of course, critical, and depends on factors such as the reduction of the defect densities in the semiconductors. The external quantum efficiencies of the InGaN-based blue LEDs have improved dramatically in the past decade, from less than 5 percent when they were first developed in the mid-1990s to around 66 percent today.[7] Green LEDs, however, which are required for lighting applications using red, green, and blue LEDs, are much less efficient than the blue and red ones, so further effort is required in this area.

Other challenges in solid-state lighting are numerous and varied. Systems based on blue LEDs in combination with yellow phosphors are very simple and cost-effective, but the quality of the light is insufficient for residential and commercial lighting applications owing to poor color rendering. The light quality will be improved in the next generation of white LEDs by using a blue LED in combination with both a green and a red phosphor, a configuration that fills the visible spectrum in a more pleasing manner. However, the blue to red down-conversion with the currently available materials is relatively inefficient, in part due to the large downshift in frequency from coupling to lattice vibrations, so new materials are currently needed. Other obstacles include the poor performance of the polymer or glass encapsulants that are used to disperse and protect the phosphors and the losses associated with poor light extraction. While new polymer or glass compositions are required to solve the encapsulation problem, nanostructured optical band gap materials may solve the latter. Other challenges are likely to stem from

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[6] Department of Energy, *Basic Research Needs for Solid-State Lighting*, Washington, D.C., 2006. Available at http://www.sc.doe.gov/bes/reports/files/SSL_rpt.pdf; last accessed September 17, 2007.

[7] Department of Energy, *Basic Research Needs for Solid-State Lighting*, Washington, D.C., 2006. Available at http://www.sc.doe.gov/bes/reports/files/SSL_rpt.pdf; last accessed September 17, 2007.

FIGURE 3.4 Applications of solid-state lighting in developing countries. The system comprises two modular 1-watt white light-emitting diode lamps; a 12-volt, 7-ampere-hour sealed lead acid battery (rechargeable and maintenance free); and a 5-watt solar panel. The system has a 100,000-hour lifetime. SOURCE: Courtesy of Light Up the World Foundation.

a shift toward ultraviolet rather than blue LEDs, since this will require yet a new generation of phosphors.

In parallel with the InGaN-based lighting development, there will be progress in making lighting and display systems using organic and polymer-based LEDs. While these may not match the lifetimes of the inorganic materials, which are aiming for 100,000 hours of continuous operation, they are likely to be much cheaper and will be preferred for area illumination requiring large emissive surfaces.

### Smart Windows

The development of smart windows based on novel nanocomposites represents an entirely different opportunity for end-use energy efficiency and an area in which CMMP is already playing an important role. For example, inorganic nanomaterials with band gaps in the near infrared (IR) could be added to polymer or glass windows in order to reduce the transmission of heat. Even more attractive, the use of *switchable* IR filters—based, for example, on thermochromic materials that show semiconductor-to-metal transitions when heated above room temperature—would enable the development of passive, smart windows for energy-efficiency applications. Nanoparticles of vanadium dioxide would be suitable for this application, since they would be optically transparent in the visible range and have an insulator-to-metal transition at 67°C.

### Other Energy Conservation Opportunities

There are many other areas in which CMMP can contribute to energy conservation. One of the most intriguing but elusive of these is the use of high-temperature superconductors to reduce losses from power transmission and increase the grid capacity. A recent report from the Department of Energy[8] argues that the electric power grid is in a critical condition and is likely to worsen as the demand increases. Transmission losses in the grid are now almost 10 percent. Superconductivity offers powerful new opportunities for restoring the reliability of the power grid and improving its capacity and efficiency. This will require the discovery of a new generation of ductile superconductors that have higher critical temperatures, sustain higher currents, and are cheaper to fabricate. The search for a room-temperature superconductor is certainly one of the elusive "holy grails" for CMMP, as is the quest for a better understanding of the mechanism of high $T_c$ superconductivity.

Other, more immediate possibilities include improving the power efficiency of computers by inventing new materials for the current computing paradigms and by developing new computing paradigms based on optical signaling and low-power computing. Improvements in power supplies would also have an impact. For example, present power supplies run at 60 to 70 percent efficiency levels in converting alternating current to low-voltage direct current. It is estimated that increasing the efficiency to 80 percent would save more than 1 percent of the electricity used in the United States.[9]

In the area of new materials, CMMP researchers are contributing to the development of plant-based plastics (bioplastics) for potential use in markets such as the car industry; however, the low strength and durability of bioplastics have proven their application to be challenging. Additionally, CMMP researchers are working on new materials for buildings that incorporate embedded sensors, self-

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[8] Department of Energy, *Basic Research Needs for Superconductivity*, Washington, D.C., 2006. Available at http://www.sc.doe.gov/bes/reports/files/SC_rpt.pdf; last accessed September 17, 2007.

[9] S. Ashley, "Power-Thrifty PCs," *Sci. Am.* **290**, 31-32 (2004).

healing composites, and responsive materials for inexpensive monitoring and self-diagnostic capabilities.

## CONCLUSIONS

While it is hard to exaggerate the seriousness of the global energy challenge, the required sense of urgency in U.S. society with respect to this challenge is not yet apparent. There are no quick or singular solutions to meeting the growing global energy requirements; the cost-effectiveness of solar energy remains unresolved, the efficiency of the photochemical splitting of water is still very poor, fuel cells suffer from longevity problems, bioethanol and biodiesel fuels compete with the food chain, and society has still not embraced nuclear energy. A sustained effort on a broad range of options is therefore required. The aggressive development of renewable energy sources must be accompanied by an equally determined effort to reduce energy consumption and waste across all sectors. The Committee on CMMP 2010 believes that a substantial increase in funding for energy-related education and research would set the United States on the path to solving this technological challenge. Priority research areas should include photovoltaic cells, fuel cells, hydrogen generation and storage, thermoelectrics, catalysis, nuclear power, solid-state lighting, and batteries. Crosscutting areas benefiting a variety of energy-related options include new materials development, catalysis science, membrane design, nanoscience advances, and advances in materials design and the modeling of materials properties. New materials will be particularly important in meeting this challenge, and the committee looks forward to the recommendations of the current National Research Council study on "Assessment of and Outlook for New Materials Synthesis and Crystal Growth" for realizing this need.

# 4

# What Is the Physics of Life?

The study of living matter poses special challenges for condensed-matter and materials physics (CMMP) because the constituent biomolecules are far more complex than the atoms or molecules that form most materials. Researchers are just beginning to see how understanding of materials can be extended to living systems and to recognize the organizing principles that govern living matter. Already, burgeoning understanding is leading to an unprecedented degree of collaboration between CMMP scientists and biologists, on problems ranging from why proteins misfold and form unwanted structures in diseased tissues, as in Alzheimer's disease, to how the brain works. CMMP will continue to catalyze advances in biology and medicine by providing new methods for quantitative measurement, from rapid genome-sequencing techniques to novel medical diagnostics. At the same time, the study of biological systems broadens the horizons of physics. The unparalleled specificity and robust functioning of biomolecular systems, such as those that enable viruses to assemble or cancer cells to spread, generate new theoretical ideas and inspire the creation of novel materials and devices. Finally, a fundamental characteristic of physics, especially CMMP, is its ability to analyze complex systems by identifying their essential and general features. This conceptual approach has the potential to be indispensable in sifting through the vast trove of accumulating data to tackle the origins of the ultimate emergent phenomena: life and consciousness.

## OVERVIEW

Physics and biology were not always separate subjects. In the 19th century, Helmholtz, Maxwell, Rayleigh, Ohm, and others moved freely among problems that are now distinguished as being parts of physics, chemistry, biology, and even psychology. At the beginning of the 21st century, there is a renewed sense of excitement at the interface between physics and biology. Many biologists believe that we stand on the threshold of another revolution, in which biology will become a more quantitative science, a science more like physics itself. At the same time, many physicists have come to view the profound challenges posed by the phenomena of life as much more than opportunities for the "application" of known physics to biology; rather, these striking phenomena encourage the stretching of the boundaries of CMMP and physics itself. This is leading to the blossoming of biological physics as a branch of physics, confronting the phenomena of life from the physicist's unique point of view. The Committee on CMMP 2010 emphasizes that the challenge here is not for physicists to become biologists, but rather for the physics community to reclaim for its own some of the most inspiring parts of the natural world and to seek an understanding of living systems that parallels the profound understanding of the inanimate world.

One cannot overstate the role that the experimental methods of physics have played in contributing to the solution of problems posed by biologists, especially in the second half of the 20th century, and the committee expects that these developments will continue (see Chapter 8). Looking ahead, however, the most important opportunities at the interface of physics and biology arise because physicists bring a different perspective to the phenomena of life. Faced with these same phenomena, biologists and physicists ask different questions and expect different kinds of answers. The goal in this chapter is to communicate the excitement that now surrounds these physicists' questions about life and to point toward the areas where the most dramatic future developments might occur. Placed in the context provided by the interactions between physics and biology in the 20th century, it is likely that these developments will reshape fundamental understanding of some of the most striking of natural phenomena and expand our ability to exploit this understanding in solving practical human problems. Given the extremely broad range of problems currently being addressed at the interface between physics and biology, the committee cannot pretend to give a complete account of the current state of the field. Instead, in what follows, it focuses on a few conceptual themes and explores how these themes run through a wide variety of phenomena. The committee's choices are intended to be illustrative, not canonical.

## AN INTRODUCTORY EXAMPLE: HIGH FIDELITY WITH SINGLE MOLECULES

One of the central problems faced by any organism is to transmit information reliably at the molecular level. This problem was phrased beautifully by Schrödinger in "What Is Life?," a series of lectures given (in 1943) in the wake of the discovery that genetic information—our very identity as individual humans and the inheritable identity of each individual organism—really is encoded by structures on the scale of single molecules, not large collections of molecules as one might have expected. The history of these ideas and the involvement of physics and physicists in the rise of molecular biology have been recounted many times. The focus here is on problems that remained unsolved long after the basic facts of deoxyribonucleic acid (DNA) structure and the genetic code were established. As described below, the resolution of these issues involved the appreciation that there is a common physics problem that the organism needs to solve in order to carry out its most basic functions.

As everyone now learns in high school, genetic information is stored in the DNA molecule. DNA is a polymer made from four types of subunits: the "bases" adenine (A), thymine (T), cytosine (C), and guanine (G); the sequence of bases along the polymer defines the genome, the full instructions for building the organism. In the double-helical structure of DNA there are two intertwined strands, and the structures of the bases are such that if one strand contains the base A, then on the other strand it is most favorable to find the base T, and similarly if one strand contains C the other base will most likely contain G. This structural complementarity provides the basis for the information stored in DNA to be copied each time a cell divides.

The idea of a molecular template involves a wonderful interplay among biology, chemistry, and physics, with implications reaching from DNA replication to modern attempts at the self-assembly of nanostructured materials. But structural complementarity cannot be the whole story. Looking carefully at the bond energies involved, the difference between a correct (A with T or C with G) pairing of bases and an incorrect pairing can be as small as 10 times the thermal energy at room temperature. All else being equal, this means that if polymerization of DNA proceeds to equilibrium, the probability of an incorrect base pairing is $\exp(-10)$, or ~0.0001. But this would be a disaster: since even simple bacteria have millions of bases in their DNA, each time a bacterium divided to make two bacteria there would be hundreds of errors. For humans, with billions of base pairs in our genome, there would be roughly one hundred thousand mistakes as we pass our genetic inheritance to our children. In fact, error rates can be as low as one mistake per generation.

The problem of precision also arises when the cell needs to "read" the information coded in the DNA. Now a single strand of DNA provides a template for the synthesis of a slightly different polymer, ribonucleic acid (RNA), but the idea is the same. The messenger RNA also has a sequence of bases, and these are read once more, now in groups of three, to determine the sequence of amino acids in proteins, yet another kind of polymer inside the living cell. In each of these several steps from DNA to protein, the cell must distinguish one molecule from another to find the correct base or the correct amino acid to incorporate into the growing polymer; in each case the structures and bond energies are not enough to explain the very low error rates that are achieved in living organisms.

That these different systems are spoken of as having a common problem of precision in molecular synthesis is itself an insight from physics, specifically from the work of Hopfield in 1974. Historically, DNA replication, the transcription of DNA into RNA, and the several steps of translation from RNA to protein all were different subfields, each with its own complex phenomenology. Hopfield realized that there was a common problem that cuts across these different layers of biological function. In a sense, the problem that he identified is the old problem of Maxwell's demon. In the 19th century, Maxwell imagined a container filled with gas (as with the air in the room where you are sitting), in which was a little demon who would see individual molecules arriving at the wall of the container, would measure their speed, and if they were moving fast enough would open a trapdoor into another chamber. After a while, the second chamber would be filled only with molecules moving at high speed, and thus it would be warmer than the original container; this temperature difference then could be used to do useful work. Apparently the little demon has made something out of nothing, violating the second law of thermodynamics. More generally, any demon who could sort molecules—not just by their speed, but also by their identity—with perfect accuracy would violate the second law, and we know (since the second law really is true!) that the demon must therefore pay some cost in energy in exchange for the ability to sort molecules. Hopfield realized that what cells needed to solve their problem of accuracy was something like Maxwell's demon, with the attendant energy cost—living organisms must pay, in energy, for their ability to convey information so precisely from one molecule to another.

It had been known before 1974 that each example of accurate molecular synthesis involved a complex sequence of chemical reactions. Hopfield argued that this complexity could be organized once one understood that the key step was energy dissipation: in each case, a chemical reaction that seemingly wastes energy really is essential in allowing the system to proofread, and thus to correct errors. Further, because errors are unlikely, the processes that allow for error correction seem like rather minor side branches in the overall flow of molecules, until one realizes their essential function. Hopfield's theory of kinetic proofreading, along with the related ideas of Jacques Ninio, made many successful experimental predictions, and the essential idea of kinetic proofreading has proven correct. Subsequent theorists have suggested yet more examples in which biology achieves paradoxically precise function at a molecular level and thus in which some version of proofreading may be at work, from the specificity of cellular signal transduction to the untangling of the strands of the double helix.

Recent work has seen a dramatic demonstration of proofreading, with the direct observation of the individual molecular events in which mistakes are corrected. This work is part of the continuing development of techniques for observing biological processes at the single molecule level, often using optical trapping methods (Figure 4.1). Several generations of improvements in the design of such optical traps have made possible the observation of stepping motions of the RNA polymerase as it reads the DNA to synthesize messenger RNA; the steps are 3.4 angstrom (Å), the distance from one base to the next along the DNA double helix. Even more dramatically, this stepwise walking can reverse, and the frequency of such backtracking is increased when the surrounding solution contains higher concentrations of the "wrong" nucleotide bases. Almost certainly this reflects the elementary steps of proofreading. Techniques based on fluorescence energy transfer between nearby molecules are giving glimpses of the proofreading steps in translation from messenger RNA to protein, again at the level of single molecules.

## ORGANIZING OUR THOUGHTS AND OPPORTUNITIES

The great discovery of modern biology has been the existence of universality at the molecular level: All organisms use the same rules for reading the information coded in their DNA, and most if not all of the functional molecules act as interchangeable parts. This is a startling confirmation of Francois Jacob's dictum that "what is true for [the bacterium] *E. coli* is true for the elephant," and appeals to the physicist's desire for universal explanations. But what makes life alive is not

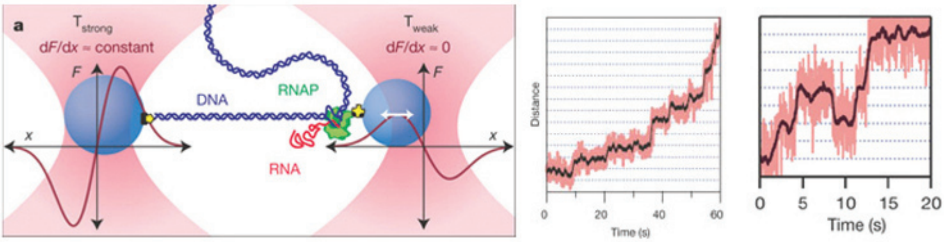

FIGURE 4.1 Watching a single molecule read the genetic code. A high-precision, double optical trap (left) makes it possible to observe a single ribonucleic acid (RNA) polymerase (RNAP) molecule as it "walks" along deoxyribonucleic acid (DNA) to synthesize the messenger RNA. A strong trap holds a bead attached to one end of the DNA molecule, and a weak trap holds a bead with the RNAP molecule attached; the distance between the beads changes as the molecule moves, and is monitored by interferometry. In the two panels to the right, it can be seen that the motion occurs in steps close to the 3.4 Å spacing between bases along DNA (indicated by the dashed lines), and there are occasional backward steps. Backward motion is enhanced under conditions in which errors are more likely, as would be expected if these backward steps were associated with proofreading. SOURCE: E.A. Abbondanzieri, W.J. Greenleaf, J.W. Shaevitz, R. Landick, and S.M. Block, "Direct Observation of Base-Pair Stepping by RNA Polymerase," *Nature* **438**, 460-465 (2005).

single molecules—it is the way they interact and work together. The next challenge thus is to discover universal principles at this system level. This problem has captured the imagination of many physicists, who are looking at systems ranging from bacteria to brains. As in the example of kinetic proofreading, this search cuts across many different levels of biological organization. In the subsections that follow, two of these conceptual challenges and how they appear in different contexts are discussed: noise in biological systems and balancing fine-tuning and robustness. Because physicists still are searching for principles, these examples are intended to be illustrative rather than exhaustive.

## NOISE IS NOT NEGLIGIBLE

The great poetic images of classical physics are those of determinism and clockwork. They come from the era of science that produced the first precision machines, and to a large extent modern efforts begin by constructing elements—for example, the submicron circuit elements on a modern chip—that approach the image of clockwork and determinism as closely as possible. Strikingly, life operates far from this limit. Interactions between molecules involve energies of just a few times the thermal energy, and biological motors, including the molecular components of muscles, move on the same scale as Brownian motion. Biological signals often are carried by just a few molecules, and these molecules inevitably arrive randomly at their targets. Human perception can be limited by noise in the detector elements of sensory systems, and individual elements in the brain, such as the synapses that pass signals from one neuron to the next, are surprisingly noisy. How do the obviously reliable functions of a life emerge from under this cloud of noise? Are there principles at work that select, out of all possible mechanisms, the ones that maximize reliability and precision in the presence of noise?

### Molecule Counting in Chemotaxis

It is a remarkable fact that single-celled organisms such as bacteria are endowed with sensory systems that allow them to move in response to a variety of signals from the environment, including the concentrations of various chemicals. This process, called chemotaxis, has been an enormously productive meeting ground for physics and biology. In particular, problems of noise are central to understanding chemotaxis.

To begin, one has to understand how bacteria swim. Fluid mechanics predicts that changing the size of a moving object is equivalent to changing the viscosity of the fluid; what matters is a combination of parameters (size, speed, and viscosity) called the Reynolds number. A micron-sized bacterium swimming in water has the same Reynolds number as that of a human swimming through (slightly) wet concrete. Thus, life at low Reynolds number is very different from everyday experience. As always in physics, interesting problems in one domain have deep connections to other fields. Thus, the problem of self-propulsion at low Reynolds number has a formulation in terms of gauge theories of the sort used to describe the interactions of elementary particles, and a deeper understanding of low Reynolds number flow has been critical to the development of practical microfluidic devices.

Bacteria are propelled by long, wispy appendages called flagella (Figure 4.2). One of the most startling discoveries about the physics of life was that these flagella are not "waving" in the water, but actually rotating, driven by nanometer-sized protein motors; power is provided by the difference in chemical potential for hydrogen ions between the inside and outside of the cell. This might seem like a curiosity;

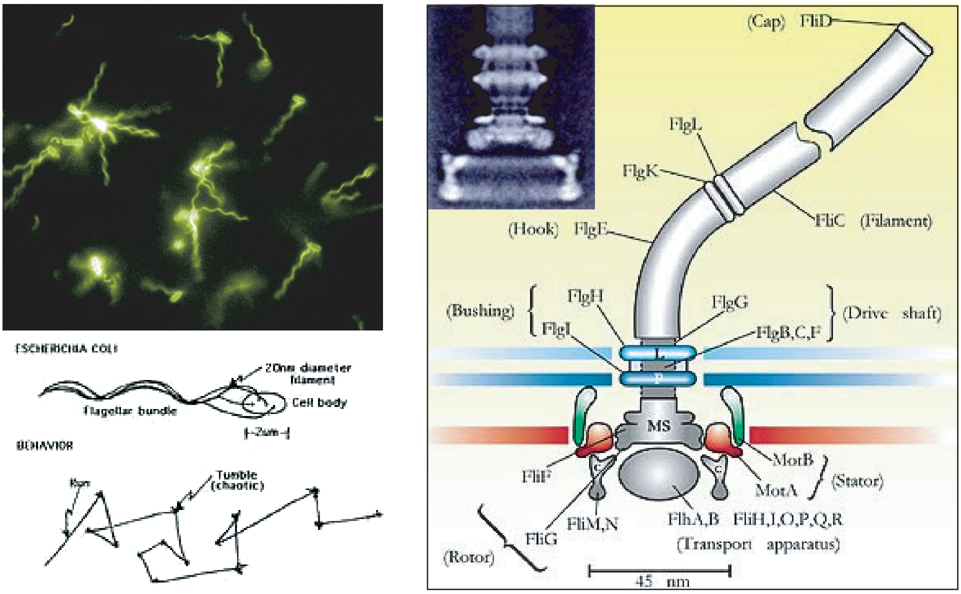

FIGURE 4.2 Bacterial motility. (Upper left) Fluorescently labeled flagella can be seen emanating from the cell bodies of *Escherichia coli*. (Right) A schematic view of the rotary motor, which is located at the base of each flagellum. The motor contains hundreds of parts, assembled from more than 20 different protein components, some of which are labeled here. The inset shows an image of the motor reconstructed from cryoelectron microscopy. (Lower left) When the motors spin together in the counterclockwise direction (as viewed from outside the cell), a stable bundle forms and propels the cell forward. When one or more of the motors spin in the clockwise direction, the bundle is disrupted and the cell tumbles and makes little forward progress. The switching between forward and tumbling motion causes the cell to undergo a (potentially biased) random walk. SOURCES: (Upper left and right [drawing]) H.C. Berg, Harvard University. (Right [inset]) D.J. DeRosier, Brandeis University. (Lower left) L. Turner, Harvard University.

after all, muscles move because of linear (not rotary) displacements of one molecule relative to another, and the energy for this motion is provided by adenosine triphosphate (ATP) (not protons)—a molecule that is widely used in biochemical reactions that need energy in order to go forward. But all living cells synthesize ATP using the chemical potential difference for protons across a membrane, and the enzyme that carries out this synthesis rotates as it performs its function. Thus, proton-driven rotation is the central step in energy flow for all cellular processes. The intellectual path from the peculiarities of low Reynolds number fluid mechanics to the essence of energy flow in cells provides a remarkable example of the interaction between physics and biology.

But why is noise so important? On the scale of bacteria, the transport of molecules is dominated by diffusion, that is, by random motion. Because the concentrations of interesting molecules in the environment are small, and differences in concentration over the scale of microns are even smaller, this randomness is not negligible: even if a bacterium can count every molecule that arrives at its surface, its estimate of whether its environment is rich or poor will be of limited precision. Bacteria themselves are so small that they become disoriented by their own rotational Brownian motion within roughly 10 seconds. Thus, these cells need to make decisions quickly, which limits their ability to average out the effects of noise. The result is that bacteria do not have access to a reliable signal that, for example, would allow them to measure whether the concentration of sugar is higher at their right or their left. The only available strategy is to measure changes of concentration in time along their path, to see if things are getting better or worse. Direct observation of bacterial swimming using a tracking microscope revealed that they indeed swim along roughly straight paths, just long enough to see the disorienting effects of Brownian motion. These straight paths (runs) are interrupted by discrete events (tumbles), after which the cell picks a new direction almost at random. When runs take the cells up the trail of an attractive chemical (or down the trail of a repellent), the time until the next tumble is longer. Quantitative analysis demonstrates that reliable changes in run length occur when the differences in concentration along the run are just slightly larger than the random shot noise in the arrival of molecules via diffusion. This means, in effect, that the cell is counting every single molecule that arrives at its surface, reaching the ultimate in sensitivity.

Running and tumbling correspond to different directions of rotation of the flagellar motor, which can be observed more directly in tethered cells. Such experiments show clearly that cells are responding to changes in time, and that the arrival of one additional molecule at the cell surface produces a substantial (~10 percent) change in the probability of clockwise rotation, which triggers tumbles. This probability depends on a "processed" version of the input chemical signals, comparing an average of the concentration over the last second to the average over the previous 4 or 5 seconds. If the cell averaged for much less time, noise would then dominate the signal, while much longer times would be useless because of the disorienting effects of Brownian motion. In this sense, the bacterium's behavioral strategy is matched to the physics of its environment.

Genetic techniques have identified a cascade of molecular events that lead from receptors at the cell surface to the rotational bias of the flagellar motor. Combining methods from molecular biology and physics, one can engineer bacteria that produce fluorescent analogs of these molecules and then use a variety of optical methods to observe the individual steps of this amplifying cascade. At the front end of the system, theorists have proposed that sensitivity can be enhanced further by collective interactions among the receptor molecules, and these ideas are being tested through experiments using fluorescence resonance energy transfer to detect associations between pairs of molecules in the cascade. At the output, the motor responds directly to a particular protein; using fluorescence correlation spectroscopy one can measure the absolute concentration of these molecules (~1,000 per bacterium) and show that the motor is extraordinarily sensitive, making a complete transition from clockwise to counterclockwise rotation in response to just a 10 percent change in concentration. The committee expects that, in the next decade, the collaboration between theory and experiment will result in a clear physical picture of how bacteria achieve their ultimate sensitivity to individual molecular events.

### Noise in the Regulation of Gene Expression

Every cell in a person's body has the same DNA; what makes the cells in the brain different from the cells in the liver is that different sets of genes are expressed as proteins. As an embryo develops, each cell makes decisions to express or not to express each gene, and the sequence of these decisions determines the identity of the cell in the adult organism. Once the organism has developed, each cell has to modulate the expression level of certain genes, making more or less of particular proteins depending on the circumstances, and this same problem arises even in single-celled organisms. To a large extent, the signals that the cell uses to regulate the expression of genes are themselves proteins, called transcription factors, which bind to specific sites along the DNA and enhance or repress the transcription (reading of DNA into messenger RNA) of nearby genes. For many years it has been clear that noise must be interesting in these processes because the relevant molecules are present in very small numbers. In the present decade, a convergence of ideas and methods from physics and biology has made it possible to turn these vague suspicions into precise experiments.

If one looks at a large number of bacteria in a test tube, expression levels of particular genes vary widely, but some of this variation may be in response to uncontrolled signals in the environment. What one really wants to know is how accurately a single bacterium (for example) can adjust the expression level of one gene, given that all inputs are fixed. One major experimental advance with respect to this question was to engineer a bacterium that uses the same transcription factor to regulate the expression of two genes, one coding for a green fluorescent protein and one coding for a red fluorescent protein (Figure 4.3). Genuine noise in the response to the transcription factor thus is converted into a change in color of the bacterium, shifting the red/green balance, while changes in other variables contribute only to "common mode" variations in the overall brightness of the cells, not to changes in color. Observing these genetically engineered bacteria with state-of-the-art light microscopy demonstrated that the intrinsic noise in gene expression could be as small as 10 percent. This was startling, since the broad distribution of expression levels seen in populations of cells had reinforced the notion that biological systems are very noisy, perhaps so noisy that cells could do no more than to turn genes on and off. In fact, cells have access to a "dial" that can be set accurately to many distinct expression levels.

Quantitative measurements of the way in which noise levels vary as a function of the mean expression level have driven theoretical efforts to dissect the contribution of different noise sources. Dynamic measurements are revealing the correlation times of different noise sources, with important consequences for theory. Different experimental strategies provide fluorescence signals related not just to protein concentration but also to the concentration of messenger RNA (mRNA); this has made it possible to see the transcription of mRNA molecules one by one and the resulting bursts of translation of mRNA into protein, giving a very detailed view of noise in these distinct steps. When cells divide, proteins are apportioned to the daughter cells at random; observation of this randomness makes it possible to get an absolute count of the number of molecules in the cell, putting the whole discussion of noise on an absolute scale. Given such absolute measurements, physicists can start to ask if the precision of gene expression is limited by physical principles, as with the example of molecule counting in chemotaxis.

Many genes are part of regulatory feedback loops, leading in some cases to multiple stable states that correspond to different "lifestyles" of the cell; noise causes spontaneous transitions among these states, and there is a substantial effort to characterize the interplay between deterministic and noisy dynamics in such systems. In testimony to the unity of physics, the theoretical methods used to understand spontaneous transitions among states of genetic regulatory circuits are borrowed from the instanton methods that were developed in statistical physics and quantum field theory. Multistable systems can be thought of as memory devices, and this "epigenetic" memory can be transmitted from generation to generation. Explorations in this field thus will characterize the capacity for information transmission beyond the genome itself.

While the initial studies of gene regulation focused on the "simplest" systems (bacteria), more complex biological systems now seem accessible to physics

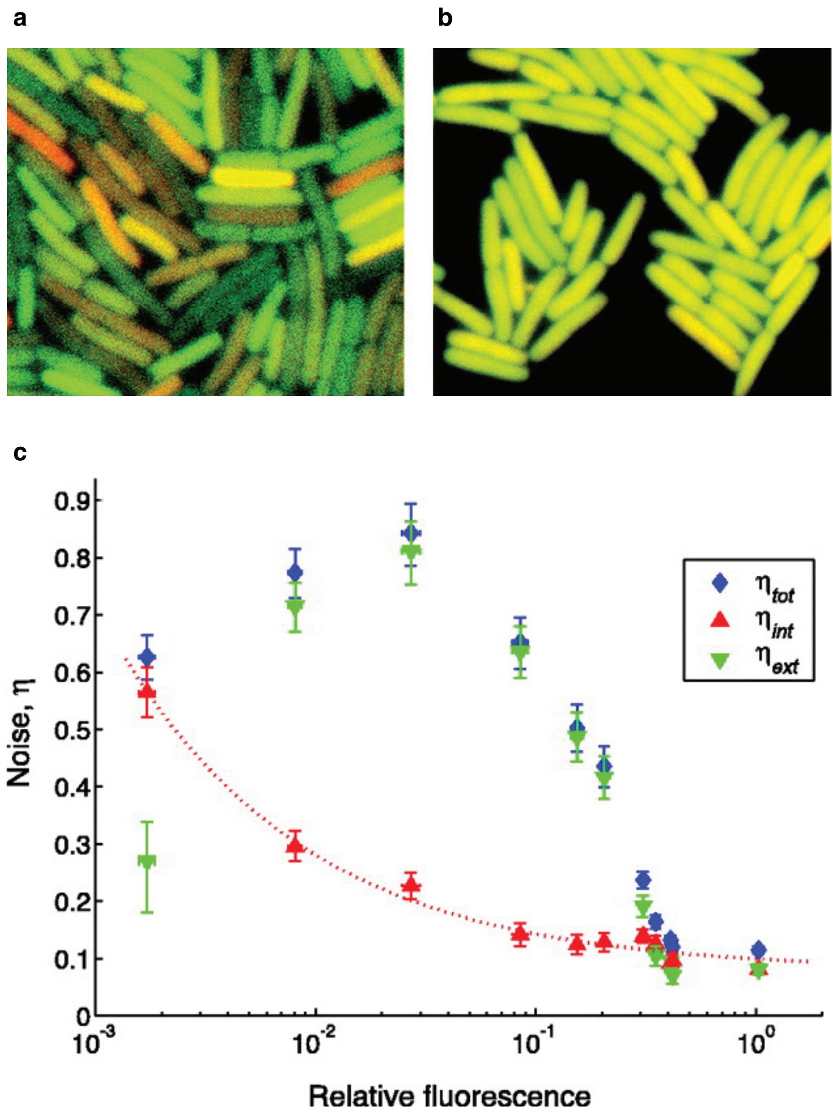

FIGURE 4.3 Intrinsic and extrinsic noise in gene expression. *Escherichia coli* are engineered to produce two different fluorescent proteins with different colors, but the expression of both proteins is controlled by the same signals. In a population of bacteria under nominally fixed conditions, there are shown (a) wide variations both in the total brightness and the color, suggesting that there is a substantial amount of noise in the system. Under conditions leading to greater expression, and hence brighter images (b), the variations in color are smaller, indicating that the control over expression level has become much tighter. (c) The noise is quantified by the fractional standard deviation in protein concentration, and this is separated into extrinsic components (that change the expression of both proteins) and intrinsic components. As explained in the text, the intrinsic noise can be quite low, so that expression levels can be set by the cell with roughly 10 percent accuracy. SOURCE: M.B. Elowitz, A.J. Levine, E.D. Siggia, and P.S. Swain, “Stochastic Gene Expression in a Single Cell,” *Science* **297**, 1183-1186 (2002). Reprinted with permission from the American Association for the Advancement of Science.

experiments. Perhaps the most dramatic examples are in the problem of embryonic development. One of the great discoveries in the modern era of molecular biology is that the spatial structure of organisms has its origins in spatial patterns of expression for particular genes that are visible in the embryo at very early times after fertilization of the egg (Figure 4.4). For a physicist, these results pose many questions: How is it possible for these patterns to scale with the size of the embryo, so that the different parts of the adult organisms remain in correct proportion even as the whole organism varies in size? What mechanisms guarantee that the spatial patterns of gene expression are reproducible from embryo to embryo? How reliably can neighboring cells in the embryo respond to the small differences in the concentration of the signaling molecules that drive these beautiful patterns? Is it possible, for example, that the precision with which a developing organism can draw boundaries between the different parts of its body is limited by the fundamental physical rules that govern the counting of individual molecules? Answers to these and other challenging questions will emerge in the next decade.

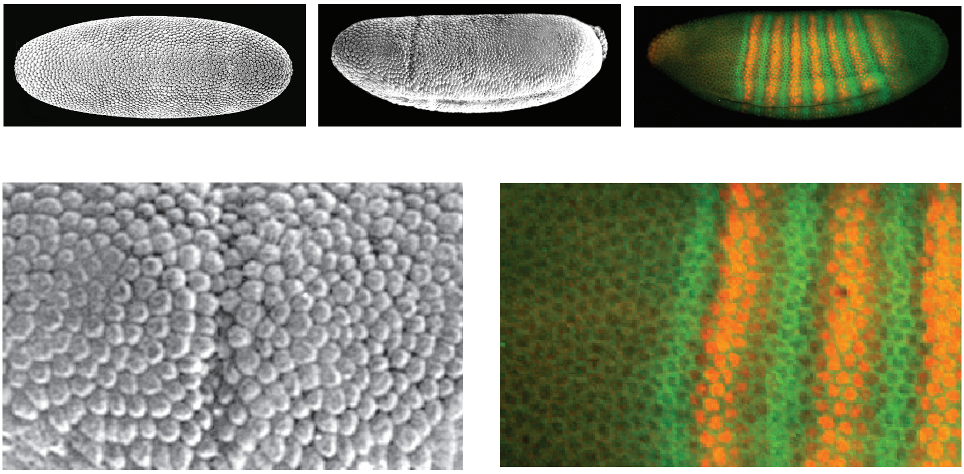

FIGURE 4.4 Genes and development in the fruit fly embryo. Images of the whole embryo, roughly 0.5 millimeter long. Two and one half hours after fertilization of the egg (top left), the thousands of cells on the surface of the embryo appear identical in an electron micrograph. Minutes later (top middle), the embryo undergoes gastrulation, folding in on itself along the bottom and making the cephalic furrow that defines the boundary of what will become the organism's head. Signals that determine the location of these structures are detectable as spatial patterns in the expression levels of different genes, two of which are made visible here in orange and green (top right). A close-up (bottom left) reveals the tight registration between the patterns of gene expression and the structural patterns such as the cephalic furrow. Additional measurements demonstrate that the stripes of gene expression correspond to the segments of the larval fly's body (bottom right). SOURCE: Images courtesy of E.F. Wieschaus, Princeton University.

## Signals and Noise in the Brain

Sitting quietly in a dark room, a person can detect the arrival of individual photons at his or her retina. This observation has a beautiful history, with its roots in a suggestion by Lorentz in 1911. The exploration of photon counting in vision reaches from the analysis of human behavior down to the level of single molecules, with many physics problems at every level. For example, it is not just that one can count single photons; the reliability of counting seems to be set by "dark noise" in the photodetector cells of the retina, and this noise in turn is dominated by thermal activation of the molecule (rhodopsin) that absorbs the light and whose structural response to photon absorption is the initial trigger for vision. The ability of the visual system to count single photons, down to the limits of thermal noise, inspires a consideration of the reliability of our perceptions more generally.

Absorption of a photon by one of the roughly 1 billion rhodopsin molecules in a photodetector cell results in a small pulse of current flowing across the cell membrane. The path from rhodopsin to the current involves a cascade of biochemical reactions that can be thought of as "molecule multipliers": when one rhodopsin molecule is activated by absorbing a photon, it catalyzes the conversion of many molecules from one state to another, these molecules act as catalysts for another reaction, and so on, until there is a relatively macroscopic change in concentration of a small molecule that binds to channels in the cell membrane and gates the flow of ions (see the discussion of ion channels below). But the number of molecular events that rhodopsin catalyzes depends on the time that it spends in the activated state, and this time must vary randomly each time a photon is absorbed by a different individual molecule. In fact, the variability of the current that flows in response to a single molecule is relatively small (~10 to 20 percent). Perhaps the most interesting possibility is that this problem is solved before it starts—rather than having rhodopsin exit its activated state by a single, necessarily random step (as in radioactive decay), the shutoff of rhodopsin activity could involve many steps, so that the random times required for each of the multiple steps average out to generate a much more precisely defined lifetime. The rhodopsin molecule in fact has a tail with multiple sites that can be modified by the attachment of a phosphate group, and it had long been known that this phosporylation is critical to the shutoff of rhodopsin activity. One can engineer rhodopsin molecules that have different numbers of phosphorylation sites, and reinsert the genes for these engineered molecules into the genome so that the photodetector cells of the retina actually make the modified molecules. The result is that the variability of the single photon response is larger in molecules that have fewer sites, and quantitatively the variance is the inverse of the number of sites, as predicted theoretically. This shows how nature has selected a very special, and seemingly complex, mechanism to do something simple—changing the state of a molecule in many steps rather than just one—in just such a way as to enhance the precision of the system beyond naïve expectations based on the random behavior of single molecules. Similarly subtle strategies for noise reduction in other processes remain to be discovered.

The example of photon counting encourages researchers to look for other examples in which the function of the nervous system may approach fundamental limits set by noise. Recent work along these lines includes the demonstration that, under certain conditions, the fly's visual system can estimate motion with a precision limited by noise in the receptor cells of the compound eye, and that this noise in turn is dominated by photon shot noise. Making optimal estimates in the presence of noise requires some prior hypotheses about what to expect, and it has been suggested that illusions—in particular, illusory motion percepts—can be understood, perhaps even quantitatively, as violations of these hypotheses. Effective priors are matched to the statistical structure of real-world signals, and this has led to a flowering of interest both in the characterization of these statistics—an effort that borrows heavily from the conceptual tools of CMMP—and in the neural response to such rich dynamic inputs. In a different direction, it has been suggested that human strategies for movement may be determined by the need to minimize the impact of noise in the control of muscles, optimizing the precision with which one can reach for a target. Noise also limits the capacity of neurons to carry information about the outside world, and it has been suggested that the coding strategies adopted by the brain may serve to make maximum use of this capacity; again this involves a matching of neural computation to the structure of its inputs. Miniaturization of the brain's components creates additional problems of noise, and hence there is pressure to make efficient use of the available space; several groups are exploring the possibility that brains may literally be shaped by the search for optimal wiring and packing. All of these different ideas of noise, optimization, and matching to the environment are under active investigation; the committee expects substantial developments over the next decade.

Many simple sensory inputs (such as a skeleton drawing of a cube) have multiple interpretations, and perceptions switch at random among these, presumably driven by noise somewhere in the nervous system. The origin of this noise is unknown, but the fact that perception fluctuates when the physical input to the visual system is constant has made possible a new kind of experiment, in which one searches for neurons whose dynamics are correlated with the subject's conscious impression of the image rather than the physical image itself. This is a far cry from Lorentz's original thoughts about photon counting, but perhaps not so far from Helmholtz's grand dream of a natural science that unifies the objective and subjective views of the physical world.

## FINE-TUNING VERSUS ROBUSTNESS

Living systems occupy a special corner in the space of all possible physical systems. On the one hand, random combinations of the microscopic parameters will not work: random sequences of amino acids will not make proteins that fold into functional structures, random biochemical networks would have chaotic dynamics, and randomly connected networks of neurons are unlikely to correspond to a brain that thinks and remembers. On the other hand, surely not every parameter needs to be finely tuned; alternatively, if fine-tuning is necessary, then there must be some as-yet-uncharacterized layer of dynamics that achieves this tuning more robustly. Physicists have identified this tension between fine-tuning and robustness in several different biological contexts.

### Protein Folding and the Space of Sequences

Proteins are polymers built from amino acids. A typical protein is approximately 200 monomers in length, and with 20 different amino acids, the number of possible proteins is enormous. Over the entire history of life on Earth, only a vanishingly small fraction of these possible polymers has been made. Unlike most polymers, proteins "fold" into compact, nearly unique three-dimensional structures. One formulation of the "protein folding problem" is to predict the three-dimensional structure that is adopted by proteins with a particular amino acid sequence. This is a physics problem, but a complex one, because there are many degrees of freedom and the interactions themselves are highly structured. But there are more general questions: Why do proteins adopt a well-defined, compact structure at all? Is the limited set of proteins observed in nature an accident of evolutionary history, or derivable from physical principles?

Some amino acids are polar or even charged, and hence have favorable (hydrophilic) interactions with water. Other amino acids are nonpolar, or oil-like, and have unfavorable (hydrophobic) interactions with water. These interactions drive proteins toward a state in which the hydrophobic amino acids are packed in a dense core, while the hydrophilic amino acids form a shell contacting the surrounding water. But this simple structure can be frustrated by the fact that the different amino acids are linked, covalently, along the length of the polymer. Indeed, a result from statistical mechanics states that a random polymer in which different monomers have competing interactions will be so frustrated that it forms a glass, with many distinct structures having nearly equal energy. This suggests that the ability of proteins to fold into unique structures already restricts dramatically the set of allowed sequences.

In the theory of disordered systems, a core area of CMMP, the intuitive notion of "frustration" has become a precise mathematical concept. Are the sequences that occur in natural proteins those which actually minimize frustration in this precise sense? If so, the dynamics leading from random unfolded structures to the compact folded structure will be a smooth, downhill slide on some coarse-grained, effective free-energy surface; rather than there being a specific pathway that the protein must follow, many different paths all flow to the unique ground state. These ideas of a smooth "energy landscape" and minimal frustration grow directly out of investigations on problems in CMMP, and over the past decade this theoretical picture of protein folding has scored important successes in connecting directly to a wide variety of experiments.

Ideas from statistical physics also have been important in defining the "inverse folding" problem: given a particular compact protein structure, is there an amino acid sequence that folds to this structure as its ground state? In simplified models, some structures are not realizable, others require very specific sequences, and a special set of structures comprises the ground states of many different sequences. These "highly designable" structures have much in common with real protein structures, and this line of research has generated predictions for new proteins that have since been synthesized.

Taken together, these results suggest that the sequences and structures of proteins are not frozen accidents of history, but rather are predictable from physical principles: the minimizing of frustration and the maximizing of designability. The minimizing of frustration "tunes" the system to a particular set of possible sequences, but the choice of maximally designable structures means precisely that structures will be robust to substantial sequence variation. Thus, the protein folding problem provides a prototype for the understanding of fine-tuning versus robustness in biological systems. Importantly, modern experimental methods make it possible to explore, quantitatively, large ensembles of sequences; the committee thus expects a rich interaction between theory and experiment over the next decade.

### Ion Channels and the Computational Function of Neurons

In the wires leading to a home appliance or in the chips in a computer, electrical currents are carried by electrons moving through solids (metals and semiconductors). In biological systems, currents are carried by ions, such as potassium, sodium, calcium, and chloride, moving through water. Every living cell has a membrane that surrounds it, defining what is "inside" the cell and making it possible for the cell to control its chemical environment. The physical properties of the membrane are such that it cannot be easily penetrated by ions, and hence it provides a huge resistance to the flow of current. But there are special protein molecules in the membrane, called channels, that allow specific ions to flow into and out of the cell. Most channel molecules can take on several different structures; some structures are "open" and some are "closed," so that current flow can be gated on or off. Further, the membrane also contains pumps, so that the concentration of ions is different on the inside and outside of the cell, forming an effective battery that will drive currents once the channels open. Finally, the opening and closing of channels is sensitive to the voltage or electric field across the membrane. The combination of ionic batteries, voltage-gated channels, and the capacitance of the cell membrane creates complex electrical circuits that are capable of many functions. These circuits can filter and amplify incoming signals, they can oscillate to generate rhythms, and they can generate pulses that propagate along the fingerlike extensions (axons) that reach from one cell to another; these pulses are called action potentials or spikes, and provide the brain's internal language for communication. These dynamics are generated in different cells using different combinations of channels, leading researchers to ask whether particular functions depend on the fine-tuning of these combinations.

It is worth noting that the path to our modern understanding of ion channels depended upon many ideas and methods from physics: The concept of channels emerged from mathematical models of the electrical circuit formed by the axon membrane. These models made quantitative predictions about the flow of particular ions, which were tested using radioactive tracers. For channels to open and close in response to voltage across the membrane, thermodynamics requires that the open and closed states have different charge distributions, so that changes in the state of the channel itself should be accompanied by small currents, and these were observed. Because the channels are individual molecules, they each can make random transitions between their open and closed states, and this should generate an electrical noise in the cell with properties that can be predicted from statistical mechanics; this noise was observed. Finally, with advances in electronics, it was possible to measure the currents that flow through a single channel molecule and to observe the discrete transitions as these molecules open and close. In parallel with these advances, x-ray diffraction has revealed the detailed atomic structure of these remarkable molecules.

By 1990, the understanding of channels had reached a significant state, allowing scientists to write down essentially exact equations that describe a neuron's functional electrical behavior. These dynamics depend on how many channel molecules are present in the membrane; a cell might contain 9 or 10 different kinds of channels, chosen from many hundreds of channel proteins encoded in the genome. Perhaps surprisingly, the mathematical models predict that small changes in the balance among the different kinds of channels can lead to qualitatively different electrical behavior, for example converting a neuron that generates a simple rhythm into one that generates a complex syncopated beat. This is disturbing, not least because the parameters of the model cannot be set by evolution, or once and for all during the course of the brain's development; cells are always "choosing" how many molecules of each protein to make and how these molecules should be distributed throughout the cell. A team of physicists and biologists took these problems seriously and argued that neurons must have mechanisms to monitor their own electrical activity and feed these signals back to the processes that regulate the expression of particular channel molecules and/or their placement in the membrane. They showed theoretically that plausible implementations of this idea could provide robust stabilization of the functional values of the cell's parameters. Very quickly this general idea was confirmed by experiments showing that neurons could be ripped from their natural environment and placed into solutions with very different concentration of ions, and then after some time they would recover their original rhythms by expressing a different combination of channels. Quite literally, it seems as if the cell "knows" its function and can check to see that it is doing the right thing.

The idea of feedback to stabilize the correct numbers of ion channel proteins has launched a whole new field of experiments. In addition to exploring molecular mechanisms of this feedback, analogous phenomena have been discovered in the dynamics of the synapses or connections between neurons. More generally one can think of learning mechanisms in the brain as operating not just to master genuinely new things, but also to "tune" neural circuits continuously so that they maintain their proper functions. New generations of physical measurements that allow researchers to see directly the molecular events at synapses are probing the rules that underlie such continuous learning (Figure 4.5). Recent excitement has focused on the fact that these learning rules are sensitive to the detailed timing of action potentials, responding differently to sequences of spikes that have different causal relations. Theoretical approaches, often grounded in the methods of CMMP, are being used to understand the consequences of these rules for whole networks of neurons. For (seemingly!) simple problems—such as the ability of the nervous system to remember how much force must be applied to the eyes to compensate for rotation of the head—there are major experimental efforts under way to make connections all the way from the submicron events at single synapses, to the collective dynamics of the relevant networks, to the plasticity of behavior in the whole organism, with each step having important interactions with theory. It is reasonable to expect that, in the next decade, the dichotomy of robustness versus fine-tuning will be replaced by a dynamical model of how the brain robustly tunes itself.

## Adaptation

As one steps from a dark room into bright sunlight, one's eyes respond with an enormous transient that can be literally blinding; after a few moments, however, the world comes back into focus; the same phenomenon happens in reverse as one steps back into the dark. Over some range, one's image of the world is largely invariant to the absolute intensity of light, instead highlighting variations in space and time. Similarly, a person feels a sudden pressure on the skin, but if this pressure remains constant, the person gradually becomes unaware of it. Although the human brain makes important contributions to these percepts, important aspects

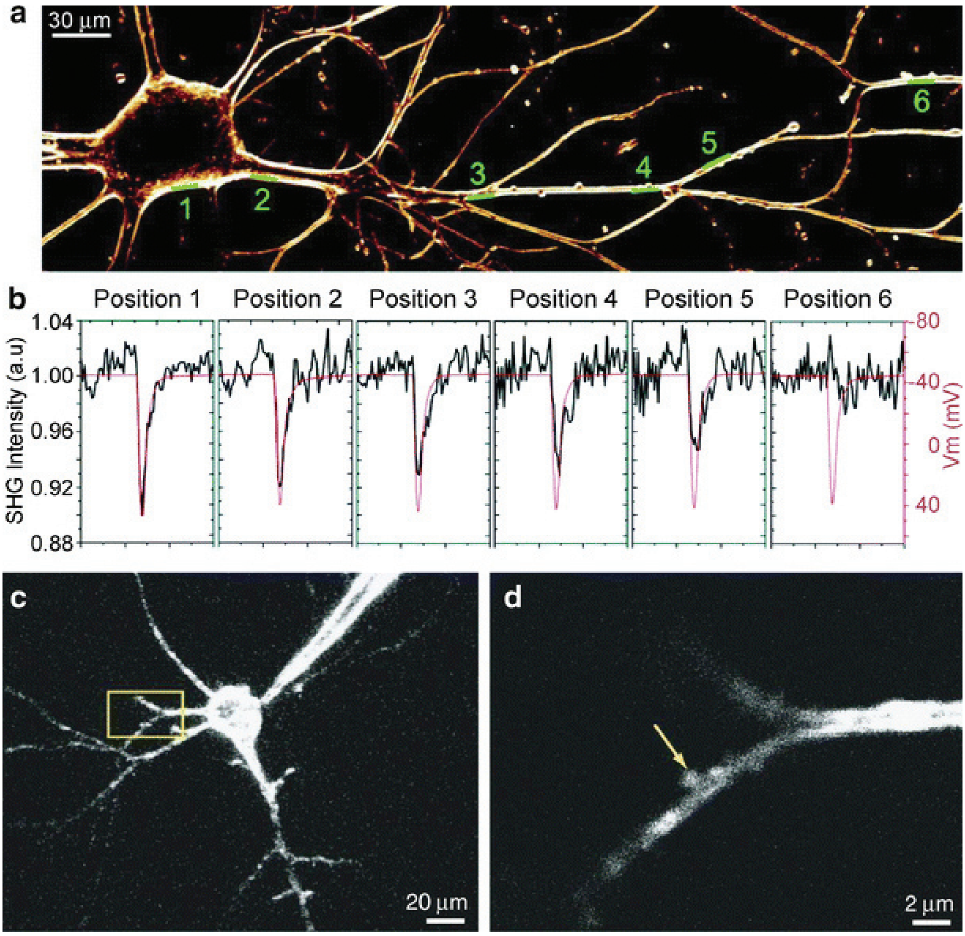

FIGURE 4.5 Physicists have developed a wide variety of methods for making the electrical and chemical activity of neurons literally visible under the microscope. Here, molecules dissolved in the cell membrane generate second harmonics when stimulated by long-wavelength light, but the efficiency of second harmonic generation (SHG) depends on the voltage difference across the membrane. (a) Image of a single neuron isolated from the sea slug Aplysia and growing in a dish. When the cell generates an action potential, this can be monitored by an electrode placed in the cell body (red traces in b), but the resulting electrical signals also are visible by measuring the intensity of second harmonics (black traces in b). Electrical signals in the cell body (Position 1) are carried for hundreds of microns (to Position 5), but not to the farthest reaches of the cell (Position 6). Turning to a cell from the cortex of a mammalian brain (c), one sees the cell body (now impaled by an electrode) and a tree of dendrites. (d) Zooming in shows the bulb or spine along the dendrite where another cell connects to this one. Observing electrical and chemical signals in these submicron structures gives direct access to the messages that cells use in changing the strengths of their interconnections, the fundamental step in learning. SOURCE: G.J. Stuart and L.M. Palmer, “Imaging Membrane Potential in Dendrites and Axons of Single Neurons,” *Pflugers Archiv*, **453**, 403 (2006).

of adaptation can be seen in the responses of the single cells that are responsible for the initial conversion of sensory input into the electrical impulses that constitute the internal language of the brain. Strikingly analogous phenomena occur even in bacteria as they migrate in chemical gradients (chemotaxis, as discussed above). A sudden increase, for example, in the concentration of sugar results in a large change in the way that bacteria swim, but eventually this change dissipates; thus, bacteria never mistake a good life for one that is getting better.

In all these systems, the relaxation to an "adapted" state is a competition between some rapid process that embodies the response to a sudden change and a slower process that acts with opposite sign. In the case of bacteria, 30 years of genetics, biochemistry, and molecular biology brought researchers to the point at which these processes can be identified with the actions of particular protein molecules. But then the strengths of the competing excitation and adaptation processes will depend on how many molecules of each protein are present. Does cancellation between excitation and adaptation then require the bacterium to have exactly the right numbers of these molecules? Does this mean that adaptation can never be perfect? Remarkably, quantitative experiments indicate that adaptation in bacterial behavior really is perfect. Closer examination of the biochemical network that processes the chemotactic signals showed that, if the proteins involved had certain specific properties, it would be possible to achieve perfect adaptation without fine-tuning of the number of proteins. Combining experimental physics methods for quantitative observation of bacterial swimming with molecular biology methods for engineering bacteria that make different amounts of the relevant proteins, this prediction of "robust perfect adaptation" was confirmed.

Encouraged by the example of adaptation, a number of theoretical physicists have explored the problem of robustness in other biochemical networks. In the developing embryo, for example, one would like to know how it is possible for networks of genetic regulatory interactions to generate reproducible spatial structures despite inevitable variations in external conditions. In a similar spirit, the cycle that leads to cell division has been analyzed to identify the classic "states" described by cell biologists as robust attractors of the underlying dynamics. In a slightly different direction, theorists have explored statistical mechanics in the space of network parameters, with the "energy" of reproducing known functional behaviors trading against the entropy that quantifies our intuition about robustness. Interestingly, a similar energy/entropy trade-off has been used to describe the mathematics of learning in brains and machines. Perhaps the ideas of robustness will lead, over the next decade, to a more precise theory, in the spirit of statistical physics, of how evolution, learning, and other regulatory mechanisms select functional biological networks out of the vast range of possible networks.

## FULFILLING THE PROMISE

We are in the midst of an explosion of activity at the interface of physics and biology. More than in any previous generation, today's physicists are learning "the facts of life" and asking new and different questions about these remarkable phenomena. As in other areas of physics, technically challenging, quantitative experiments are making precise our qualitative impressions of these phenomena, and this new experimental power provides fertile ground to test increasingly sophisticated theories. The breadth of this activity is enormous, from the dynamics of single molecules to perception and learning in the brain and from networks of biochemical reactions in single cells to the dynamics of evolution.

We have passed the point at which the interaction between physics and biology can be viewed as "merely" the application of known physics. Rather, the conceptual challenges of the phenomena of life are driving the emergence of a biological physics that is genuinely a subfield of physics. Guiding the growth of this field and taking full advantage of the enormous range of opportunities are major challenges for the research community, not least in terms of how it educates itself and its students (see Chapter 8). The committee is optimistic that the coming decade will see at least the outlines of a "physics of life" that brings together the many exciting threads of current research at the borders of physics and biology. The goal is nothing less than the unification in understanding of the animate and inanimate worlds, fulfilling the dreams of our intellectual ancestors.

# 5

# What Happens Far from Equilibrium and Why?

Isolated systems evolve toward equilibrium, a special state in which properties do not change with time. Yet much of the richness of the world around us arises from conditions far from equilibrium. Phenomena such as turbulence, earthquakes, fracture, and life itself only occur far from equilibrium. Subjecting materials to conditions far from equilibrium leads to otherwise-unattainable properties. For example, rapid cooling is a key process in the manufacture of the strongest metallic alloys and toughest plastics. Processes that occur far from equilibrium also create some of the most intricate structures known, from snowflakes to the highly organized structures of life. While much is understood about systems at or near equilibrium, scientists are just beginning to uncover the basic principles governing systems far from equilibrium. Breakthroughs in this area of condensed-matter and materials physics (CMMP) research will affect virtually every discipline in the physical sciences, life sciences, and engineering.

## THE IMPORTANCE OF FAR-FROM-EQUILIBRIUM PHENOMENA

We live in a world of evolving structures and patterns. When energy is continually supplied to systems with many interacting constituents, the outcome generally differs strikingly from the unchanging state that characterizes equilibrium. From the molecular processes on the nanoscale that form the basis of life, to the dynamically changing climate on this planet, to the clustering of matter within the universe as a whole, a myriad of phenomena owe their existence to being not just slightly away from equilibrium, but far from it (Figure 5.1). Far-from-

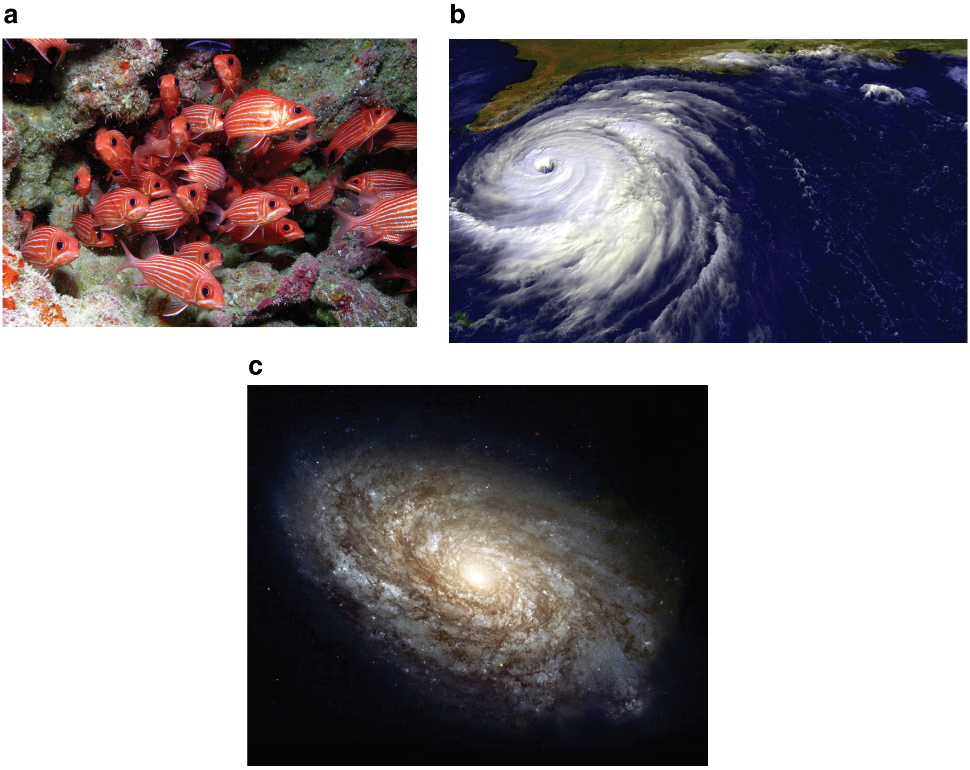

FIGURE 5.1 (a) Swarming schools of fish, (b) swirling storms, and (c) galaxies are all examples of systems formed and evolving far from equilibrium. SOURCES: (a) Department of the Interior. (b) Laboratory for Atmospheres, National Aeronautics and Space Administration. (c) National Space Science Data Center, National Aeronautics and Space Administration.

equilibrium conditions also significantly alter the behavior of ordinary fluids and solids. Dramatic examples occur when fluid flow turns turbulent or when solids give way and fracture (Figure 5.2). Both turbulence and fracture generate patterns of amazing complexity that not only completely change the materials properties but also redistribute energy across a whole hierarchy of nested structures, ranging from the microscopic to the macroscopic scale. Far-from-equilibrium processes span a similarly immense range of timescales, from electronic transitions at the subnanosecond scale, to glassy relaxation too slow to measure with any technique, to the age of the universe.

Far-from-equilibrium behavior is not confined to special conditions or certain types of materials. Instead, it arises across the entire spectrum of condensed-matter and materials physics in a host of problems of fundamental interest. Far-from-equilibrium phenomena also benefit and plague us in technology and in everyday life. Indeed, some of the most complex outcomes of behavior far from equilibrium

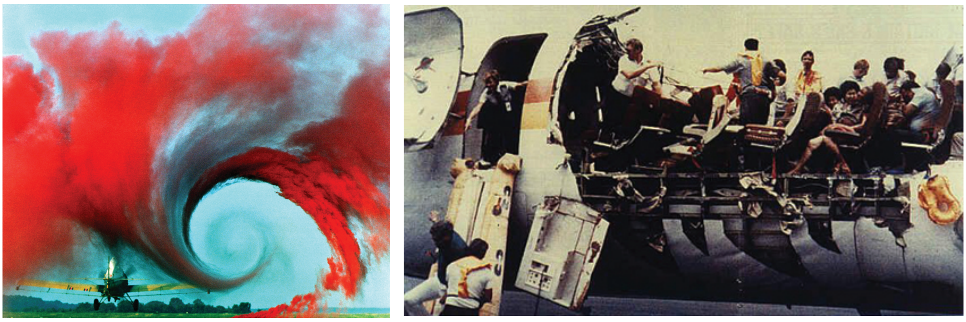

FIGURE 5.2 The need to control far-from-equilibrium behavior. (Left) Turbulent airflow produced by the wingtips of a small airplane (visualized by red smoke). (Right) Disastrous effect of materials fatigue and eventual fracture. SOURCES: (Left) Langley Research Center, National Aeronautics and Space Administration. (Right) Hawaii State Archives.

emerge in situations familiar in everyday experience. For example, we can see turbulence in cloud patterns as well as in a bathtub; we take advantage of glassy behavior in nearly all plastics but suffer from it in traffic jams; we exploit the breaking up of a stream of fluid into droplets with fuel injection and ink-jet printing but also find it in every leaky faucet. The reach of far-from-equilibrium phenomena extends even farther, to many systems of profound societal importance. In the past decade, CMMP researchers have begun to tackle far-from-equilibrium behavior governing the workings of systems ranging from the economy to ecosystems and the environment.

### Key Themes Defining the Scope of the Challenge

Two important themes define the scope of the challenge. They run as persistent motifs through a description of the current status of CMMP far from equilibrium. The first theme is that far-from-equilibrium behavior is ubiquitous. The breadth of phenomena investigated makes the study of far-from-equilibrium systems an inherently interdisciplinary field that forges connections between the CMMP community and researchers in biology, chemistry, applied mathematics, geology, meteorology, and engineering. Far-from-equilibrium physics is connected intimately to both fundamental scientific challenges and cutting-edge materials processing. And, far-from-equilibrium physics underlies a wide range of phenomena outside the traditional boundaries of CMMP, including earthquakes, hurricanes, galaxy formation, and consciousness. As a result, breakthroughs in the area have the potential for far-reaching impact across many scientific disciplines.

The second key theme is that, despite its importance, far-from-equilibrium behavior still remains largely uncharted territory. Far-from-equilibrium behavior is not a simple extension of equilibrium or near-equilibrium physics. Instead, it corresponds to qualitatively different types of behavior and response, typically associated with crossing some threshold into a new regime. In some specific cases, researchers have been able to unearth the microscopic origins of far-from-equilibrium phenomena, but still lacking is the understanding necessary to develop more comprehensive frameworks. The reasons why far-from-equilibrium phenomena often resist understanding are described below. This is followed by a discussion of problems for which robust features have been identified, both in experiment and in theory, that can serve as starting points for work over the next decade. Finally, critical needs and recommendations for achieving progress over the next decade are discussed.

## What CMMP Brings to the Table

Condensed-matter and materials physics is uniquely positioned to spearhead progress in the field of far-from-equilibrium behavior. As one of the forefront areas of interdisciplinary research, CMMP has long been a focal point for new approaches that bring together ideas from physics and other science and engineering disciplines and that connect basic science with applied research. CMMP also specializes in developing new theoretical, numerical, and experimental tools and techniques (Chapter 11) for systems of many interacting constituents. Experimental techniques that have been especially useful for probing far-from-equilibrium behavior include novel imaging tools and spectroscopic and particle-tracking methods. Many powerful theoretical and numerical techniques for studying the emergent behavior of many-particle systems near equilibrium have been generalized to systems far from equilibrium; for example, techniques originally developed for studying magnets have been extended to the flocking of birds. Perhaps the field's most valuable characteristic, however, is its penchant for searching for commonalities in wildly disparate systems. This focus led to the spectacular success of CMMP in realizing that the enormous variety of equilibrium phase transitions can be understood in terms of a few classes of behavior. This history motivates CMMP researchers to search for similar organizing principles in the even vaster array of far-from-equilibrium phenomena.

Far-from-equilibrium behavior is an important component in several of the other CMMP grand challenge areas discussed in this report. It underlies many emergent phenomena (Chapter 2) in systems ranging from the nanoscale (Chapter 6) to the macroscale, and it plays an essential role in the physics of living systems (Chapter 4). Because many far-from-equilibrium phenomena require energy in order to be driven, they are also inevitably implicated in energy consumption and conversion (Chapter 3). In quantum computing (Chapter 7), the challenge is to prepare qubits in prescribed pure quantum states. Such systems are necessarily far from equilibrium. Finally, because far-from-equilibrium phenomena are so common in everyday life and underlie so many societal concerns, they provide a rich context for education and learning, for the next generation of scientists as well as for the general public (Chapter 8).

## HOW DO SYSTEMS REACH THE FAR-FROM-EQUILIBRIUM REGIME AND WHAT MAKES FAR-FROM-EQUILIBRIUM PHYSICS DIFFICULT?

One way to keep a system from its natural state of rest and to push it into the far-from-equilibrium regime involves continual and sufficiently strong forcing. For example, the energy that continually strikes Earth from the Sun gives rise to far-from-equilibrium behavior ranging from chaotic weather patterns to the staggering diversity of life. If solar energy were no longer supplied, many systems on Earth would revert to equilibrium. Driven systems such as these not only give rise to rich and unanticipated phenomena but are also of tremendous importance to technological applications. For example, in molecular or nanoscale electronics, new phenomena arise from the response to large electromagnetic fields, currents, and mechanical stresses. As one scales the physical dimensions of matter to the nanometer scale, the applied fields that drive the system away from its equilibrium state are amplified, while the scattering that allows relaxation back to equilibrium is suppressed. As a result, such devices often operate in the far-from-equilibrium regime, unlike conventional semiconductor devices at the micron scale, which typically operate much closer to equilibrium.

Conditions far from equilibrium also provide a route for controlling a larger variety of patterns and for assembling structures from the nanoscale on up at growth rates much faster than would be possible with near-equilibrium approaches. Importantly, far-from-equilibrium processes can achieve structural and dynamical richness even with the simplest of ingredients, such as the intricate dendritic growth realized in snowflakes (Figure 5.3).

Other systems are trapped far from equilibrium because they simply cannot relax back to equilibrium even after all driving forces have been removed. This happens for many materials vital to industrial society, including glasses, powders, foams, and most plastics, which attain their properties from being intrinsically caught in far-from-equilibrium states (Figure 5.4). These materials exhibit structural properties that, under equilibrium conditions, would identify them as liquids; yet they can behave like solids.

Processes occurring far from equilibrium are beginning to force researchers to rethink some of the foundations of condensed-matter and materials physics. Yet even today, most of the knowledge about how systems with many constituent particles behave and evolve is based on considerations valid only close to equilibrium.

FIGURE 5.3 Far-from-equilibrium growth in nature: the snowflake. SOURCE: Image courtesy of Kenneth Libbrecht, SnowCrystals.com.

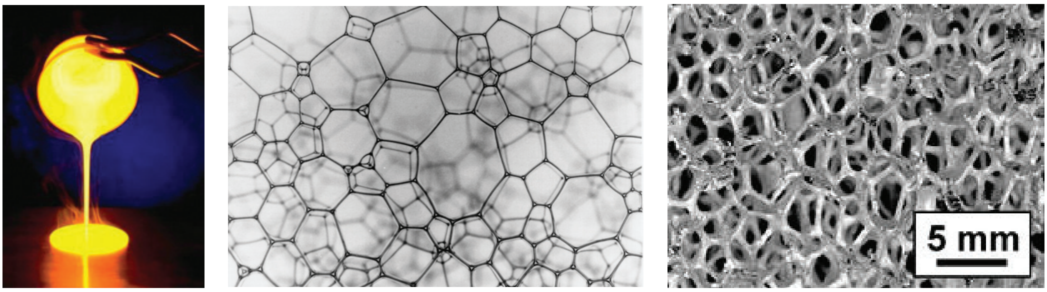

FIGURE 5.4 Glasses and foams are examples of important materials that are generically in states far from equilibrium. (Left to right) Molten glass freezing into a solid, soap foam, and open-cell aluminum foam. SOURCES: (Left) Savannah River National Laboratory, Department of Energy. (Middle) D. Durian, University of Pennsylvania. (Right) D.C. Curran.

CMMP researchers know much more about systems near equilibrium and have developed a powerful formalism, statistical mechanics, to predict the emergent, collective behavior of many-particle systems. This framework has allowed CMMP researchers to understand a large number of phases of matter, the origins of many of their properties, and the nature of transitions between them. However, this framework applies only to situations in which a system is thermally and mechanically in balance with its surroundings, and thus it covers only a small subset of the phenomena observed around us and confronted in applications.

One conceptual difficulty posed by systems far from equilibrium thus arises from the absence of established theoretical frameworks. However, by virtue of being far from equilibrium, such systems also pose additional challenges. They are typically *nonlinear:* that is, their response to perturbation is often not proportional to the magnitude of the perturbation, as for systems near equilibrium. Such systems are often *disordered:* that is, their structure is typically not crystalline, as equilibrium solids generally are. Finally, such systems are often *non-ergodic:* that is, they do not necessarily explore a large subset of the states available to them, as equilibrium systems must. As a result, even characterizing their behavior and structure leads one onto largely unfamiliar ground from the standpoint of most of CMMP.

## Far-from-Equilibrium Materials

Certain classes of materials almost always exist under conditions far from equilibrium. Many materials investigated by researchers in the area of soft condensed-matter physics fall into this category, including glasses, foams, granular materials, and dense colloidal suspensions. In all of these examples, the thermal energy supplied by the surroundings is too small to allow the systems to explore many configurations. Instead, they are trapped in configurations that structurally resemble a liquid (they are dense and highly disordered), but are unable to flow and thus behave as solids. This glassy behavior, a hallmark of many far-from-equilibrium materials, is observed for constituents ranging from molecules in glass-forming liquids to grains of sand in dunes. Since these materials cannot relax to equilibrium, they typically retain a memory of the preparation or processing conditions, a key for many technological innovations such as molded plastic parts and shape memory polymers. Transitions from far-from-equilibrium glassy states to near-equilibrium crystalline states are the basis for chalcogenide glass optical disks and phase-change memory devices.

Over the past decade, granular matter has emerged as a key prototype of a far-from-equilibrium material (see Figure 1.4 in Chapter 1). In its simplest form, granular matter consists of nothing more than a large number of noncohesive, macroscopic hard spheres interacting only at contact; yet it exhibits all the characteristics of far-from-equilibrium behavior, as discussed in the subsequent sections.

Furthermore, several ideas developed originally within the context of granular materials have by now been successfully “exported” into other areas; for example, the concept of jamming gives insight into glassy phenomena. Similarly, ideas about avalanche statistics in driven dissipative systems, investigated early on in sandpiles, have been applied to earthquakes and have led to renewed interest in flux-bundle motion in superconducting magnets.

Beyond fundamental research, a large number of industrial processes depend on the handling and transport of granular matter, from seeds and fertilizer pellets in agriculture, to ore and gravel in mining operations, to powders and pills in the pharmaceutical industry. Yet the inherently far-from-equilibrium behavior of these materials is still poorly understood and controlled. For example, in North America, new plants designed for processing granular materials initially operate at only about 50 to 60 percent of design capacity, while those designed for the handling of liquids immediately operate at nearly full efficiency. Investment in this area of CMMP would not only raise the level of fundamental understanding needed for innovative solutions to pervasive industrial problems but would also increase the pool of scientifically trained people who can contribute to the understanding of materials-processing industries.

### Far-from-Equilibrium Processing and Assembly

Many materials-processing techniques exploit far-from-equilibrium conditions for the growth and manufacture of materials that otherwise could not be fabricated. Many high-strength alloys are formed by the same rapid dendritic growth that underlies the formation of snowflakes. Some of the very strongest materials available are metallic alloy glasses, made by rapid cooling into amorphous states far from equilibrium (Figure 5.5). Lightweight, strong, and tough plastics for car bumpers and aircraft are produced by similar processes. The understanding and control of out-of-equilibrium behavior are also important for interface growth processes, as in those used to produce the huge, essentially defect-free single crystals of silicon used in the semiconductor industry.

Far-from-equilibrium processing conditions can be used to drive a system toward unique final configurations in very efficient and speedy ways. On the nanoscale this offers new advantages. For example, certain polymers (diblock copolymers) spontaneously organize themselves into extended patterns with repeat spacings in the 10 nm to 50 nm range. Such spacings are desirable for applications such as high-density magnetic storage but difficult to achieve with conventional lithographic methods (see Chapter 7). In equilibrium, these polymeric structures are typically fairly disordered and contain a large number of defects. If the systems are sheared far from equilibrium, however, the defects can be removed and the structures can order over extremely large distances. Another advantage of far-

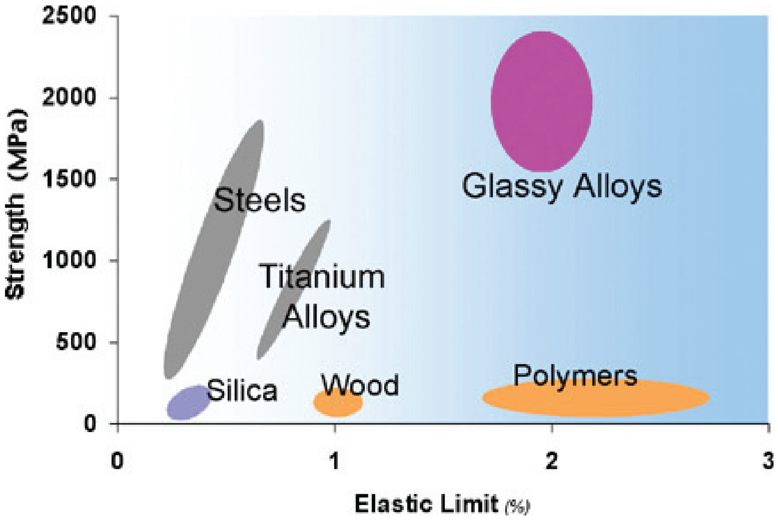

FIGURE 5.5 Far-from-equilibrium processing produces some of the toughest, highest-strength materials (glassy metal alloys). The abscissa corresponds to the yield strain, while the ordinate corresponds to the Young's modulus of the materials identified in the figure. SOURCE: Courtesy of William L. Johnson, California Institute of Technology.

from-equilibrium conditions is that small differences in the physical or chemical properties of neighboring regions in a material can be amplified; in equilibrium, diffusion tends to smooth out such differences. This property can be exploited to aggregate inorganic components, such as metallic, magnetic, or semiconducting particles, on selective polymer domains. The resulting configuration faithfully duplicates the domain pattern instead of assuming the uniform coverage found in equilibrium.

## WHAT DETERMINES BEHAVIOR FAR FROM EQUILIBRIUM?

In equilibrium, minimization of a free energy determines the preferred state, and the system reaches this state independent of the initial conditions. Far from equilibrium, systems typically exhibit a very rich set of characteristic behaviors that are not generally described by a minimization principle. What physics governs the state that a system chooses? Physicists have made considerable progress in a number of specific cases. This section discusses advances in the areas of fluids and dynamical systems and looks at the use of singularities in understanding and controlling far-from-equilibrium behavior.

## Systems with Hydrodynamic Equations of Motion

In many cases, far-from-equilibrium systems exhibit a convenient separation of length scale and timescale. In order to understand many fluid-flow problems, such as the vortex of a tornado, it is not necessary to describe the motions of individual molecules. The experience of CMMP with equilibrium systems has taught that it is often fruitful to focus on the long-length-scale, long-timescale behavior. This so-called hydrodynamic approach has been the basis of success in describing a number of systems far from equilibrium. Once the basic differential equations that describe the long-length-scale and -timescale behavior are known, such as the Navier-Stokes equation for fluid flow, an astounding range of far-from-equilibrium, nonlinear behaviors can be tackled. These behaviors include the erratic fluttering of flags in the wind (Figure 5.6), the flapping of a bird's wings, and the breaking of water waves on a beach. Similar descriptions also apply to complex fluids under flow, a frontier area that is only beginning to be explored.

Finally, the hydrodynamic approach can be applied to a wide range of phenomena not associated with fluids at all, such as the braking of gravity waves on a collapsing white dwarf, the flocking of birds and other organisms, and the development of single-celled amoebae into multicellular organisms. Another example is found in semiconductor heterostructures in which electron density waves are confined to the sample edge. There, strong electronic correlations are predicted to produce shock waves that resemble roll clouds in the atmosphere. Many more examples are provided by the physical, chemical, and biological systems that exhibit pattern formation, in which a uniform system develops patterns in space and/or time by being driven out of equilibrium.

The idea that the dynamics of a system with many degrees of freedom can be dominated by the interaction of only a few (such as those at long length scale and timescale) is an important CMMP contribution that motivates the study of simple dynamical models in order to gain insight into complex phenomena. Models such as the Lorenz model and other climate models include only a few degrees of freedom, yet successfully capture qualitatively many features of Earth's climate. Similar approaches are used to gain insight into the origin of Earth's magnetic field, mantle convection, Jupiter's red spot, and the cycle of solar flares.

The challenges in tackling this class of problems lie in the identification of the few crucial degrees of freedom that must be retained and in the complexity of the resulting equations of motion. Much progress has come from a close coupling of analytic theory with large-scale computer simulations, informed by experiments; access to the fastest supercomputers will become increasingly important over the next decade. As the understanding of complex interacting dynamical systems and the power of computational resources increase, one great challenge will be to apply

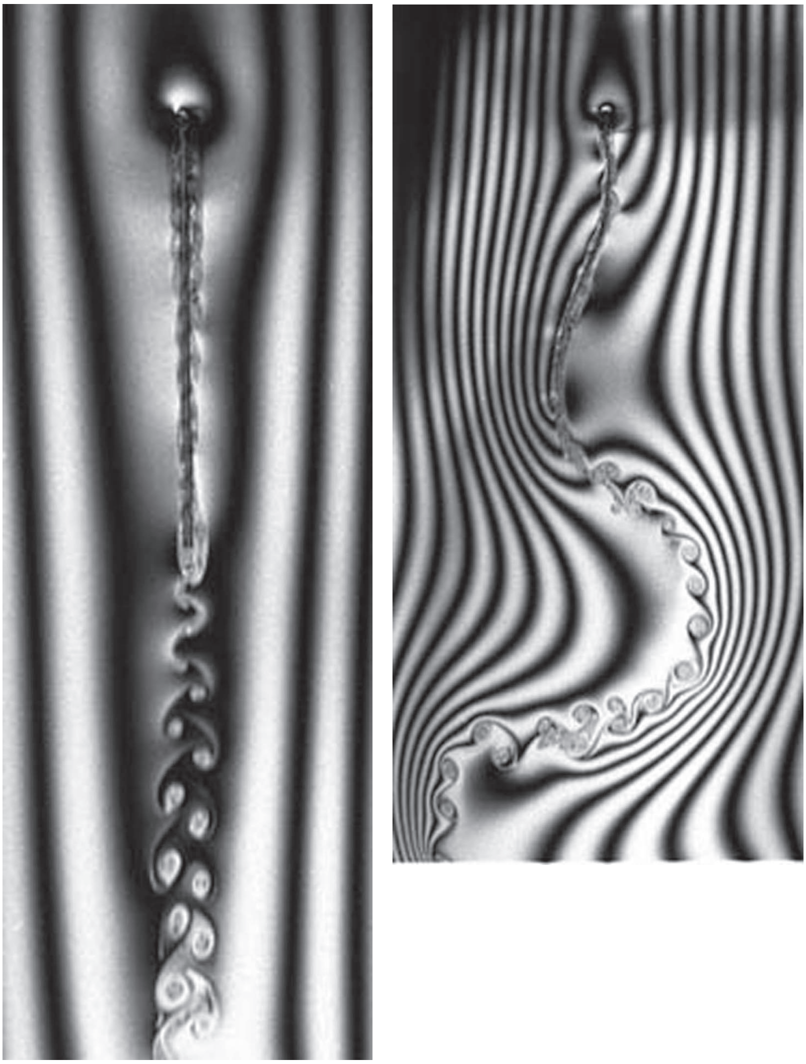

FIGURE 5.6 Modeling the fluttering of flags in the wind: the transition from steady (left) to fluttering (right) motion, visualized by imaging fluid flow around a filament tied to a post (circle at the top). SOURCE: J. Zhang, S. Childress, A. Libchaber, and M. Shelley, “Flexible Filaments in a Flowing Soap Film as a Model for One-Dimensional Flags in a Two-Dimensional Wind,” *Nature* **408**, 835-839 (2000).

this knowledge and computing power to global warming, as CMMP researchers are beginning to do.

## Turbulence and Fracture

Many far-from-equilibrium phenomena pose special challenges because they involve a multitude of length scales and timescales that interact and thus all become important. Large-scale turbulence is connected directly to flow behavior at scales many orders of magnitude smaller; macroscopic fracture patterns depend intimately on the local configuration of molecular bonds in front of the crack tip (Figure 5.7). In problems such as turbulence, hydrodynamic equations apply but become impossible to solve. Theoretical techniques used in CMMP to study equilibrium critical phase transitions, such as the renormalization group, can be useful here. These techniques are designed to understand how physics at small length scales or timescales affects behavior at somewhat larger length scales or timescales,

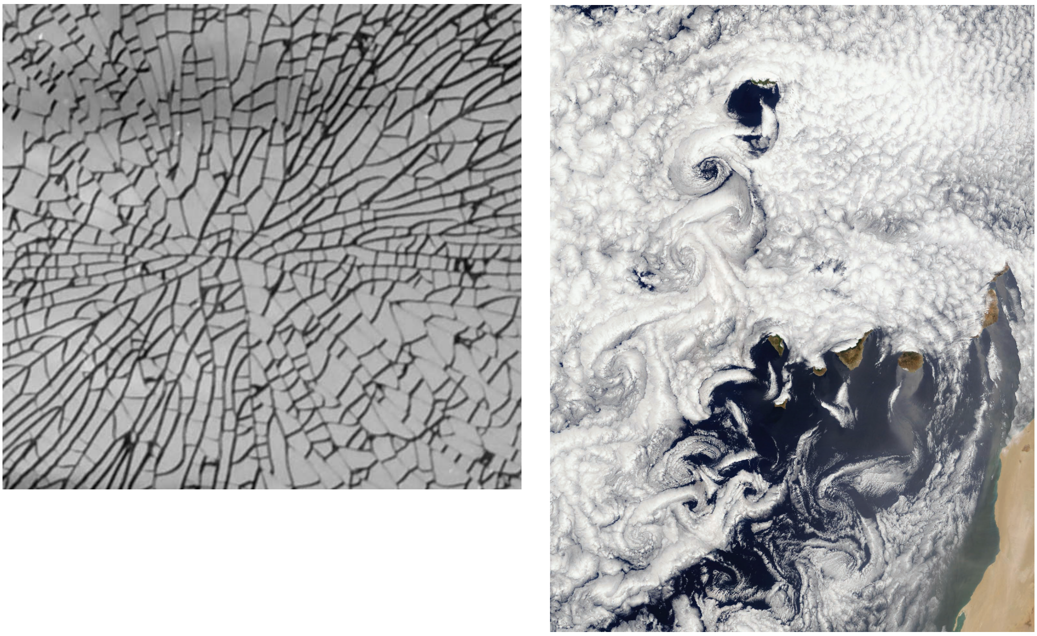

FIGURE 5.7 Far-from-equilibrium behavior often involves processes interacting over a large range of length scales and timescales, leading to characteristic patterns such as the ones observed in the fracture of a glass (left) and in turbulent cloud formations (right). SOURCES: (Left) John C. Barry, PicaMS Pty Ltd. (Right) Visible Earth, National Aeronautics and Space Administration.

and so on, ultimately leading to an understanding of how a wide range of length scales or timescales interact with one another.

The focus here is on turbulence, which is one of the most common far-from-equilibrium phenomena in the environment and in industrial processes. Turbulence produces complex flow structures that modify the transport of momentum, mass, and heat, thereby creating a wide variety of both wanted and unwanted effects: a means for rapid mixing of reagents in industrial processes but also parasitic drag in pipe flow and, on a larger scale, catastrophic weather patterns such as hurricanes. Very similar unstable flow structures are produced during the extrusion of polymers or pastes through an orifice, in slow flows of complex fluids such as polymer solutions, and in slow sedimentation of particles at high concentration in a fluid. Thus, the mechanisms underlying turbulence appear to be remarkably general. Ideas from turbulence have even been applied to finance. Despite the ubiquity and importance of turbulence, however, how it develops is not understood well enough to control or prevent it in many cases. The onset flow rate and the nature of the onset of turbulence are still puzzling; turbulence often sets in gradually, in stages, but in many cases, including simple pipe flows, turbulence sets in prematurely for reasons that remain vexingly elusive. Finally, despite much progress during the past decade or two, the nature of the fully turbulent state still poses many open problems. In this state, long-lived, long-length-scale coherent structures play an important but still poorly understood role. In the next decade, new particle-tracking techniques for imaging fluid elements during turbulent flow should shed light on many of these long-standing questions.

### Singularities

In many circumstances, especially under extreme mechanical loading or shearing conditions, materials are driven so far from equilibrium that they change their shape irreversibly. This happens every time a liquid splashes and breaks up into droplets, a piece of glass fractures, a sheet of paper crumples, or a car crashes. Such catastrophic events are typically connected with deformations or failure modes that act at the smallest possible scales and yet affect the overall shape. Consider a slowly dripping faucet with water that is just about to pinch off into a drop. What sets the shape of drop and of the neck by which it hangs just before breaking off? It turns out that these shapes are controlled completely and at every stage by only one spot along the neck—namely, where the neck is thinnest. This type of behavior is *scale invariant*—an image of a neck gives no clue as to the overall size of the neck. In other words, the breaking apart into a drop is controlled by a local singularity, in this case the divergence of the neck curvature. Similarly, the overall behavior of a crumpled piece of paper is determined by a small number of local spots, sharp points of very high curvature connected by a network of ridges. Such singular spots instantly transform an otherwise floppy sheet into a structure that can bear loads and absorb shocks (Figure 5.8, left panel).

Similar scale invariance occurs at singularities such as those at critical phase transitions in equilibrium systems. Over the past decade, CMMP researchers have built on the foundation of equilibrium phase transitions to identify and tackle far-from-equilibrium materials under extreme conditions. These systems were previously intractable precisely because of their singularities; the triumph in the past decade has been to *exploit* singularities in order to understand how they control the behavior of such systems over a broad range. Extensions of this approach have demonstrated how the unique behavior in the vicinity of a singularity can be used to achieve unprecedented levels of processing control, which can be used, for example, to uniformly encapsulate live cells prior to transplantation (Figure 5.8, right panel). The extreme mechanics associated with singularities are likely to become increasingly important. They also are prime examples of how, far from equilibrium, the evolution of structure and dynamics are often inseparable.

### Robustness as a Design Principle

In the past decade, ideas from engineering and biology have led CMMP researchers to explore a mechanism of state selection very different from equilibrium free-energy minimization. Many far-from-equilibrium systems have been designed, either by deliberate engineering or through evolution and natural selection, to be

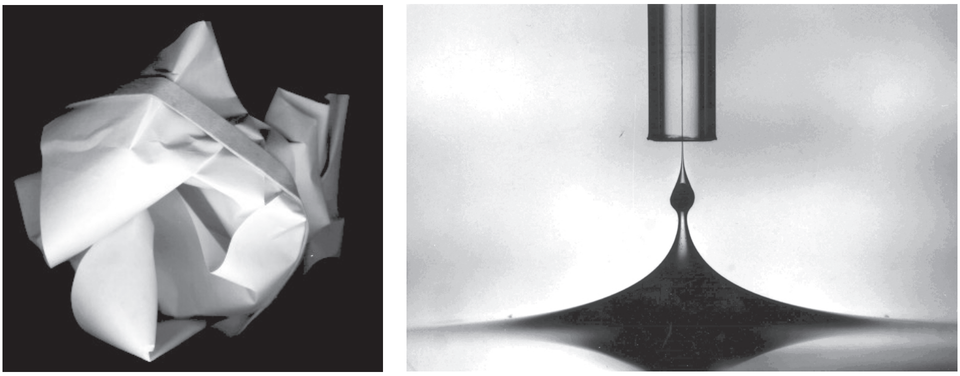

FIGURE 5.8 Using singularities to control materials' properties. (Left) Crumpling a piece of paper stiffens it and allows it to absorb shock. (Right) Particles are entrained, for encapsulation purposes, into the near-singular flow when an interface between two fluids (here, oil and water) is deformed by extruding the oil with a pipette. SOURCES: (Left) T.A. Witten, University of Chicago. (Right) S.R. Nagel, University of Chicago.

robust to perturbations. For example, cars are now designed with complicated internal networks involving many components, backup mechanisms, and adaptive feedback loops to ensure reliable operation under a wide range of environmental conditions. Likewise, biological networks, such as those that enable white blood cells to pursue invading bacteria, have evolved to be insensitive to biochemical changes in their components. In the past decade, CMMP researchers have realized that maximization of robustness can be viewed as a mechanism of state selection in interacting networks. This opens up a vast array of systems that can be studied using the tools of CMMP, ranging from circadian clocks to the Internet and from the human immune system to financial markets (Figure 5.9).

One interesting common feature of systems designed for robustness is that their complexity renders them vulnerable to rare, unexpected perturbations. For example, the network of interconnected species in the world's oceans has adapted over millennia to be remarkably stable despite the vast number of perturbations that can occur. Yet a small change of acidity in ocean waters produced by increased carbon dioxide in the atmosphere may trigger mass extinctions of species. Even far-from-equilibrium systems, such as materials under stress, which have not evolved or been specifically designed, can exhibit similar vulnerabilities, such as fracture, owing to the history of their formation and the complexity of interactions among the many atoms or molecules that constitute them.

FIGURE 5.9 Examples of evolving network structures far from equilibrium. (Left) Map of interacting yeast proteins. (Right) Internet nodes. SOURCES: (Left) H. Jeong, S. Mason, A.-L. Barabási, and Z.N. Oltvai, "Lethality and Centrality in Protein Networks," *Nature* **411**, 41-42 (2001). (Right) Barrett Lyon, The Opte Project.

### Predictability and Control: What Can We Learn from Fluctuations?

For systems composed of many particles in or near equilibrium, statistical mechanics says that fluctuations of observable quantities around their average values tend to be small and to have a Gaussian (bell-shaped) distribution. For systems far from equilibrium, there is no general framework such as statistical mechanics, and fluctuations tend to be distributed rather differently. The distributions are often broader than Gaussian, for example with power laws, so that large and catastrophic, but rare, events can dominate behavior. This is the case in avalanches involving sudden magnetic domain reorientations or flux-bundle motion in superconducting magnets. Similar avalanches occur in granular materials, as in landslides or mudslides, or during earthquakes (Figure 5.10). Turbulence and spatiotemporal chaos

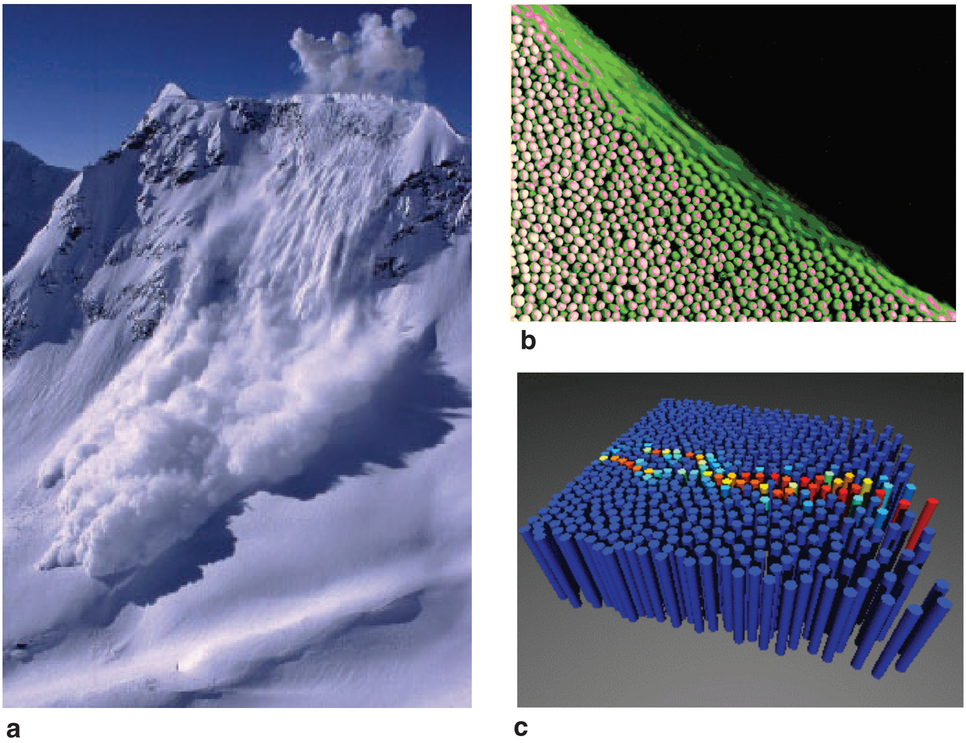

FIGURE 5.10 Large and often-catastrophic fluctuations, such as avalanches, are characteristic of many systems far from equilibrium. (a) Snow avalanche, (b) granular avalanche, (c) flux-bundle avalanche in a superconductor. SOURCES: (a) See http://www.avalanche.org; photo by Bradley White. (b) S.R. Nagel and H.M. Jaeger, University of Chicago. (c) Cynthia Reichhardt, Los Alamos National Laboratory.

also produce characteristic fluctuations in the measured quantities. The spectrum of fluctuations thus can serve as a signature of far-from-equilibrium behavior.

One of the most important questions that one can ask about a many-particle system is how it will respond to perturbations. For systems in thermal equilibrium, the fluctuation-dissipation theorem provides the answer: If the perturbation is small, the system will respond just as it does to naturally occurring fluctuations. The relationship between correlation and response depends on temperature; temperature measures the size of fluctuations relative to the response, which quantifies how hard it is to create a fluctuation. For systems far from equilibrium, temperature no longer plays such a role. However, in analogy to the thermal case, it is possible, in some cases, to define an *effective* temperature from the relationship between correlation and response. For certain classes of driven dissipative systems—such as sheared glasses, foams, or fluidized granular materials such as vibrated or gas-fluidized granular beds—there is evidence that the notion of an effective temperature can be useful in predicting behavior. Important CMMP issues are to elucidate the conditions under which effective temperatures provide a reasonable description and to determine the extent of the analogy to ordinary temperature.

### Formal Theoretical Developments

One of the great challenges of far-from-equilibrium systems is to develop a theoretical framework, akin to equilibrium and near-equilibrium thermodynamics and statistical mechanics, for tackling these systems. In the past decade, substantial progress has been made in generalizing thermodynamics and statistical mechanics to far-from-equilibrium systems. Steady-state thermodynamics takes into account the heat that is continually generated in steadily driven systems to generalize the second law of thermodynamics. Other approaches generalize the concept of entropy to zero-temperature systems, while still others generalize the fluctuation-dissipation theorem to far-from-equilibrium systems. A new thermodynamic result has made it possible to extract equilibrium free-energy differences from far-from-equilibrium processes. As a result of these developments, the field of nonequilibrium thermodynamics and statistical mechanics is gathering additional momentum.

### Getting (Un-)Stuck: Jammed States and Jamming Transitions

The prototypical example of a jammed state is a glass, a state that has both fluid- and solid-like attributes: It has the amorphous structure of a liquid, yet responds to an applied stress as a solid responds. All liquids will form glasses upon cooling if crystallization can be avoided (for example, by cooling rapidly enough), and for complex fluids such as polymers, the transition to a glass (plastic) is nearly impossible to avoid. As a liquid is cooled, the time required to reach equilibrium, the relaxation time, increases, and the response of the system to perturbations becomes more and more sluggish until it is immeasurably slow. At this point, the system is called a glass. The increase of relaxation time is continuous, but it occurs over an incredibly narrow range of temperature, so that lowering the temperature by 10 to 20 kelvin can increase viscosity and relaxation time by 10 orders of magnitude. Because the relaxation time exceeds any measurable timescale as the glassy state is approached, a glass by definition is a system far from equilibrium.

Similar glassy states are found not only in ordinary liquids but in many electronic systems in the presence of disorder, including interacting electron spin systems (spin glasses) or systems of interacting magnetic flux bundles (vortex glasses). They also occur whenever particles of any size congregate at sufficiently high concentrations. For example, micelles or colloids in dense suspensions, lubricants trapped between surfaces, bubbles in foams, and candies in a jar all get trapped in glassy states (Figure 5.11). The onset of glassy behavior is easily observed in an hourglass filled with sand: A fluid-like stream of grains falling through the central neck is rapidly quenched into a solid-like heap that retains the stream's amorphous structure but, unlike a fluid, supports a finite angle of repose. However, once the particles become macroscopic as in the case of sand grains, temperature is no longer effective in facilitating escape from the glassy state. Instead, mechanical fields such

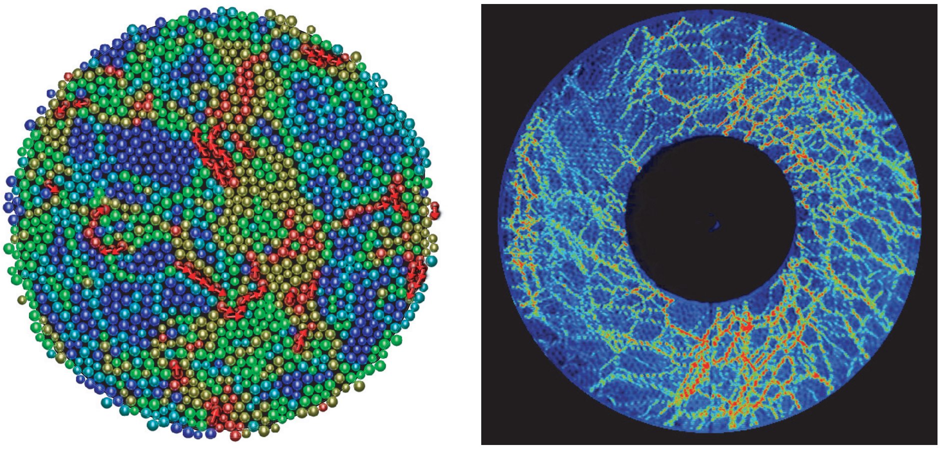

FIGURE 5.11 In systems at or near the jamming transition, network-like structures are formed dynamically, such as chains of particles experiencing high contact forces in slowly sheared granular systems (left) and strings of particles whose motion is correlated in a gas-fluidized granular bed (right). SOURCES: (Left) D. Howell and R.P. Behringer, Duke University. (Right) A.S. Keys, A.R. Abate, S.C. Glotzer, and D.J. Durian, "Measurement of Growing Dynamical Length Scales and Prediction of the Jamming Transition in a Granular Material," *Nat. Phys.* **3**, 260-264 (2007).

as stress or vibration can take over this role and unjam the system. The suggestion that temperature and stress can act similarly in systems close to the onset of rigidity has led to the introduction of a more general framework, the concept of jamming. This concept describes the cooperative phenomenon of jamming in terms of the interplay of three key parameters: random thermal motion, applied forcing, and geometrical constraints (Figure 5.12).

The idea of a general jamming transition, applying to both thermal and nonthermal systems, has put the spotlight on some of the most long-standing problems in condensed-matter physics, such as the glass transition. Because the jammed state is out of equilibrium, even the most basic questions about any jamming transition remain intensely controversial. Is there a true thermodynamic transition, at which the relaxation time diverges? Or is there a dynamical transition to the jammed state, where the relaxation time diverges with no thermodynamic signature? Or is there no transition at all, so that the relaxation time only truly diverges at zero temperature or mechanical driving? It is because these fundamental questions

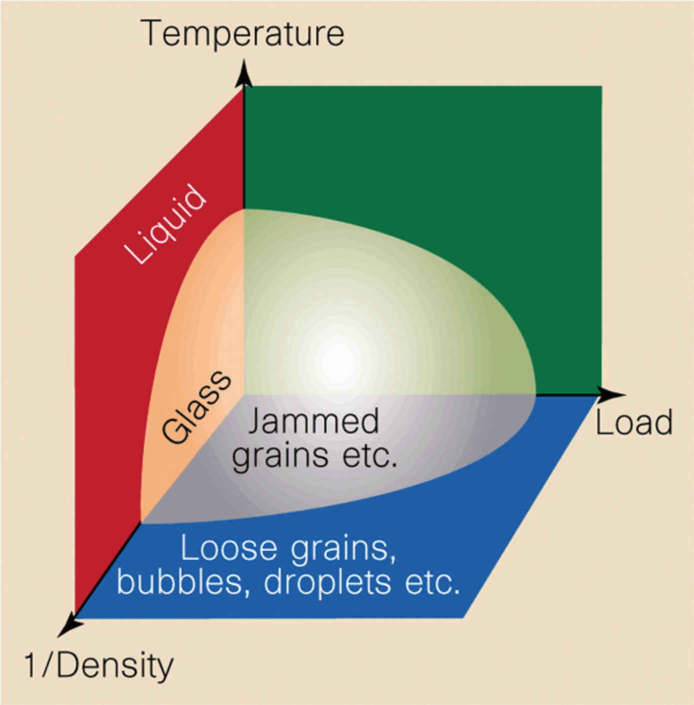

FIGURE 5.12 Jamming phase diagram, delineating the conditions under which a multitude of systems become rigid and solid-like. Inside the jammed region (grey), these systems are far from equilibrium. SOURCE: A.J. Liu and S.R. Nagel, “Nonlinear Dynamics: Jamming Is Not Just Cool Any More,” *Nature* **396**, 21-22 (1998).

remain unresolved that the onset of glassy behavior is generally considered one of the most intriguing unsolved problems in CMMP.

The concept of jamming has fueled an explosion of new interactions and crosscutting research between previously separate communities working on the glass transition, gelation, granular materials, foams, and dense colloidal suspensions. It also has driven much fruitful interaction between condensed-matter physicists and engineers in this field.

## THE NEXT DECADE

Far-from-equilibrium behavior is emerging as one of the major challenges within CMMP and beyond. The importance of making progress in this field is underlined by several key facts. First, far-from-equilibrium behavior is not rare but ubiquitous, occurring from the nanometer scale on up, in daily life as well as in high-technology applications. Second, it connects directly to critical, national needs for the next decade, affecting a large fraction of the manufacturing base as well as the U.S. economy, climate, and environment. The committee emphasizes that far-from-equilibrium behavior cannot be understood simply through small modifications of equilibrium physics. Because it differs so strikingly and at the same time represents largely uncharted intellectual territory, it provides exciting opportunities for major scientific breakthroughs.

CMMP researchers are tackling ever-bigger and -broader problems in far-from-equilibrium phenomena. This expansion drives critical needs. Currently, research on far-from-equilibrium phenomena is fragmented into small subfields. These are typically divided along the types of materials or specific phenomena studied—for example, fracture in solids or turbulence in fluids. The field of far-from-equilibrium physics is vast, and it is unlikely that any one organizing principle will work for all far-from-equilibrium systems. Nonetheless, there is great value in identifying *classes* of systems that might have common underlying physics or that might be tackled by common methods. There have been few incentives to adopt such broader approaches, but this will be increasingly required in order to make progress.

Recent work within the CMMP community has set the stage for fresh approaches to long-standing problems concerning far-from-equilibrium behavior by introducing new model systems such as granular matter, new unifying paradigms such as jamming, new organizing principles such as robustness, and new formal approaches such as steady-state thermodynamics. The community is also finding important connections to a wide range of other fields, both within and outside physics, connections that are likely to amplify the impact of CMMP even further. Over the next decade it will be critical to find ways to stimulate new links and nurture crosscutting approaches.

# 6

# What New Discoveries Await Us in the Nanoworld?

Nanometer-scale materials straddle the border between the molecular and the macroscopic. They are small enough to exhibit quantum properties reminiscent of molecules but large enough for their size and shape to be designed and controlled. Furthermore, many of the atoms in a nanoscale object are on the surface, available to catalyze chemical and biological reactions and altering nearly every material property. For example, nanocrystals of semiconductors can melt at temperatures hundreds of degrees lower than the temperatures at which bulk materials melt, allowing thin films to be recrystallized with a hair dryer instead of a furnace. Carbon nanotubes and quantum dots form single-electron transistors that turn from on to off with the addition of a single elementary charge. The potential of nanoscale materials is almost limitless, but scientists must first overcome two fundamental challenges. The first is physical: How does one generically control the identity, placement, and function of every important atom in a nanoscale solid and then assemble them into real-world systems? The second is conceptual: How does one attack problems too big to be solved by brute force calculation but too small to be tackled by statistical methods? Meeting these challenges will transform the study of nanoscale materials from a frontier science to a mature discipline and will have a revolutionary impact on fields from materials to information and from energy to biology.

## WHY NANO?

Nanoscience and nanotechnology have the potential to revolutionize science and technology in ways that will make the world 50 years from now unrecognizable compared with today. The field can be seen as the logical continuation and combination of three separate trends in science that are all intersecting at a common point, opening the doors to revolutionary concepts and capabilities. The three trends are these: (1) the continuation of Moore's law and the nonstop shrinking of electronic circuitry, (2) the rapid advances in molecular biology that have completely changed people's understanding of life over the past 30 years, and (3) the evolution of chemistry from the study of single atoms and molecules to the fabrication and exploitation of very large complexes such as quantum dots and proteins. This scientific "perfect storm" will change the world profoundly over the coming decades.

When scientists and engineers created the first human nanotechnology, the integrated circuit (see Figure 1.5 in Chapter 1), it redefined the modern world. In actuality, it is a very limited technology, focusing on just a few materials (silicon, copper, gallium arsenide, and so forth) patterned by a single class of lithography-based techniques, and aimed at one major goal, the manipulation of electronic information. The goal of nanoscience is to perform the fundamental scientific studies needed to create even more nanotechnologies, ones capable of manipulating matter, energy, and light the way that integrated circuits manipulate electrons. Scientists are thus laying the foundations for the next set of revolutions. Nature shows what is possible (Figure 1.5). Using carbon-based building blocks such as deoxyribonucleic acid (DNA), proteins, and lipids, life creates self-replicating complex structures that can harvest energy, store information, and control matter, from the atomic scale to the macroscale. Will we someday be able to duplicate and improve on the incredible abilities of life? Will we someday be able to build complex, functional (and beautiful) structures from nothing but a patch of dirt and a splash of sunlight?

To progress down the path, researchers must face a huge number of challenges. First, they must learn to construct and quantitatively understand the basic nanoscale building blocks, discussed below. For example, the energy levels for an electron spiraling down a nanotube (Figure 6.1) are quantized like those in an atom, but these quantum properties are designable: The levels can be tuned by choosing the diameter and chirality of the nanotube. The next decade will see an explosion of designable nanostructures, along with new techniques to probe them and new ideas to understand them. As researchers master these nano-building blocks, they face an even greater challenge: How does one connect these blocks into larger assemblies, and how does one predict the properties of these assemblies? In other words, how does one create the kind of complex, functional structures such as the nanopore discussed in the following section? At the end of the chapter, the new experimental and theoretical tools necessary to make these revolutions happen are discussed.

The kinds of technologies that are being envisioned seem almost like science fiction. As an example, consider the quest to replace the complementary metal oxide

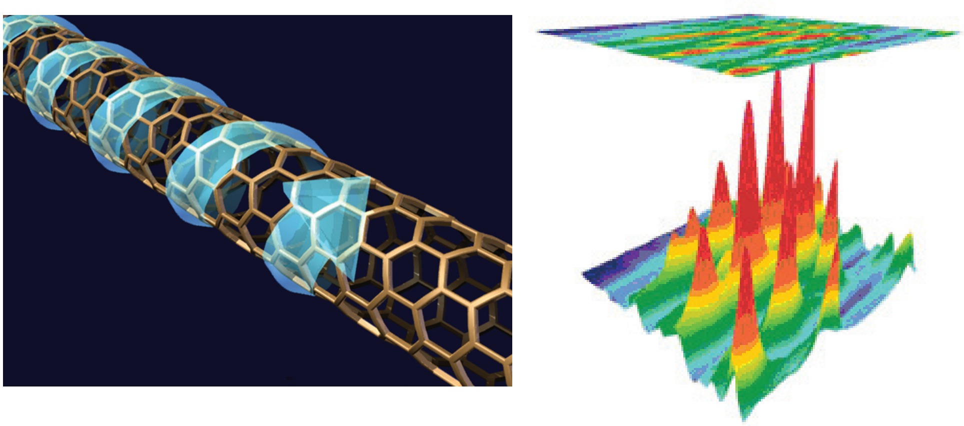

FIGURE 6.1 (Left) Electron spiraling down a nanotube. The nanotube energy levels are quantized, as in an atom, so that every nanotube species has a different fluorescence peak determined by its diameter and chirality, as shown in the right panel. SOURCES: (Left) P.L. McEuen, Cornell University. (Right) R.B. Weisman, Rice University.

semiconductor (CMOS) transistor with a device that is a nanometer in scale, suggesting that there may be many more orders of magnitude in microcircuit scaling still ahead of us. In the area of novel materials, nano ultrastrong, low-weight materials will enable more fuel-efficient cars and aircraft that are lighter, stronger, and cheaper. Cancers may be cured by multilayer nanoparticles that become activated by penetrating infrared or terahertz radiation. Personalized medicine will become a reality, allowing each of us to have a map of our own genomes so that doctors can tailor therapeutic solutions to the individual's makeup.

## NANOSCALE STRUCTURES: HOW DO WE BUILD THEM?

The starting point of nanoscience is its fundamental building blocks—the balls, sticks, and sheets out of which more complex structures will be made. These are analogous to atoms or molecules in traditional condensed-matter and materials physics (CMMP)—the fundamental units from which solids are constructed. These building blocks are examined first, and then their assemblies are explored in later sections. The building blocks are most easily categorized by how they are constructed. The first approach is by carving up larger-sized materials, reducing their size along one or more directions to make quantum wells, wires, and quantum dots. An alternative approach is to grow a nanoscale version of a bulk material to the desired shape. The final category consists of chemically or biologically synthesized molecules or molecular assemblies that have no macroscopic counterpart.

Biological examples include lipid membranes; linear, information-carrying structures such as DNA; and protein functional elements. Historically, these approaches have lived in separate disciplines: electrical engineering for lithography; materials science, physics, and solid-state chemistry for growth; and chemistry for molecular synthesis. A key goal in the coming decade will be to train scientists who are capable of combining all of these approaches.

### Patterning at the Nanoscale: Lithography and Self-Assembly

Modern lithographic techniques allow researchers to pattern materials into devices with dimensions down to approximately 30 nanometers (nm), approximately 100 atoms across. These techniques have been the foundation of the modern integrated circuit, creating devices such as the transistor shown in Figure 1.5 in Chapter 1. This relentless miniaturization has allowed engineers to pack the equivalent complexity of a city landscape on a fingertip-sized chip. These same lithographic and patterning procedures are now being applied to the manufacture of a wide range of nanomechanical, microfluidic, and nanobiological devices.

The major challenges facing lithography are many, some of which are discussed in later sections. The first is to reproducibly create structures at 10 nm and below. At this scale, the intrinsic fluctuations in the material—the size of an individual polymer molecule in the resist or the detailed properties of the surface of a material—become important. Figure 6.2 shows one application that requires precisely controlled features at the nanometer-scale—a nanopore in a silicon wafer designed to sequence DNA. The DNA passing through the pore blocks it, resulting in a change in the conductance through the nanopore that depends on the chemical identity of the base pairs in the pore. This novel approach to sequencing DNA could revolutionize biology and health care, but it is currently beyond the range of existing lithographic technology.

A second challenge is to be able to pattern a wide variety of nanoscale materials. Lithographic processes were initially developed for "tough" inorganic materials such as silicon, metals, and glass that can withstand harsh solvents and high temperatures. However, most organic and biological materials cannot withstand the processing conditions used for standard lithography. New techniques are being developed, such as stamping and dip pen-nanolithography, to directly write such soft molecules such as lipids, DNA, and proteins. There have been notable successes already, such as lithography for the creation of DNA and protein arrays, and the impact has been extraordinary. Scientists are still at the beginning of this revolution that applies the power of nanofabrication to problems in chemistry and biology.

Self-assembly involves the organization of a group or subunits, such as atoms, molecules, or particles, into a larger aggregate, or structure, characterized by a length scale many times the size of the individual units. Forces that "drive" self-assembly

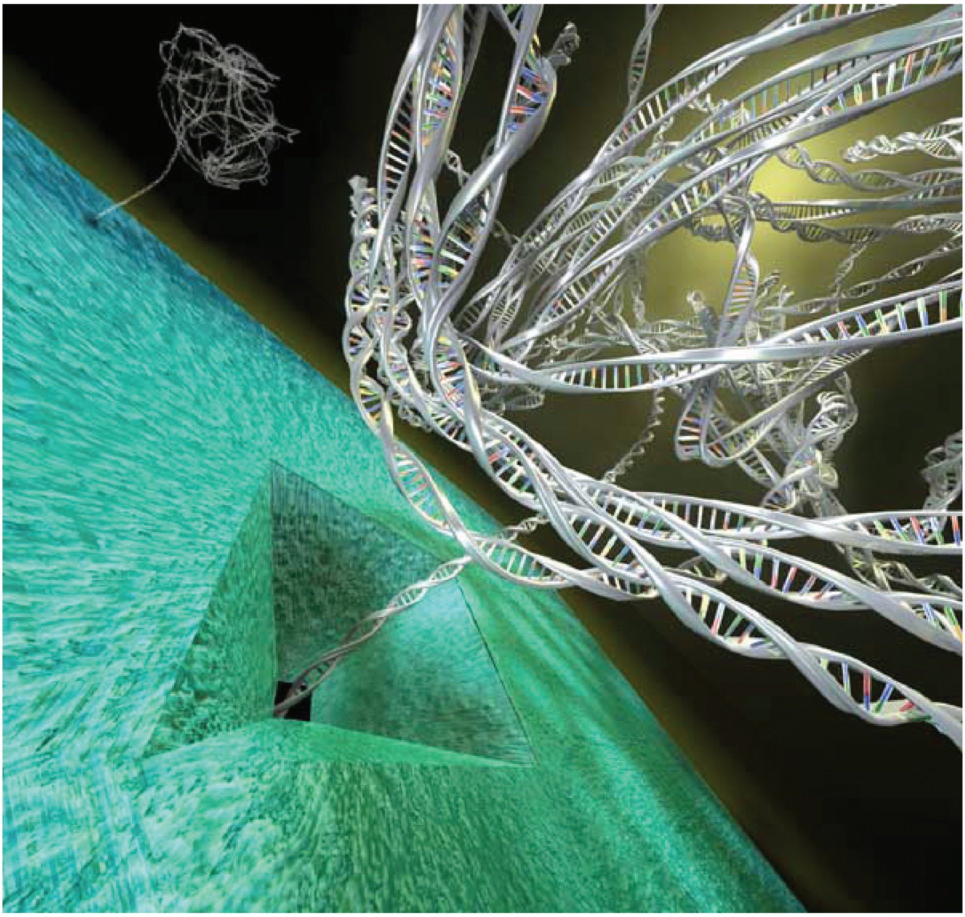

FIGURE 6.2 Artist's rendition of a nanopore fabricated in a silicon wafer used for studying DNA. The nanopore is created by a combination of lithography and controlled annealing. SOURCE: Courtesy of C. Dekker, Delft University of Technology.

are varied, depending on the system, and include van der Waals, electrostatic, capillary, hydrogen-bonding, and other types of thermodynamic, noncovalent forces. The organization of quantum dots and/or nanoparticles into crystalline order, the formation of micellar and other mesoscale structures by surfactant systems, and the formation of block copolymer systems are examples of self-assembly. The self-assembly of copolymers (amorphous, rod-coil, and so forth), synthesized with varying functionalities (electronic, optical, magnetic, and so forth), results in the formation of various geometric structures (spheres, cylinders, lamellae, and so forth) on nanometer length scales determined by the size of the molecules.

Combinations of self-assembly and patterning enable the control of the structure of materials over different length scales. Block copolymers, which possess highly ordered structures such as cylinders, with high lateral regularity can be placed on surfaces. The patterns can serve as templates for etching and for growth or synthesis to enable building structures such as nanowires.

### Controlling Growth at the Nanoscale

Fabrication by lithography has been likened to building a bridge by carving it out of a block of steel. An alternative approach is to directly grow the nanoscale structure of interest in the desired size and shape. The past decade has seen tremendous progress in this area. First, researchers have created new types of heterogeneous layered materials in which the properties of the interfaces are controlled with atomic precision, as shown in Figure 6.3. Stunning progress has been made in the growth of nanowires and quantum dots. In the past decade, researchers have created transistors, p-n junctions, heterostructures, lasers, and so forth, in one-dimensional semiconductor wires. Quantum dots grown by a variety of techniques are now used in many applications, from solar cells to biological markers.

Another important class of building blocks is based on an intrinsically two-dimensional material, graphene (also discussed in Chapter 2), consisting of a sheet of carbon atoms bonded in a honeycomb-like pattern. These sheets can be rolled to create nanotubes (Figure 6.1) or wrapped to create $C_{60}$ and related small molecules. The properties of carbon nanotubes have received tremendous attention over the past decade, but a major roadblock looms for applications. There are still no protocols to grow precisely positioned, structurally identical carbon nanotubes of a desired length, diameter, and chirality. Similarly, techniques to create single-sheet graphene layers are in their infancy. A revolution in the understanding and control of growth is needed to reliably create structures with atomically precise characteristics and move these remarkable new materials from the laboratory to the marketplace.

### Molecular and Biological Building Blocks

The building blocks discussed above typically consist of one or a few types of atoms arranged in a rigid, usually periodic fashion. Chemistry and biology provide building blocks that are much more varied, and they can readily mix different functions. Nature, in particular, plays a very different game. Its structures are much more dynamic, assembling and disassembling in response to small changes in their environment. For example, the double-stranded DNA helix unzips at modest temperatures, separating into individual strands that are key to DNA's ability to duplicate itself. Furthermore, the sheer diversity of chemical and biological

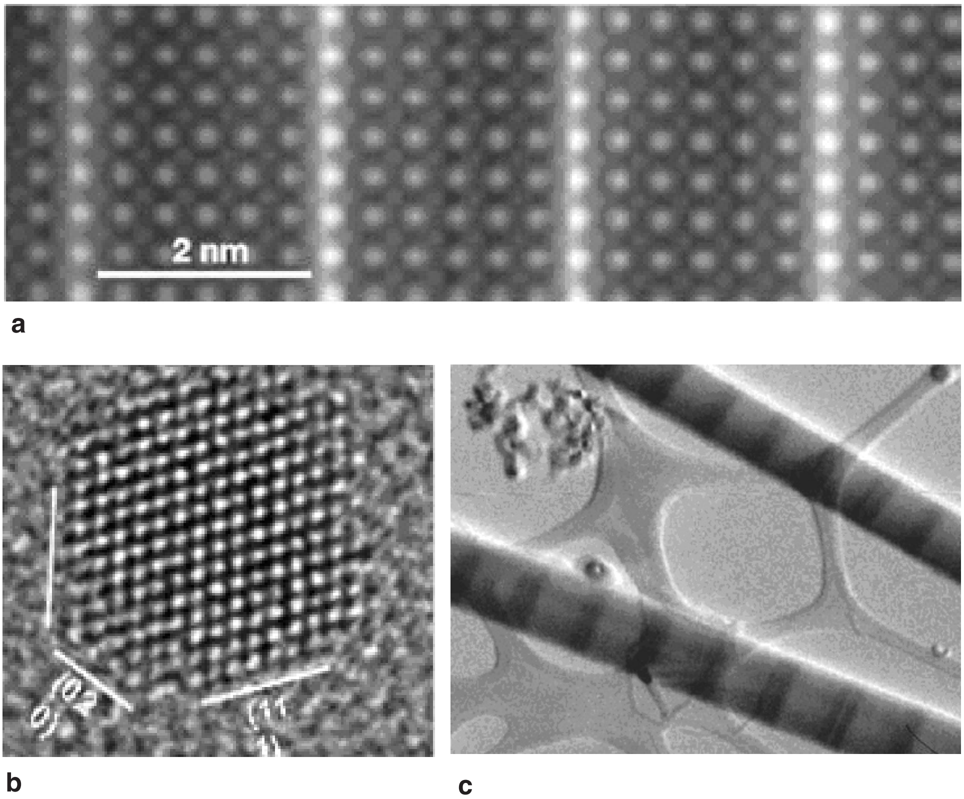

FIGURE 6.3 Crystalline inorganic material building blocks. (a) A complex oxide multilayer. (b) Semiconductor nanocrystal. (c) Nanowire heterostructures. SOURCES: (a) Courtesy of H.Y. Hwang, University of Tokyo. (b) Courtesy of Y. Zhu, Brookhaven National Laboratory. (c) Courtesy of P. Yang, University of California at Berkeley.

building blocks is staggering. For example, viruses can present literally millions of peptides that can specifically attach to almost any surface, biological or inorganic. This power has recently been used to recognize, bind to, and nucleate the growth of nanoscale building blocks.

The inherent functionality and diversity of these building blocks can be directly used, but they can also be taken as inspiration. From the point of view of biology, current inorganic building blocks are exceedingly primitive. The future challenge is to create nanoscale building blocks with built-in functionality—ones that can move, change, and assemble in specific ways. The way that nature does this is astounding—constructing machines out of a linear string of elements that folds itself into useful shapes. Researchers are nowhere near being able to perform such subtle and difficult feats, but they are learning how to co-opt nature's toolbox, as shown in Figure 6.4. Researchers have developed algorithms that can design DNA sequences that will assemble into arbitrary two-dimensional shapes. The assembly is massively parallel, in this case creating 50 billion smiley faces in a single test tube.

## STUDYING NANOSTRUCTURE BUILDING BLOCKS: THE ATOMIC PHYSICS OF NANOSCIENCE

Understanding the properties of individual atoms lies at the heart of the physics and chemistry of solids. Similarly, a thorough and complete understanding of the properties of nanoscale building blocks is central to the field of nanoscience and

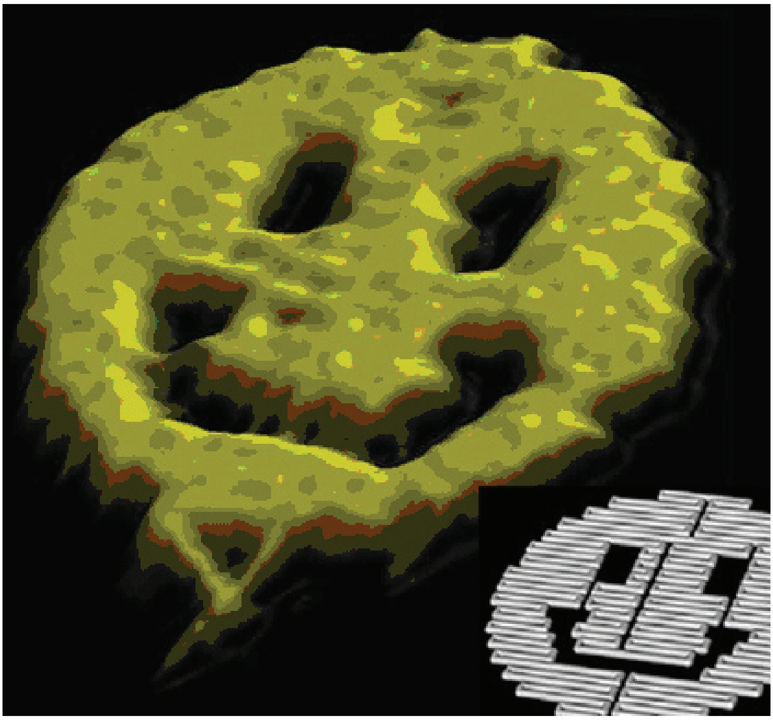

FIGURE 6.4 Rationally designed DNA assembly of a complex nanoscale structure. SOURCE: Courtesy of P.W.K. Rothemund and N. Papadakis, California Institute of Technology.

is an emerging area in atomic, molecular, and optical (AMO) physics.[1] It is also a necessary first step toward technological applications.

The understanding of the basic properties of nanoscale structures has grown extraordinarily over the past decade. Many of the basic phenomena have been carefully worked out. In small conductors, the charge of a single electron can regulate electron flow, resulting in the single-electron transistor. The optical properties of nanocrystals, nanowires, and quantum wells can be continuously and carefully controlled. Similarly, the mechanical, magnetic, and thermal properties of individual nanostructures have been explored. The coming decade will see this basic understanding pushed to the limits, addressing cases in which simple ideas break down, such as when the correlations between electrons in a nanostructure become dominant. Physicists will also explore the quantum manipulation of spins, states, and even entire physical structures. Finally, researchers will begin to engineer nanosystems that combine functions—for example, ones that can absorb a photon and convert it efficiently into electrical or chemical energy (see Chapter 3).

### Quantum Manipulation

One major goal of nanoscience is to controllably and coherently manipulate information stored in quantum states; this capability is important for applications ranging from controlling chemical reactions to quantum computing (see Chapter 7). Already, scientists can create quantum dots and add electrons to them one by one, as shown in Figure 6.5. Each dot can serve as a quantum bit, and researchers have already demonstrated that the quantum state can be read out or transferred to a neighboring dot coherently. These are initial steps on the way to a scalable quantum computer, but enormous hurdles remain to be overcome. One is controlling the sources of "decoherence," the unwanted interaction of a quantum bit with its environment. A second, more fundamental hurdle, is that of understanding the nature of the ground states and correlations between interacting electrons, which can open up the possibility of new types of quantum objects for manipulation, from Cooper pairs to fractionally charged quasi-particles with exotic quantum properties (see Chapter 2).

Another fascinating quantum realm is that of quantum "mechanics," that is, the properties of nanomechanical systems. Researchers are on the verge of measuring the quantum fluctuations of a mechanical beam, demonstrating that the quantum rules of behavior can apply to objects consisting of millions of atoms. Also of interest are the interactions between different kinds of quantum systems—single electrons interacting with a mechanical resonator, or a single quantum dot coupled

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[1] National Research Council, *Controlling the Quantum World: The Science of Atoms, Molecules, and Photons*, Washington, D.C.: The National Academies Press, 2007.

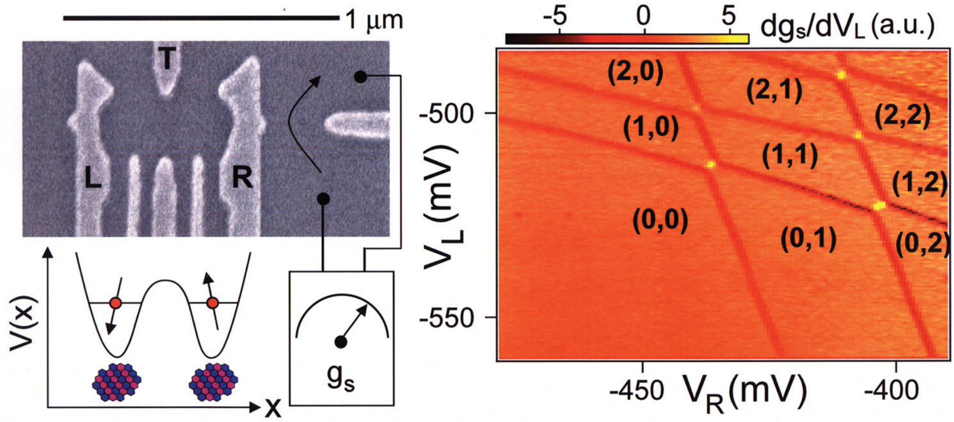

FIGURE 6.5 (Left) Lithographically patterned coupled quantum dot molecule formed in a GaAs/AlGaAs heterostructure. Using voltages applied to the gates, a double-well potential is created in which individual electrons can be trapped in the left- or right-hand well. The charge state of the molecule is read out using the quantum point contact to the right of the confining gates as a sensor. (Right) Measured "charge stability diagram" of the molecule, where the pairs of numbers (a,b) indicate the number of electrons in the left- and right-hand wells. The slanted lines indicate places where the charge state changes. SOURCE: Courtesy of C.M. Marcus, Harvard University. Adapted from J.R. Petta, A.C. Johnson, J.M. Taylor, E.A. Laird, A. Yacoby, M.D. Lukin, C.M. Marcus, M.P. Hanson, A.C. Gossard, "Coherent Manipulation of Coupled Electron Spins in Semiconductor Quantum Dots," *Science* **309**, 2180 (2005) and J.R. Petta, A.C. Johnson, A. Yacoby, C.M. Marcus, M.P. Hanson, and A.C. Gossard, "Pulsed-Gate Measurements of the Singlet-Triplet Relaxation Time in a Two-Electron Double Quantum Dot," *Phys. Rev. B* **72**, 161301 (2005).

to the quantized light modes of a microfabricated structure. Researchers are at the beginning of a new era in quantum manipulation; the next decade will be decisive in determining how far and how fast this new field can grow.

### Controlling Light: Nano-Optics

Since the wavelength of visible light is on the scale of 1 micron, nano-optics sounds like a contradiction in terms. However, researchers have recently shown that a variety of cleverly designed nanostructures can confine or guide light on a scale smaller than previously thought possible. Using either dielectric waveguides on a silicon chip or metal structures whose plasma excitations guide light, researchers are bringing light down to the nanoscale for applications ranging from biomolecular detection to information processing.

Also, researchers have recently used nanowires, nanotubes, and quantum dots to create and detect light on the nanoscale. The ultimate goal is to perform detection and information processing at the single-photon limit.

## Probing Molecular Machines

Biological nanomachines (see Chapter 4) accomplish remarkable tasks, from reading and writing information in a single molecule to converting sunlight to energy. How do these machines accomplish their objectives? New techniques to tug on individual molecules using optical tweezers or to measure the light coming out of a single molecule using ultrasensitive fluorescence microscopy are answering these questions. For example, consider the virus shown in Figure 6.6. How much force is required to pack the DNA inside the capsid shell? Studies using optical tweezers to tug on the DNA as it is drawn into the capsid head provide the answer. The virus's rotary motor exerts 60 piconewton-scale forces that compress the DNA to 6000 times smaller than its normal volume. The internal pressure thus generated is later used to launch the DNA into the cell targeted by the virus.

The next 10 years should see explosive growth in the kinds of techniques capable of exploring biological functioning on the nanoscale (see Chapter 11), leading to a revolution in understanding of the detailed physical operation of biological

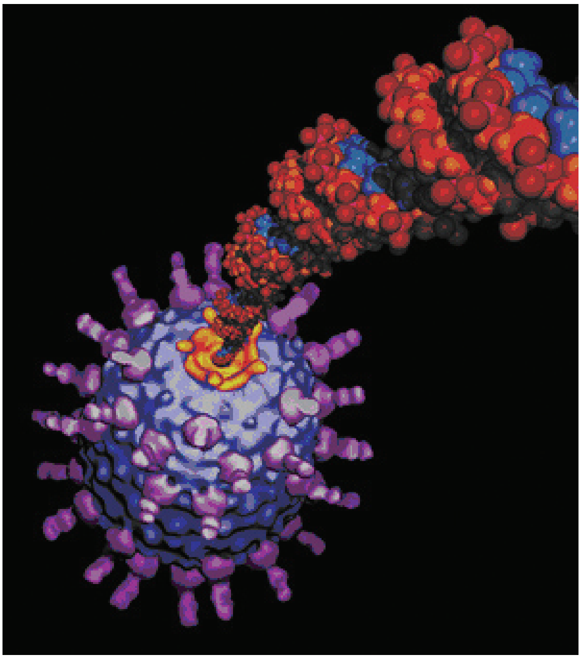

FIGURE 6.6 Artist's conception of DNA being packed inside a virus capsid by a molecular motor. SOURCE: D.E. Smith, S.J. Tans, S.B. Smith, S. Grimes, D.L. Anderson, and C. Bustamante, "The Bacteriophage Φ29 Portal Motor Can Package DNA Against a Large Internal Force," *Nature* **413**, 748-752 (2001).

machinery. This research is critical for the life sciences and health industry (for example, understating the mechanisms of viral infection). Equally important, studies of biomolecular nanotechnology will help to understand the physical principles, design rules, and structural motifs for creating new kinds of nanoscale functional entities.

### Combining Different Properties

The next 10 years will see major advancements in structures in which different nanoscale properties interact. Notable examples have already been demonstrated. In small magnetic devices, torques exerted by spin-polarized electrical currents have been developed as a new way to switch ultrasmall magnetic bits. Single-electron transistors have been used as readouts to measure the quantum properties of mechanical oscillators and electromagnetic resonators. The optical absorption of nanoparticles and carbon nanotubes has been used to deliver local pulses of heat to destroy cancer cells. These important first steps point the way to a rich new science and technology, moving beyond the paradigm of controlling and making use of one property at a time. For example, new complex oxide materials promise tremendous integrated control over electronic, magnetic, and optical properties. Again, biology is the master to which researchers can aspire (see Chapter 4). The absorption of photons triggers a complex cascade of electronic, chemical, and physical rearrangements that result in the production of ion gradients and energy-storing molecules. Can researchers too understand and control nanoscale processes with similar sophistication, and furthermore can they expand the suite of available materials far beyond biology's limited choices?

## ASSEMBLING THE BLOCKS: THE CONDENSED-MATTER PHYSICS OF NANOSCIENCE

The previous sections looked at the building blocks of nanoscience, their fabrication, and their properties. This section turns to assemblies of these building blocks—the condensed-matter physics of nanostructures. This subject has the potential to produce truly revolutionary results, allowing researchers to create designer solids with both practical and scientific applications. There are two central questions to address: How does one build the assemblies? What properties will they have?

### Ordered Arrays

Detailed models of atoms arranged on periodic lattices comprise the central paradigm of condensed-matter physics. They allow CMMP researchers to understand everything from electrical and thermal conductivity to the color of solids.

Both the lattice structure and the nature of the atom(s) in the lattice combine to determine its properties, but the choices are limited by the elements in the periodic table. Individual nano-objects with carefully tailored properties promise to act as “artificial atoms” and to vastly expand the repertoire. However, creating periodic solids composed of nanoscale objects has proven to be quite a challenge. With atoms, all the individual subunits are identical, and they readily build extended, nearly perfect arrays. Only recently have objects such as nanocrystals been synthesized with the level of uniformity needed to create such well-ordered “artificial” crystals. Figure 6.7 shows a binary solid created from mixing two different types

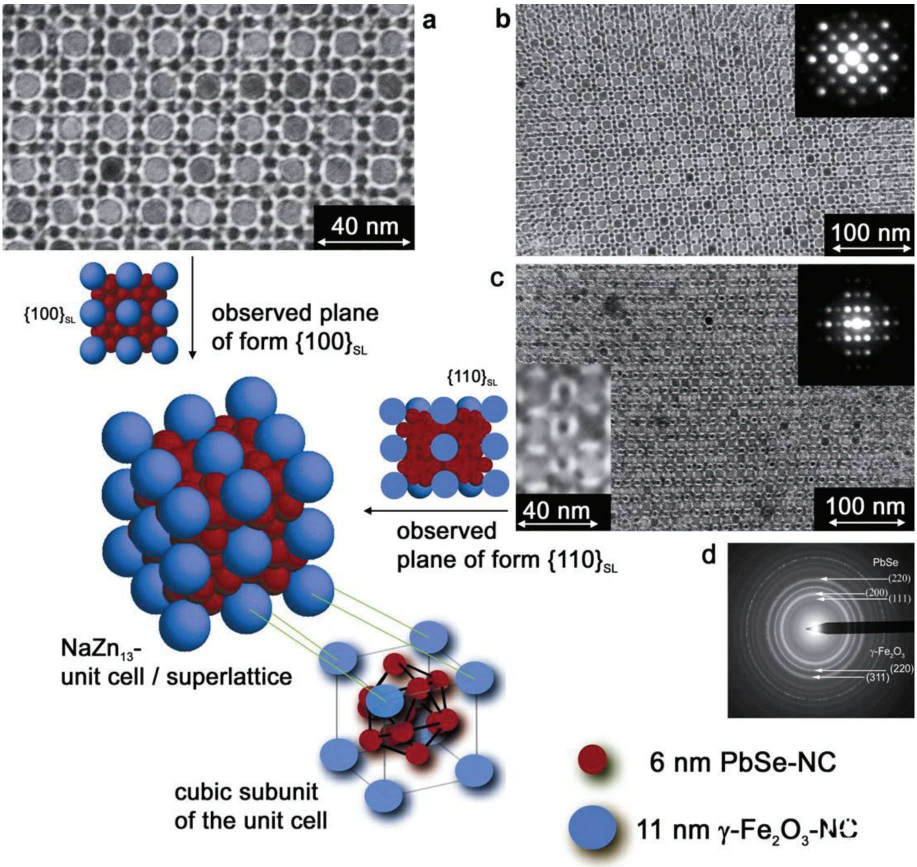

FIGURE 6.7 Well-ordered binary crystals formed from two nanocrystal subunits. In this structure, 13 6-nm-diameter PbSe semiconductor nanocrystals (quantum dots) arrange themselves, with each 11-nm $Fe_2O_3$ magnetic nanocrystal a close-packed AB13 lattice. This new magneto-optic “metamaterial” captures the novel properties of both nanocrystal systems and allows exploration of new phenomena that emerge from the interaction of the nanoscale building blocks. The repeat unit in this colloidal crystal contains almost 5 million atoms. SOURCE: Courtesy of C.B. Murray, University of Pennsylvania.

of nanocrystals. This development opens up the way for artificial nanoscale solids whose properties reflect the coupled states of the individual nano building blocks. These metamaterials will have electric optical, thermal, and magnetic properties carefully tailored both for real-world applications and as a laboratory to test theories of condensed-matter physics. For example, optical metamaterials may make possible lenses with resolution beyond the standard limits of wave diffraction. So far, these properties have only been partially achieved—creating metamaterials that will have these properties over the visible spectrum will be a major challenge for the coming decade.

### Arbitrary Structures

The periodic structures described above are among the simplest examples of nanoscale assemblies. Of equal interest are nonperiodic geometries, from the relatively simple nonrepeating linear structure of a DNA molecule to the full-blown complexity of an integrated circuit or a cell. Lithography offers one flexible route to achieve complexity, but it is subject to the materials and dimensional limitations discussed above. Another approach is to use the lock-and-key properties of chemical or biological molecules as a kind of smart glue to link nano-objects to each other or to attach them to specific locations in a lithographic environment. Recent examples include two-dimensional DNA templates that can be a breadboard to which other nano-objects are attached.

Another possibility is to assemble the nano-objects using external forces. Researchers have developed techniques using holographic optical traps to manipulate simultaneously hundreds of micron-scale beads and to control, cut, solder, and place individual nanowires. Similarly, circuits to create electric or magnetic forces have been used to manipulate and assemble nano-objects. All of these, however, are difficult to push to the true nanoscale. Researchers need revolutionary new approaches to assembling arbitrary patterns at the nanoscale reproducibly, routinely, and reliably.

## SMALL PROBES AND BIG IDEAS: CRITICAL NEEDS FOR A NANO FUTURE

The past decade has seen tremendous progress in the field of nanoscience, but in a very real sense researchers are still poking around in the dark. They still do not have adequate tools to see and feel at the nanoscale—to determine the positions and function of all the elements (atoms, electrons, electric and magnetic fields) in a nanoscale solid. Similarly, they do not have a complete set of intellectual tools to interpret what they see. Their needs range all the way from simple models that capture the essence of phenomena to detailed simulations that can accurately predict behavior and guide experiment (see Chapter 11).

## Better Eyes

One of the most pressing needs is techniques to see where all the atoms are and what they are doing inside a nanostructure. While in some cases this is now possible (scanning tunneling microscopy of surface atoms is a prime example), in general the nanoscientist must infer what his or her sample looks like and how it operates on the basis of a limited amount of direct evidence. Is it possible to do better? For example, can electron or x-ray diffraction measurements be performed on individual nano-objects, from nanotubes to proteins? Particularly needed are new ways to look at the workings of nanoscale structures in their natural environment (e.g., in liquids). Recommendations detailed in Chapter 11 will help realize these needs and those detailed below. An example of recent progress is shown in Figure 6.8: Optical images with much higher resolution than the wavelength of light

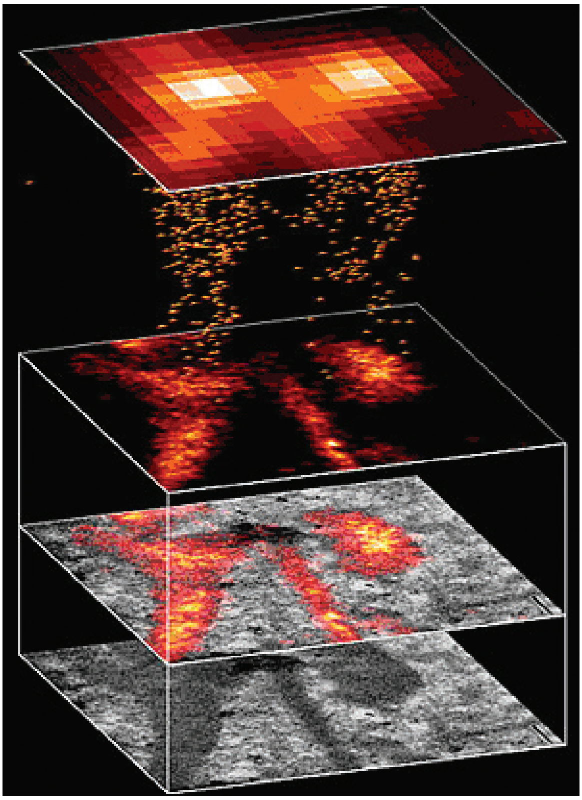

FIGURE 6.8 Photoactivated localization microscopy—PALM—yields nanometer-resolution fluorescence images of biological structures. SOURCE: Courtesy of H. Hess, Howard Hughes Medical Institute.

are obtained by a new kind of fluorescence microscope where individual fluorophores are turned on one by one and their positions accurately measured.

## Improved Sensing

More than knowing where all the atoms are, researchers also want to know their charge, local magnetic properties, chemical identity, and so forth. While scanning probe techniques have provided revolutionary images of the properties of nanostructures, this has only scratched the surface, so to speak. What is needed is the continued development of tools that can probe the local properties in new ways. A recent success, over 10 years in the making, was the first detection of a single electron spin using an atomic force microscope. It took years of concentrated effort by world-class scientists to bring this to fruition. It illustrates the importance of long-term commitments to research, as well as the potential problems with the changing landscape of the industrial research laboratories.

## A Greater Understanding

The final pressing need is for an increased understanding of the fundamental properties of nanostructures, as well as knowledge of the most appropriate design rules for creating nanoscale systems. First, a set of simple paradigms to describe nanoscale phenomena is needed. Many of these models are now well developed—single-electron charging, conductance quantization, and so forth—but more remain to be discovered and sorted out. For example, how does one understand systems in which the nuclei in a structure no longer move much more slowly than the electrons, as in a usual solid? How does one cope with nanostructures in which the motions of the electrons are strongly correlated and the independent particle picture breaks down (see Chapter 2)?

Another pressing need is for a set of new analytic and computational tools to allow researchers to address ever-more-complex nanoscale systems (see Chapter 11). This is important in order to continue the evolution of the field from a descriptive to a predictive discipline. A huge part of the challenge of dealing with a complex system is in integrating the separate computational and calculational techniques used to describe different aspects of the problem—the combination of approaches that address the electronic, structural, and optical properties in a unified way, for example.

# 7

# How Will the Information Technology Revolution Be Extended?

Extrapolation of Moore's law suggests that in the next 20 to 30 years, electronic circuit elements will shrink to the size of single atoms. Even before this fundamental limit is reached, electronic circuits will have to operate in a new regime in which quantum mechanics cannot be ignored. New approaches to communications and information processing will have to be invented, and condensed-matter and materials physics (CMMP) will work with other disciplines to enable this transition. Among the many avenues already being explored in CMMP are devices based on spin rather than charge, molecular-scale circuit elements fashioned from carbon nanotubes, and novel computational engines based on biomolecules such as deoxyribonucleic acid (DNA). Perhaps most exotically, quantum information science envisions computation and communication based not on the familiar laws of classical physics but instead on the often counterintuitive laws of quantum mechanics. The familiar binary "bits" of today may tomorrow be replaced by arrays of quantum bits, or "qubits," capable of encoding vastly more information. CMMP, the science that helped launch the information age, will play a pivotal role in determining its future.

## THE ROAD AHEAD

Information technology (IT) pervades modern life. It is worth trillions of dollars per year in the global economy.[1] About half of the productivity growth in

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[1] Dale W. Jorgenson, *Econometrics, Volume 3: Economic Growth in the Information Age*, Boston, Mass.: MIT Press, 2002.

the U.S. economy is now attributed to information technology. Seminal inventions such as the transistor, the hard disk drive, and the communications laser eventually enabled the rise of the Internet, a watershed event in modern history. Indeed, some have compared the impact of the Internet to that of the printing press in extending broad access to information that was previously available only to the privileged.

The great force behind this modern industrial revolution has been miniaturization—the repeated shrinking of the devices that process, store, and communicate information. To extend the IT revolution, new devices will have to be invented. Smaller devices tend to be faster. More important, they tend to be cheaper because many more devices can be manufactured at the same time. More devices per dollar mean more function per dollar, and ever-more-affordable function has enabled the industry to expand its products from yesterday's mainframe computers to today's bewildering array of consumer products. Virtually every electronic product contains at least one microprocessor, and game machines now pack the computational power of supercomputers from just a few years ago.

The devices of IT have not just "shrunk." They have shrunk in an exponentially compounding fashion. In 1965, it was noted that the number of transistors that could be built on a single silicon chip was doubling every few years. This doubling trend has roughly persisted over the past 40 or so years, elevating the trend to the status of a "law"—Moore's law. But Moore's law is not unique in IT. Analogous exponential doubling trends have been noted for information storage capacities of hard disk drives, digital communication rates, and many other key performance indicators of IT. Over time, such powerful trends can change the world. For example, since the introduction of the hard disk drive about 50 years ago, the areal density of information storage has increased by a factor of roughly 100 million. The resultant dive in the cost of information storage has been a key enabler for the rise of the Internet and the explosive growth of electronic commerce.

What is required to drive such powerful trends? It is the repeated reinvention of the devices that store, process, and communicate information. For instance, the introduction to hard disk drives in 1998 of read-head sensors based on the giant magnetoresistance (GMR) effect greatly accelerated the above-mentioned doubling trend in information storage capacity. GMR is a subtle collective effect in magnetic materials, unknown to physics before 1988. It is striking that GMR was put to practical use in almost all computers manufactured worldwide by the late 1990s. Harnessing the effect for information technology involved the development of practical methods for manufacturing multilayered structures consisting of thin ferromagnetic films separated by metallic spacers of precisely controlled nanometer-scale thickness. A magnetic field passing through such a structure determines whether the magnetic moments of adjacent ferromagnetic films are aligned parallel or antiparallel. Through the phenomenon of spin scattering, this alignment gives rise to low and high states of electrical resistance, respectively, corresponding to the 0 and 1 states of binary digital information. Thus, this "spin valve sensor" can translate the changing reversals of magnetization stored on a spinning hard disk surface into the electrical signals needed for digital information processing. Technologists found that these sensors could be readily miniaturized, allowing ever-smaller regions of magnetization to represent information on a hard drive. These developments contributed substantially to the huge drop in the cost of information storage in the past 15 years and the rapid rise of the Internet.

Now, sparked by new developments in condensed-matter and materials physics, magnetic sensors for hard disk drives are being reinvented again. Figure 7.1 shows a schematic of a GMR spin valve structure as originally utilized in the late 1990s and a schematic of the new magnetic tunnel junction (tunnel valve) sensor that is enabling disk drive manufacturers to further reduce the cost and increase the speed of information storage. Replacing the metallic spacer of the GMR structure with an electrical insulator means that electrons can pass between the two ferromagnetic layers only by quantum tunneling. Recent advances in materials physics now allow the tunneling rate to be made exquisitely sensitive to a magnetic field, providing a new generation of sensors for hard disk drives.

This complex interplay between the discovery of new physics and progress in miniaturization is not limited to magnetic sensors for hard disk drives. Figure 7.2 shows the current transition to higher-storage-density perpendicular magnetic recording from the traditional longitudinal geometry. This transition is being aided by the above-described improvements in magnetic sensors, but it also depends on

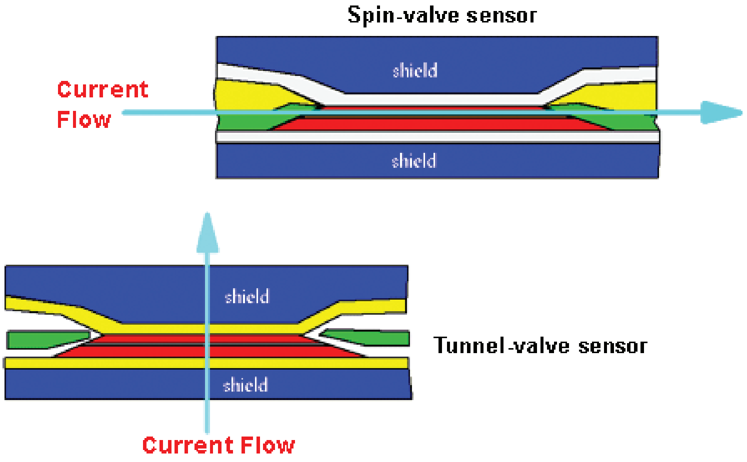

FIGURE 7.1 (Top) Giant magnetoresistance (GMR) spin valve with the current flowing in the plane of the film. Two ferromagnetic layers are separated by a nonferromagnetic metallic spacer layer. The magnetoresistance is higher when the two magnetic layers have their magnetization aligned in parallel (high state, or binary “1”) and lower when antiparallel (low state, or binary “0”). (Bottom) A tunnel magnetoresistance (TMR) spin valve is indicated where the spacer is a nonmagnetic insulator and the current flow is perpendicular to the plane of the film structure. SOURCE: Courtesy of Hitachi Global Storage Technologies, Inc.

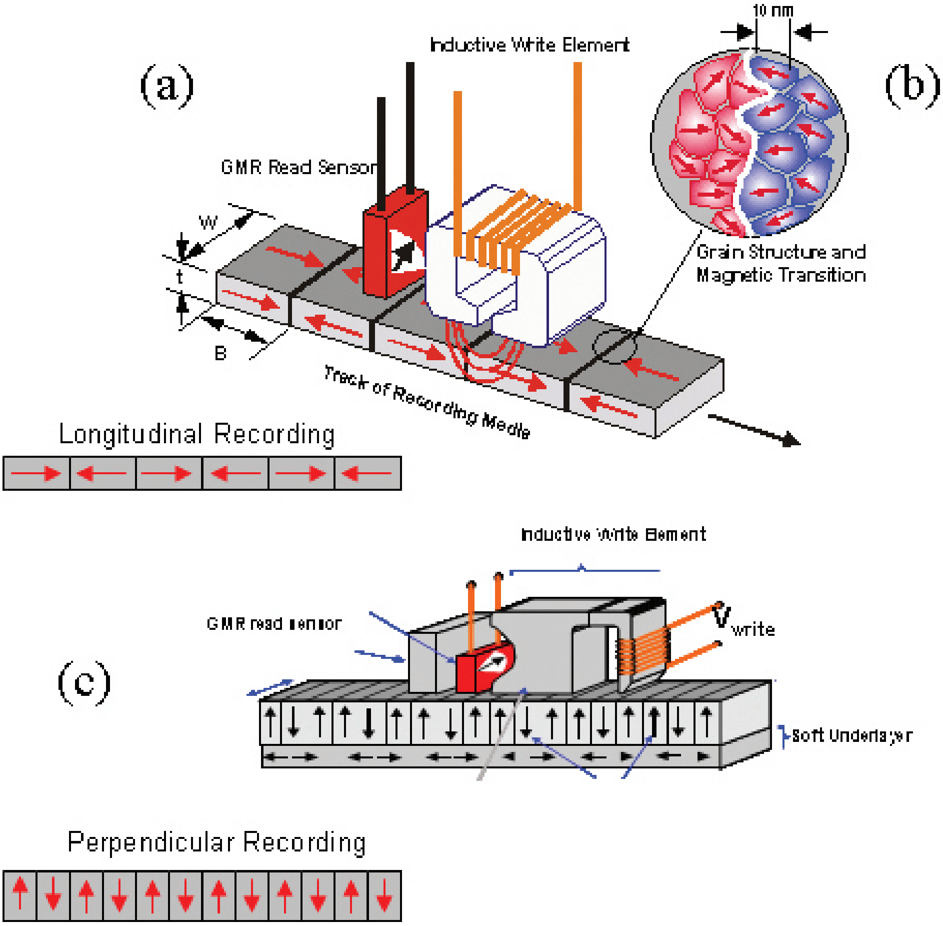

FIGURE 7.2 (a) Schematic illustration of a longitudinal recording system with a read and write head flying above the recording medium: *t* is the medium thickness; *W*, the width of the recorded track; and *B*, the bit size. (b) Schematic of magnetic alloy longitudinal recording layer showing amorphous grain boundaries as white and an average grain size of 8.5 nm. (c) Schematic illustration of a perpendicular recording system with a read and write head flying above the recording medium. The magnetization of the media is perpendicular to the films, and a soft magnetic underlayer is below the medium to enhance the perpendicular write fields from the head. SOURCE: Image courtesy of E. Fullerton, University of California at San Diego; based on G. Srajer, L.H. Lewis, S.D. Bader, A.J. Epstein, C.S. Fadley, E.E. Fullerton, A. Hoffmann, J.B. Kortright, K.M. Krishnan, S.A. Majetich, T.S. Rahman, C.A. Ross, M.B. Salamon, I.K. Schuller, T.C. Schulthess, and J.Z. Sun, “Advances in Nanomagnetism Via X-Ray Techniques,” *J. Magn. Magn. Mater.*, **307**, 1-31 (2006).

other distinct and dramatic advances in the understanding of micromagnetic materials and structures. Indeed, the development of magnetic storage, the transistor, the optical communications laser, and other key devices of IT are all marked by the *repeated* introduction of new materials and by improved device structures based on new physical principles.

Over the long run, even the key devices have themselves been repeatedly supplanted and replaced by new (smaller, faster, cheaper) devices. Before there was random access memory based on the silicon transistor, magnetic core memories were dominant. Today they are found only in museums. The mechanical mechanisms of the first commercial tabulators were replaced by electromechanical relays and then by vacuum tubes. Commercial computing began to take off when tubes were replaced by discrete bipolar transistors and then by integrated circuits based first on bipolar transistors and then on more efficient field-effect transistors (FETs). History thus suggests that the key devices of IT may be reinvented again. There are also good scientific reasons to believe that this can happen; in order to extend the growing benefits of the IT revolution for several more decades, researchers must strive to make it happen. This is because the "old" established devices are nearing their physical limits.

According to the *International Technology Roadmap for Semiconductors*,[2] hard limits to the further miniaturization of the transistor are fast approaching. In particular, undesired power dissipation, such as that caused by quantum mechanical tunneling, is already limiting further advances in speed; many believe it will limit further advances in miniaturization within a decade. Similarly, the physics of magnetism is beginning to limit advances in hard disk drive technology. In particular, the volume of the magnetized regions that store each bit ("0" or "1") of digital information cannot be shrunk below what is known as the superparamagnetic limit. Smaller magnets cannot retain their magnetic order long enough to be useful for the permanent storage of information. Figure 7.3 shows a high-resolution magnetic force microscopy image of magnetic bits tightly arranged along tracks in a magnetic recording medium.

To extend the IT revolution, new devices for processing, storing, and communicating information will have to be invented. The new devices will very likely be based on new materials and exploit physical principles that condensed-matter physicists are just beginning to explore. Some devices may operate in a new regime in which quantum mechanics will be embraced. New molecular-scale structural elements such as carbon nanotubes and organic spin valves and semiconductor nanowires and nanocrystals are of great interest for the new devices. This is because low-atomic-number elements, such as carbon, should cause less undesirable spin-

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[2] Available at http://www.itrs.net/Links/2006Update/FinalToPost/00_ExecSum2006Update.pdf; last accessed September 17, 2007.

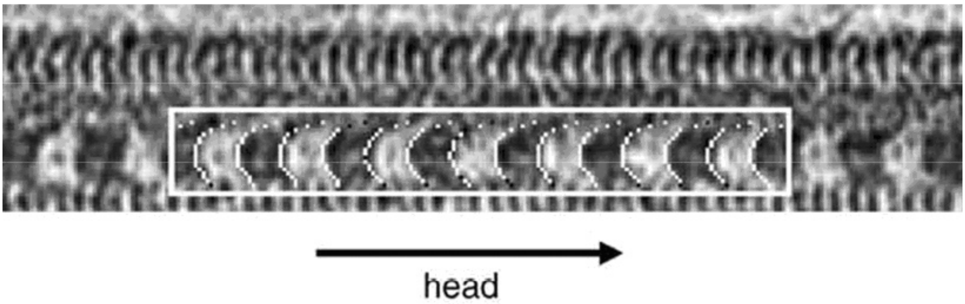

FIGURE 7.3 Have you ever seen a magnetic bit? Shown here is a high-resolution magnetic force microscopy image of magnetic bits arranged along tracks, as in magnetic recording media. The upper track is a square-wave bit pattern written at 1024 kilo-flux reversals per inch (kfci), and the bottom track is at 240 kfci. The upper track corresponds to a transition-to-transition distance of only 24.8 nm, which matches the maximum transition density used in a 36 Gbit/cm$^2$ areal density demonstration. For comparison, the micron marker is the same length that a magnetic bit was in 1989. The white lines in the box, generated by an analysis program, indicate the average transition shape. The arrow indicates the direction of the head motion during the write process. SOURCE: A. Moser, C. Bonhote, Q. Dai, H. Do, B. Knigge, Y. Ikeda, Q. Le, B. Lengsfield, S. MacDonald, J. Li, V. Nayak, R. Payne, M. Schabes, N. Smith, K. Takano, C. Tsang, P. van der Heijden, W. Weresin, M. Williams, and M. Xiao, "Perpendicular Magnetic Recording Technology at 230 Gbit/in$^2$," *J. Magn. Magn. Mater.*, **303**, 271-275 (2006).

orbit scattering in spin-based device structures. Thus, the information contained in electron spins can be propagated over longer distances. Figure 7.4 shows one example of how this new physics is being explored for potential applications in IT.

Novel computational strategies based on the self-organizing properties of biomolecules such as DNA have also been demonstrated, and approaches based on the manipulation of molecular configuration are being explored. Perhaps most exotically, quantum information science envisions computation and communication based not on the familiar laws of classical physics but instead on the sometimes counterintuitive laws of quantum mechanics. The familiar binary "bits" of today may tomorrow be replaced by arrays of quantum bits, or "qubits," capable of encoding vastly more information. Condensed-matter and materials physics, the science that helped to launch the information age, will likely play a pivotal role in determining its future.

Thus, the next decade is one of transition as this burning issue is confronted: How will we extend the IT revolution? What device will allow the storage of massive amounts of information more compactly than can be done with the hard disk drive? What device will allow the processing of information faster and cheaper than can be done with the silicon FET? These ubiquitous devices are the fruits of basic research in condensed-matter and materials physics stretching back to the 1930s and 1940s. The current form of these devices is the result of many decades of R&D

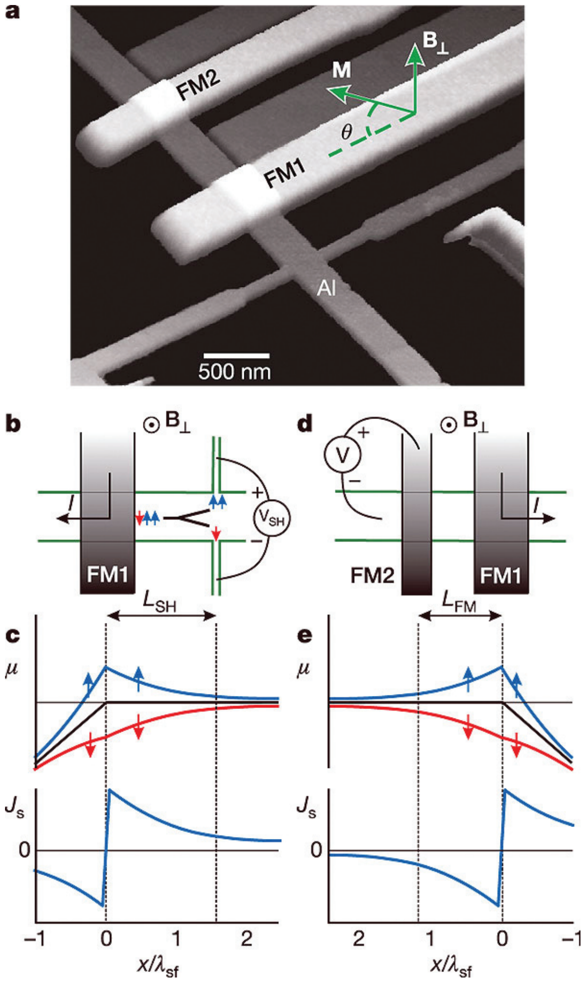

FIGURE 7.4 Spintronic device example involving the detection of the spin Hall effect utilizing a lateral spin transistor-type geometry. (a) An atomic force microscopy image of the device, which consists of a thin aluminum Hall cross that is oxidized and in contact with two ferromagnetic electrodes of different widths (FM1 and FM2). (b) The measurement, where a current *I* is injected out of FM1 into the Al film and away from the Hall cross. A spin Hall voltage ($V_{SH}$) is measured between the two Hall probes. $V_{SH}$ is caused by the separation of up and down spins due to the spin-orbit interaction in combination with a pure spin current. The top panel of (c) shows the spatial dependence of the spin-up and -down electrochemical potentials $\mu$, while the black line represents $\mu$ in the absence of spin injection. The bottom panel of (c) illustrates the associated spin current $J_s$. The polarized spins are injected near $x = 0$ and diffuse in both Al branches in opposite directions. The sign change in $J_s$ reflects the flow direction. (d) A spin-transistor measurement for device characterization, where *I* is injected out of FM1 into the Al film and away from FM2. An output voltage V is measured between FM2 and the left side of the Al film, where (e) depicts the same quantities as in (c). SOURCE: S.O. Valenzuela and M. Tinkham, "Direct Electronic Measurement of the Spin Hall Effect," *Nature*, **442**, 176 (2006).

and manufacturing experience. Many engineers and scientists believe that further rapid improvements will be possible for another 10 years or more. Replacing them with devices that can be smaller, faster, cheaper, and more reliable is an awesome challenge, but there are good scientific reasons to believe that this challenge can be met (see Figure 1.6 in Chapter 1). Doing so in a timely fashion will require increased investment and societal focus in the coming decade.

## NEW DEVICES FOR MASS STORAGE OF INFORMATION

Since the physics of magnetism sets limits on the further development of hard disk drive technology, future devices for the mass storage of information may store information differently. "Scanning-probe storage" holds the promise of storing information at a bit density approaching the density of atoms on a surface—perhaps a thousand times the areal density that will be obtainable with magnetic storage. Since the Nobel Prize–winning invention of the scanning tunneling microscope in the 1980s, a plethora of scanning probe techniques for the atomic-scale imaging, characterization, and modification of surfaces have been developed by condensed-matter physicists. While laboratory instruments already demonstrate a very limited ability to write and read information with atomic resolution, commercial development sacrifices "ultimate" storage density in favor of speed and reliability.

To overcome speed limits in reading and writing information with a single scanning probe tip, arrays of thousands of tips are being developed, along with the multiplexed electronics to read and write from many tips in parallel. Researchers have reported rapid and reliable operation of many parallel scanning probe tips at storage densities of 120 gigabits (Gb; 120 billion bits) per square centimeter—several times the storage density of today's hard disk drives. Operation of single tips at storage densities of 0.6 terabits (Tb; 0.6 trillion bits) per square centimeter suggests that the technology can be extended. For such prototypes, the scanning probe tips store information in the form of tiny indentations in a thin polymer film.

Various industrial and academic research groups are pursuing a variety of other classes of materials and storage mechanisms. Experimental storage densities of *several hundred trillion bits per square inch* have been demonstrated by some research groups. However, understanding the atomic-scale interactions between probe tips and a variety of storage media and storage methods is key to realizing the enormous promise of this nascent information storage technology. That challenge will keep members of the CMMP community busy for many years to come.

## NEW SOLID-STATE MEMORY DEVICES

Solid-state memory devices are used for information storage when hard disk drives are too slow or bulky. Today there are several distinct varieties of solid-state memory in widespread use. Static random access memory (RAM) is used when speed is of paramount importance. A circuit consisting of six FETs stores one bit of digital information. Static RAM retains information only as long as power is supplied. Dynamic random access memory is the dominant memory in computers. Slower than static RAM but still far faster than a hard disk, dynamic RAM represents information as electronic charge stored on a capacitor integrated with a single FET. Dynamic RAM loses its information rapidly through charge leakage and must be intermittently refreshed while in use. Like static RAM it loses its information as soon as the power is turned off. *Nonvolatile memory* represents information as electronic charge trapped in insulating films built into specially designed FETs. Charge-retention times are typically about 10 years. This is the memory that is used in the memory cards of commercial MP3 players, digital cameras, and many other consumer products.

All of these memory devices are based on the silicon FET, and all represent (or store) digital information in the form of packets of electronic charge. All are thus limited in their potential for further miniaturization by the same basic physical principles. The emerging memory devices being explored by condensed-matter physicists and electrical engineers will not have the same physical limits because they represent the information in physically different ways.

Ferroelectrics provide one example of a solid-state memory device. These materials possess ordered electric dipoles. Ferroelectric memory devices are based on complex oxides that can exhibit large polarizations under the influence of an electric field. A digital “0” or “1” is represented by a persistent polarization corresponding to a structural change in the material in which a central ion in the building block of the crystal structure moves to an off-center location. Ferroelectric memories are already used in some consumer devices, such as smart cards. They are also being explored as a promising medium for scanning probe information storage. There are many scientific challenges in understanding and controlling ferroelectric effects in nanoscale structures. The issue of perfecting thin insulating barriers of high-dielectric-constant materials is a challenge shared by the magnetoelectronics community in its quest to harness the magnetic tunnel junction effects (described below). More broadly, it encompasses the issue of exploring coherent interfaces and the physics of hybrid structures in general.

Magnetic random access memory represents a digital “0” or “1” by the high or low electrical resistance of a magnetic tunnel junction. The basic concept of the magnetic tunnel junction goes back decades, but continuous and rapid advances in the physics of nanostructured magnetic materials are just beginning to make it practical as a memory device. The first commercial magnetic RAM memory chip was recently announced in the United States. Magnetic RAM is nonvolatile—in other words, it retains its information even when the power is turned off. Magnetic RAM easily exceeds silicon FET-based nonvolatile memories—the kind used in cameras and MP3 players—in terms of write speed and durability. It may eventually replace many of the established memory devices, but that will require further invention and discovery. In particular, the recently demonstrated spin-transfer switching effects may eventually endow magnetic RAM with an unrivaled combination of speed, low power consumption, and low cost. But, while magnetic RAM might seem like an obvious path to the future, technology and the marketplace can be fickle; many competing technologies are vying for future acceptance.

For example, phase-change memory is another nonvolatile memory in the late stages of commercial development. Information is represented as a change in the resistance of a material that can be rapidly switched between amorphous (high-resistance) and crystalline (low-resistance) phases. The phase change is driven by appropriately timed electrical heating pulses. With good prospects for shrinking devices to very small dimensions, phase-change memory is seen as the successor to silicon nonvolatile memory in the rapidly growing consumer electronics market. The chalcogenide materials that enable it are thus under intense exploration and development. Still, the physics of phase changes in structures with dimensions on the order of 10 nm and smaller is just beginning to be explored.

While the commercialization of magnetic RAM and phase-change memory are most advanced, many other new memory devices are being explored in universities and industrial laboratories. A partial list of commercial development efforts includes memories based on changes in the conductivity of complex metal oxides, electrochemical reactions in small molecules, and electromechanical deformations of molecular-scale structures. All of these approaches to future memory devices are nonvolatile, and none stores its information in the form of a packet of electronic charge. None is wed to a silicon substrate, although for now, the circuits that read and write the information to each memory device must be based on silicon FETs.

## NEW DEVICES FOR PROCESSING INFORMATION

While some new memory devices are beginning to enter the market, no new device for *processing* information is at a remotely similar state of development. The coming decade will be one of exploring many pathways. While some approaches outperform others in certain aspects, no one knows the best overall solution at this time. But just as the transistor, more than any other invention, enabled the explosive growth of IT in recent decades, so would the invention of something “smaller, faster, and cheaper” enable further explosive growth in the capabilities and applications of IT.

The search for new logic device concepts is driving research into new materials and novel physical systems. The terminology to describe these areas stems from the word electronics—as in spintronics, orbitronics, plasmonics, and so forth—names that evoke a sense of imminent technological applications. In reality, the technological applications of these scientific developments are still quite uncertain. However, the research is drawing the interest of top scientists in a way that reminds some observers of the excitement in the early days of solid-state electronics. The following examples should convey a sense of some of the innovative paths that lie ahead.

Spintronics, also known as magnetoelectronics, represents a break with silicon technology because it is based on magnetic materials, possibly including magnetic semiconductors. Processing information that is represented by spin orientation offers intriguing possibilities for nearly dissipationless computing. For example, under the right conditions, spin precession can rapidly switch the spins from one orientation to another, while dissipating only a small fraction of the energy stored in the system. This possibly can reduce or avoid wasteful heating that occurs in electrical circuitry. Understanding spin dynamics in nanoscale structures provides an enormous basic challenge, because geometric confinement and physical proximity of these materials can endow them with extraordinary properties. Many basic questions need to be addressed. Can the spin-transfer effects being developed for magnetic memory devices also be employed in logic devices (see Figure 7.5)? Will further advances in materials allow these effects to be harnessed in low-power devices? Also, the extension of spin-transfer effects within antiferromagnetic

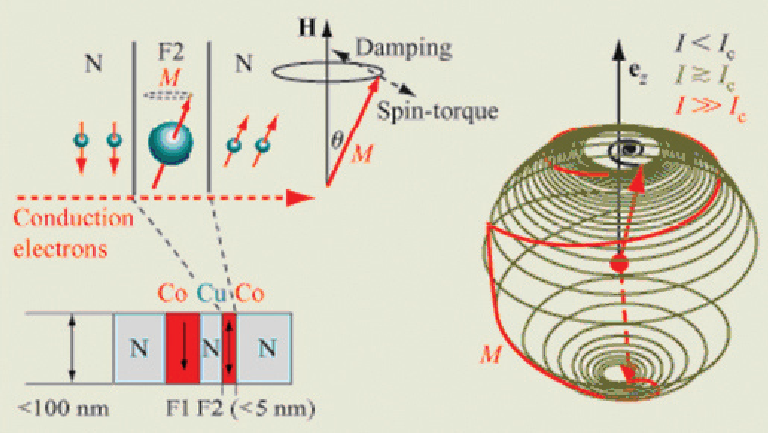

FIGURE 7.5 Illustration of spin-transfer effects and associated spin dynamics. The magnetic field H is aligned along the z-direction, collinear with the magnetic easy axis which has a uniaxial anisotropy, where M denotes the magnetic moment. The red trajectory at the right shows how a spin-polarized current of sufficient magnitude can switch the magnetization orientation via the spin-transfer effect. SOURCE: J.Z. Sun, "Spin Angular Momentum Transfer in Current-Perpendicular Nanomagnetic Junctions," *IBM J. Res. Dev.*, **50**, 81 (2006).

structures remains relatively unexplored. Voltage-induced switching of magnetic domains remains another avenue to explore. Indeed, obtaining a truly comprehensive understanding of magnetism in nanoscale structures would be a major breakthrough and is a challenge that might result in one or more Nobel Prizes.

Multiferroics are yet more-exotic materials, including nanoscale composites, that merge magnetic (ferromagnetic) and ferroelectric effects. This enables the switching of a magnetic bit via an electric field rather than a magnetic field, or the switching of a ferroelectric polarization via a magnetic rather than an electric field pulse. Multiferroics may thus help to realize useful spintronic devices that can be made very small. Magnetic fields are inherently nonlocal in nature, and hence as device density increases, stray magnetic fields can adversely affect neighboring bits. Multiferroics may offer a way to surmount the hurdle. At the same time, basic physical properties, such as the coupling of the order parameters, present intrigue for the theorist and experimentalist alike.

A still more speculative and less well traveled field is the nascent study of orbitronics, in which silicon retains its central role. Theoretical studies predict that electric fields can be used to create orbital currents in the absence of conventional charge currents. The orbital angular momentum is transmitted perpendicular to the direction of electron movement, making an orbital Hall effect. The excitement is that the orbital current can be dissipationless and robust against disorder. Experimental tests and realizations remain for the future.

Photonics and plasmonics offer the promise of new logic devices based on light. At present, photonic devices such as the semiconductor laser are used for digital communication over relatively long distances—from a few meters to thousands of kilometers. The smallest photonic devices are generally limited by light diffraction effects to dimensions somewhat greater than the wavelength of the light that is used. Plasmonics seeks to go beyond the diffraction limit of light and to explore new device concepts in subwavelength structures. Particles in electromagnetic fields provided by light can develop resonant charge oscillations (plasmons) that can be propagated and manipulated. It is hoped that this approach can take optical devices into the nanometer realm. A major challenge is to integrate photonic and electronic circuits, intimately linking communications and information processing on a single chip, as envisioned in Figure 7.6.

The emergence of metamaterials, or negative index-of-refraction materials, also opens new areas of optics and optical materials for physical exploration, as discussed in Chapter 6. The implications for applications are in the area of wireless communication. The quest is not only to explore such exotic phenomena but to shrink the structures so that they operate at shorter wavelengths. It has been said that negative refraction is a subject with constant capacity for surprise, with innocent assumptions sometimes leading to unexpected and profound consequences. While the roots of modern geometric optics can be traced back to the work of

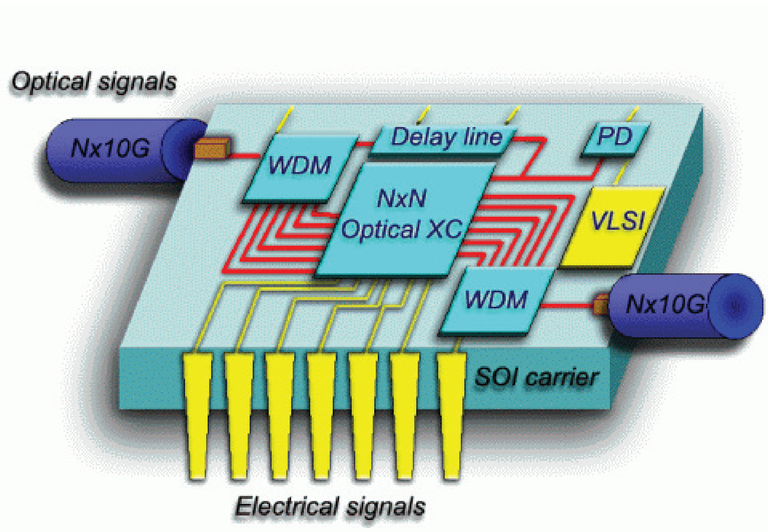

FIGURE 7.6 Schematic of a futuristic silicon chip with monolithically integrated nanophotonic and electronic circuits. The convergence of electronics and photonics is on the cutting edge of integrated circuit research. The goal is to perfect the materials and processes in order to integrate on a chip ultracompact nanophotonic circuits for manipulating light signals similar to the way that electrical signals are manipulated in present-day computer chips. The example shown is an N-channel multiple of signals from a germanium photodetector, where the performance is monitored via complementary metal oxide semiconductor (CMOS) very large scale integrated (VLSI) logic circuitry integrated onto the optoelectronic chip. SOURCE: Image courtesy of IBM Corporation.

Willebrod Snell in the 17th century, the 21st century is ripe for new insights and breakthroughs.

Molecular electronics, sometimes dubbed moletronics, are devices that are constructed at the ultimate size limit of single molecules and in which single electrons are transported, rather than currents of ensembles of electrons flowing in circuitry. In the future, the microscopic theory of electronic transport should move well beyond the knowledge presented in today's most advanced textbooks. At the present time, the effects of Coulomb blockade and percolation through nanoscale particle arrays are being pursued. For example, densely packed arrays of organic-ligand-coated gold nanocrystals have been reported to belong to a new class of artificial solids with tunable electronic transport properties. Such properties stem from single-electron charging and quantum confinement energies at the level of individual particles, mediated by couplings to neighboring particles. The particles are so small that a single electron can block the tunneling of another electron onto the same particle or require the next electron to be of opposite spin as dictated by the Pauli principle. Thus, the physics of Coulomb blockades and the Pauli exclusion principle are experiencing a rebirth of interest. As in this example, such developments in molecular electronics are also motivating fabrication based

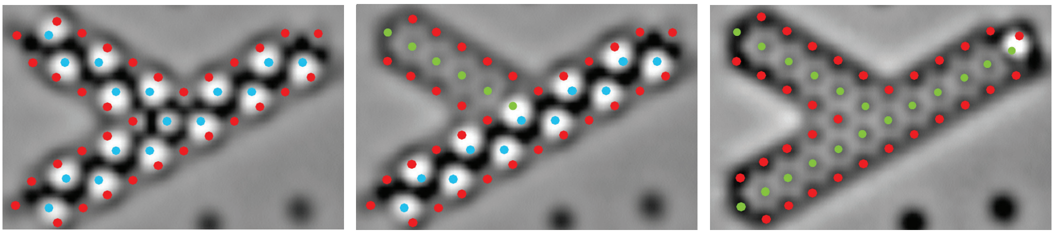

FIGURE 7.7 Logic components on a molecular level: Logic AND gate based on carbon monoxide (CO) cascade on a copper surface. The blue, red, and green circles represent, respectively, CO molecules that are going to hop, that are not going to hop, or that have already hopped to their final location. (Left) Initial state of CO molecules. (Middle) The result of a cascade that propagates after triggering one input. (Right) The final configuration, in which all of the CO molecules have hopped to their final locations. SOURCE: Images courtesy of IBM Corporation.

on self-assembly rather than lithography, and thus they encompass major integrated challenges that span the physical, chemical, biological, and manufacturing sciences.

A second example at the ultimate limit of miniaturization involves the molecular cascade of CO on a copper surface to form a logic AND gate. The system is laboriously configured by means of scanning tunneling microscope manipulation of the CO molecules to form the initial state, as shown schematically in Figure 7.7.

## QUANTUM COMPUTING

No matter what device concepts are pursued, smaller devices must eventually embrace a profound change in the way we think about computing. Present devices average the behavior of a great many quantum particles. Make any of these devices small enough and there will be only a few quantum particles in the system. In this limit, the laws of quantum mechanics manifest themselves most vividly, as has also been discussed in the National Research Council's atomic, molecular, and optical physics decadal survey.[3]

Thus, researchers need to traverse the threshold and look beyond the limits of classical physics. Quantum computing should have broad applications across scientific disciplines. An application of immediate interest, however, involves the factoring of large numbers into primes, a capability that is key to breaking current cryptographic protocols. In principle, a quantum computer should be expo-

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[3] National Research Council, *Controlling the Quantum World: The Science of Atoms, Molecules, and Photons*, Washington, D.C.: The National Academies Press, 2007.

nentially faster at this task than a conventional computer. To illustrate the point, consider that, while a classical computer composed of a three-bit register can store only one of eight possible numbers at a given moment in time, a quantum computer with three qubits can store all eight simultaneously, owing to the coherent superposition of states possible in quantum systems. Once the register is prepared, the quantum computer can perform many different calculations in parallel. Now imagine going from three qubits to ten to a hundred. The basis for enabling such operations is to assemble arrays of quantum coherent nanoscale objects to serve as the qubits and logic gates of the quantum computer. Solid-state approaches to building qubits include, for example, the confined electron spins in semiconductors and the superconducting currents in Josephson junctions. For example, an alternating-current-voltage pulse applied to one of two Josephson junction qubits connected by a capacitor can cause the two qubits to becoming entangled and oscillate between two combined states, if the energy differences between the "0" and "1" states are equal in both qubits. The characteristic oscillation frequency is analogous to that of a quantum state of an atom; hence the circuit is referred to as containing "artificial atoms." See Figure 7.8 for a representation of a qubit that could be used in such a circuit.

Unlike in classical computers, in quantum computers the bits are prepared in an initial state, interact with one another to entangle, and must then be read out while still in a coherent state. Many novel pathways are being pursued, including the use of biological templates such as DNA strands, to serve as a backplane to secure the qubits in place. The challenges of addressing readout and quantum error correction have stimulated theorists and experimentalists alike and will continue to do so well into the future. The effort to build practical quantum devices is driving unprecedented progress in the ability to measure and control physical systems. The new capability will impact science and society well beyond the currently perceived boundaries of IT. Quantum computing might disrupt the status quo by making present-day encryption methods obsolete because of its potential to rapidly break conventional codes. But simultaneously, it holds promise of providing quantum encryption schemes that are fundamentally unbreakable.

## CONCLUSIONS

In summary, the rise of IT has powered an ongoing transformation of the global economy and modern society. It has changed manufacturing, finance, communications, commerce, entertainment, education, and science itself. Today's world has thus been shaped tremendously by "old" inventions such as the transistor and the hard disk drive. But the continued growth of IT will depend on new inventions.

Advances in IT are intimately connected to advances in the rest of the CMMP grand challenge areas. The new materials for future IT applications will likely

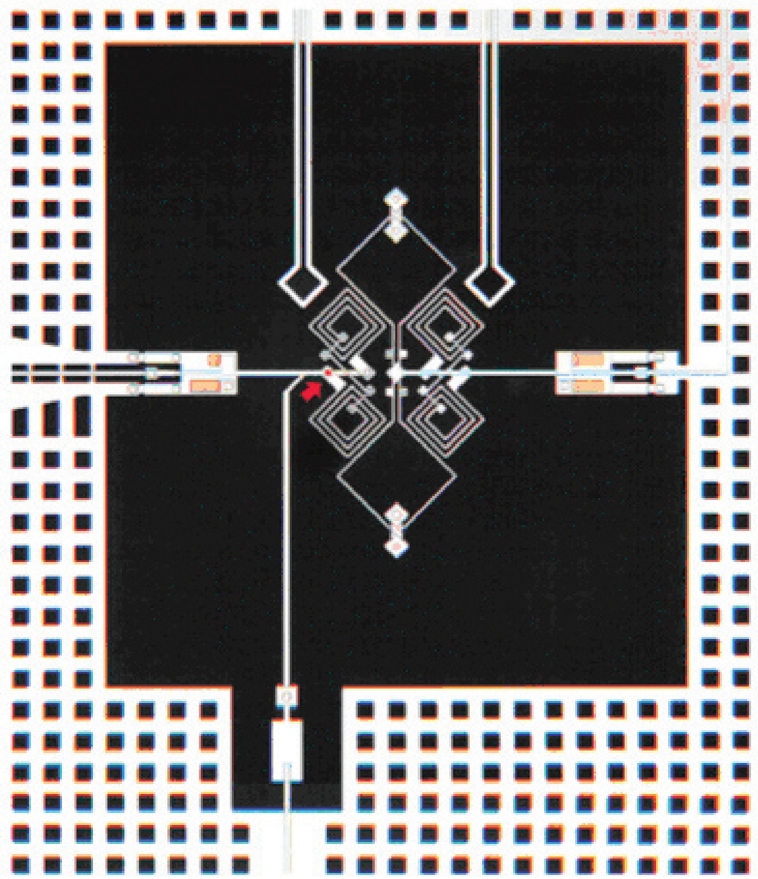

FIGURE 7.8 Josephson junction devices might be used in future quantum computers. The optical micrograph shows an "artificial atom" about the size of a human hair made with a superconducting circuit. The red arrow points to the heart of the qubit—the Josephson junction device that might be used in a future quantum computer to represent a "1," a "0," or both values at once. SOURCE: Courtesy of R. Bialczak and J.M. Martinis, University of California at Santa Barbara.

embrace the emergent behavior discussed in Chapter 2. Also, the exploration of the nanoworld, described in Chapter 6, will be critical, as will the availability of advanced measurement techniques and major characterization and computational facilities (Chapter 11). Foremost will be the new understanding captured by the conceptual theories that are in the process of being formulated to develop understanding of new states of condensed matter.

What is expected of the industrial, academic, and national laboratory sectors of the research community in the next decade to extend the information technology revolution? Industrial laboratories must aggressively pursue new partnerships with the academic and national laboratory communities to promote critical, pre-competitive research that will lay the basis for future IT technologies (see Chapter 9 and the concluding recommendation). The Nanoelectronics Research Initiative, a consortium of microelectronics companies and state and federal agencies funding university research, is one possible example for the future. Universities and national laboratories can lower barriers to the creation of innovative start-up companies. Such companies can offer uniquely flexible environments for the creative development of new products aimed at new IT markets. The national laboratories can expand their tradition of stewardship of major characterization facilities for the research community at large. The scientific sophistication and technical complexity of new projects requires staffing, planning, and investment at a higher level than in prior eras. Such powerhouse teams of researchers will be capable of flexibly configuring into large interdisciplinary working groups to pursue scientific challenges in information technology, helping maintain U.S. leadership in this key industry.

To scientists, it is exhilarating to explore new materials and physical processes with the hope of extending for future generations the benefits of the IT revolution that scientists and the public alike have had the good fortune to experience in their lifetimes. The case for strong investments in CMMP information technology research is compelling.

# 8

# The Impact of Condensed-Matter and Materials Physics Research

## IMPACT ON SOCIETY

Condensed-matter and materials physics (CMMP) is remarkable for the breadth and depth of its impact on society as well as on other scientific disciplines. While it is not possible to review all of these connections exhaustively, in this chapter a few examples in the areas of education, the economy, energy, and medicine and health care are used to illustrate the major impact that CMMP has had, and continues to have, on U.S. society.

### Education

Condensed-matter and materials physics describes and shapes the world we see. It is critical to educate a new generation with a deeper understanding of the role of CMMP (and of science in general) in society. Yet few people ponder the quantum mysteries of the magnet on their refrigerator or realize that they are working against entropy when they stretch a rubber band. Many people benefit from the torrent of new and improved electronic devices, but few are aware that these products are the fruits of a rich and coherent scientific discipline characterized by an inseparable mix of fundamental and applied research. Limited public awareness and understanding of science constitute an increasing danger to U.S. economic security and are most dramatically reflected in the current crisis in primary and secondary school science education. The CMMP community must now extend educational efforts not only to improve general scientific literacy but also to increase the pool of students interested in science and engineering. It is critical to infuse a new generation of scientists with the knowledge, skills, creativity, versatility, and sense of wonder needed to meet the challenges ahead.

Along with the six scientific challenges for CMMP that are identified in this report, the challenge to educate the next generation of scientists and citizens is equally important. In further refinement of this challenge, the Committee on CMMP 2010 identified three key issues: how to educate the next generation of CMMP researchers, how to attract talented people to the field, and how to increase the scientific literacy of the general public and of school-age children. These three issues are addressed below.

Regarding the education of the next generation of CMMP researchers, the research community perceives that significant changes have occurred in the field during the past decade and that these changes have had and will continue to have implications for the education of this next generation. Growing interdisciplinarity at the frontiers of CMMP is evident in all the scientific challenges discussed in this report, including the nanoworld, emergent and far-from-equilibrium phenomena, energy for the future, the physics of life, and the evolution of the information age. This interdisciplinarity is manifested as a broadening of the interface between CMMP and other areas of physics and also other disciplines, such as chemistry, biology, mathematics, and computer science. More exposure to these fields is therefore needed in the undergraduate and graduate educational programs of students who might be seeking careers in CMMP. Such interdisciplinary education should include both formal course work and hands-on exposure to how research is done in these fields, as well as an introduction to the vocabulary and culture of these diverse fields as they are now practiced in their interface with CMMP. This new emphasis is believed to be essential for working at the cutting edge of CMMP in the coming decade and beyond.

The great challenge that faces the academic community thus is to create an undergraduate curriculum that balances the need for breadth against the depth of the traditional physics culture, from which the community draws its strength. Innovative, experimental approaches to this problem should be encouraged, as should more flexible curricula that can transmit at least part of the physicist's intellectual style to students considering careers in areas such as business, finance, and law. There is a strong sentiment that the achievements and experience level of students receiving undergraduate and graduate degrees in U.S. universities must be very thorough and fully competitive with their counterparts in the best universities worldwide. The implementation of these new educational directions for students and faculty in an exciting way, without increasing the length of undergraduate, graduate, and postdoctoral programs, is a significant challenge.

Attracting top-level talent to CMMP is identified as the second significant challenge to the field. It is expected that transforming the undergraduate educational experience to be more interdisciplinary and more flexible, while emphasizing educational achievement and research leadership at the highest levels, will help attract high-level talent to the U.S. CMMP research enterprise. Emphasis on rewarding hands-on research experiences at the undergraduate level is regarded as a critical component in exposing young people to the excitement and intellectual rewards of CMMP research. The committee recommends that the Research Experience for Undergraduates (REU) program that is now working well be further expanded. Thoughtful mentoring and attention to young people in the classroom and research laboratory are also regarded as important ingredients in effective career development in the changing environment that CMMP faces, both in supporting the intellectual development of the field and in providing more opportunities to young people in developing their independent but CMMP-related careers in the United States. Finding more pathways for rewarding careers for young people in the changing landscape of CMMP-related careers in industry, in national laboratories, and in other sectors remains a challenge for the community. To make academic careers more attractive, efforts are needed to increase the probability of funding new research proposals so that more time is devoted to doing research rather than to writing proposals seeking funding for it. Enhancing the degree to which CMMP researchers can work on the topics in which they are genuinely most interested, as opposed to those most in fashion with the funding agency, was identified as another way that academic CMMP careers could be made more attractive and more scientifically productive.

Increasing the scientific literacy of the general public remains a high-priority challenge, especially for the CMMP community, because CMMP involves so many captivating and often everyday phenomena that are of great general interest. At the same time, the general public is largely unaware that CMMP is the science behind many of the technological marvels that they take for granted. Introducing interesting CMMP phenomena at all levels of science teaching, from "gee-whiz" talks in the local public library to science classes in elementary school and the undergraduate lecture hall, is an opportunity that the CMMP community should not miss. Through common examples of CMMP occurring in daily life, from the growth of soap bubbles to the beautiful symmetry of ice crystals, the imagination of young people can be captured to increase their interest in science and to improve their retention of scientific concepts. Such examples could also be used by science teachers seeking to focus more on presenting fundamental concepts than on preparing students to pass standardized tests. For more advanced students in high school and college and for the general public, more attention to current interesting examples of CMMP should be introduced in order to achieve similar educational objectives. Examples such as the physics behind the operation of a cellular telephone, or the dynamics of biological motion in a zebra fish, or why nanoscience offers promise of better utilization of renewable energy sources will resonate and inspire. Indeed, CMMP affects daily life and influences important societal and governmental decisions concerning issues such as energy policy, industrial competitiveness, and the preservation of the global environment. Increased public appreciation of this interplay between CMMP and society is sure to pay dividends to the nation.

The CMMP community believes that the level of science education in high schools needs to be elevated in order to decrease the gap between high school science and introductory college-level courses. Not only does this gap present a hurdle to enthusiastic future scientists, but it also scares away undergraduates who are less certain that science and engineering will figure largely in their careers. Strong input from the focus groups that were convened for the CMMP 2010 study indicated a great desire for CMMP participation in outreach programs, kindergarten through grade 12 (K-12) education, and increased public understanding of science. Nonetheless, the present system, in which the quality of outreach programs is a criterion for the evaluation of scientific research grants, confuses two conceptually distinct goals to the point that neither is optimally served. The Committee on CMMP 2010 therefore concluded that outreach, K-12 education, and undergraduate science education initiatives should be supported by supplemental or stand-alone grants administered by separate National Science Foundation (NSF) and Department of Education programs. Further discussion between the funding agencies and the CMMP community is needed on how best to implement this common goal.

## The Economy

The impact of science and technology on economic growth and the quality of life has been tremendous over the past hundred years. Technology has now replaced capital and the workforce as the major growth factor in developed countries and in developing nations as well. While there is a variation in the quantitative value assigned to economic growth owing to science and technology, all agree that science and technology are the principal factors in the past and continued growth of national economies. Usually, the impact is determined by subtracting the effect of capital and labor and attributing the remaining economic growth to research and development (R&D). A summary by Boskin and Lau gives a range of 25 to 50 percent, depending on how the education of workers is included.[1] Whatever the impact, most economic regions have large and growing efforts in research in all scientific fields in the belief that it will impact economic growth. The growth in research in CMMP has been especially large in Southeast Asia and Western Europe.

The U.S. CMMP research effort is conducted in government laboratories, industrial laboratories, and universities. The industrial laboratories grew from

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[1] Nathan Rosenberg, Ralph Landau, and David Mowery, *Technology and the Wealth of Nations*, Palo Alto, Calif.: Stanford University Press, 1992, p. 32.

a start in the late-19th century, with major investments following World War II. The national policy on government laboratories was set by Vannevar Bush in the report *Science, The Endless Frontier*,[2] initiated by President Roosevelt and presented to President Truman in 1945. The U.S. research universities benefited from wartime investments and the destruction of research institutions in many other countries in the 1940s. Today, the United States leads the world in investment in R&D and as a result, many believe, has a major market position in key industries. However, this situation is changing, as other economic regions are making large government investments with the conviction that these investments will lead to additional economic growth and perhaps market leadership in the key industries of the 21st century.

The period from 1940 to 1980 in the United States saw the federal government as the leading investor in R&D. After 1980, U.S. industry's investment exceeded that of the government and is now more than two-thirds of the national R&D effort.[3] However, most of the industrial R&D effort is focused on product development, with less than 10 percent going to fundamental research. The U.S. economic leadership, measured in gross domestic product (GDP) per person or in total dollars, is unquestioned. The portion of that leadership owing to R&D is not widely acknowledged. However, there is no question that physics research, and especially CMMP research, has had a major impact on almost every aspect of life today. Examples range from the invention of the transistor/integrated circuit and the laser to their application in personal computers and supercomputers and the instrumentation that is used to diagnose and treat disease—for example, computer-aided tomography, positron emission tomography, and magnetic resonance imaging. Tools developed by physicists are also essential to the advancement of science in other fields, such as astronomy, biology, chemistry, and many of the life sciences.

CMMP has been one of the leading contributors to economic advances and better health care and life style. The electronics industry alone is about a $1.5 trillion business worldwide, based principally on technology arising from CMMP research, some done more than 50 years ago.[4] A NASA report estimated that the direct contributions of granular materials and fluids processing alone account for roughly 5 percent of the GDP and almost one-third of the manufacturing output of the

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[2] Vannevar Bush, *Science, The Endless Frontier*, Washington, D.C.: U.S. Government Printing Office, 1945.

[3] National Science Foundation, Division of Science Resources Statistics, *U.S. R&D Increased 6.0% in 2006 According to NSF Projections*, NSF 07-317, Arlington, Va., 2006. Available at http://www.nsf.gov/statistics/infbrief/nsf07317/; last accessed September 17, 2007.

[4] David C. Mowery and Nathan Rosenberg, *Paths of Innovation*, New York: Cambridge University Press, 1998, p. 175.

United States alone (about $850 billion per year).[5] Thus, better understanding of far-from-equilibrium behavior (Chapter 5) can lead to better packing of granular materials with large economic benefit. Other applications such as financial systems, health care, and education are major economic areas in which CMMP research has had an effect. The CMMP research underlying these areas has been recognized by a significant number of Nobel Prizes (see Chapter 9) and many other awards. It is clear that there has been a significant impact of CMMP research on society and the economy. For continued growth in the world's economy and the improvement of health care, research in the fundamental aspects of CMMP, both experimental and theoretical, is essential.

## Energy

The introduction to the energy challenge in Chapter 3 of this report outlines the energy and environmental issues that will face society during the 21st century. Recent reports from the United Nations climate panel[6-8] estimate with 90 percent certainty that average global temperature increases during the second half of the 20th century were due to anthropogenic greenhouse gas emissions, and they predict further increases in temperatures during the 21st century accompanied by substantial rises in sea level. Even if greenhouse gas emission can be stabilized, atmospheric carbon dioxide ($CO_2$) levels will take hundreds of years to return to their pre-industrial level.

Against this backdrop, the United States will face some difficult decisions concerning its energy policy. With U.S. oil and gas resources dwindling, it will be tempting to place more emphasis on power generation from coal, especially because the nation has massive coal assets, which represent more than 25 percent of the world's recoverable reserves. At the present time, approximately 50 percent of U.S. electricity is produced from coal, and this could certainly be increased.[9] Coal, therefore, could present a partial solution to the nation's burgeoning energy

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[5] Paul Chaikin and Sidney Nagel, *Report on the NASA Soft and Complex Condensed Matter Workshop*, 2003. Available at http://gltrs.grc.nasa.gov/reports/2003/CR-2003-212618.pdf; last accessed September 17, 2007.

[6] Intergovernmental Panel on Climate Change, Working Group I Report, *The Physical Science Basis*, 2007. Available at http://ipcc-wg1.ucar.edu/wg1/wg1-report.html; last accessed September 17, 2007.

[7] Intergovernmental Panel on Climate Change, Working Group II Report, *Impacts, Adaptation and Vulnerability*, 2007. "Summary for Policymakers" available at http://www.ipcc.ch/SPM13apr07.pdf; last accessed September 17, 2007.

[8] Intergovernmental Panel on Climate Change, Working Group III Report, *Mitigation of Climate Change*, 2007. "Summary for Policymakers" available at http://www.ipcc.ch/SPM040507.pdf; last accessed September 17, 2007.

[9] For further U.S. energy statistics, see http://www.eia.doe.gov; last accessed September 17, 2007.

needs, but the inevitable production of greenhouse gases from the use of coal as a fuel makes this strategy very unattractive from an environmental perspective unless the $CO_2$ emissions can be ameliorated. Another viable option would be to generate more electricity from nuclear power, but here there are societal concerns about safety, nuclear waste disposal, and security. So what are the alternatives to oil, gas, coal, and nuclear power? Renewable energy sources, such as solar, wind, and hydroelectric power, have low carbon emissions but currently contribute only about 6 percent to the energy supply in the United States. Clearly there will have to be major changes in U.S. energy policy if the nation is to make a significant effort to reduce greenhouse gas emissions.

The CMMP community cannot solve the political and economic issues that surround the energy challenge, but it can aspire to creating technological breakthroughs that will provide lawmakers with more options. For example, progress in the area of $CO_2$ sequestration could substantially reduce the environmental impact of using coal for power generation, and the development of closed-loop nuclear fuel cycles could mitigate concerns about nuclear waste disposal.[10] Improvements in the efficiency of solar cells may make the price of solar energy competitive with that of energy from fossil fuels, and success in the areas of hydrogen generation and storage could make the hydrogen economy a reality. The possible use of hydrogen as a fuel is complex from an emissions standpoint, because it depends on how the hydrogen is produced. About 95 percent of the current hydrogen production derives from natural gas, so the carbon content of the natural gas ultimately ends up as $CO_2$. The greater efficiency of fuel cells compared with internal combustion engines mitigates the level of emissions, but hydrogen must be efficiently generated from solar energy or by electrolysis based on hydroelectric or nuclear power to be a viable fuel. The use of ethanol or diesel fuel from natural sources is similar in that, while these sources are renewable, the required processing and infrastructure will nevertheless contribute greenhouse gas emissions. An exciting long-term goal in the fuels area would be to make renewable liquid fuels from $CO_2$ and sunlight through a water-gas shift reaction with carbon monoxide as an intermediate, but many difficult obstacles remain in this pathway.

With respect to the energy challenge, an area of great societal concern, the CMMP community has an exciting opportunity to make major contributions based on new materials, new systems, and advanced computation and modeling. For it to be able to do so, it is necessary that there be a broad research investment strategy, based on multiple energy technologies: oil, gas, coal, solar, wind, nuclear, biofuels, hydroelectric, thermoelectric, and so forth. This is, of course, an interdis-

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[10] For a description of research and development needs, see the Technology Roadmap for Generation IV Nuclear Energy Systems, available at http://gif.inel.gov/roadmap/pdfs/gen_iv_roadmap.pdf; last accessed September 17, 2007.

ciplinary challenge that will require close cooperation between CMMP and other disciplines. In addition, given that the energy challenge is clearly a global issue, the area also presents an opportunity for international collaboration on these different technologies.

## Medicine and Health Care

Condensed-matter and materials physics has a long history of seeding not only developments in fundamental biology—the progression from the early work on x-ray diffraction from crystals to the invention of molecular biology comes to mind here—but also in the practice of medicine. This trend has been accelerating, involving more people and entailing larger consequences over the past decade. While this trend is well known, it is still worth noting a few examples of recent progress. In particular, there has been widespread adoption of reliable home pregnancy tests based on gold nanoparticles, routine magnetic resonance imaging—employing ever-improving superconducting magnets and other hardware and software, but also nanoparticle-based contrast enhancement—of everything from tumors to brain function, and the development of new materials to increase the lifespan of surgical implants.

The committee expects similarly rapid progress in the coming decade, especially given the growing emphasis on interdisciplinary and translational (laboratory bench to bedside) research at universities and hospitals. Important areas will be nanotechnology, photonics, novel x-ray sources and optics, superconducting devices, and tissue engineering. Nanotechnology is of particular interest, as it has captured the public imagination with its tremendous potential for diagnostics, public health, and therapeutics. Indeed, two of the examples listed in the preceding paragraph as recent advances demonstrate that nanotechnology has already arrived in clinical medicine. Today, there are journals with “Nanomedicine” in their titles, and a look at such journals as well as more established publications shows the huge scope of activity, on themes ranging from the targeting of tumors by functionalized nanoparticles to single (or few)-molecule detection using nanomechanical and nanophotonic devices instead of chemical amplification. The reverse side of therapeutics is toxicology, which will be essential for the further take-up of nanotechnology, and especially nanoparticles, in the clinic and elsewhere. The underlying science here will be cell physiology at the nanoscale, and many of the tools to be used, including electron and scanning probe microscopes, will be provided by condensed-matter physics.

At a more general level, health care is facing several major simultaneous challenges. The most important is to bring affordable personalized health care to all, thus finally reaping the fruits of the genomics revolution. Many secondary but nonetheless large challenges also exist, ranging from the drug pipeline crisis in the pharmaceutical industry to the evolution of bacteria to circumvent antibiotics. While it would clearly be an exaggeration to claim that CMMP will play the leading role in meeting these challenges, its contributions will nevertheless be very important. Sensors embodying novel transduction mechanisms, such as field-effect transistors with chemical modulation of gate voltages, micro- and nanofluidic reactors made according to recipes developed for the computer and telecommunications industries, and sensitive but inexpensive magnetometers are among the many technologies that condensed-matter physicists and materials scientists will be called on to develop for clinical and pharmaceutical use.

Indeed, what the committee foresees is a merger of the health care and information technology sectors, with the mobile phone network eventually being the platform for diagnostics and the real-time management of therapies. The hope is that there will finally be a Moore's law for health care provision, with productivity increases finally exceeding spending increases as insatiable demands for ever-better prevention and treatment are met. Because of the associated demands for miniaturization and quantitative rigor as well as the fact that medicine ultimately deals with the materials systems of life, there are tremendous opportunities for contributions from CMMP, and especially from subfields such as soft matter and nanometrology. There are also less immediately obvious subfields that will contribute to meeting the needs of health care; these include even the area of devices for quantum encryption, which might find use in ensuring the confidentiality of the exchange of patient records.

## IMPACT ON OTHER SCIENTIFIC DISCIPLINES

CMMP plays a vital role in other disciplines of science in two ways. First, CMMP technologies, such as materials and devices ranging from nonlinear organic materials to charge-coupled-device detectors, are ubiquitous in laboratories throughout the scientific enterprise. Second, as science expands and the disciplinary boundaries blur, concepts originating in CMMP—for example, fermion pairing or the statistical mechanics of biological molecules (Chapter 4)—find increasing relevance. Examples of the impact of CMMP on other subfields of physics and on other disciplines are illustrated by atomic, molecular, and optical (AMO) physics; nuclear and high-energy physics; astronomy; chemistry; biology; and information technology and computer science.

### Atomic, Molecular, and Optical Physics

Scientific and technological connections between CMMP and atomic, molecular, and optical physics are historically strong, principally because of similarities between the energy and length scales of the two fields. Laser and optical technology, developed primarily within the AMO community, has wide application in CMMP research for materials characterization and processing. While lasers are the most prominent and wide-reaching connection so far, the recent development of methods to trap and cool atoms into the nano-kelvin regime also has the potential to affect CMMP profoundly, by enabling the realization of some of the most fundamental models of condensed-matter physics.[11]

Lasers have long been used to characterize materials by a variety of techniques. Photoluminescence spectroscopy, for example, is widely employed to measure band gaps and to identify defects and impurities. Sensitivities down to the single-molecule level have been achieved. Ultrafast laser technology, with pulse durations in the femtosecond regime, can reveal critical information about charge carrier dynamics, such as relaxation processes, needed for the characterization of semiconductor materials for the potential application of these materials in devices. Femtosecond pulses are also used in time-resolved photoemission spectroscopy to determine surface states and relaxation processes in solids, and they can be used to study structural phase transitions in real time. Bound electron-hole pairs, known as excitons, may be created by the laser excitation of semiconductors and their dispersion properties measured using laser spectroscopy. Laser-induced light scattering is also commonly used to characterize the distribution of particles in random and diffuse media. Laser technology is routinely employed in CMMP research to process and anneal materials.

While CMMP benefits from laser technology developed by the AMO community, optical materials developed by CMMP scientists are essential to many laser applications. Nonlinear optical materials, for example, have profoundly affected almost all applications of lasers. Newly developed organic and polymer nonlinear materials, a forefront area of investigation in CMMP, are being integrated with semiconductors and used for optical information processing and data storage.

Fundamental connections between the AMO and CMMP communities have grown recently owing to developments in ultracold atomic research. In the past 10 years, laser cooling and evaporation techniques have been employed by AMO physicists to cool composite atomic bosons, such as $^{87}$Rb and $^{7}$Li, as well as the fermions $^{40}$K and $^{6}$Li. Temperatures in the nano-kelvin regime are routinely achieved. At these temperatures, quantum-state occupancy is of order unity, and the gases may undergo Bose-Einstein condensation or fermion pairing into a superfluid state, phenomena long ago discovered and explained by CMMP scientists in the context of superconductivity and superfluidity of liquid helium $^{4}$He and $^{3}$He.

An emerging theme is that systems of ultracold atoms may be used as idealized and highly tunable model systems for fundamental problems in condensed-

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[11] For additional detail, see National Research Council, *Controlling the Quantum World: The Science of Atoms, Molecules, and Photons*, Washington, D.C.: The National Academies Press, 2007.

matter physics. Their utility as model systems derives from the fact that they are inherently "clean," with no uncontrolled defects, impurities, or disorder, and that their physical properties, such as density, temperature, geometry, and perhaps most importantly, interaction strength, are widely tunable. By imposing an optical lattice formed by the interference of laser beams, periodic potentials in various dimensions and geometries may be created, thus simulating an underlying crystal lattice (Figure 8.1).

Spurred by prior discoveries in CMMP, recent experiments with ultracold atoms have been remarkably successful in modeling important problems in condensed-matter physics, including the observation of the superfluid to Mott insulator transition, the Bose-Einstein condensation to Bardeen-Cooper-Schrieffer (BEC-BCS) crossover, vortex lattices, and the Josephson effect. Several of these are examples of emergent phenomena and are discussed in more detail in Chapter 2. The Mott insulator, which arises in periodic structures with strong on-site repulsion, is an example of strong particle correlations resulting in a dramatic change in the macroproperties of the gas. It was realized with cold atoms by imposing an optical lattice onto a Bose-Einstein condensate.

The BEC-BCS crossover in paired fermions is a concept going back more than 25 years in the CMMP community, where it was first realized that there is an intimate connection between BCS pairing, the underlying mechanism of superconductivity and superfluidity in $^3$He, and Bose-Einstein condensation of composite bosons that are created by binding two fermions. Although apparently quite different, the BEC and BCS regimes are just the extreme limits of a continuum. In the BEC limit, the superfluid corresponds to a condensation of tightly bound bosonic molecules, while in the BCS limit, pairing is a many-body phenomenon involving correlated but spatially diffuse pairs of fermions of opposite spin. Probing the crossover requires that the strength of interaction between particles be varied, which can be accomplished with ultracold atoms using a Feshbach resonance.

The effect of pairing when the two spin states have unequal Fermi energies has long been of interest to CMMP. Exotic new phases with broken-space symmetries

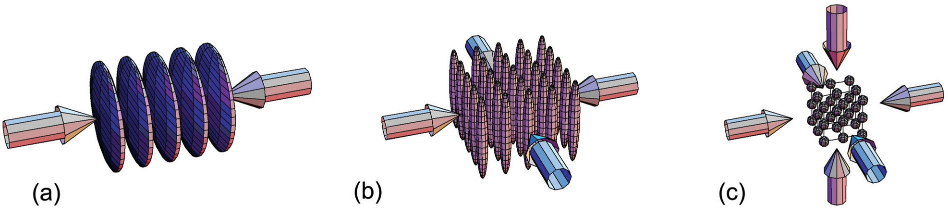

FIGURE 8.1 Optical lattices in (a) one dimension, (b) two dimensions, and (c) three dimensions may be used to create arrays of confined atoms in lower dimensions. SOURCE: E. Mueller, Cornell University.

were predicted more than 40 years ago but have been difficult to confirm owing to the fundamental incompatibility of magnetism with the usual forms of superconductivity. In contrast, making unbalanced mixtures of atomic Fermi gases is straightforwardly accomplished by driving radio-frequency transitions between the states. New experiments have begun to explore the phase diagram. The relevance of these experiments goes beyond CMMP, as unbalanced pairing is expected to be an important ingredient in the quark-gluon plasmas formed in high-energy collisions of heavy nuclei and could also play a central role in understanding neutron stars (see the following subsection on connections between CMMP and nuclear and high-energy physics).

As discussed in Chapter 2, strong correlation effects often manifest themselves in lower dimensions, where particle interactions can more easily dominate the kinetic energy. Atoms confined to lower dimensions can be achieved using various optical lattice configurations. For example, two counter-propagating laser beams can divide a cloud into a number of quasi-two-dimensional sheets (Figure 8.1b). The two-dimensional Kosterlitz-Thouless transition, a transition to a superfluid state without Bose-Einstein condensation previously studied in CMMP in connection with interacting spin systems, was realized with cold atoms using this configuration. Four lasers in a plane can be used to make a square array of ultracold atoms confined to quasi-one-dimensional tubes (Figure 8.1a), which has promise to realize the exactly solvable model of an interacting one-dimensional gas of fermions. One of the most significant outcomes of strong correlations is the emergence of quasi-particles that are no longer the single-particle-like excitations of the conventional Landau-Fermi liquid theory, as discussed in Chapter 2. A one-dimensional Fermi gas, which should exhibit a separation of the single-particle spin and charge degrees of freedom, may provide a highly idealized system for studying this remarkable effect. One of the most significant opportunities for CMMP would be the realization of the Hubbard model, in which particles can hop from lattice site to lattice site, interacting repulsively on doubly occupied sites. While the Hubbard model is the most prominent model of high-temperature superconductors, it is still not known for sure whether it reproduces the essential properties of these materials. One can envision that systems of ultracold atoms, acting as highly tunable quantum simulators, can resolve this and other similarly vexing issues in CMMP in the near future.

These growing connections between CMMP and AMO physics have blurred the boundaries where these two fields intersect. Increasingly, young CMMP physicists, particularly theorists, are engaging in ultracold atom research. Similarly, AMO physicists are applying their expertise to CMMP-related investigations. An indication of the growing interconnection is that an increasing fraction of the program of the American Physical Society's annual March Meeting, the traditional venue for presenting CMMP research, is being devoted to ultracold atom physics. Federal funding agencies, in particular the Department of Defense, have recognized the intellectual fervor developing at this interdisciplinary boundary by establishing new funding initiatives. Some university physics departments have already introduced new graduate-level courses to prepare students for interdisciplinary CMMP/AMO research, and more are in development. As in other areas of scientific research, interdisciplinary research can be very productive scientifically, but it also challenges the existing infrastructure to adapt to changes.

### Nuclear and High-Energy Physics

CMMP has had a significant impact on nuclear and particle physics over the years, ranging from the development of advanced detector materials to fundamental studies of nuclei, neutron stars, and elementary particles. Examples of detector technology made possible by CMMP research include ultrapure silicon wafers used for charged-particle detection, avalanche photodiodes, and large, very pure crystal scintillation materials. Such connections are not unexpected, since nuclei, as well as the vacuum, as complex many-body systems, present intellectual challenges with many similarities to those of condensed-matter physics. For example, the shell structure of nuclei owes its existence to the Pauli exclusion principle lengthening mean free paths of nucleons near the Fermi surface, in precisely the same way that electrons in normal metals often behave as nearly free particles. Indeed, corrections to free-particle behavior, seen in experiments on nuclei in which particles are removed or added, are understood in the same way as in condensed-matter systems such as metals.

The discovery of the BCS theory of superconductivity had an immediate impact on nuclear physics: Cooper pairing of neutrons and of protons explained many features of the single-particle excitation levels, as well as the larger-than-expected spacing of the energies of states of rotating nuclei in terms of a reduced moment of inertia—the analog of the Meissner effect in superconductors.

In neutron stars—in essence, giant nuclei with masses somewhat greater than that of the Sun, and the driving engines of pulsars and related high-energy astrophysical phenomena—the neutron liquid is expected to be superfluid, and the proton liquid, superconducting. The superfluidity in rotating stars gives rise to vortices, as in superfluid liquid helium, whose sporadic motions explain the observed sudden speedups (glitches) of pulsars. Indeed, elucidation of the properties of neutron stars, as well as of other astrophysical systems including the early universe, has depended considerably on techniques—for example, transport theory—previously developed for condensed-matter systems.

The ideas of BCS theory have also been extended to quark-gluon plasmas, the liquid of quarks and gluons that constituted matter in the early universe prior to a few microseconds after the big bang, the matter that is produced in ultrarelativistic heavy-ion collisions, and that may possibly be present in neutron stars. Cold quark-gluon plasmas are predicted to have a rich structure of Cooper-paired states, which could influence observed properties of neutron stars.

More generally, the concept of the spontaneous breaking of symmetries, which arose in describing condensed-matter systems such as antiferromagnets and superconductors, has come to play a dominant role in elementary particle physics. For example, the internal symmetry of the standard model of strong and electroweak interactions is spontaneously broken as the temperature in the early universe falls. This breaking leads to a finite expectation value of the Higgs field in the vacuum, which is responsible for the masses of the fundamental quarks, vector bosons, and leptons—analogous to the way the Anderson modes of a superconductor develop a finite frequency gap in a superconductor.

The intellectual flow between work on condensed-matter and nuclear systems has in fact been in both directions. Research in one area frequently inspires new insights and approaches in other areas. For example, work on vortices in neutron stars has led to new insights into Bose-Einstein condensates, superfluids, and superconductors. Similarly, studies of neutron matter have led to new insights into the behavior of strongly coupled atomic clouds, and into the general properties of superfluid Fermi gases. Current areas of study include questions about the similarity of the transition between Bose-Einstein condensation and BCS pairing in condensed matter and the deconfinement transition of dense hadronic matter; the observed low viscosity of strongly interacting quark-gluon plasmas and condensed atomic clouds; and BCS pairing of imbalanced Fermi seas in superconductors, trapped fermionic atomic clouds, and quark-gluon plasmas.

In addition, expertise developed for condensed-matter systems, such as quantum Monte Carlo computational techniques and techniques of many-body theory at finite temperatures, have played important roles in modern nuclear physics, leading, for example, to exact Green's function Monte Carlo calculations of the levels of all nuclei up to mass number eight.

### Astronomy

The contribution of CMMP to astronomy and experimental astrophysics is hard to overstate. Virtually every modern telescope, whether observing gamma rays, visible photons, or radio waves, has a sophisticated solid-state detector at its focus. At optical wavelengths, silicon charge-coupled-device (CCD) arrays long ago supplanted photographic plates, in much the same way that they have recently done in ordinary photography. In the millimeter band (which includes the cosmic microwave remnants of the big bang and accounts for most of the electromagnetic energy in the universe), semiconductor diode detectors and, more recently, superconducting transition-edge sensors are used for photometric observations.

Heterodyne mixers based on superconducting tunnel junctions are now in wide use for high-resolution studies of molecular absorption lines. At very high energies, NASA's Chandra X-ray Observatory, launched aboard the space shuttle in 1999, uses silicon CCD detectors to study gamma-ray bursts and other spectacular astronomical events.

The catalog of the various solid-state detectors in use in modern astronomy is a very long one, and a thorough review would be inappropriate here. Instead, a single new detector concept that promises to have a large impact on astronomy in the coming decade is discussed: the so-called kinetic inductance detector (KID). The KID is a particularly appropriate example, since it relies on aspects of non-equilibrium superconductivity that themselves are not far from the research cutting edge in CMMP.

The heart of a KID consists of a small strip of superconducting metal forming the inductor of a resonant "tank" circuit embedded in a conventional transmission line. On resonance (at typically ~10 GHz), the tank circuit loads down the transmission line and reduces its transparency, an easily detected effect. A remarkable property of a superconductor is that the inertia of moving Cooper pairs within it contributes significantly to its inductance. Incoming photons, with energies larger than the superconducting energy gap, tear apart a number of Cooper pairs and thus modify this inductance. This in turn shifts the resonant frequency of the tank circuit and changes the transmission through the line.

The KID concept has a number of key advantages. Perhaps most important is its straightforward extension into an array geometry. Pixelated array detectors are essential in modern astronomy and astrophysics, in part because in many cases the noise in individual detector elements is actually due to photon-counting statistics, not to external amplifier noise. Detector arrays gather more photons and thus increase the net signal-to-noise ratio. The resonant tank circuit and transmission line of the kinetic inductance detector are readily fabricated by conventional lithographic means. It is therefore easy to embed many resonant circuits in the same transmission line, each designed with a slightly different resonant frequency. In this way a detector array can be made, and each "pixel" can be rapidly addressed via a simple frequency multiplexing scheme. In addition, kinetic inductance detectors are sensitive over an extremely broad energy band, from the very low energies characteristic of the cosmic microwave background to the very high energies encountered in x-ray astronomy.

The connections between CMMP and astronomy and astrophysics are certainly not limited to detector technology. There are many fundamental scientific connections as well. (Connections between CMMP and astronomy, astrophysics, and cosmology are discussed in the previous subsections.) For example, the classic CMMP concepts of superfluidity and superconductivity are quite relevant to the internal structure and dynamics of neutron stars. Similarly, the notion of spontaneous symmetry breaking discussed in Chapter 2 in the context of phase transitions in condensed matter is also a cornerstone of our understanding of the very early universe, just moments after the big bang. Finally, neutron stars and other astrophysical objects are, in effect, laboratories for the study of materials under conditions (ultrahigh density, magnetic field, and so forth) that no terrestrial laboratory will ever replicate.

## Chemistry

Advances in a number of areas of CMMP have had an important impact on developments in chemistry, especially in the areas of materials chemistry and physical chemistry. In the area of computation, the importance of density functional theory—which is now used extensively by chemists to calculate the electronic structures of materials and by polymer physicists to calculate the structure of polymer molecules in solutions and melts—was recognized by the sharing of the Nobel Prize in chemistry by physicist Walter Kohn in 1998. In the field of soft condensed matter, theoretical concepts and methods from statistical physics such as percolation theory, renormalization group, scaling, (self-consistent) field theory, disordered systems (quenched disorder, spin glasses), and to some extent liquid-state physics, have had an enormous impact on macromolecular science. Ideas taken from the understanding of systems such as Ising models and magnetism, for example, are now applied to the interpretation of phase transitions in polymer mixtures and block copolymers.

CMMP has also had a very great impact on the chemistry of materials through the development of advanced characterization tools, such as light sources for synchrotron x-ray diffraction and extended x-ray absorption fine structure studies, neutron sources for diffraction, spectroscopic and small-angle scattering studies, and advanced transmission electron microscopes for high-resolution imaging. Instruments based on the scanning tunneling microscope (STM), for which Rohrer and Binnig won the Nobel Prize in physics in 1986, have made key contributions to the chemistry of nanomaterials in recent years. In particular, the atomic force microscope (AFM), which uses broadly the same principle as that used by the STM but does not require the sample to be conducting, is now used ubiquitously by chemists and others to obtain images of surfaces with atomic resolution.

Sometimes, of course, the fundamental developments in physics take many years to make their mark. The discovery of nuclear magnetic resonance (Nobel Prize in physics, 1952) only gradually developed into one of the most powerful characterization tools in organic chemistry, polymer science, and molecular biology, but finally led to several Nobel Prizes in chemistry (e.g., 1991, 2002), as well as the 2003 Nobel Prize in physiology or medicine for the development of magnetic resonance imaging (MRI).

The symbiotic nature of the relationship between CMMP and chemistry is reflected in the fact that synthetic chemists have enabled some of the most exciting advances in condensed-matter physics in recent years. Advances in conducting polymers and molecular electronics over the past 25 years were initially launched by the synthesis of polyacetylene films in the laboratory of Shirakawa in Japan. Subsequent collaborations between physicists and chemists led to the electrical characterization of this and related materials, and the resulting explosion of work in the area is now impacting technologies as disparate as biosensors and photovoltaic cells. Similarly, the discovery of buckminsterfullerene, $C_{60}$, in the Chemistry Department at Rice University in 1985 (Nobel Prize in chemistry, 1996) provided the impetus for the identification of carbon nanotubes in 1991 and arguably for the dramatic advances in nanoscience witnessed during the past decade.

In the hard condensed-matter area, the lanthanum cuprate high-temperature superconductors, for which Bednorz and Muller received the 1987 Nobel Prize in physics, were first synthesized by chemists in France and Russia in the 1970s and 1980s, although the remarkable electronic properties of these materials were not appreciated at the time. The same can be said for magnesium diboride ($MgB_2$), which was synthesized by chemists as early as 1954, but it was not until 2001 that the exciting superconducting properties of $MgB_2$ were revealed; 6 years later it is already being developed for use in a new generation of superconducting magnets for MRI.

Physics and chemistry will continue to be inextricably linked, and many exciting future discoveries in the CMMP area will be found at the interface between these two important fields. It is essential that this interface be nurtured by bringing chemists and physicists together at interdisciplinary research centers such as the NSF Materials Research Science and Engineering Centers and the Department of Energy Nanoscale Science Research Centers. It is also important to recognize the role of national facilities, such as the neutron and light sources, in providing opportunities for scientists from different disciplines to discuss their findings and different perspectives on CMMP research. Finally, the committee would like to stress the importance of such interfaces in education, as discussed elsewhere in this report.

### Biology

The experimental methods of CMMP have had an enormous impact on biology and medicine, and the committee expects that this will continue and grow in the coming decade. While the discussion of the challenges to CMMP researchers in biology (Chapter 4) emphasized new questions that physicists ask about living systems, this subsection focuses on the application of CMMP techniques to questions posed by biologists; for the impact of CMMP on medicine and health care, see the earlier discussion in this chapter.

One of the lasting legacies of the revolution that created molecular biology is the idea that biological function is linked tightly to molecular structure; nowhere is this more obvious than in the case of deoxyribonucleic acid (DNA). This link makes the determination of molecular structures a central problem in biology. Roughly 50 years have passed since the first protein structures were solved using x-ray crystallography. Today, many biologists look forward to the day when they will be able to determine the structure of all proteins at atomic resolution. This grand effort, sometimes referred to as structural genomics, is conceivable only because of dramatic improvements in the performance of synchrotron light sources (see Chapter 11). The increased brilliance of these sources means that data collection is faster, that radiation damage is reduced, and that smaller crystals are sufficient. At the same time, a number of groups are investigating the physics of protein crystallization itself, in an attempt to increase the efficiency of this most problematic step in sample preparation. Finally, as with all fields of science, mastery over the physics of semiconductor devices has driven the dramatic improvements in computational power that make solving a complex molecular structure a routine calculation. Thus, the biologists' dream of a complete catalog of biomolecular structures is being enabled by the technology generated in the CMMP community.

For the CMMP community, some of the most striking aspects of magnetic resonance involve relaxation processes: how spins exchange energy with each other and with their surroundings, and how these interactions build a bridge between the coherent quantum dynamics of isolated spins and the dissipative behavior of macroscopic samples as they come to thermal equilibrium. It is the understanding of these relaxation processes that has made magnetic resonance such a useful tool in investigating biological systems.

In proteins, the fact that energy transfer or cross-relaxation between two spins depends on their spatial separation means that relaxation experiments can measure, more or less directly, the distance between atoms even as the protein tumbles freely in solution. These distance measurements can be combined to generate accurate three-dimensional structures with nearly the same accuracy as that of x-ray diffraction but without the need to form crystals. Improvements in high magnetic field techniques will extend the range of applicability of these methods to yet larger molecules.

The bulk of any living organism is water, and the easiest magnetic resonance signal to detect is thus from the water protons. But the relaxation dynamics of these protons is sensitive to their environment, responding even to relatively subtle changes such as the oxygen content of blood. The beautiful brain images seen even in the popular press are derived from this subtle effect: when cells in a particular region of the brain are more active, they use more oxygen, and the change in oxygenation level of the blood flowing to these regions changes the relaxation time of the proton spins. Images of spin-relaxation time thus provide an image of neural activity, literally showing which regions of the brain are involved in particular tasks or even particular thoughts. Functional magnetic resonance imaging, as it is called, has evolved in roughly 15 years from a physics experiment into a standard technique for psychology laboratories. While knowing which areas of the brain are involved in a process does not describe how things work, the images that emerged from this work have completely changed the language for discussion of cognition, and in this sense are beginning to transform our view of ourselves as humans.

Optical microscopy is a venerable technique that has undergone a renaissance in the past decade, especially in its application to biological systems. Lasers have made confocal microscopy commonplace, and scanning multiphoton fluorescence microscopies have made it possible to reach deep into tissues such as the brain and observe dynamics on the micron and submicron scales, revealing, for example, the continual making and breaking of connections between neurons as animals learn about their environment. Microscopy using evanescent waves makes it possible to focus on events within 100 nanometers of the cell surface, and near-field scanning probes provide even higher resolution. Recent developments combine scanning microscopy with photo-switchable probes to literally count every molecule of a given class. Related ideas combine surface microscopies (either optical or electron microscopy) with laser ablation to provide detailed, three-dimensional structures of fixed tissue, holding out the potential to revolutionize the study of anatomy in general and the “wiring diagram” of the brain in particular.

### Information Technology and Computer Science

In this subsection, the intellectual connections between CMMP and information technology and computer science are discussed. The economic connections are discussed in Chapter 7 and earlier in this chapter. CMMP has contributed enormously to the development of devices for information technology; it has made modern computers possible. These contributions are outlined further in Chapter 7. Less obviously, statistical physics concepts developed in CMMP in order to understand complex and emergent phenomena in materials have also contributed to the development of computer science. The Metropolis algorithm and Monte Carlo methods, which compute properties by the judicious sampling of possibly favorable configurations, were first used in nuclear physics and further developed in condensed-matter physics. They were the first of a broad class of methods than can be used to find approximate but very accurate solutions to difficult search problems.

More sophisticated search algorithms followed, motivated by the need to analyze systems which have many distinct and unrelated configurations that are comparably favorable. The simulated annealing algorithm of Kirkpatrick, Gelatt, and Vecchi is a generalization of a Monte Carlo method, inspired by slow cooling techniques in crystal growth, for examining the possible states of many-body systems. In this method, once the system has found one favorable configuration, it can draw energy from a thermal reservoir to jump away and search further for more favorable configurations of distinct character. Such Monte Carlo methods have since been applied to classic optimization problems in computer science such as the traveling salesman problem.

The Swendsen-Wang algorithm, another method for making large jumps to explore distinct classes of configurations to identify favorable ones, has been applied to problems such as graph partitioning and computer vision. Studies of the spin glass problem—the problem of calculating the lowest energy state of a disordered system—have contributed to understanding in the theory of computational complexity. For a spin glass, like many other so-called nondeterministic polynomial problems, the running time of all known algorithms increases exponentially with the size of the problem, and the challenge is to determine if there is no algorithm for which the running time is polynomial rather than exponential. Correlation and scaling laws from statistical mechanics are used to describe and understand the structure and emergent behaviors of large computer networks. Concepts of self-organized collective behavior from CMMP are now at the frontier of computer science and robotics, as researchers strive to find general rules for the emergence of sophisticated collective behavior from networks of computing agents interacting by simple rules.

Finally, it has become clear in recent years that the theory of the transmission and processing of intact quantum states represents a profound extension of the classical theories of information and computation, significantly altering the assessment of the kind and quantity of physical resources needed to solve various computational problems. The developing theory already has some applications to cryptography, and, if general-purpose quantum computers can be built, a large class of optimization problems will be solvable in a time proportional to the square root of the time presently required. A few problems, such as factoring of large integers, would be sped up even more. Thus, the theoretical study of quantum computation has become a new and vital branch of both computer science and theoretical physics, and the CMMP research community is making enormous contributions to the development of the new devices that will be required in the future for practical quantum computing.

## INTERDISCIPLINARY RESEARCH IN CMMP

Increasingly, the nature of CMMP research is becoming more interdisciplinary, and its scope is broadening. CMMP researchers are jointly working with other physicists in areas such as atomic, molecular, and optical science and particle physics, and with researchers in other disciplines such as chemistry, biology, and astronomy. CMMP approaches are being applied to problems ranging from energy conversion to information technology to biological systems and other far-from-equilibrium systems such as the climate. If the United States is to continue to be a leader in these scientifically and economically important areas, funding agencies should support the emerging interdisciplinary research that underpins them. However, the current organizational structure at funding agencies is based on subfield boundaries established decades ago. This structure hinders individual researchers from venturing into nontraditional, rapidly evolving areas. The first of the committee's two recommendations below is intended to promote more efficient approaches toward advancing emerging interdisciplinary research areas. This recommendation is further supported by and discussed in a general context in the National Research Council report *Facilitating Interdisciplinary Research.*[12]

## RECOMMENDATIONS

> **Recommendation:** Funding agencies should work to develop more-effective approaches to nurturing emerging interdisciplinary areas for which no established reviewer base now exists. The CMMP community should organize sessions at national meetings to engage funding agencies and the community in a dialogue on best practices for proposal review and for the support of nontraditional, rapidly evolving areas.
>
> **Recommendation:** Outreach, K-12, and undergraduate science education initiatives should be supported through supplemental or stand-alone grants administered by separate National Science Foundation and Department of Education programs, instead of through individual research grant awards. In the present system, the quality of outreach programs is a criterion in the evaluation of NSF/Division of Materials Research grants. The present approach confuses two conceptually distinct goals to the point that neither is optimally served. The funding agencies and the research community both want outreach programs to succeed, and they should confer to determine how best to implement an effort to achieve that goal.

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[12] National Academy of Sciences, National Academy of Engineering, and Institute of Medicine, *Facilitating Interdisciplinary Research*, Washington, D.C.: The National Academies Press, 2005.

# 9

# Industrial Laboratories and Research in Condensed-Matter and Materials Physics

## HISTORY OF INDUSTRIAL RESEARCH LABORATORIES

The 20th century was an era of large, well-funded corporate research laboratories focusing on research in the physical sciences and related engineering disciplines. General Electric (GE) Laboratories founded in 1900, Bell Laboratories founded in 1925, IBM T.J. Watson Laboratories founded in 1945, and Xerox Palo Alto Research Center (PARC) founded in 1970 are examples of major corporate-funded laboratories that encouraged large groups to work on long-range research. Breakthroughs such as x-ray tubes, transistors, lasers, cellular telephones, graphical user interfaces, and other technologies that define the beginning of the 21st century were the result, as summarized in histories of the industrial laboratories.[1] Some Nobel Prize–winning contributions from industrial laboratories are summarized in Table 9.1.

These powerful corporate laboratories, harboring some of the greatest scientists and engineers of the time, were enabled by the market dominance of their parent corporations. GE, Xerox, and IBM dominated lighting, copiers, and computers, respectively. Kodak, Polaroid, and Westinghouse had similar histories. As a government-regulated monopoly, AT&T ran the telephone network. These companies generated large amounts of cash that enabled them to invest in the future with fundamental, long-term research. The results have been stunning. Fundamental

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[1] Richard S. Rosenbloom and William J. Spencer, eds., *Engines of Innovation: U.S. Industrial Research at the End of an Era*, Boston, Mass.: Harvard Business School Press, 1996.

TABLE 9.1 Some Nobel Prize–Winning Contributions from Industrial Laboratories

| Activity | Corporate Sponsor | Name of Researcher(s) and Date of Prize |
|---|---|---|
| Surface chemistry | GE Laboratories | Langmuir, 1932 |
| Electron diffraction | Bell Laboratories | Davisson and Thomson, 1937 |
| Transistor | Bell Laboratories | Bardeen, Brattain, and Shockley, 1956 |
| Maser-laser | Bell Laboratories/Columbia University | Townes, Basov, and Prokhorov, 1964 |
| Quantum tunnel junctions | IBM T.J. Watson Laboratories/ GE Laboratories | Esaki and Giaever, 1973 |
| Theory of disordered materials | Bell Laboratories | Anderson, Mott, and van Vleck, 1977 |
| Cosmic microwave background radiation | Bell Laboratories | Penzias and Wilson, 1978 |
| Scanning tunneling microscopy | IBM Zurich Research Laboratory | Binnig and Rohrer, 1986 |
| High-temperature superconductivity | IBM Zurich Research Laboratory | Bednorz and Mueller, 1987 |
| Quantum Hall effect | Bell Laboratories | Laughlin, Stormer, and Tsui, 1998 |
| Integrated circuit | Texas Instruments | Kilby, 2000 |

SOURCE: See http://nobelprize.org.

inventions, such as the transistor from AT&T, the semiconductor diode (or communications) laser from IBM and GE, and many others enabled the revolution in consumer electronics, information technology, and digital communications that is still sweeping the world today. Ironically, the global changes sparked by these and many other inventions have, over decades, weakened U.S. industrial research in the physical sciences.

In particular, information technology has been a key enabler of globalization and its resulting intensified economic competition. Information technology has upset natural monopolies in communications and computers and is sweeping entire job categories, products, and industries into the dustbin of history, even as it creates new ones. Newer industrial research laboratories established by Microsoft, Google, IBM, and others focus principally on software, systems, and services. This has also been the growth direction for some of the longer-established industrial laboratories. And some of these new software-focused laboratories have been set up in other countries to attract local talent and to improve understanding of and participation in rapidly growing local markets. In sum, these changes have led to the downsizing or elimination of some once-great industrial laboratories and have greatly reduced the focus on physical sciences research in others.

In addition to generating countless inventions that have driven the U.S. economy, this core of industrial laboratories has also provided large numbers of scientific and technological leaders to industry, academia, national laboratories, and the government. This training ground for future leaders in science, education, and policy is also diminished by the changes in the industrial laboratories. After a century of scientific and technological leadership, the consequences to the U.S. economy and national pride of going from best-in-class to technology followers would be devastating. So, what research organizations and institutions will drive innovation in the physical sciences for the next hundred years?

In the decades following World War II, the federal government was the major provider of U.S. funds for research and development (R&D). Since 1980, the industrial investment has exceeded the government investment and today represents over two-thirds of the national effort. However, the bulk of the industrial investment in R&D is in incremental improvements to existing products, while longer-range research has declined; today it almost certainly represents less than 10 percent of the industrial investment (see, for instance, the discussion in Chapter 10 of Figure 10.15). The federal government is now the larger investor in fundamental long-range research, and this is especially true in condensed-matter and materials physics (CMMP). Other investment in U.S. R&D comes from foundations, states, and private individuals. This funding is increasing, and today some of the longer-range work in CMMP comes from state sources. The states of New York, California, and Texas have been leaders in this area.

The sharp rise of venture capital in the 1990s is also changing the face of R&D investments. Some of today's venture-funded start-up companies are pursuing research models that they hope will be more efficient than the older model of the centralized industrial research laboratory. Through the licensing of intellectual property from universities at low rates and the hiring of the graduate students who generated that intellectual property, these companies strive to translate academic research rapidly into product innovations that they can license to large companies. Note, however, that these companies do not themselves, as a rule, pursue basic or long-term research.

The Bayh–Dole Act (or University and Small Business Patent Procedures Act) of 1980 (Public Law No. 96-517) has also contributed to changes in R&D investment practices. It reversed the presumption of title so that universities, small businesses, or nonprofit institutions pursuing government-funded research can elect to pursue ownership of a resulting invention before the government. The act thus encouraged universities and small companies to pursue the licensing and development of such inventions. However, some observers maintain that the act has encouraged some universities to be very protective of all potential intellectual property development and that this practice has hindered university-industry research partnerships.

## FILLING THE GAP: NEW APPROACHES TO LONG-TERM RESEARCH

With reduced participation by industrial laboratories, breakthroughs resulting from long-term research must increasingly come from universities, national laboratories, and/or industry-led consortia. For example, the National Nanotechnology

Initiative (NNI) led to the creation of the Department of Energy (DOE) Nanoscale Science Research Centers (NSRCs), which represent an organizational innovation—an effort to include university students, faculty, and industrial researchers in government-funded, interdisciplinary centers focused on nanoscience. The NSRCs thus differ in some significant ways from other DOE beamline-based facilities. The five NSRCs collectively are similar in cost to a single large DOE synchrotron, in terms of cost for construction (about $380 million total) and operation (about $100 million per year).[2] As for the large DOE facilities, users from any institution (in the United States or elsewhere) may submit a proposal that is peer-reviewed for science to be done at the facility.

For the DOE NSRCs to re-energize long-term basic research in CMMP, they need, in addition to "user" facilities, a large in-house base of world-class scientific talent. This staff should be challenged to foster great new ideas. It is not yet clear that the new research institutions are focusing sufficiently on nurturing a creative intellectual environment. While these centers represent a significant investment in an important emerging scientific research area, to be successful they must also attract and serve the needs of many industrial users, including start-ups and small companies. Can the ownership of intellectual property from the research provide protection to an organization developing commercial products? Is there a pathway for product development from the research, and does the government policy on indemnification restrict participation in the centers? There will undoubtedly be other questions that arise as work is performed at the NSRCs. If successful in producing research results and structured for other organizations to bring those research results quickly to market, these centers can serve as a model for future government-university-industry cooperation. However, due to the newness of these centers, the research community awaits further experience with their operation before drawing conclusions from this experience.

A second possibility for replacing some of the CMMP physics research done by the U.S. industrial laboratories is to enhance the research sponsored by industry in research universities. Today, U.S. industry funds less than 10 percent of university research, although the funding varies greatly by institution, with some of the better-known universities having greater than 30 percent of their research funded by industry.[3] The focus of much of this research is in engineering and business schools and little is in physics or materials research.

An example of industry-university cooperative research is the Semiconductor

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[2] Details on the construction and operation budgets of the DOE NSRCs can be found at http://www.sc.doe.gov/bes/archives/budget/BES_FY2008budget.pdf; last accessed September 17, 2007.

[3] National Science Foundation, Division of Science Resources Statistics, *Where Has the Money Gone? Declining Industrial Support of Academic R&D*, NSF 06-328, Arlington, Va., 2006. Available at http://www.nsf.gov/statistics/infbrief/nsf06328; last accessed September 17, 2007.

Research Corporation (SRC) founded by the U.S. Semiconductor Industry Association (SIA) in 1982. The SRC cultivated a pivotal cultural change for the semiconductor business, sharply raising the funding of relevant university research and the transfer of university research results into the semiconductor industry. Talented faculty members have received incentives to tackle outstanding semiconductor industry research problems and to train students who then seek employment with semiconductor companies. For about 25 years, much of the SRC funding has gone to engineering departments and has addressed incremental improvements to established devices and manufacturing process technologies. However, given increasing industry concern that transistor technology is approaching fundamental physical limits, some SRC programs are beginning to focus on long-term research in CMMP. One of these is the Focus Center Research Program (FCRP); another is the Nanoelectronics Research Initiative (NRI).

The SRC-FCRP consists of five centers, each composed of research groups from several geographically dispersed universities with funding from a subset of the SRC member companies and the Defense Advanced Research Projects Agency (DARPA). The FCRP research portfolio is longer term and higher risk than older SRC programs. A portion of this portfolio is aimed at exploratory materials and devices. The SRC-NRI consists of three major research centers with lead schools located in New York, Texas, and California. Funding comes from six of the leading U.S. semiconductor manufacturers and various state governments. NRI has also teamed with the National Science Foundation (NSF) to provide additional joint funding of existing NSF-funded research centers. NRI research focuses on new materials and device concepts that might someday replace the field-effect transistor as the foundation of information technology. The new materials might not be semiconductors. The new devices may operate by as-yet-undiscovered physical principles. This is a remarkable development, motivating top condensed-matter physicists to explore exotic physical systems with the goal of revolutionizing an entire great industry. For more on the motivation for this research, see Chapter 7.

In the SRC programs, there is broad and intimate contact between the engineers and scientists in the SRC member companies and the university students and faculty. The research directions are set by the university faculty with input from the SRC members. This process has been nurtured and modified over nearly 25 years and is considered a major success by universities and by the global semiconductor industry. It could serve as a model for enhancing condensed-matter and materials research in physics, chemistry, and materials science departments.

Finally, it might be possible to form research consortia that would involve international companies that would profit by funding university research and having increased interaction with students and faculty. There are consortia today in many economic regions around the world that have involved cooperative R&D. In the United States, SEMATECH was initially an effort by the semiconductor industry to solve short-term research needs. As part of this program, there was a $10 million program to fund SEMATECH Centers of Excellence at several U.S. universities. In 1995, SEMATECH became an international organization and withdrew from U.S. federal funding, permitting funding of research internationally. In Europe, the Interuniversity Microelectronics Consortium has both short- and long-term research in several universities. In Japan, there has been a history of cooperative efforts in semiconductors and computers. The pharmaceutical industry has a history of funding university research. Again, while much of this research is focused on short-term results, some of the consortia are investing in longer-range work that will be of interest to CMMP scientists and offer examples of possible future funding possibilities.

## CONCLUSIONS

The United States has lost a major source of innovation in CMMP with the changes that occurred in the great industrial laboratories of the 20th century. Replacement of this source of invention and leadership will be a major challenge. As described above, new research models are being tried. These include cooperative university-industry agreements, new interdisciplinary centers at the national laboratories that welcome university and industry researchers, and a variety of university-government-industry research consortia. There are undoubtedly other possibilities as well. The current approaches described here are focused on electronics and information technology, but other CMMP research areas that serve society can also benefit and advance from these approaches, such as energy research. These new approaches to long-term research are expected to evolve over the next decade, so the next decade will be one of exploration (see also related discussions at the end of Chapter 7).

It would be highly desirable for the physics community and the federal government to establish mechanisms to measure and compare the effectiveness of these evolving models for conducting scientific research—particularly those that are funded primarily by the government. Can we as a nation make the organizational and funding mechanisms work well for this new purpose—for creating scientific and technological breakthroughs and providing future scientific leadership? The national laboratories were not originally formulated to capture commercial economic dominance, and universities historically have existed to advance knowledge, not to develop new products. The semiconductor industry's effort in SRC and particularly in the new NRI program is one model to look to for lessons for introducing change. The DOE Nanoscale Science Research Centers are another example of this new mode of research. An evaluation of efforts such as these could identify the positive lessons to apply in the future about how to provide funding to stimulate vigorous innovation in CMMP research from which the United States reaps major economic rewards. Further, the DOE should evaluate the new NSRCs by metrics that include success in attracting a diverse set of industrial users and by other metrics as highlighted in the previous section. The National Nanotechnology Coordination Office, in its arrangement of the triennial review of the NNI, should evaluate all NNI-funded centers and networks of centers by similar metrics. For further discussion, see Chapter 11.

## RECOMMENDATION

> **Recommendation:** The Office of Science and Technology Policy (OSTP) should convene a study with participation from the Department of Energy, the Department of Defense, the National Science Foundation, and the National Institute of Standards and Technology, the physics community, and U.S. corporations to evaluate the performance of research and development (R&D) activities that might replace the basic science previously done by the large industrial laboratories and the contributions that those laboratories made to the training of future scientific leaders and educators. This next decade will involve a series of new approaches to long-term R&D designed to recapture the ability to work on large difficult projects based on fundamental CMMP research. Such an evaluation should be an ongoing activity of OSTP, since it may be several years before the performance of these activities can be adequately evaluated.

# 10

# Structure and Level of the Current Research Effort

Condensed-matter and materials physics (CMMP) is the largest and, in its scope, most diverse subfield within all of physics. By its nature, CMMP is also fundamentally a crosscutting research enterprise; it connects a multitude of subfields within physics, from semiconductors to biological physics, and it links physics with a multitude of other disciplines, from engineering to computer science to applied mathematics. This chapter looks at the available data for assessing the current level of federal research support, the demographics of the field, and the research output as measured by publications. Where data were available, the Committee on CMMP 2010 also compares the United States with other countries.

## FEDERAL FUNDING FOR CMMP RESEARCH

Federal support for CMMP research activities occurs through several funding venues, supporting work at universities and national laboratories. Agencies were asked to provide data for the past 10 years on funding levels, grant sizes, and success rates, as well as on the demographics of the CMMP-supported programs. Additional questions concerned the number and size of centers and of facilities supported. The breadth and range of research activities falling under CMMP make it difficult to arrive at a clean breakdown, especially since the federal agencies delineate their programs differently and much of the research is interdisciplinary. Besides condensed-matter physics and condensed-matter and materials theory, CMMP-related programs include aspects of ceramics, metals, polymers, electronic materials, and solid-state chemistry. More recently, nanoscience and nanotechnology have emerged as areas with a large and inherent overlap with CMMP activities. For the funding trends discussed here, the committee has made an effort to focus on CMMP-related physics efforts.

The primary funding sources in terms of the total amount of funds allocated for CMMP research over the past 10 years have been the National Science Foundation's Division of Materials Research (NSF DMR); the Department of Energy Basic Energy Sciences (DOE BES); the Department of Defense Army Research Office, Air Force Office of Scientific Research, and Naval Research Laboratory (DOD ARO, AFOSR, and NRL, respectively); and the National Aeronautics and Space Administration's Materials Physics and Condensed-Matter Physics programs (NASA MP and CMP).

The total funding for CMMP basic research from the sources listed above has varied little over the past 10 years. When corrected for inflation, using Office of Management and Budget (OMB) deflators, the net increase over this period is roughly 10 percent. Figure 10.1 gives the overall funding level for CMMP basic research at universities in inflation-adjusted fiscal year (FY) 2006 dollars. The total amount of support shown in this figure, roughly $600 million per year, includes the direct funding of research through grants to individual investigators and small

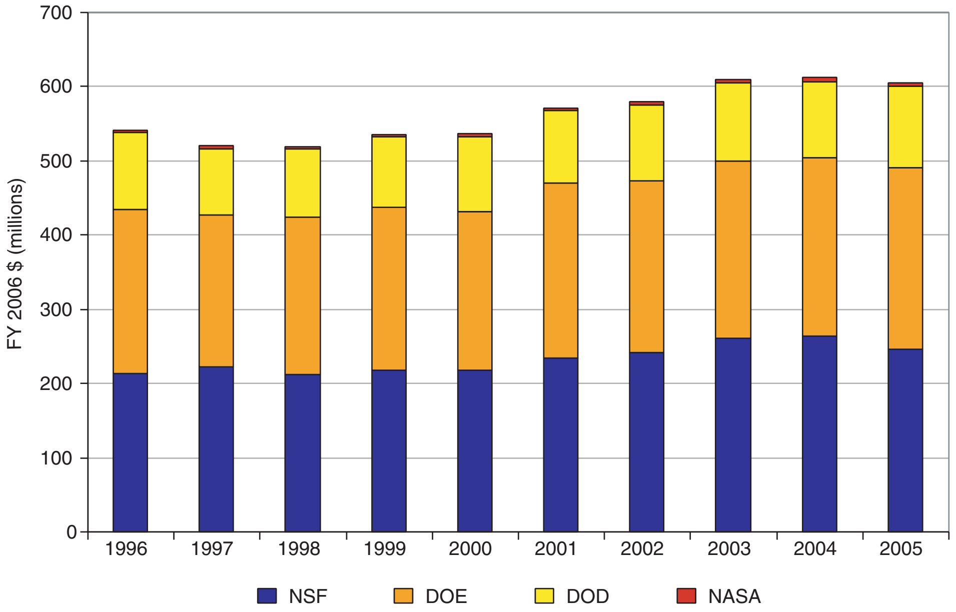

FIGURE 10.1 Federal investment in condensed-matter and materials physics basic research in terms of inflation-adjusted FY 2006 dollars. SOURCE: Data supplied to the Committee on CMMP 2010 by the respective agencies.

groups of investigators (such as Focused Research Groups at NSF) both at universities and national laboratories, and NSF DMR support for research centers such as the Materials Research Science and Engineering Centers (MRSECs), Science and Technology Centers (STCs), and Nanoscale Science and Engineering Centers (NSECs). In addition to the research support shown in Figure 10.1, CMMP benefits from investments by the federal government through the support of national laboratories, including the new DOE nanocenters, and investments into the construction and maintenance of large facilities, such as facilities for x-ray and neutron scattering, electron microscopy, high magnetic fields, and large-scale computation. These facilities are discussed in more detail in Chapter 11.

It is important to note that within each agency, individual program areas have evolved during the past 10 years, with some growing at modest amounts and others declining somewhat. However, there are situations in which downward fluctuations in specific programs of several agencies occur at the same time, thereby threatening whole areas of CMMP. This is particularly critical for smaller research efforts and emerging areas. During the past couple of years this has happened, for example, for research on colloids and granular materials. In other instances, whole programs have been eliminated, such as NASA CMP (at the end of 2006). Specific research areas strongly dependent on these funding sources are now in jeopardy in the United States.

For research at universities, a major cost factor is the support of graduate students. A survey by the Committee on CMMP 2010 of nine state and private universities indicates an average increase over the past 10 years of about 5 percent per year in the cost per graduate student, as charged to federal grants related to CMMP research. This increase includes the salary, health fees and tuition, and overhead. As pointed out in the National Research Council (NRC) study on the Materials Research Science and Engineering Centers,[1] the use of this deflator more realistically captures the actual costs associated with carrying out research at universities. In the present report, the committee identifies this deflator with the funding "buying power." Figure 10.2 indicates that, using this measure, the overall support for CMMP research has steadily declined over the previous decade. The NRC study *Midsize Facilities* also found that instrumentation costs over the past 10 years have risen far more quickly than inflation.[2] Since the actual cost of doing research is closely tied to the cost of supporting personnel, such as graduate

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[1] National Research Council, *The National Science Foundation's Materials Research Science and Engineering Center Program: Looking Back, Moving Forward*, Washington, D.C.: The National Academies Press, 2007.

[2] National Research Council, *Midsize Facilities: The Infrastructure for Materials Research*, Washington, D.C.: The National Academies Press, 2006.

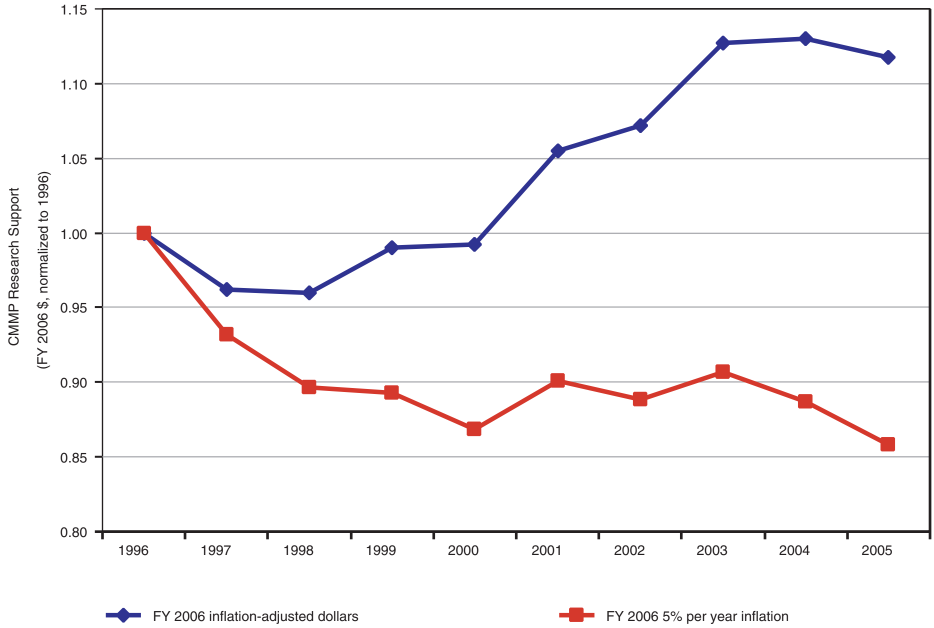

FIGURE 10.2 U.S. funding for basic research in condensed-matter and materials physics (CMMP), in FY 2006 dollars, normalized to 1996. The top curve takes inflation into account by using the Office of Management and Budget deflator (the same data as for Figure 10.1 are used). The bottom curve uses the average yearly increase in costs to support a graduate student (5 percent) as the deflator. This clearly indicates that CMMP research support experienced a decrease in “net buying power” over the past decade.

students, and instrumentation, CMMP research in the United States can only stay competitive if the level of funding increases in a commensurate way.

Within individual programs, funding can be delineated by support for individual investigators (or small teams), support for facilities, and support for larger groups such as research centers. Figure 10.3 gives this breakdown for NSF DMR for the past 10 years.

It is clear from these figures that, in NSF DMR, the support for individual principal investigators (PIs) has closely tracked overall DMR growth. Both have grown so modestly that, in taking the graduate student cost inflation into account, the “buying power” of an NSF grant has decreased (see Figure 10.2). For centers, the funding trend has been even worse, as they have been essentially flat-funded in inflation-adjusted dollars.

At DOE BES, grant support for CMMP research has also increased, from $181 million in 1996 to $220 million in 2006. This corresponds to an approximate 20 percent increase in as-spent dollars over the time period. Hence, when the

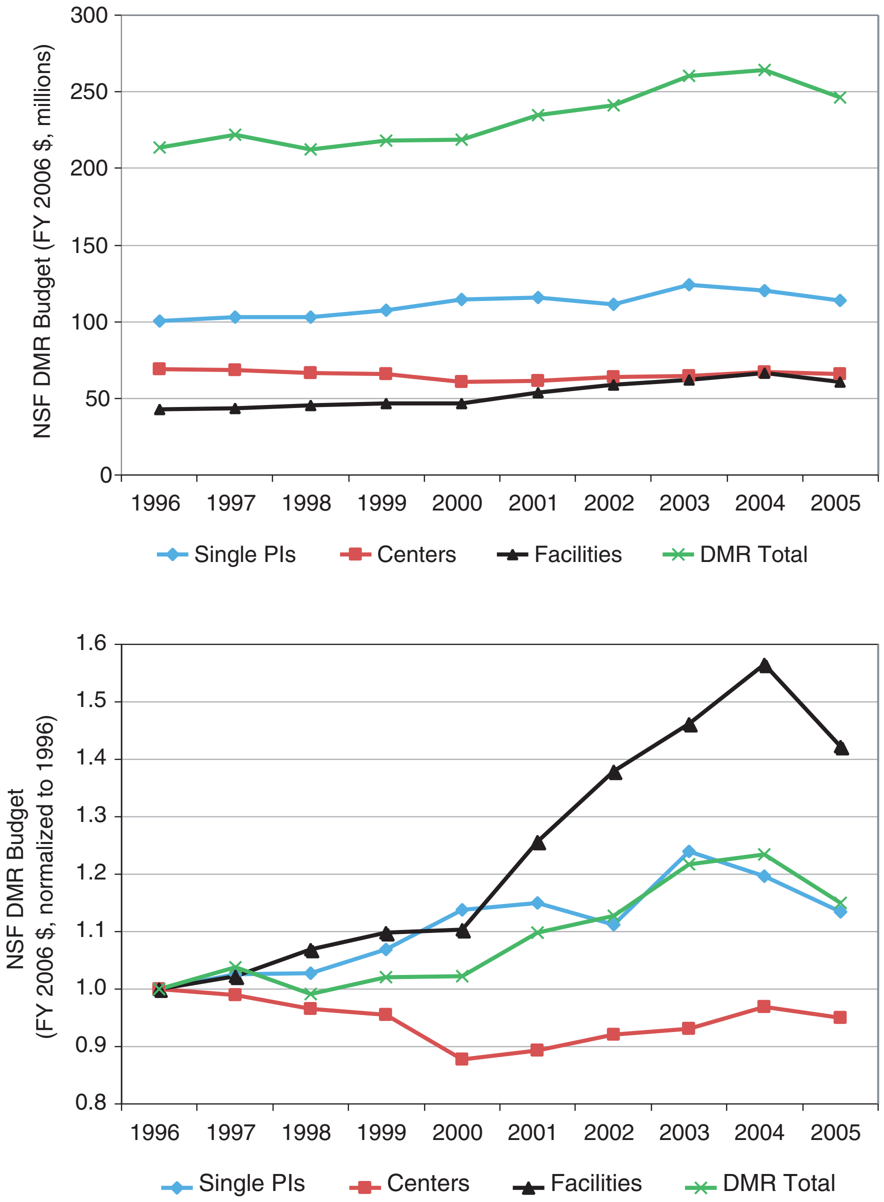

FIGURE 10.3 The National Science Foundation Division of Materials Research (NSF DMR) funding profile for the past 10 years. The data are in inflation-adjusted FY 2006 dollars. (Top) Funding levels for the identified programs (data provided by NSF). (Bottom) These same funding levels normalized to 1996 levels. Note that the data shown for facilities include the Major Research Instrumentation and Instrumentation for Materials Research programs, which support small teams of principal investigators (PIs) in addition to supporting large-scale NSF facilities.

increasing cost for supporting a graduate student is factored in (5 percent per year on average, based on the past 10 years), the net “buying power” has declined.

## FUNDING SUCCESS RATES

The essentially flat federal funding for CMMP basic research over the past 10 years, coupled with an overall increase in the number of grant applications, has led to an increase in pressure on grant allocations. A modest increase in average grant size for DOE and NSF (discussed below) thus implies a significant drop in success rate, defined as the ratio of the number of grants awarded by a program to the number of applications (Figure 10.4).

For NSF DMR, the average success rate dropped precipitously over the past 5 years, from 38 percent in 2000 to 22 percent by 2005. Success rates for applications by new investigators, that is, investigators not supported by NSF within the 5 years prior to the application, have always been lower, but until 2001 they were in the 20 percent range. For NSF DMR, the two rates track each other very closely (see Figure 10.4, bottom); success rates for “new investigators” have fallen from 28 percent in 2000 to 12 percent in 2005. At DOE BES, new grant applications to the Division of Materials Sciences and Engineering (DMS&E) have had fairly steady average success rates of around 25 to 30 percent over the past decade (Figure 10.5). Success rates for renewal applications, however, during 2000 to 2005 dropped from percentages in the high 90s to 87 percent for condensed-matter physics and materials chemistry (CMP and MC), and to about 62 percent for materials and engineering physics (MEP). Because the DOE, unlike NSF, actively encourages, or discourages, full proposals on the basis of previously submitted “white paper” preproposals, success rates reported by the DOE tend to be significantly higher than at NSF. This makes these drops in funding success rates especially significant.

As success rates drop, the effort spent by PIs in preparing more grant applications and the effort spent by the funding agencies in managing and reviewing increased numbers of applications become a burden on the federal funding system. Certainly when success rates drop as low as 10 percent, the overall amount of energy spent in the application process becomes counterproductive. As the data show, the CMMP research community is now reaching this point for new applications at NSF DMR and is heading in the same direction for established PIs. These are extremely worrisome trends.

As the above data for the increases in submitted proposals and concomitant drops in success rates indicate, there is tremendous pressure on the CMMP funding system. This pressure is further increased by the loss of the premier industrial laboratories. However, the importance, vigor, and increasing breadth of CMMP, as outlined in this report, demonstrate that the field is healthy and indeed poised

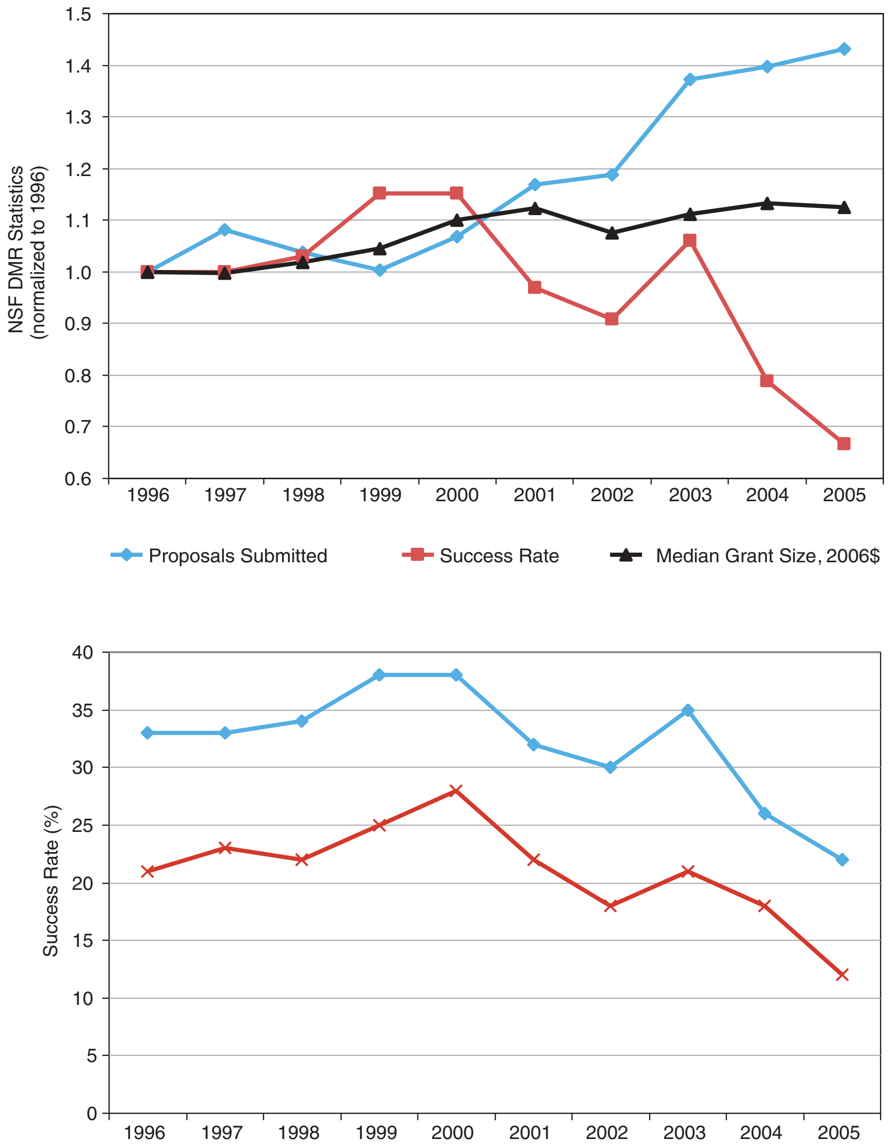

FIGURE 10.4 Grant proposals, success rates, and grant sizes for the National Science Foundation Division of Materials Research (NSF DMR). (Top) DMR statistics normalized to 1996. Shown are the number of proposals submitted, the median grant size (in inflation-adjusted FY 2006 dollars), and the success rate for established principal investigators (PIs) (same as the upper curve in the bottom panel). (Bottom) Success rates for PIs (average over all DMR programs). The upper curve represents success rates for PIs who received funding from the NSF within the previous 5 years, while the lower curve represents PIs new to NSF.

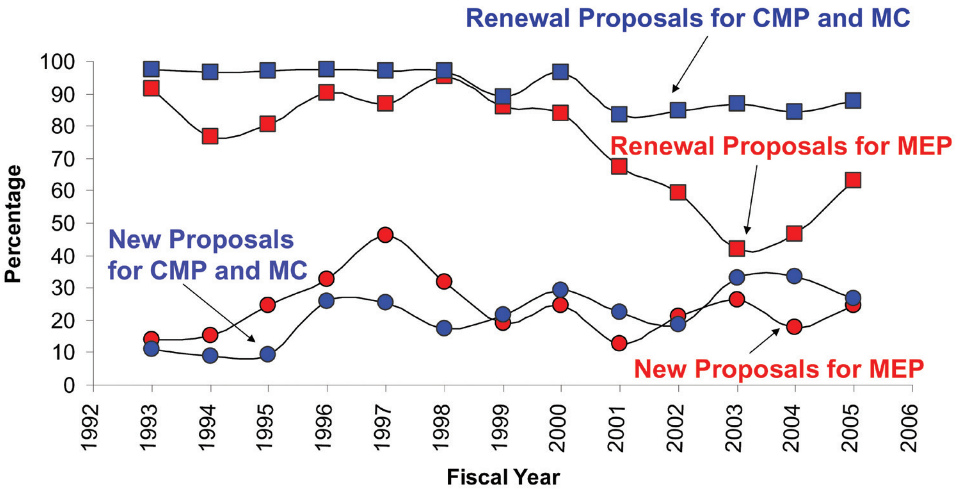

FIGURE 10.5 Success rates for new and renewal proposals at the Department of Energy (DOE) Basic Energy Sciences' Division of Materials Sciences and Engineering as analyzed using the Information Management for the Office of Science database. NOTE: CMP, condensed-matter physics; MC, materials chemistry; MEP, materials and engineering physics. SOURCE: DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

to grow. Recent reports[3,4] strongly recommend an increase in the funding of the physical sciences, such as CMMP, to the level of a doubling in the funding over a 10-year period to maintain U.S. economic innovation relative to the rest of the world. When considering the increasing costs of doing CMMP research in terms of graduate student support, a doubling of funding levels over 10 years would represent a growth of approximately 20 percent over a decade. The committee believes this growth level to be necessary for the United States to sustain a competitive position in CMMP worldwide, also taking into account the need to nurture the new subfields that are developing at the interdisciplinary frontiers between CMMP and other physics subfields and other disciplines.

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[3] National Academy of Sciences, National Academy of Engineering, and Institute of Medicine, *Rising Above the Gathering Storm: Energizing and Employing America for a Brighter Economic Future*, Washington, D.C.: The National Academies Press, 2007.

[4] Domestic Policy Council, Office of Science and Technology Policy, *American Competitiveness Initiative: Leading the World in Innovation*, Washington, D.C., 2006. Available at http://www.whitehouse.gov/stateoftheunion/2006/aci/aci06-booklet.pdf; last accessed September 17, 2007.

## GRANT SIZES

Over the past 10 years, the median grant size has increased moderately. For NSF DMR, it rose from $84,000 to $112,000 (see Figure 10.4), and for DOE BES it rose from approximately $120,000 to $150,000 per year. However, costs associated with research at universities have outpaced inflation. As discussed above, the committee's survey of state and private universities indicates an average increase of 5 percent per year in the cost per graduate student. Median-size grants today often can only support one graduate student in full, plus the costs of materials and supplies and of small pieces of equipment.

## INTERNATIONAL DATA

The committee endeavored to obtain data to compare the overall funding trends for CMMP in the United States with those in other countries. The breadth and diversity of the CMMP enterprise and the different venues for funding CMMP-related activities in different countries made this difficult. However, funding for various nanoscience and nanotechnology initiatives abroad can provide a basis for an estimate of the increasing rate of CMMP funding in foreign countries. Figure 10.6 provides such data for four Asian countries, indicating a wide variation in funding trends over the 5-year period, with China showing the largest percentage increase (more than a factor of two) and Japan showing the smallest increase (about 10 percent). The data are corrected for economic inflation within each country and normalized, to provide an estimate of recent increases in the "buying power" related to total expenditures. A comparison of research output in terms of publications is described later in the chapter.

## DEMOGRAPHICS OF CMMP

According to data compiled by the American Institute of Physics (AIP), after the rapid and historic increase in the number of U.S. physicists after World War II, the number of Ph.D. degrees peaked around 1970 (see Figure 10.7). The peaks and valleys in recent decades are influenced by many factors, including changing perceptions of job opportunities in physics, changes in the number of foreign students enrolling in U.S. graduate programs, and changes in the number of those receiving physics bachelor's degrees in the United States and in the proportion of those who choose to continue with graduate study in physics. Economic and political changes also have an effect on degree production, along with available funding for physics research. The substantial 25 percent decline in Ph.D. production over the past decade has ended with a sharp increase in the number of degrees conferred in the class of 2005. Following the large gains seen in first-year Ph.D.

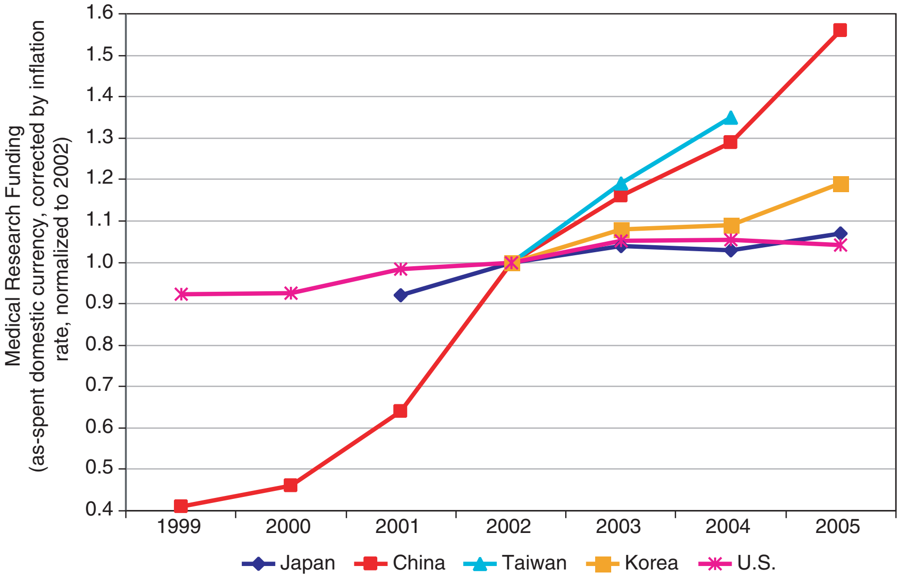

FIGURE 10.6 International trends in funding of materials science, normalized to 2002 with correction for inflation rates of each country (data provided by colleagues in each country). Since each country has a different way to categorize research, the research topics included in the figure vary, depending on the country. The committee was unable to locate data for Europe.

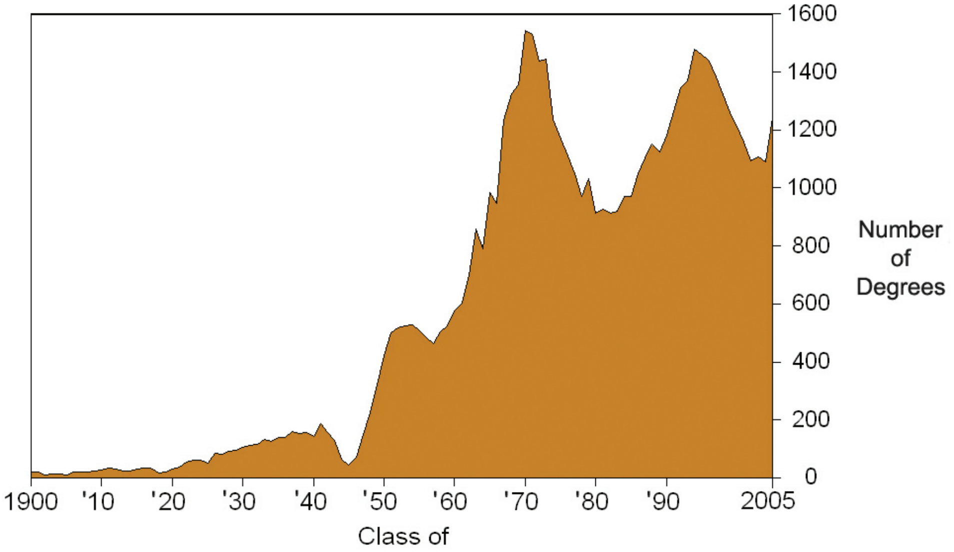

FIGURE 10.7 The number of physics doctorates conferred in the United States, 1900-2005. SOURCE: American Institute of Physics, *Enrollments and Degrees Report*, College Park, Md., 2006. Available at http://www.aip.org/statistics/trends/reports/ed.pdf.

student enrollments from 1998 to 2003, increases in physics Ph.D. production are expected in future years.

Over the preceding decades, CMMP has been the largest subfield of physics in the United States and worldwide. The number of Ph.D. degrees issued in CMMP over the past 20 years is compared to other subfields in Figure 10.8. The decline in CMMP Ph.D. degrees from the mid-1990s to 2003 mirrors the decline in total physics degrees over the same period. These data were obtained from the NSF through the Survey of Earned Doctorates, in which new doctoral recipients are asked to identify their primary field of dissertation research from a list of categories. This survey has about a 95 percent response rate from new doctoral recipients. In the 2004 survey, "Applied Physics" and "Biophysics" were introduced as new categories (the committee chose to include applied physics as part of CMMP, but to graph biophysics separately). Doctoral recipients in these areas prior to 2004 likely chose "Physics, General" or "Physics, Other" as their field of dissertation research, thus de-

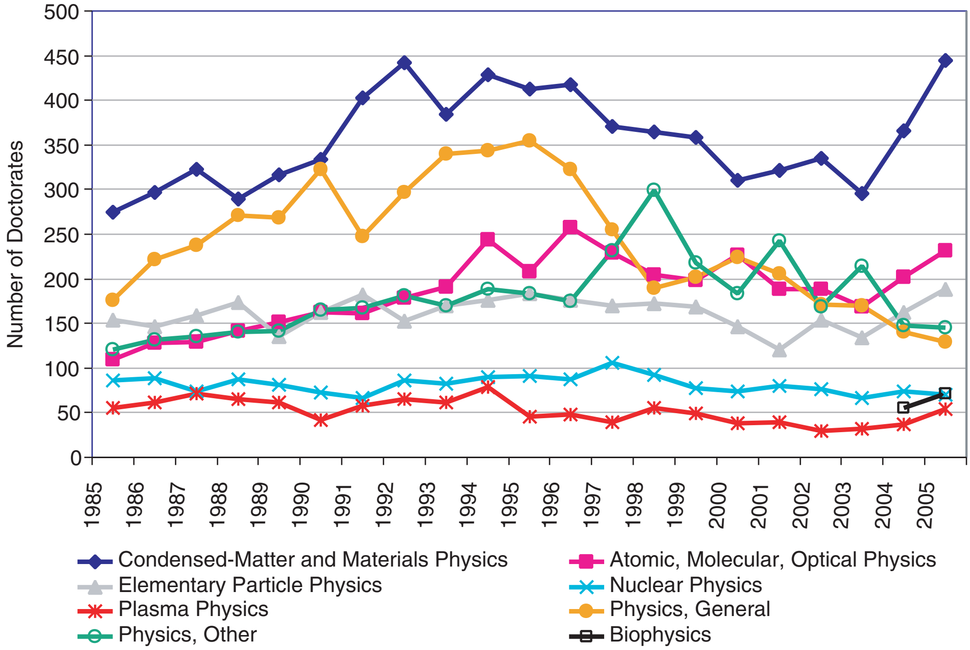

FIGURE 10.8 Physics doctorates awarded by subfield, 1985-2005. Condensed-Matter and Materials Physics includes Solid-State/Low-Temperature Physics, Polymer Physics, Fluids Physics (category discontinued in 2004), and Applied Physics (new category in 2004). Biophysics is a new category as of 2004 and is shown separately here. SOURCES: National Science Foundation, *Selected Data on Science and Engineering Doctorate Awards: 1994*, NSF 95-337, Arlington, Va., 1995; and National Science Foundation, *Science and Engineering Doctorate Awards: 2005*, NSF 07-305, Arlington, Va., 2006.

creasing the CMMP count. Because of these variations in the categorization of dissertation research, the data in Figure 10.8 can only give an approximate indication and are likely an underestimate of the number of Ph.D. recipients in CMMP.

### Women and Underrepresented Minorities in CMMP

Data from the American Institute of Physics Statistical Research Center show the number of degrees granted to women from 1978 to 2005 (see Figure 10.9). While the total number of women entering physics each year has reflected, to some extent, the ups and downs in total degrees granted, the dominant trend is a steady rise in the fraction of degrees granted to women, from about 6 percent of Ph.D. degrees in 1978 to about 14 percent of Ph.D. degrees in 2005.

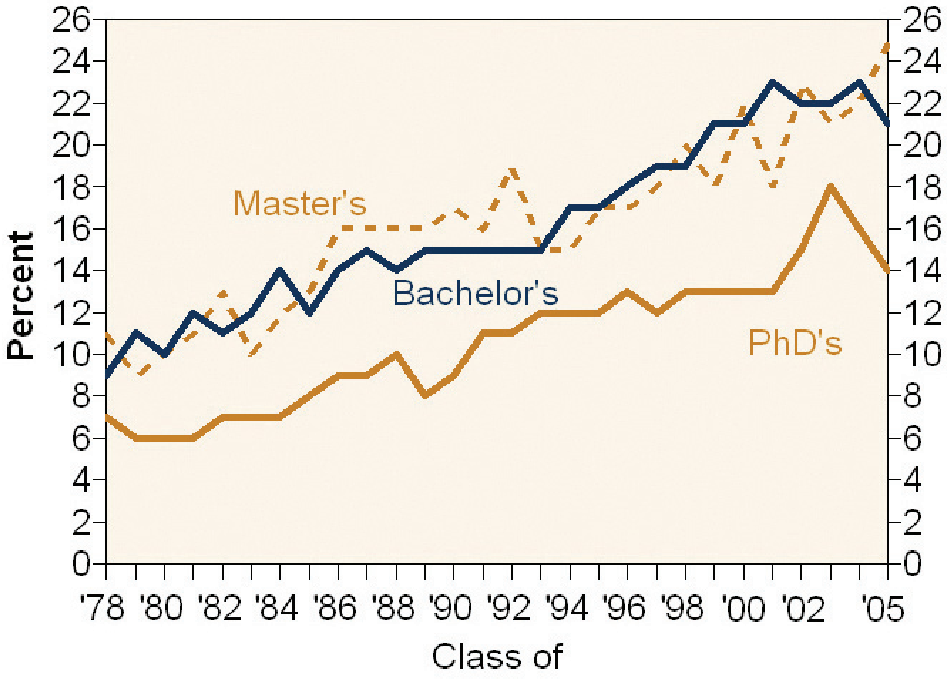

FIGURE 10.9 Percentage of bachelor's degrees, master's degrees, and doctorates in physics earned by women, 1978-2005. NOTE: A form change occurred in 1994 resulting in a more accurate representation of women among holders of a bachelor's degree in physics. Some of the increase in 1994 only may be a result of that change. SOURCE: American Institute of Physics, *Enrollments and Degrees Report*, College Park, Md., 2006. Available at http://www.aip.org/statistics/trends/reports/ed.pdf.

Data from the AIP Statistical Research Center (see Table 10.1) also show a significant increase between 2000 and 2004 in the number of African-American and Hispanic university faculty, particularly those working in Ph.D.-granting departments. Much of this increase is due to one institution, Florida Agricultural and Mechanical (A&M) University, a historically black university, which switched from granting the master's degree as its highest degree to granting Ph.D.'s.

However, African-Americans, Hispanics, and women remain underrepresented compared with their representation in other disciplines. Figure 10.10 shows just how imbalanced the situation still is for women faculty. In 2006, approximately 40 percent of all physics departments in the United States count fewer than two women among their faculty.

As the largest Ph.D.-producing physics subfield, CMMP has both an obligation and an opportunity to improve this situation. Data compiled by NSF show a rise in the number of degrees granted to women in CMMP (see Figure 10.11; NSF physics subfield categories are discussed above in the section "Demographics of CMMP"). The number of degrees granted to women roughly doubled over the period from 1986 to 2005, with a peak around 1996, which mirrors a peak in total CMMP doctoral degrees around the same time. Over the same period, the percentage of CMMP Ph.D. degrees earned by women increased steadily from around 8 percent in 1986 to around 14 percent in 2005. This is a very encouraging trend, but the CMMP community must continue to encourage women to enter the field and continue to knock down remaining obstacles to their advancement.

Several efforts within CMMP are actively increasing the participation by women and underrepresented minorities. In particular, the NSF Materials Research Science

TABLE 10.1 Percentage of Physics Faculty Who Are African-American and Hispanic and Number of African-American and Hispanic Physics Faculty by Degree-Granting Department, 2004 and 2000

| | Percentage of Physics Faculty | Highest Degree Granted by Department | | |
|---|---|---|---|---|
| | | Ph.D. | Master's | Bachelor's |
| Number of departments | | | | |
| Total number of physics departments in 2004 | | 185 | 72 | 503 |
| 2004 Faculty | | | | |
| African-American | 2.0 | 64 | 29 | 78 |
| Hispanic | 2.7 | 107 | 56 | 60 |
| 2000 Faculty | | | | |
| African-American | 1.8 | 38 | 41 | 62 |
| Hispanic | 2.0 | 81 | 32 | 42 |

SOURCE: American Institute of Physics, *2004 Physics and Astronomy Academic Workforce Survey*, College Park, Md., 2005. Available at http://www.aip.org/statistics/trends/reports/awf.pdf.

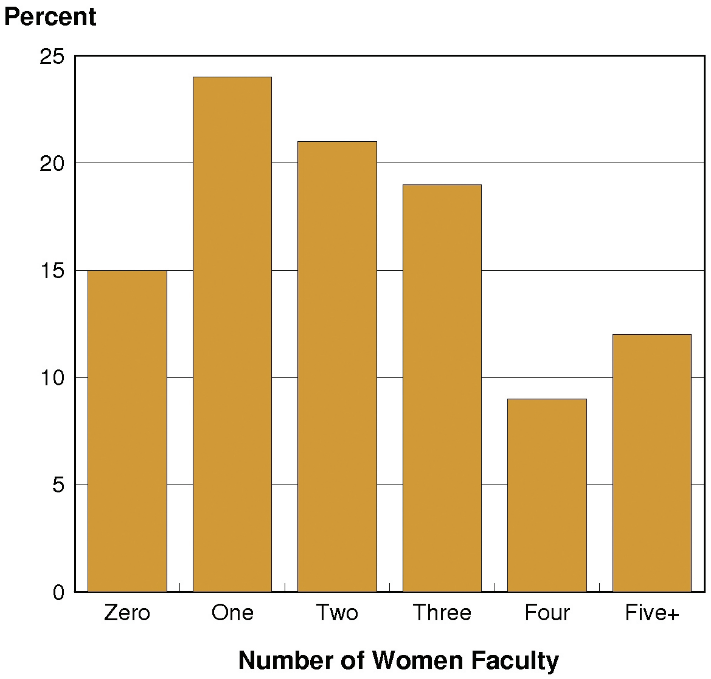

FIGURE 10.10 Percentage of Ph.D. physics departments, by number of women faculty in professorial ranks, 2006. SOURCE: American Institute of Physics, *2006 Physics and Astronomy Academic Workforce Survey*, College Park, Md., 2007.

and Engineering Centers are playing an important role in CMMP in attracting and retaining women and minorities. Averaged over all MRSECs in 2005, about 13 percent of MRSEC faculty were women and 3 percent were from underrepresented minorities. At the level of graduate students participating in MRSECs, the numbers are 27 percent and 5 percent, respectively (for a detailed discussion, see the NRC MRSEC report[5]). MRSECs are also helping to address the pipeline issue through their K-12 outreach programs and, at the college level, their Research Experience for Undergraduates programs. In addition, NSF DMR recently initiated the Partnerships for Research and Education in Materials program that seeks to enhance diversity by stimulating long-term partnerships between minority-serving institutions and DMR-supported centers and facilities. Together, these efforts provide CMMP

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[5] National Research Council, *The National Science Foundation's Materials Research Science and Engineering Center Program: Looking Back, Moving Forward*, Washington, D.C.: The National Academies Press, 2007.

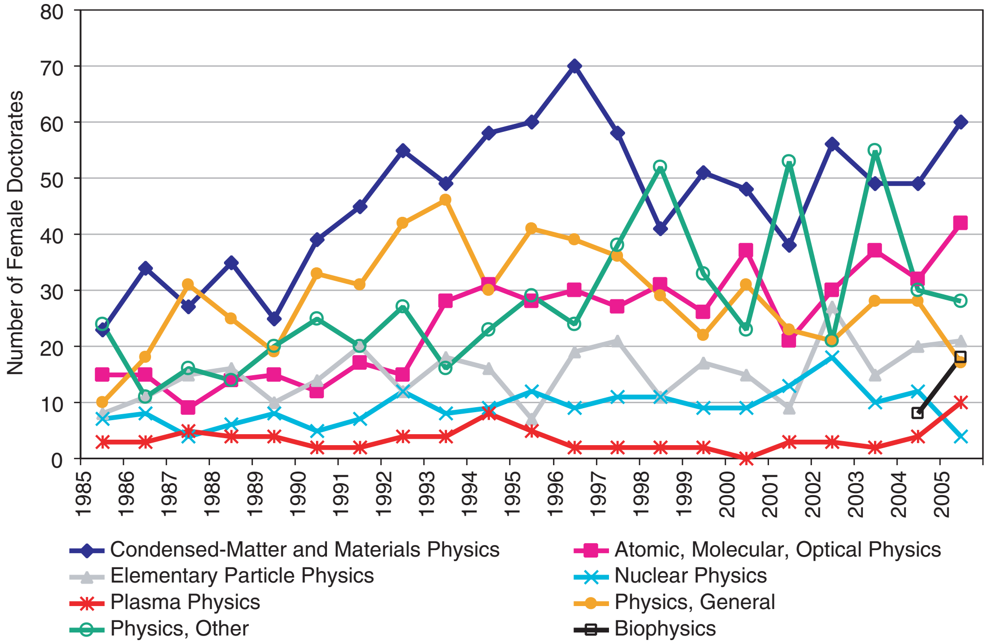

FIGURE 10.11 Physics doctorates awarded to women, by subfield, 1985-2005. Condensed-Matter and Materials Physics includes Solid-State/Low-Temperature Physics, Polymer Physics, Fluids Physics (category discontinued in 2004), and Applied Physics (new category in 2004). Biophysics is a new category as of 2004 and is shown separately here. SOURCES: National Science Foundation, *Selected Data on Science and Engineering Doctorate Awards: 1994*, NSF 95-337, Arlington, Va., 1995; and National Science Foundation, *Science and Engineering Doctorate Awards: 2005*, NSF 07-305, Arlington, Va., 2006.

with a leading role in increasing the number of women and underrepresented minorities in physics.

## Doctoral Degrees in Physics by Citizenship

In contrast to the ups and downs in total Ph.D. production discussed earlier, data compiled by the AIP Statistical Research Center show a steady decline in the proportion of physics Ph.D. degrees granted by U.S. universities to U.S. citizens over the period from 1966 to 2005 (see Figure 10.12). This decline has been compensated for by a steady rise in the proportion of degrees granted by U.S. universities to citizens of other nations. In past decades, many of these advanced degree holders have remained in the United States to pursue employment opportunities. Now, with rapidly improving opportunities outside the United States, many are

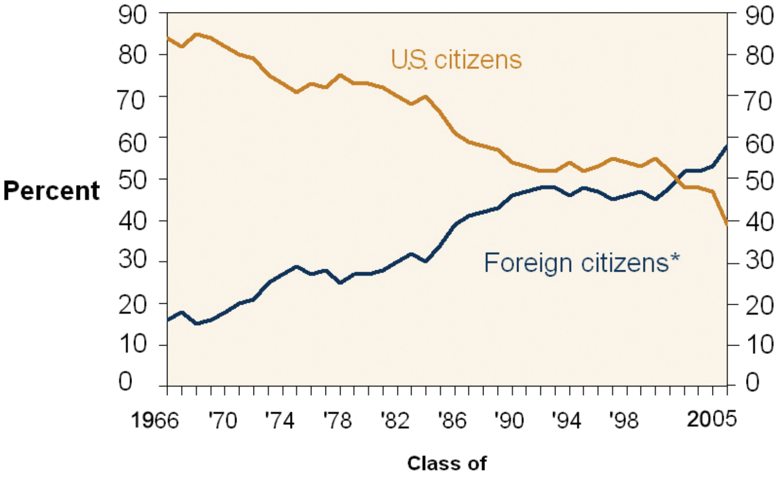

FIGURE 10.12 Citizenship of individuals granted physics doctoral degrees by U.S. universities, 1966-2005. SOURCE: American Institute of Physics, *Enrollments and Degrees Report*, College Park, Md., 2006. Available at http://www.aip.org/statistics/trends/reports/ed.pdf. Foreign citizens include individuals with permanent residence and those with temporary visas.

taking their knowledge and creative energies elsewhere. This is, no doubt, a positive development for the world, but some have predicted undesirable consequences for the U.S. economy as high-paying research and development (R&D) jobs move to other countries and the United States loses clear leadership in various fields of science. However, this downward trend in Ph.D. degrees granted to U.S. citizens is expected to reverse soon. According to the AIP (see Figure 10.13), the number of U.S. citizens enrolling as first-year graduate students was up nearly 50 percent from the recent low in 1998. It should therefore follow that the number of Ph.D. degrees awarded to U.S. citizens in coming years will grow sharply. Degree production in the subfield of CMMP is expected to follow the same course.

## PUBLICATION TRENDS

The Committee on CMMP 2010 considered the number of articles published in scholarly journals as a good proxy for scientific productivity. The committee obtained data for the numbers of articles published by and submitted to several journals of the CMMP-relevant American Physical Society and the American Institute of Physics. Comparisons between the United States and other countries and between academia, industry, and national laboratories can be made with these data. The committee's most important observations and conclusions are described below.

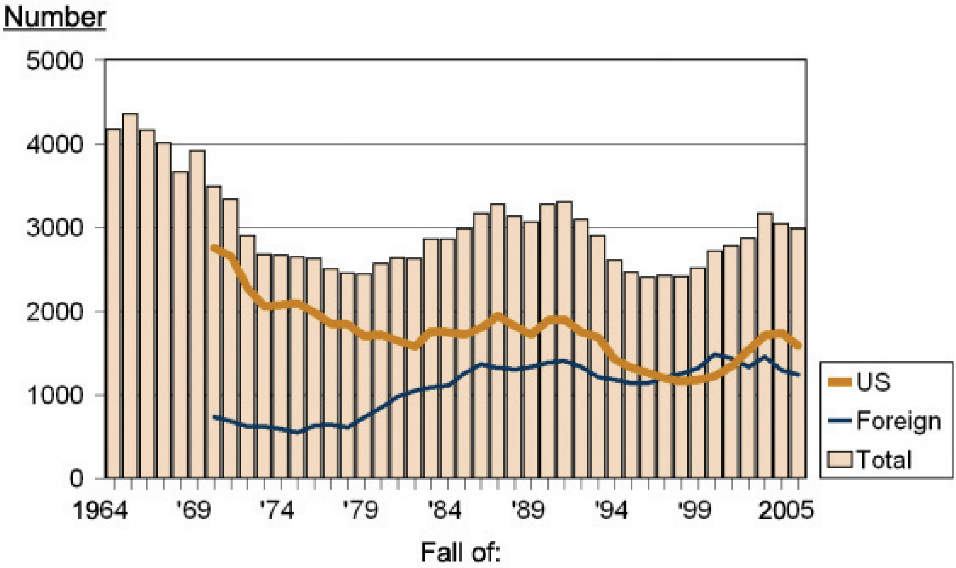

FIGURE 10.13 First-year U.S. and foreign graduate physics students, 1964-2005. NOTE: A change in wording on the 2000 questionnaire resulted in more accurate data on first-year graduate students. This change was responsible for 3 percent of the reported 8 percent increase in total first-year students between 1999 and 2000. SOURCE: American Institute of Physics, *Enrollments and Degrees Report*, College Park, Md., 2006. Available at http://www.aip.org/statistics/trends/reports/ed.pdf.

Figure 10.14 compares the combined numbers of articles originating in the United States with those coming from the rest of the world. The committee bases this comparison on two journals that capture the core disciplines within CMMP: *Physical Review B*, whose subject areas include hard condensed-matter and materials physics, and *Physical Review E*, which covers statistical, nonlinear, and soft-matter physics. While the number of publications contributed from the United States has remained essentially flat for the past 13 years, publications from the rest of the world nearly doubled. The United States has lost ground to both Western Europe and Asia during this period, as shown in Figure 10.14. Articles originating in the United States constituted the largest component at the beginning of the period, but the United States was overtaken by Western Europe in about the middle of the past decade. The committee emphasizes that the publication trends are recent (since 1993) and occur long after the reestablishment of Western Europe after World War II.

If the current trends continue, the United States will also be overtaken within the next decade by Asia, consisting of primarily Japan and China, and to a lesser extent, South Korea. In fact, articles submitted to *Physical Review B* and *Physical*

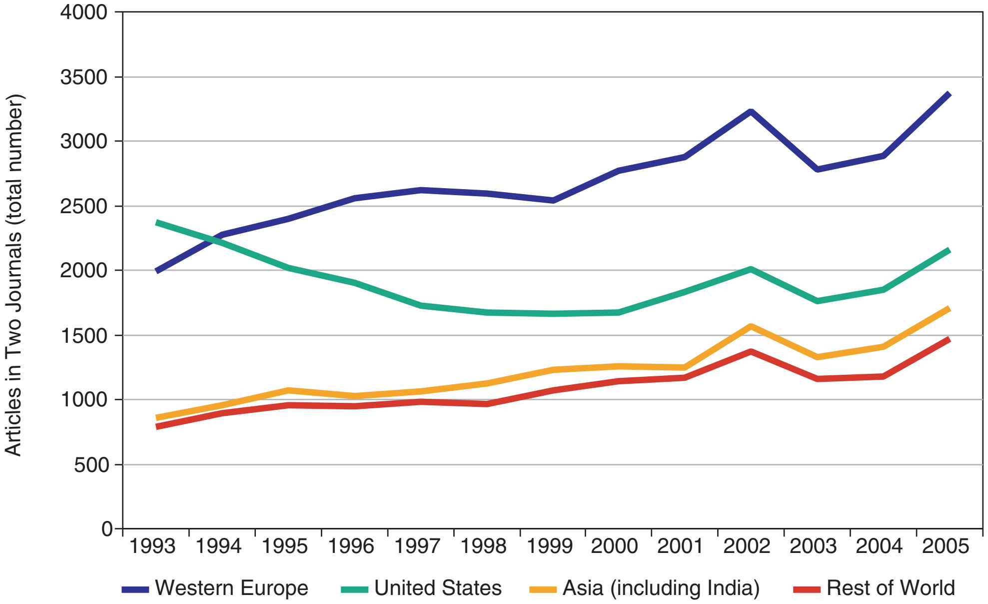

FIGURE 10.14 Comparison among the United States and other regions of the world in the total number of articles published in *Physical Review B* plus *Physical Review E* for the past 13 years (1993-2005). SOURCE: Publication data supplied to the Committee on CMMP 2010.

*Review E* by scientists from Asia already exceed those from the United States, but the article rejection rate for Asia is currently larger than that for the United States. The committee acknowledges that the growth of CMMP research in Asia in the next decade is indeed expected because of the growths of Asian nations' economies. A general trend across all the journals surveyed, however, is that the rejection-rate gap between the United States and the rest of the world has narrowed, and continues to narrow, presumably reflecting a relative improvement in scientific quality of the rest of the world relative to the United States, although the quality of the U.S. publications remains high as judged by publication citations, as discussed below.

Publication data can also expose shifts in activity at industrial and national laboratories. Figure 10.15 is a plot of the numbers of publications by several notable U.S. industrial laboratories in *Physical Review B*. The data reveal a precipitous drop in publications between 1996 and 2001 by the two major industrial research laboratories, Bell Laboratories and the IBM Research Centers, indicating a dramatic drop in CMMP basic research being performed at these institutions. Bell Laboratories, in particular, experienced an eight-fold decrease in publications in just 5 years, followed by a slight increase in output for the past 5-year period. Data for the national laboratories do not exhibit any particularly significant trends.

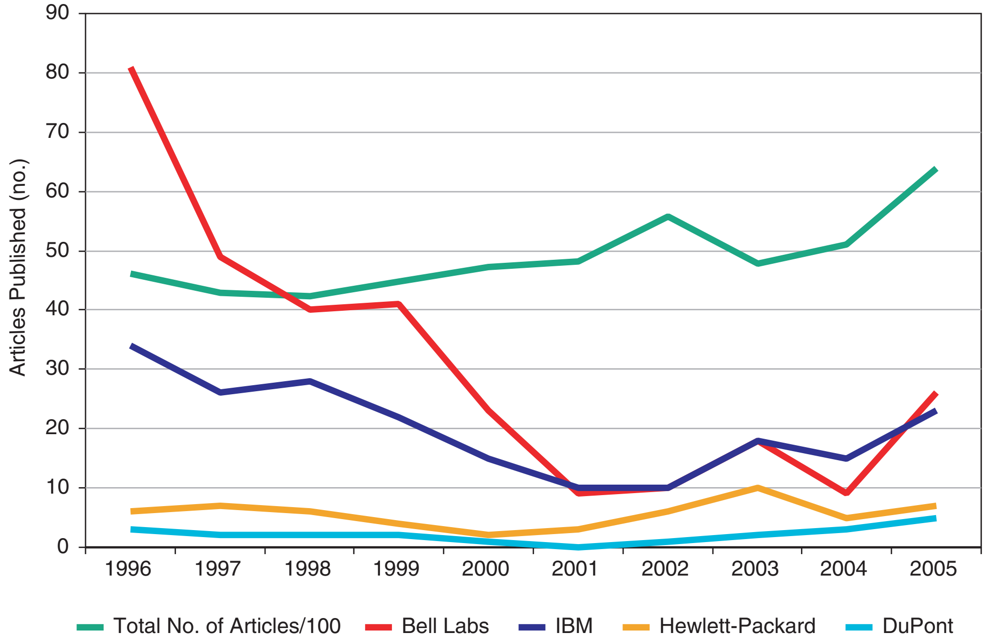

FIGURE 10.15 Numbers of articles published in *Physical Review B* by major industrial laboratories in the past 10 years (1996-2005), compared to the total number of articles (divided by 100 to fit on the same graph) published in the same journal.

In addition to looking at the geographical distribution of CMMP publications in leading U.S. journals, the committee also tried to assess the quality of the U.S. output. Here the picture is rather more encouraging. For example, although the U.S. share of the overall output in journals such as *Physical Review B* and *Physical Review E* has fallen in absolute terms during the past decade, the fraction of U.S. papers in the top 100 cited publications has remained approximately constant. The committee concludes from this observation that the quality of work in the nation's leading CMMP research groups remains world-class, even if the total output is flat. There is no room for complacency, however, as it is also clear that the impact of publications from emerging nations such as China is growing rapidly.

CMMP publications are one source of evidence that individual investigators and small numbers of collaborators dominate advances in the field. Furthermore, CMMP research at large facilities also tends to be done by individual groups or by small groups of collaborators. CMMP researchers view large facilities as a means to do individual or small-group research, and the publications from using large facilities still have a small number of authors.

## RECOMMENDATIONS

The Committee on CMMP 2010 bases the following recommendations on its assessment regarding the most efficient use of resources and projected growth in funding for the field of 7 percent per year over the next 10 years. This rate of growth reflects levels recommended in the president's *American Competitiveness Initiative*,[6] which seeks a doubling of the physical science research budget of NSF, DOE, and the National Institute of Standards and Technology in 10 years. In some cases, improved research quality and efficiency can be obtained through changes in the structure of funding. In other cases, additional funding is necessary in order to retain current expertise and to nurture emerging fields of science. Some new facilities are also required to advance science and to keep the U.S. research effort at the forefront.

What is critical for success in the coming decade is strong support for research at the single- and few-investigator level. Centers and national facilities provide the infrastructure, but they will be useless without a strong community of scientists pushing the science and technology forward.

The field of CMMP is large, heterogeneous, and complex. It progresses through the integration of a large number of small breakthroughs rather than by a few high-profile achievements. Unlike some other fields of science, these breakthroughs are predominately made by small teams following their particular visions rather than by large groups pursuing a limited number of specific, clearly defined goals. This means that strong support at the individual-investigator level is *essential*. The proposed doubling of the physical sciences budget, with particular focus on supporting individual investigators (by increasing both average grant size and the number of awards), would be an excellent first step toward accomplishing this goal.

As described above, the funding situation in CMMP has made it difficult for researchers to focus on their research programs. The reduced success rates for proposals, the reduction in buying power of grants, and the increasing number of submitted proposals have changed dramatically over the past 10 years. The prospects are particularly dim for young scientists and for those entering for the first time a field in which funding success rates are approximately 10 percent. It is also difficult for researchers involved in interdisciplinary research to obtain support. Finding the correct funding agency and program for work that lies between physics and engineering or physics and chemistry or biology has been difficult. The recommendations below to the National Science Foundation, the Department of

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[6] Domestic Policy Council, Office of Science and Technology Policy, *American Competitiveness Initiative: Leading the World in Innovation*, Washington, D.C., 2006. Available at http://www.whitehouse.gov/stateoftheunion/2006/aci/aci06-booklet.pdf; last accessed September 17, 2007.

Energy, and the CMMP community are aimed at maintaining U.S. innovation in CMMP research.

> **Recommendation:** Strong support should be maintained for individual and small groups of investigators, which are historically the primary source of innovation in CMMP. The ratio of support for individual and small groups of investigators relative to support for centers and facilities should not decline in the next decade.
>
> **Recommendation:** The average success rates for the funding of proposals should be increased to more than 30 percent over the next 5 years in order to give junior scientists the opportunity to obtain research results before the tenure decision and to enable currently funded researchers to maintain continuity in their research programs.
>
> **Recommendation:** The size of grants to individual and small groups of investigators should be increased to maintain the buying power of the average grant and to retain scientific talent in the United States.
>
> **Recommendation:** The CMMP community should work to improve the representation of women and underrepresented minorities in CMMP through mentoring; providing flexible working conditions, day-care opportunities, and viable career paths; and developing outreach programs targeted to students and the public and aimed at increasing the numbers of prospective researchers.
>
> **Recommendation:** The Faculty Early Career Development awards and other research grant awards should be made on the basis of research criteria, not education and outreach. Providing financial incentive for education and outreach activities would more effectively engage the community and encourage the best programs. The committee recommends a separate program for funding outreach and education (see Chapter 8 for further discussion of this recommendation).

# 11

# Tools, Instrumentation, and Facilities for Condensed-Matter and Materials Physics Research

The quest to observe, predict, and control the arrangements and motions of the particles that constitute condensed-matter systems is central to the condensed-matter and materials physics (CMMP) enterprise. The constituent particles span an enormous range of sizes—from electrons and atoms to macromolecules—and their motions span a correspondingly immense range of timescales. As a result, the experimental, computational, and theoretical tools required to study them are extremely diverse. Many of these tools are developed by individual research groups; other tools, such as synchrotron x-ray and neutron scattering, are developed at large-scale national laboratory facilities. Technical innovations that extend the limits of measurement and prediction lie at the forefront of CMMP research. For example, scanning probe microscopes were developed to image surfaces at scales too small to be resolved by ordinary optical microscopy, and they immediately transformed the fundamental understanding of surface science. Moreover, the benefits of new techniques often stretch far beyond condensed-matter physics; scanning probe microscopes have now evolved into universal tools at the nanoscale for the physical and life sciences. Experimental condensed-matter tools underlie many noninvasive medical diagnostics, while theoretical and computational tools from CMMP, such as local electron density approximations and numerical simulation methods, are now used by pharmaceutical companies. The past decade has seen the advent of promising techniques, such as coherent and pulsed x-rays, novel optics based on exotic materials, multiscale modeling, and topological approaches to the study of magnetic and superconducting materials. As CMMP researchers seek to answer fundamental questions about materials, they will continue to design tools, or adapt tools for new applications, that will benefit CMMP, other scientific disciplines, and society at large.

## TOOLS AND INSTRUMENTATION FOR CMMP RESEARCH

Measurement techniques designed to probe the properties of matter at smaller length, time, or energy scales or with greater quantitative resolution and sensitivity advance the forefront of condensed-matter and materials physics research. Likewise, techniques designed to synthesize high-quality materials with precisely controlled structures underpin many great CMMP discoveries. By pushing the boundaries of materials fabrication and measurement forward, experimental CMMP researchers have uncovered new phenomena that were often unanticipated. These discoveries have not only transformed CMMP, but they themselves have led in turn to new ways to manipulate and image matter, crucial to many new technological advances with a broad range of applications.

New computational and theoretical techniques that push forward the boundaries of prediction also play a prominent role in advancing CMMP. To some extent, theory and computation are interlinked—theory nearly always forms the basis for new approximations or algorithms that substantially increase the efficiency of computations. Conversely, numerical computation is often indispensable in theory. Theoretical innovations, such as the application of field theories to condensed-matter systems and linear response theory have not only allowed researchers to tackle previously intractable problems, but, like many of the greatest experimental and computational techniques, have also changed the landscape of CMMP by revealing unexpected phenomena or deep, previously hidden connections among phenomena. As discussed later, computation can dramatically amplify the power of analytical tools. Indeed, the first electronic digital computer itself was built in order to carry out theoretical CMMP calculations.

The research community is at the brink of an era in which powerful computer simulations will be integrated into measurement tools, enabling the extraction of information in unprecedented detail from measured quantities. Simulations will extend the reach of analytical theoretical techniques, connecting conceptual developments to experimental measurements. The results will guide researchers through the realms of materials possibilities so vastly expanded by the ability to control the structure of the material at the nanoscale. Closing the loop, new detectors and devices will be made possible by new, purposefully designed, functional materials to further increase the power of measurements. Some of these breakthroughs will be made in single-investigator laboratories and, following the example of the scanning tunneling microscope, will turn into commodity instruments. Other advances will rely on the unique powers of staggeringly expensive large-scale instruments and teams of experts supported by large national facilities; these tools will need to be broadly available and "user friendly" for a wide cross section of researchers. Thus, all agencies supporting CMMP research should provide strong instrumentation programs to enable the research work in the CMMP field to be carried out efficiently and well. There is a need for keeping the infrastructure supporting CMMP research at universities up to date and for providing modern instruments for the training of the next generation of researchers.

## Instrumentation in CMMP Research

CMMP researchers have a track record of developing new measurement tools that have enabled advances not only within CMMP, but also in other areas that encompass the physical, chemical, biological, and medical sciences. Indeed, the continued development of techniques with sufficient spatial resolution and sensitivity to measure structure, composition, and properties of condensed-matter over various length scales (from nano to macro), dimensionalities, and timescales is essential. During the past decade there have been significant advances in the use of tools in imaging, scattering, and spectroscopy. In this section, the Committee on CMMP 2010 briefly highlights advances in some of these areas.

### *Imaging Techniques*

Imaging techniques provide structural images, direct and indirect, and property maps. Microscopy alone and microscopy combined with tomographic techniques are the most commonly used techniques to create images in two and three dimensions, respectively. Recent developments in x-ray microscopy, based largely on improvements of the fabrication of the optics, have enabled the observation of molecular length-scale height variations on a surface. Image measurements are now accomplished over an area of many microns, with a resolution of 200 nanometers (nm) and a step height of 0.6 nm with this technique. X-ray imaging has also enabled imaging at greater depths within a sample than is possible with electrons. With third-generation synchrotron sources, it is possible to study opaque objects using hard x-rays, while soft x-rays are used for soft materials and to probe near the surface of materials. X-ray beams can be focused to dimensions on the order of 100 nm to enable better resolution; the limiting resolution with x-rays is yet to be reached.

A new development involves imaging by neutrons. Imaging is based on the notion that neutrons are characterized by a de Broglie wave packet with a spatial distribution that is sufficiently large to permit interference, very much in the same way as light. With the development of appropriate "optics," including transmission gratings based on differences in neutron-capture cross sections and incoherent scattering cross sections, two-dimensional images of various materials can be created. In fact, a three-dimensional image, based on the scattering length density distribution, can be reconstructed.

While scanning probe techniques have become ubiquitous in CMMP and have had an enormous impact on the understanding of materials, particularly at the nanoscale, many challenges remain. The inability to scan large areas of samples rapidly and issues related to thermal drift remain to be solved. Other issues awaiting resolution relate to the interpreting of data that are influenced by interactions between the cantilever tip and the sample. In the future, further progress in instrumentation and data analysis, smaller cantilevers together with better deflection sensors, and improved sample-preparation techniques will lead to greater sensitivity and resolution. Multifunctional cantilevers, wherein a local "field" is applied while simultaneously probing the local response of the system, are part of a future strategy to ensure the increased impact of these techniques in the understanding of nanoscale properties. More sophisticated detection systems to enhance sensitivity further and improved computer algorithms for data interpretation and analysis will increase the utility and wide accessibility of these techniques that are so essential to modern CMMP materials characterization.

### *Scattering Techniques*

Scattering is also used to provide information about the structure and dynamics of condensed matter. For example, diffraction techniques, the best known of the scattering processes, provide information about the long-range order of a sample, with tenths-of-a-nanometer resolution, and the use of x-rays, combined with information gleaned from neutron measurements, has led to a better understanding of the crystallography of complex macromolecules. Neutron scattering has grown in recent years as a regular tool for the characterization of samples. Neutron scattering techniques provide information about dynamics from $10^{-12}$ seconds to seconds and structure at length scales from 0.1 nm to $10^3$ nm. Neutrons convey information about interatomic forces on the basis of measurement of the energy of the scattered neutrons. The incident intensity (flux) of neutrons and the efficiency with which the scattered neutrons are detected are key factors that determine the performance of a neutron source. The third-generation neutron sources (for example, the Spallation Neutron Source [SNS] at Oak Ridge National Laboratory) provide large increases in sensitivity that will result in better speed in data acquisition (seconds or minutes versus hours or a day, depending on the system and the information collected) and will enable measurements of lower concentrations of a given species. The latter is important because it will enable the analysis of multicomponent systems.

Other types of scattering techniques provide direct spatial depth profiling information of materials, including Rutherford backscattering spectrometry, forward recoil spectrometry, nuclear reaction analysis, and secondary ion mass spectrometry. These techniques involve the use of incident energetic ion beams; analysis of species emanating from the sample provides information about the concentration of a given species as a function of depth. The effective use of combinations of neutron and x-ray scattering with ion-beam techniques can provide more detailed information about the structure and dynamics of nanocomposites, heterostructures, and complex liquids at smaller length scales.

### *Spectroscopy Techniques*

The use of spectroscopy techniques for imaging has grown rapidly in recent years. These techniques, which have been very successful in the imaging of soft materials, including biological materials and polymers, have been invaluable. New developments that involve the use of scanning force probes, scanning force magnetic resonance (a sample is placed on a cantilever in the presence of a small ferroelectric tip which creates an inhomogeneous field that has the effect of polarizing the spins in the sample) have enabled the three-dimensional imaging of an individual atom as well as single spins.

Infrared and Raman techniques have been used to image samples based on a vibrational signature associated with a molecule. Researchers have been successful in using the Raman effect, inelastically scattered light that is shifted in wavelength relative to the incident wavelength, to improve the sensitivity of the identity of certain molecules within a sample. Surface-enhanced Raman scattering has laid the foundation for the development of surface-enhanced spectroscopies that include surface-enhanced fluorescence and surface-enhanced infrared spectroscopy. The latest developments include single-molecule surface-enhanced Raman spectroscopy and tip-enhanced scanning near-field optical microprobe Raman spectroscopy.

### *Simultaneous Measurement Capabilities*

New strategies that involve in situ characterization of materials using x-rays or neutrons are becoming routine. Specifically, some research groups use x-rays or neutrons to measure the properties of materials (dynamics structure, phase transitions, and so on) that are simultaneously subjected to external perturbations (stress, temperature, and various kinds of fields). With the use of tomographic techniques, information about the interior of samples can now be learned without the need to section them destructively for analysis with transmission electron microscopy (TEM) or scanning probe techniques. The availability of these combined techniques enables increased spatial and temporal resolution and rapid data acquisition. In some cases the duration of measurements could be reduced from tens of hours to minutes.

Another significant advance is the use of scanning force techniques in conjunction with other techniques for learning about properties, such as electrical conductivity and magnetism, in unprecedented detail at the nanoscale. Instruments are approaching the stage at which the resolution of joint probes is comparable to atomic force microscope measurements of topography. In situ TEM capabilities are also being developed to enable the direct observation of changes in atomic arrangement (structure) of a material while it simultaneously experiences external perturbations owing to changes in temperature, mechanical stresses, or electric fields. This is a powerful technique that is currently exploited by a number of electron microscopists. The development of more sophisticated theory and multiscale algorithms that enable better use of experimental data to characterize samples will be a continuing challenge.

## Computation in CMMP Research

As the materials and phenomena of interest have become increasingly complex, computation has emerged as an essential tool in the process of interpreting experimental data and analyzing theoretical models. Over the past decade or two, computational CMMP has developed fully into a branch of study in its own right, on a par with experimental and theoretical CMMP.

From the beginning, computational CMMP has not only allowed researchers to confront previously insoluble problems but has also provided a means to discover new phenomena. There are two paradigms in computational CMMP. One extends the power of theoretical modeling by numerical solution of "simple" models, both classical and quantum, which capture the essential physics of the system of interest. These results are used either directly in interpreting and predicting experimentally observed phenomena or as an aid to "pencil and paper" analysis by developing and validating approximations to study models that cannot be solved exactly. The second paradigm is the direct solution of the quantum mechanical equations to make quantitative predictions about the behavior of particular materials at the atomic scale. In both, breakthroughs in the development of theory and algorithms, aided by enormous increases in computer speed and memory, have enabled dramatic progress in the past decade.

Techniques developed for the numerical investigation of simple models have had widespread applicability beyond CMMP. Monte Carlo methods are now standard tools in all fields of science and engineering and are even used in industrial contexts. Some recent approaches that have promise for significant impact in CMMP are phase retrieval methods and new forms of Monte Carlo algorithms, including ones that can evolve dynamically. New field theoretical algorithms are having increasing impact. With the density matrix renormalization group (DMRG) method, significant progress has been made toward eliminating the "sign problem" bottleneck, ubiquitous in numerical studies of systems of interacting electrons; this method has also had a significant impact in quantum chemistry, quantum information theory, and nuclear and high-energy physics.

With these methods, it is now possible quantitatively to study models that capture aspects of the essential physics of materials with strongly correlated electrons, such as complex oxides, including the high-temperature superconducting cuprates and magnetoresistive manganites, and two-dimensional electron gases. Figure 11.1 shows an example of the rich variety of ground-state orderings that have been observed in models of the cuprates with the DMRG method.

Methods for the direct solution of the underlying quantum mechanical equations allow quantitative, material-specific, first-principles prediction of structure and properties. The ongoing development of efficient algorithms allows the study of ever-more-complex structures, including crystals with very large unit cells, and nanostructured systems. New classes of algorithms and the incorporation of many-body physics allow the extension of these methods to a broader range of materials—notably, correlated electron systems with magnetic, orbital, and

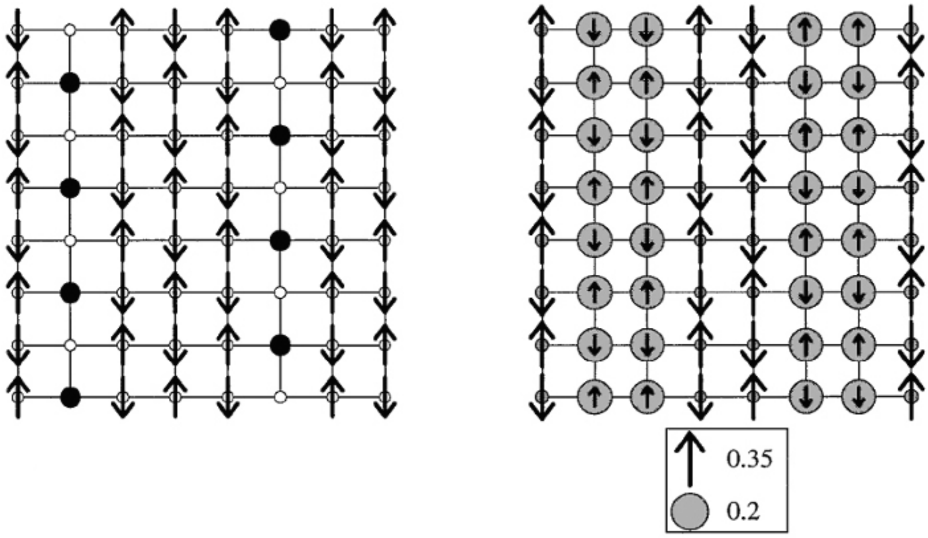

FIGURE 11.1 Plots showing the stripe ordering of the charge and spin on a two-dimensional $CuO_2$ plane in the high-temperature superconductor $(La,Nd,Sr)CuO_4$. (Left) As suggested by neutron-scattering experiments. (Right) As calculated for the t-J model using the density matrix renormalization group method. SOURCE: Reprinted with permission from S.R. White and D.J. Scalapino, "Density Matrix Renormalization Group Study of the Striped Phase in the 2D t-J Model," *Phys. Rev. Lett.* **80**, 1272 (1998). Copyright 1998 by the American Physical Society.

charge ordering, and systems under ultrahigh pressure relevant to geophysics. New capabilities are being developed to study systems in applied electric and magnetic fields and to extend computations for excited states. Such computational capability is necessary for predicting optical and transport properties. An example is shown in Figure 11.2.

The direct solution of the underlying quantum mechanical equations also plays a key enabling role in the design of new materials. In this work, the target is particular structures and properties, requiring the solution of the "inverse problem" to find a corresponding material. In an experimental framework, combinatorial solid-state methods survey the structure and properties for entire compositional ranges for complex solids containing three or more different elements. Similarly, computational methods for the prediction of structure and properties of solids now are accurate and fast enough to allow first-principles materials design, in which the

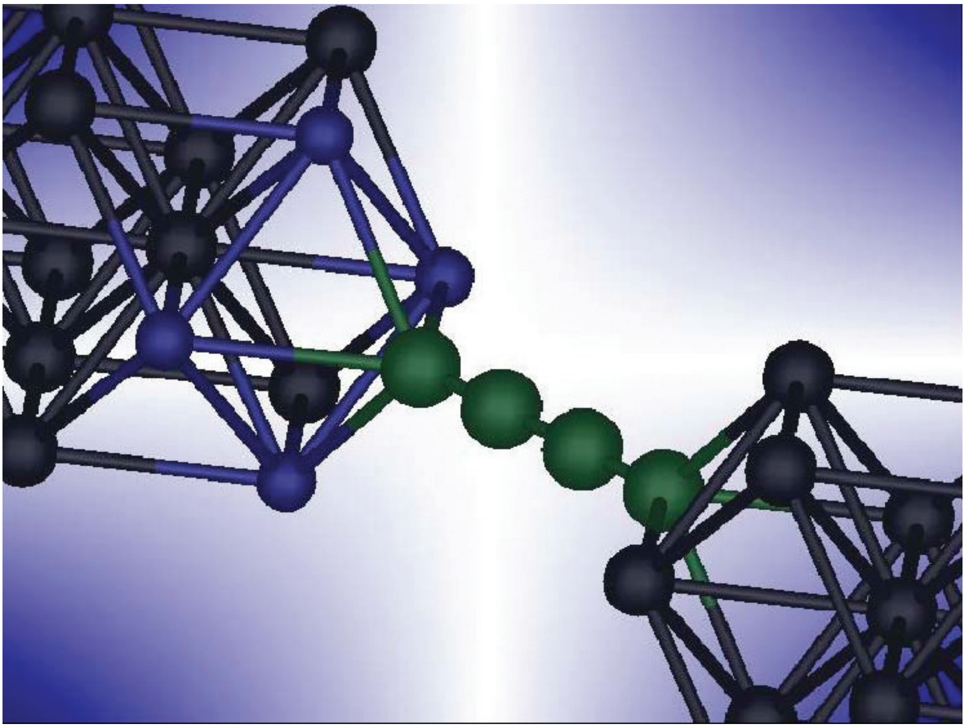

FIGURE 11.2 The current induced by varying voltages across carbon chains of varying lengths sandwiched between gold and aluminum leads can be computed using first-principles methods. The carbon nanowires differ from conventional wires in that the current is not proportional to the voltage. SOURCE: J.B. Neaton, K.H. Khoo, C.D. Spataru, and S.G. Louie, "Electron Transport and Optical Properties of Carbon Nanostructures from First Principles," *Comput. Phys. Commun.* **169**, 1-8 (2005).

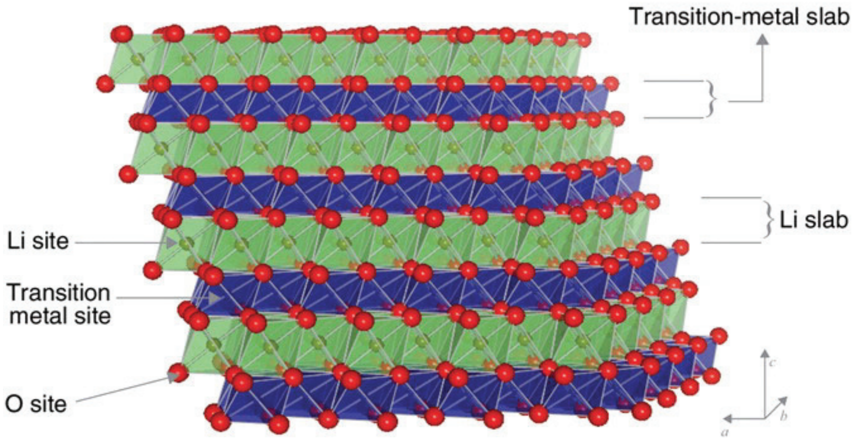

FIGURE 11.3 The structure of lithium nickel manganese oxide, a promising new battery material designed using computational methods, consists of layers of transition metal (nickel and manganese, blue layer) separated from lithium layers (green) by oxygen (red). SOURCE: K. Kang, Y.S. Meng, J. Bréger, C.P. Grey, and G. Ceder, "Electrodes with High Power and High Capacity for Rechargeable Lithium Batteries," *Science* **311**, 977 (2006). Reprinted with permission from the American Association for the Advancement of Science.

structural parameters and selected properties for large sets of real and hypothetical structures can be surveyed to identify interesting materials for new physics and applications, including room-temperature ferromagnetic semiconductors for spintronics[1] and new battery materials[2] (see Figure 11.3). By using the first-principles calculations as input into parameterizations of the composition space, searches can be extended to even larger spaces of materials. Similar principles can be applied to the design of heterogeneous materials and devices.

Much of the important physics in materials systems takes place at length scales well beyond which fully first-principles methods are practical. This range is extended by molecular dynamics simulations with parameterized interatomic potentials. The associated loss in accuracy at the atomic level is compensated by the ability to use tremendously larger numbers of atoms (100 million or more) and the ability to study the time evolution of phenomena. One area in which such computations have proved particularly valuable is in the study of mechanical properties, such as strength of materials, plastic deformation, fracture, and friction, in

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[1] S.C. Erwin and I. Zutic, "Tailoring Ferromagnetic Chalcopyrites," *Nat. Mater.* **3**, 410 (2004).

[2] C.C. Fischer, K.J. Tibbetts, D. Morgan, and G. Ceder, "Predicting Crystal Structure by Merging Data Mining with Quantum Mechanics," *Nat. Mater.* **5**, 641 (2006).

which the behavior is determined by line and planar defects that are created and propagated through the system. An example of such calculational results is given in Figure 11.4.

As impressive as such simulations are, they are still far short of macroscopic scales: a solid cube 1 micron on a side contains over a thousand times more atoms. Within the past decade, priority has been given to developing truly multiscale methods for modeling materials properties, with seamless integration of atomic scale, intermediate length scale, and continuum methods. Similar multiscale approaches are needed to treat materials physics involving time evolution (dynamics) on a wide range of timescales. While great progress has been made, additional breakthroughs are needed.

As new measurement tools are developed, computational approaches will be essential to interpreting larger amounts of data and extracting subtle signals and correlations. Simulations can be invaluable in separating artifacts from intrinsic behavior. Both in the numerical study of simple models and in first-principles

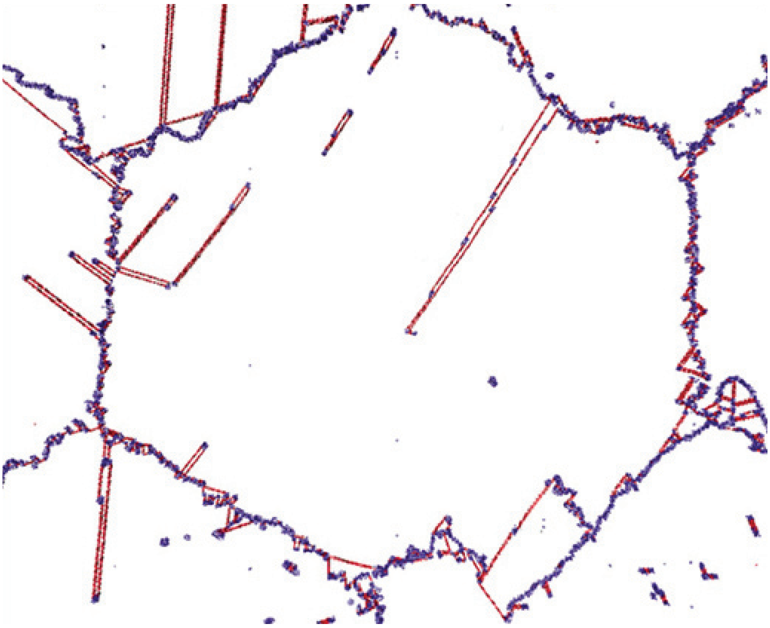

FIGURE 11.4 Snapshot from a molecular-dynamics simulation showing the behavior of nanocrystalline aluminum during deformation. The crystal grain at the center is 70 nm in diameter and is defined by clear grain boundaries (blue atoms). Deformation is seen to drive the formation of planar defects (red atoms) that start at the grain boundary and grow into the grain's interior. SOURCE: V. Yamakov, D. Wolf, S.R. Phillpot, A.K. Mukherjee, H. Gleiter, "Dislocation Processes in the Deformation of Nanocrystalline Aluminium by Molecular-Dynamics Simulation," *Nat. Mater.* **1**, 45 (2002).

simulations, novel unanticipated physical behavior can arise, giving new insights and guiding experimental investigation.

Fundamental issues need to be addressed in the next decade to build on this progress. More efficient, accurate, and broadly applicable methods must be developed to study dynamics, effects of thermal fluctuations, and excited states of materials. There are many promising avenues for further progress in techniques for studying systems with strong correlations. Particular attention should be paid to improving the conceptual and algorithmic framework for studying energy transformation in solids, such as in electromagnetic radiation, energetic particles, and heat generation. Efforts should continue to be made to increase the efficiency of algorithms by drawing on forefront research in numerical methods and computer science. New approaches to multiscale methods for spatial and temporal variations should be pursued. A concerted effort should be made to integrate simulations into experimental data analysis and help with the proper interpretation of the experimental measurements to increase the power of the developing experimental probes described in this chapter. Lastly, the push to integrate simulations into new materials design should intensify, with work continuing in parallel both on realizations for particular systems and on the development of broadly applicable tools based on knowledge gained from these collaborations.

## CENTERS AND FACILITIES IN CMMP RESEARCH

Both the complexity of scientific challenges and the resources required to conduct a successful CMMP research program have increased in recent years. A major scientific challenge to the field is how to synthesize or fabricate materials in which the electronic, atomic, and molecular organization varies spatially, and in some systems, temporally. A related challenge is how to understand principles, or rules, that govern the behavior of materials over different length scales and timescales. To address these challenges, sophisticated tools (experimental, computational, and theoretical) are needed to probe the structure and properties of materials over a wide range of length scales and timescales. For synthesis, fabrication tools such as focused ion beams, molecular beam epitaxy, and lithography have become prohibitively expensive for operation by a single principal investigator (PI). Measurement tools to probe structure and properties are also very expensive, with centers and facilities addressing many of these needs. The associated requirements to educate students on how to perform experiments using new techniques and facilities are a pressing and constantly evolving need. In this section, the committee describes the current status of the research infrastructure and its ability to address, for example, the six CMMP challenges introduced in Chapter 1 and explicitly discussed in this report. The status and role of centers and mid- and large-scale facilities in relation to single and small-group principal investigators are discussed. This chapter also contains recommendations and proposed prioritization of resources for the construction of future facilities.

Various facilities and centers involving interdisciplinary, multi-investigator research groups, with top-down, well-directed missions, now play an increasingly important role in CMMP research. National Science Foundation (NSF) and Department of Energy (DOE) expenditures for building and supporting large, multiuser facilities have thus increased considerably. However, there is a concern that the balance between support for the individual investigator and facility construction and operation is leaning too heavily toward the latter. This scenario presents a natural dilemma, since individual investigators are the users of these facilities and are the source of important scientific breakthroughs. Yet advanced instrumentation and facilities are needed to conduct the research programs of individual investigators. The committee emphasizes here that strong individual research programs, state-of-the-art equipment, and world-class facilities are all important for advancing the field of CMMP, and a proper balance in the funding of each is essential.

In addition, midsize facilities are an important part of the CMMP research enterprise and require careful management to ensure that they have a continued impact. Starting in the 1970s, NSF provided resources for central user facilities through the Materials Research Laboratories (MRL) program. Current multi-investigator research centers, such as Materials Research Science and Engineering Centers, which replaced the MRLs in the mid-1990s, and the Science and Technology Centers, are highly utilized by CMMP researchers. These centers are focused on collaborative, interdisciplinary projects as well as on education and public outreach. The centers have had a large impact on fostering the interdisciplinary aspects of CMMP.

Beyond the MRL-type mechanism for providing central facilities, “generic” multiuser facilities have existed at many institutions, available to local users for a fee. Such facilities, which generally cost in the range of $1 million to $3 million per year of operation, would provide materials characterization facilities such as nuclear magnetic resonance (NMR) spectroscopy, x-ray diffraction, or transmission electron microscopy, and are operated by their host institution. To supplement the present basic central-facility instrumentation now available at the top CMMP research universities in the United States, basic nanofacilities for the synthesis of nanomaterials and their characterization are needed. For more sophisticated and specialized nanofacilities needs, access to the DOE Nanoscale Science Research Centers (NSRCs) is available. The rising costs of sophisticated instruments, often well beyond the rate of inflation, place an increasing burden on institutions. For example, the new aberration-corrected transmission electron microscope costs approximately $4 million and requires support staff for operation and upkeep. Institutions around the world are beginning to acquire such instruments, and this certainly introduces a new metric to the cost of doing cutting-edge research in CMMP.

One crisis associated with the utility of mid-scale facilities is that some institutions have difficulty finding resources to maintain and to support such instruments appropriately once they are acquired. First, maintenance service contracts can be very expensive. Second, state-of-the-art instruments often require support staff with Ph.D.-level expertise, who are needed to train students and to help with the interpretation of data. The problem is compounded by the fact that often there is no viable career path in many institutions for Ph.D. scientists doing these jobs. Two recent National Research Council (NRC) reports highlight the problems and challenges associated with the operation of these facilities.[3,4]

In addition to funding centers and mid-scale facilities, the NSF Division of Materials Research (NSF DMR) now invests a significant portion of its resources toward funding large-scale facilities: the synchrotron facilities at Cornell University and at the University of Wisconsin-Madison, a beam line at the neutron-scattering facility at the National Institute of Standards and Technology, and the National High Magnetic Field Laboratory at Florida State University. NSF DMR should set budget priorities between single PIs and small groups, centers, and facilities. The major concern, as discussed in Chapter 10, is that federal funding for basic research in CMMP has remained essentially flat while the average success rate for proposals from single investigators has decreased dramatically in the past decade. The problem is compounded by costs associated with research at universities outpacing inflation rates. The committee believes that to fully leverage the investment in these centers and facilities, the current balance of funding between single PIs and small groups of PIs relative to centers and facilities should not decline in the future.

During FY 2004, NSF initiated a new program that expands the types of facilities available to institutions: the National Facilities (NAF) program. The NAF program supports unique experimental capabilities for materials research and a wide range of other disciplines. Resources from NSF DMR are leveraged with resources from other directorates within NSF to support the NAF program, which should accomplish the goal of extending the utility of mid-scale facilities. Another program at NSF, the Instrumentation for Materials Research-Major Instrumentation Projects, provides about $2 million to $20 million for instrumentation such as high-field magnets and beam-line instrumentation.

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[3] National Research Council, *Midsize Facilities: The Infrastructure for Materials Research*, Washington, D.C.: The National Academies Press, 2006.

[4] National Academy of Sciences, National Academy of Engineering, and Institute of Medicine, *Advanced Research Instrumentation and Facilities*, Washington D.C.: The National Academies Press, 2006.

DOE funds large-scale scientific user facilities such as light sources, neutron sources, electron microscopy facilities, and nanoscience centers. The light sources and neutron facilities provide beam lines for a wide range of materials analysis. The need for increased sensitivity and resolution (spatial and temporal) to study properties at the nanoscale or atomic scale makes the use of large-scale facilities an increasingly necessary component of CMMP research, as documented by user demand.

The interdisciplinarity of CMMP research is reflected in part by the demographics of investigators supported by NSF DMR and by DOE Basic Energy Sciences. Figure 11.5 shows the demographics of materials researchers supported by NSF DMR; besides physicists, this enterprise involves engineers, chemists, biologists, mathematicians, and researchers in other disciplines. It should be noted that the establishment of the new biomaterials program within NSF DMR is expected to further change the demographics of researchers who compete for these resources.

It is clear from the foregoing that the culture of CMMP research is being transformed in such a manner that the role of the individual principal investigator continues to evolve. In addition to the increasing role of large facilities and sophisticated instrumentation, the research problems that are now taking center stage

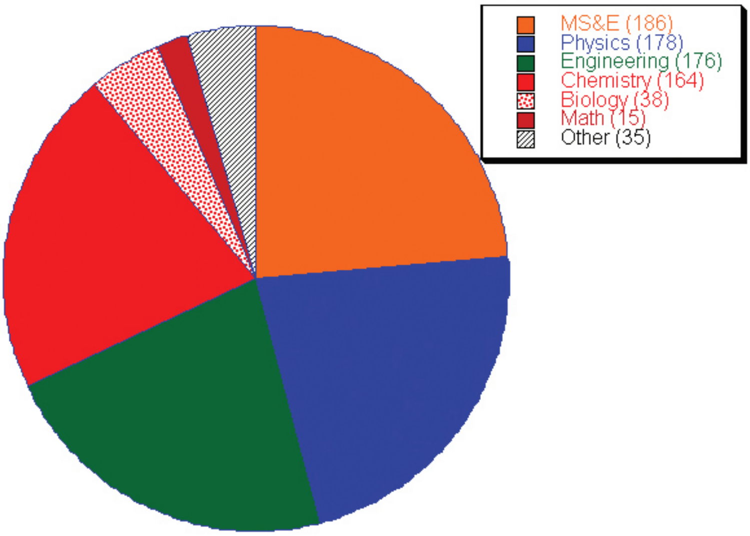

FIGURE 11.5 Faculty supported by the Division of Materials Research at the National Science Foundation in 2004 by departmental affiliation. The actual number of faculty is indicated in the parentheses in the inset. NOTE: MS&E, Materials Science and Engineering. SOURCE: National Science Foundation.

have become increasingly interdisciplinary. Centers now play an important role in meeting CMMP challenges. Nevertheless, single PIs hold the potential for making the most significant breakthroughs in science, as they have in the past. Grant sizes and success rates are beginning to impact the ability of CMMP researchers to conduct cutting-edge and high-risk scientific exploration and to train the next generation of CMMP researchers and technology developers properly. Nowadays, CMMP researchers report that they are diversifying their research portfolios for the survival of their research groups. CMMP researchers comment that diversification often means that in practice they work on certain problems only because funding is available and not because that work is where they can make the most significant difference toward advancing the field. Strong support of the individual investigator coupled with access to world-class instrumentation and facilities is needed for cutting-edge CMMP research, to train students to do such research, and to compete and collaborate with Europe and Asia to advance science and exploit societal applications of CMMP discoveries.

## SCIENTIFIC USER FACILITIES FOR CMMP RESEARCH

The Committee on CMMP 2010 was charged to "identify, discuss, and suggest priorities for construction, purchase, and operation of tools and facilities ranging from instrumentation for the individual investigator to the national user facilities." To address this charge, the committee convened a workshop with government, university, and industry stakeholders to discuss the future needs for facilities in CMMP (see Appendix C). This section focuses on the present status of user facilities for CMMP research and identifies needs for the future based on the community input received at the workshop. In turn, the committee considers here light sources, neutron sources, electron microscopy, high-magnetic-field facilities, nanocenters and materials synthesis, and high-performance computing facilities. Prioritized recommendations are provided for each class of facility (see the respective "Recommendations" subsections below), but the committee did not rank order the classes.

DOE, NSF, and the National Institute of Standards and Technology (NIST) support scientific user facilities for CMMP research. DOE is by far the largest supporter, accounting for approximately 85 percent of the investment. These agencies construct and operate light, neutron, and electron-beam sources; high-magnetic-field laboratories; and nanocenters. The facilities are available to users around the country and elsewhere, based on an equitable review process of the merits of a research proposal. The facilities are reviewed every few years with the goal of providing new techniques to users and of optimizing the use of the facilities. The types of scientific problems examined at these laboratories are diverse and include areas such as geology, magnetism, structural biology, catalysis, and many others.

## Light Sources

Many of the developments in CMMP of the past decade have depended heavily on electron-accelerator-based sources of radiation, popularly referred to as light sources. These sources vary from free-electron lasers to generate far-infrared radiation, with capitalizations on the order of $5 million, through to large-scale facilities such as the Advanced Photon Source (APS) at Argonne National Laboratory, with a replacement value on the order of $1 billion. Light sources allow the extension of the power of the optical microscope to obtain images of condensed matter at smaller and smaller distances in real space as well as in the space spanned by momentum and energy and, in what is becoming increasingly important, a mixture of the two. Examples of results from the past decade include ultraviolet photoemission work elucidating the exotic normal and superconducting states of the copper oxides, high-resolution phase contrast images of insects, pictures of nanoscale antiferromagnetic domains, and thousands of new entries in protein structure databases. Light sources can be used as nanoprobes, for imaging, diffraction, molecular crystallography, in situ high-pressure experiments, and x-ray microscopy for a wide range of novel materials.

The importance of light sources will increase over the next decade, and indeed they are indispensable to meeting all of the CMMP grand challenges simply because of the power of images obtained at the length scales ultimately responsible for macroscopic physical phenomena and underpinning the functionality of materials, devices, and organisms. In the coming decade, the committee therefore looks forward to the continuation, among other things, of diffraction studies to locate atoms in new materials and novel nanostructures with, for example, impact on the energy problem and future information technology; high-resolution photoemission to probe emergent quantum phenomena in transition metal oxides; and time-resolved studies of dynamical processes in biology. Third-generation light sources offer the possibility of single-molecule spectroscopy to determine electronic structure, oxidation states, symmetry of chemical bonds, and local atomic structure. In addition, and what will lead to a qualitatively new science, new methods are being developed to exploit higher brilliance (by many orders of magnitude) and coherence in the light sources. There is expected to be great progress in x-ray scanning probe microscopy where there are plans to reach nanometer resolution, phase contrast imaging, and, most exciting, the wholesale importation of techniques from modern pulsed (visible) optics to the accelerator-based sources. The latter will mean that researchers will be able to exploit transform-limited x-ray pulses to look at linear excitations and non-equilibrium phenomena essential for the functionality of systems ranging from biological membranes to quantum computers.

### *Current Status of Light Sources*

The world has a large variety of accelerator-based light sources. The United States has a presence in each of the major current categories of light sources, including large third-generation synchrotrons devoted to soft and hard x-rays, several free-electron lasers to produce infrared radiation, a recently refurbished second-generation x-ray synchrotron, several ultraviolet synchrotrons, several free-electron lasers to produce infrared radiation, and an x-ray free-electron laser whose construction was endorsed in the last decadal survey of CMMP and is now under construction. Therefore, the current position of the United States in this general area appears healthy and world leading.

DOE currently operates light sources to meet the needs of a large number of users, projected to be more than 10,000 investigators in the near future (see Figure 11.6). At the APS, for example, the number has increased at a relatively constant rate of about 500 users per year since 1997. It is noteworthy that the fraction of users from the life sciences has increased rapidly, from less than 10 percent in 1990 to approximately 45 percent in 2003. Physics and materials science account for just over 25 percent of the use, with materials science having twice as many users (see Figure 11.6). Most users are academics; government and industry account for a combined use of approximately 25 percent.

Light sources are primarily used for hard x-rays for scattering experiments. Spectroscopy is the second more popular use, with most of the use occurring at the National Synchrotron Light Source and the Advanced Light Source (ALS). Imaging experiments are becoming increasingly popular, particularly for soft materials (using soft x rays), with most of the work done at ALS (see Figure 11.7). The

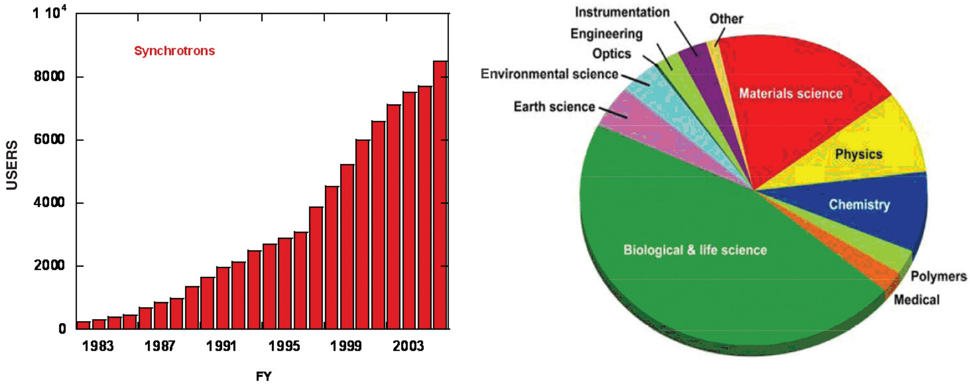

FIGURE 11.6 (Left) The number of users at U.S. synchrotron facilities, 1982-2005. (Right) The demographics of users of the Advanced Photon Source. SOURCE: Department of Energy.

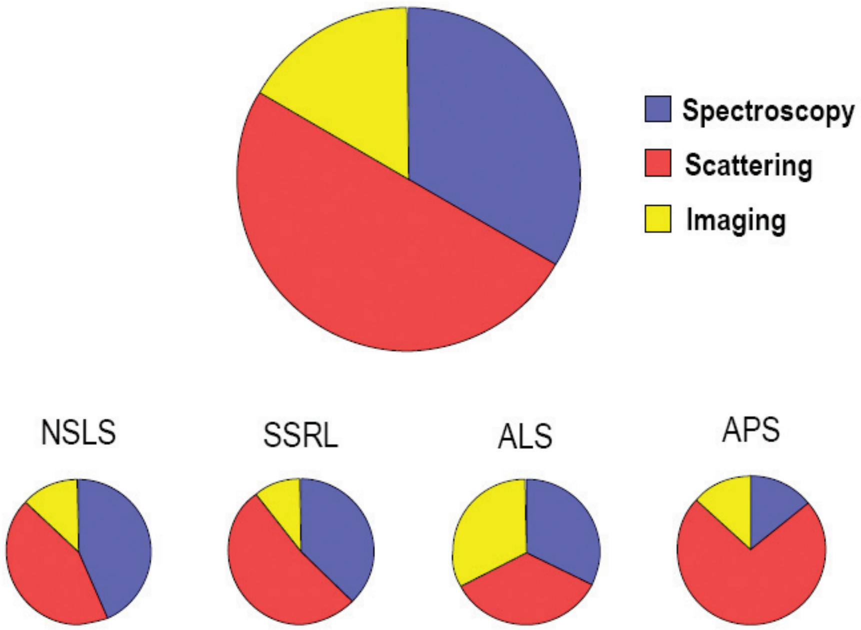

FIGURE 11.7 The types of experiments conducted at U.S. light sources. NOTE: NSLS, National Synchrotron Light Source; SSRL, Stanford Synchrotron Radiation Laboratory; ALS, Advanced Light Source; APS, Advanced Photon Source. SOURCE: Department of Energy.

primary advantage of using a beam line at a light source for these types of experiments is the improved sensitivity over other techniques.

### *Medium-Term Developments for Light Sources*

In the medium term, the U.S. position looks less secure. No synchrotron facilities currently under construction worldwide are located in the United States except one—the Linac Coherent Light Source (LCLS). Indeed, the LCLS represents the only new start in the past decade. The LCLS will be the first x-ray free-electron laser in the world, giving the United States a unique window on the first experiments in single-molecule imaging. The LCLS will therefore be a tremendous tool for meeting the challenges discussed in Chapter 4 ("What Is the Physics of Life?") and Chapter 6 ("What New Discoveries Await Us in the Nanoworld?"), and for developing the capabilities of both the CMMP and accelerator communities for a next step in the development of light sources: namely, the seeded free-electron laser. In addition, the LCLS has the potential to make large contributions to many other disciplines, including biology, atomic and molecular science, and even plasma physics. The LCLS will also, from both a technical and a community-building point of view, provide opportunities for further cross-fertilization between CMMP and its lively neighboring disciplines.

As shown in Figure 11.8, there are currently three times as many beam ports outside as inside the United States; there are about 123 beam ports in the United States now. This difference is estimated to grow to approximately seven times as many beam ports outside the United States by 2009 with the construction of new synchrotrons abroad.

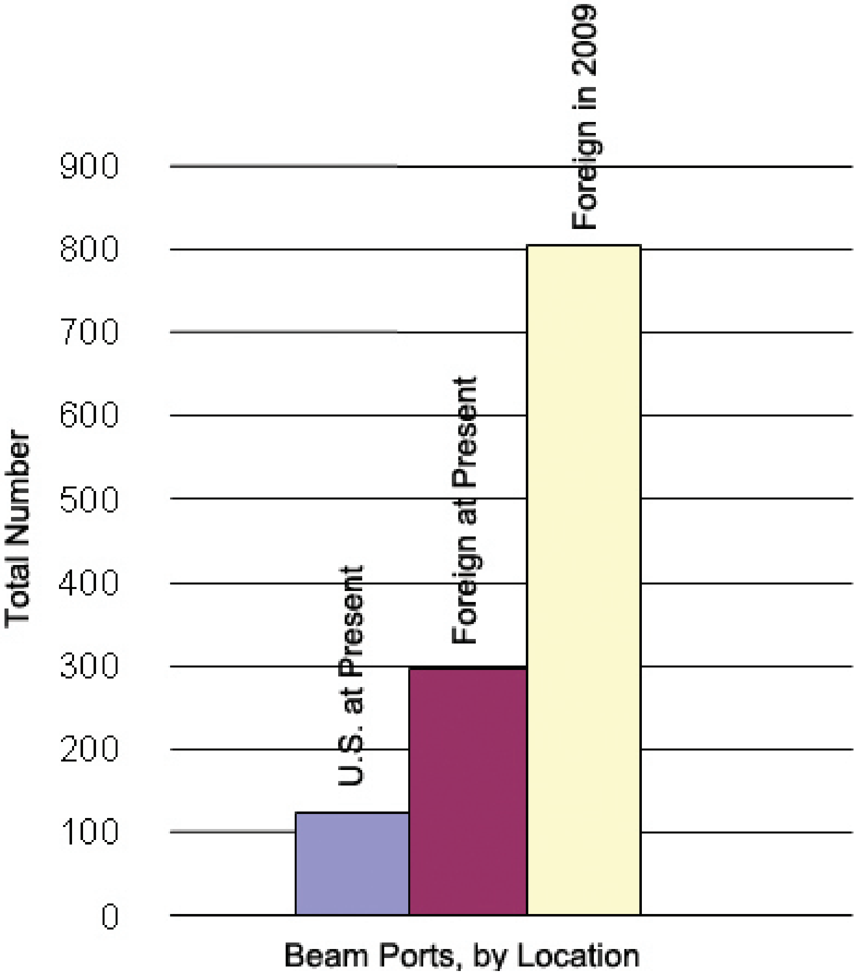

FIGURE 11.8 The total number and location of third-generation synchrotron beam ports around the world. SOURCE: Department of Energy.

It is clear that unless new initiatives are undertaken, the United States will be faced with aging and less-than-world-class infrastructure over the next decade. The impact of accelerator-driven light sources over the past decade suggests a goal of full utilization of existing third-generation sources as well as the construction of a major new source. The third-generation light sources are key tools for meeting all of the grand scientific challenges whose descriptions are at the core of this report. They provide vital information on the micro- and nanostructures emerging from simple ingredients (Chapter 2); on the materials and increasingly on the processes for energy extraction and utilization (Chapter 3); on biomolecules, membranes, and larger systems pertaining to the physics of life (Chapter 4); on nanomaterials and nanosystems (Chapter 6); and on the materials and device structures that will underpin the continuation of the information technology revolution (Chapter 7). The committee points out that slower non-equilibrium phenomena (Chapter 5) are well studied using third-generation synchrotrons, but faster, dynamic effects, especially in small structures, and also effects where coherence is important, will demand more-advanced types of light sources.

What is most exciting, though, is that the need for new infrastructure coincides with several extraordinary developments in the generation and exploitation of light at accelerators:

- Demonstration experiments on coherent beams providing holograms of nanocrystals, dynamics of magnets, polymers, and even of flames;
- The beginning of picosecond and even subpicosecond time-resolved x-ray science, with applications both in molecular and solid-state science;
- New optics, fabricated using nano- and microtechnology originally developed for the semiconductor industry, allowing phase contrast as well as more traditional scanning probe imaging;
- Worldwide growth of interest in coherent terahertz radiation for imaging, with applications ranging from security (including luggage screening) to medicine, but also for spectroscopy, especially in conjunction with high magnetic fields;
- New special-purpose sample environments, ranging from sample stages that incorporate scanning probe microscope drivers to pressure cells and series-connected hybrid magnets. Application areas opened by these sample environments range from the engineering of micro- and nanomechanical systems to Earth and planetary sciences, where high-pressure environments occur naturally but cannot be accessed directly;
- Concepts for low-cost ($5 million to $10 million) compact x-ray sources providing time-averaged fluxes and brilliance comparable to second-generation synchrotrons and short-pulse performance superior to any capabilities offered at large facilities today. The underlying operating principle is the inverse Compton effect, where a relatively low energy electron beam,

prepared in a superconducting linear accelerator, passes through a laser cavity in which the optical fields act as an undulator. If the promise of these concepts is realized, CMMP (as well as many other areas of science) will be transformed as a result of the possibilities afforded by immediate and intimate contact between the fabrication, x-ray characterization, and other characterization in the discovery and study of a new material. This will bring x-ray analysis much closer to the mainstream of CMMP characterization, in the same way that routine electrical, magnetic, and electron microscopy are used;

- Concepts for seeding x-ray lasers to produce single, transform-limited, coherent pulses rather than random sequences of closely spaced pulses as with the present self-stimulation paradigm. This will greatly enhance our ability to do high-resolution x-ray spectroscopy, but more importantly, it will allow x-rays to image non-equilibrium dynamics of condensed matter in both classical and quantum regimes. Experiments that might become possible are numerous, and range from investigations of the time-dependent changes in thin gate oxide transistors as they are switched, to measurements of time-dependent structural changes in active nanoscale biological systems such as ion channels; and
- Blossoming of interest in the energy-recovery linear accelerator concept as a method for delivering more spatial coherence and higher brilliance beams than are possible with third-generation synchrotrons. If they performed as predicted, energy-recovery linear accelerators would allow the promise of the current generation of demonstration experiments exploiting spatially coherent beams (described in the first bullet point, above) to be fulfilled for a much larger class of scientific problems.

Obvious from the list above and from Figure 11.9 are the tremendous opportunities as well as large potential costs of future light sources. Conservatively, the implementation of one exemplar of the two large concepts, namely, the seeded free-electron laser and the energy-recovery linear accelerator, as well as construction of another more conventional third-generation synchrotron light source, would cost on the order of $3 billion, and the corresponding annual operating expenses would eventually run to approximately $500 million. This means that prioritization for these facilities is especially important.

### *Recommendations for Light Sources in CMMP Research*

Informed by presentations and discussion at the CMMP 2010 Facilities Workshop (see Appendix C) and subsequent discussion by the Committee on CMMP 2010, the committee identifies the recommendations in this subsection as priorities (in the order in which they appear below) for future investment in light sources.

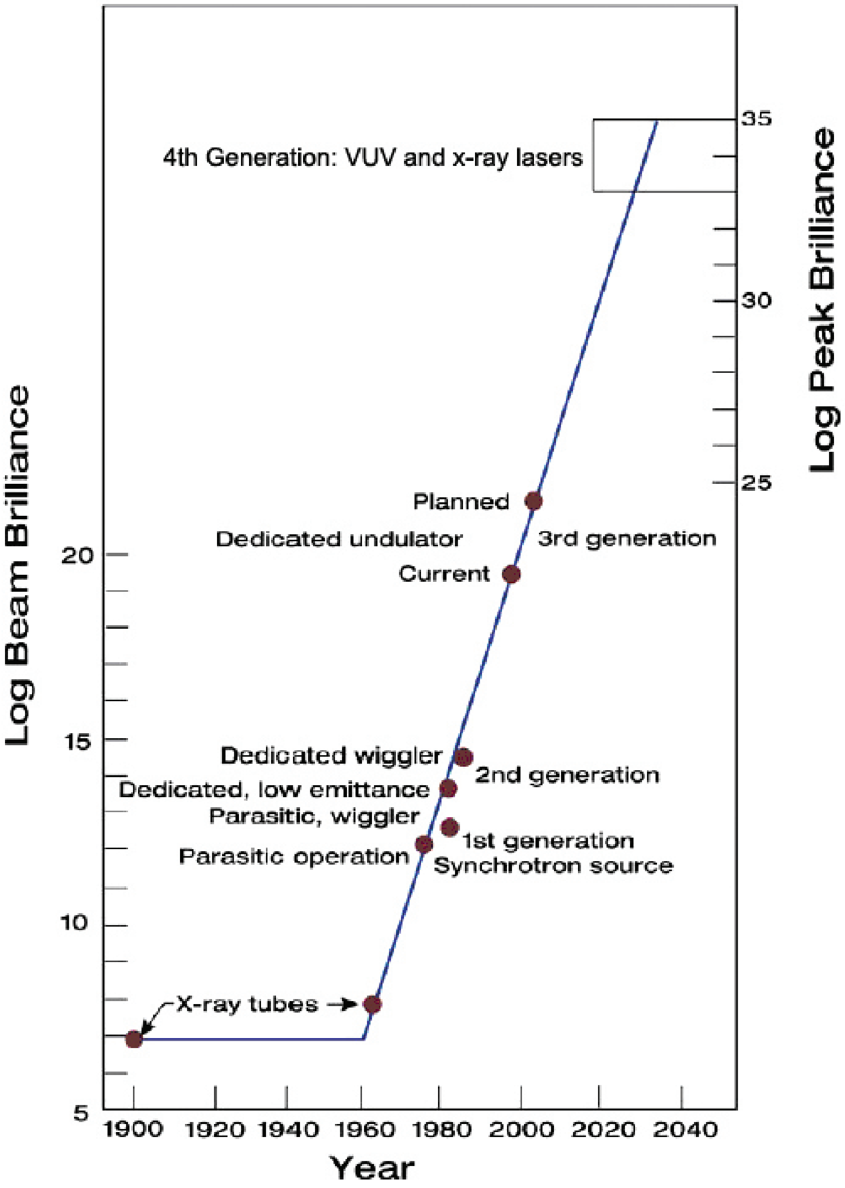

FIGURE 11.9 Increased x-ray brilliance, which measures the flux of photons per unit of phase space volume, can be achieved by combinations of increases in raw beam power and improvements in beam coherence. NOTE: VUV, vacuum-ultraviolet. SOURCE: D.E. Moncton, Massachusetts Institute of Technology.

The first recommendation is for systematic long-term planning for future U.S. light sources. The second and third recommendations are aimed at benefiting optimally from investments already made. The fourth recommendation is for planning, design, and construction of the next synchrotron facility in the next decade, and the final recommendation is to enable entry into the next phase of light sources, providing small brilliant light sources for the laboratory. A past NRC committee reached remarkably similar conclusions in 1994.[5]

A key feature of the development of light sources over the past decade has been their transformation from facilities primarily of interest to the core CMMP programs of DOE and NSF to resources pertinent to the agendas of a much broader range of government agencies and private groups, including especially those concerned with the biomedical sciences, such as the National Institutes of Health (NIH) and pharmaceutical companies. This means that even while DOE and NSF should continue in their roles as key stewards of large- and medium-scale facilities, respectively, it is essential to engage strongly with the other interested organizations for planning and funding purposes if the full potential of light sources is to be realized in the United States. It is for this reason that the committee recommends a research and development (R&D) consortium, which has the highest priority in the list below, with expertise in cutting-edge light source technology but without legacy investments and decisions to protect.

Another interesting aspect derives from the growing cost of new facilities, and the committee expects that for the very largest machines, such as a seeded x-ray free-electron laser, there will be a growing trend toward international cooperation. Nonetheless, it will be important for the United States to bring technology as well as money to the table when strategic international decisions (for example, site selection) are made; this is another reason why the committee considers the implementation of the first recommendation to be very important.

> **Recommendation:** DOE and NSF, partnering with NIH and NIST, should create a consortium[6] focused on research and development needs required for next-generation light sources. The consortium, with an independent chairperson, should include stakeholders from universities, industry, and government (both laboratories and agencies). The consortium should formulate a light source technology roadmap and make recommendations on the R&D needed to reach milestones on the roadmap for a new generation of light sources, such as seeded x-ray free-electron lasers, energy-recovery linear-accelerator-driven

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[5] National Research Council, *Free Electron Lasers and Other Advanced Sources of Light: Scientific Research Opportunities*, Washington, D.C., National Academy Press, 1994.

[6] The committee used the term "consortium" in the sense of a partnership among the stakeholders described in the recommendation for developing a light source technology roadmap. The committee expects that the "consortium" will follow federal rules for providing advice to federal agencies.

devices, and other promising concepts. The consortium should also take into account cost containment and the internationalization of research facilities. The sponsoring agencies of the consortium should fund the R&D needed to reach the milestones on the roadmap.

**Recommendation:** DOE should exploit fully the existing third-generation synchrotrons; this means utilizing the remaining straight sections at the National Synchrotron Light Source, Stanford Positron Electron Accelerating Ring, Advanced Light Source, and Advanced Photon Source, and recapitalizing obsolete beam lines at all four facilities. This also means proceeding with the high-magnetic-field sample environment for APS. In addition, it means providing personnel and consumables for beam lines in accord with best international practice. New beam lines and instrumentation should be added according to need.

**Recommendation:** DOE should complete and fully fund the operations of the Linac Coherent Light Source.

**Recommendation:** DOE should prepare an engineering design for and then begin construction of a major new light source in the United States such as the National Synchrotron Light Source II (NSLS-II). The NSLS-II design should follow a trend in regional synchrotron light sources of employing more moderate beam energies but, through use of more sophisticated insertion devices, achieving good spectral coverage, including the x-ray region. Because the accelerator and instrumentation design goals for NSLS-II are very challenging and a significant extrapolation of the current state of the art, it would be desirable to have an open, transparent, and independent review of the engineering design.

**Recommendation:** DOE and NSF should create opportunities for $5 million to $10 million facilities with suitable operating funds to take advantage of compact x-ray sources and infrared free-electron lasers. The associated scientific possibilities are enormous, in the first case making medium-intensity x-ray beams as accessible as high-end electron microscopes, and in the second case, providing tunable, high-intensity radiation in a part of the electromagnetic spectrum with rapidly growing technological and scientific relevance.

## Neutron Sources

New materials will play a pivotal role in solving some of the societal issues that face the world in the 21st century. These issues include the development of clean and abundant sources of renewable energy, the availability of sufficient potable water, and the protection of the environment from anthropogenic activity. The newest generation of materials is only just beginning to creep into our daily lives, but it is already clear that some will have a major impact. For example, wide band gap semiconductors based on gallium nitride will clearly provide the basis for solid-state lighting devices that consume far less electricity than conventional lighting such as incandescent and fluorescent lamps do. Conducting polymers may well play a major role in the search for affordable and efficient solar energy.

Against this backdrop of materials discovery and deployment, it is important to understand the central role that major facilities have played in underpinning the knowledge of new materials and accelerating their progress toward real applications. Neutrons are important in the world of both organic and inorganic materials. For example, following the discovery of high-temperature cuprate superconductors in 1986, neutrons were immediately deployed in order to understand the structures of these exciting materials and to explore the relationship between magnetism and superconductivity. Several of the early papers from major facilities became citation classics, such as work on the structure of $YBa_2Cu_3O_{7-x}$, that on magnetic fluctuations in $La_{2-x}Sr_xCuO_4$, and the study of stripe correlations in copper oxide superconductors. Small-angle neutron scattering played a central role in understanding polymer chain structure and conformation. The same pattern repeated itself when bulk samples of buckminsterfullerene, $C_{60}$, were synthesized in the early 1990s. The power of neutron scattering was immediately harnessed to characterize the structure of the buckminsterfullerene and to study the properties of the new superconducting fulleride derivatives that were discovered immediately afterward. Recent achievements include in situ imaging work at NIST on water movement in hydrogen fuel cells (Figure 11.10), studies of electronic phase segregation and short-range order in transition metal oxides, and polarized neutron reflectometry applied to spintronic materials. Other recent achievements involved the use of neutron reflectivity to study block copolymer thin films. Neutron spin echo techniques provided new insights into polymer chain dynamics and transitions.

There can be no doubt that neutron sources and related major facilities will make major contributions to all of the grand challenge areas identified in this report. History shows that with each new generation of advanced materials, the power of the nation's major facilities is used to address some of the key scientific and technological issues.

The neutron is a unique probe for studying condensed matter. Its penetrating power enables it to probe large objects up to 1,500 kilograms in weight, making it suitable for characterizing defects in macroscopic engineering structures. At the atomic level, the magnetic moment of the neutron makes it sensitive to the spin and orbital properties of transition metal ions in important materials such as highly magnetoresistive oxides. And the unique sensitivity of neutrons to the location and

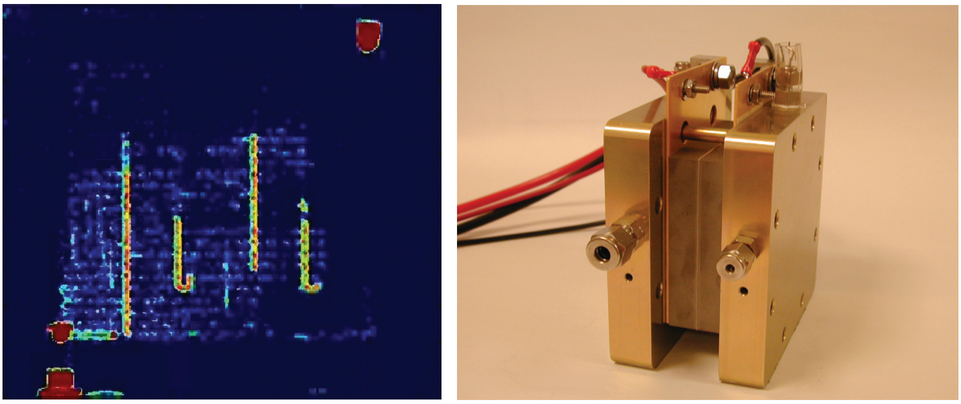

FIGURE 11.10 (Left) Image of water motion in the channels of a hydrogen fuel cell. (Right) The corresponding fuel cell. SOURCES: J.P. Owejan, General Motors Corporation, and the National Institute of Standards and Technology.

motion of hydrogen atoms will continue to be unmatched for studies of hydrogen storage materials, catalysts, polymers, and biomaterials.

### *Current Status of Neutron Sources*

The neutron community in the United States is entering an exciting period. The commissioning of the Spallation Neutron Source and the refit of the High Flux Isotope Reactor (HFIR), both located at Oak Ridge National Laboratory (ORNL), will bring leadership-class source capability back to the United States for the first time in more than 30 years. SNS will be a factor of 8 times more intense than the ISIS spallation facility in the United Kingdom, which is currently the most intense spallation source in the world. Furthermore, the new generation of instruments, with their improved optics and detectors, will give a further advantage, leading to an overall gain in signal of 20 to 100 times. In terms of reactor sources, the HFIR facility is comparable in power to the high-flux beam reactor at the Institut Laue-Langevin in Grenoble, France, albeit with fewer beam lines and instruments, so the combined source capability at ORNL will be best-in-class.

Scientific leadership, of course, is not simply dependent on source intensity but also on the development of innovative instruments, versatile sample environments, powerful data-analysis infrastructure, and the recruitment of talented and energetic instrument scientists. Even more, of course, it depends on the creativity of the science community in employing these instruments.

However, even with the advent of SNS, the United States remains beam-line and instrument poor compared with Europe. In 2010, for example, there will be about 170 neutron instruments in Europe, compared with only 70 in the United States. In addition, the rate of growth of neutron sources in the Asia-Pacific region will likely surpass the capabilities in the United States within the next decade. For example, China is building three new neutron sources, the Japan Proton Accelerator Research Complex is being completed in Japan, there is a major reactor upgrade in Korea, and a new Australian research reactor has recently started up. In the light of the 1997 closure of Brookhaven National Laboratory's High Flux Beam Reactor (HFBR) and the possible closure of Argonne National Laboratory's Intense Pulsed Neutron Source (IPNS) in 2009, it is essential that the remaining facilities at NIST and the Los Alamos Neutron Scattering Center (LANSCE) at Los Alamos National Laboratory be sustained at internationally competitive levels and that the remaining expertise at Brookhaven and Argonne National Laboratories be retained and harnessed.

One very positive development in the U.S. neutron community over the past 15 years has been the growth of the user base (Figure 11.11). In particular, the overall number of users has increased from approximately 650 in 1990 to more than 1,500

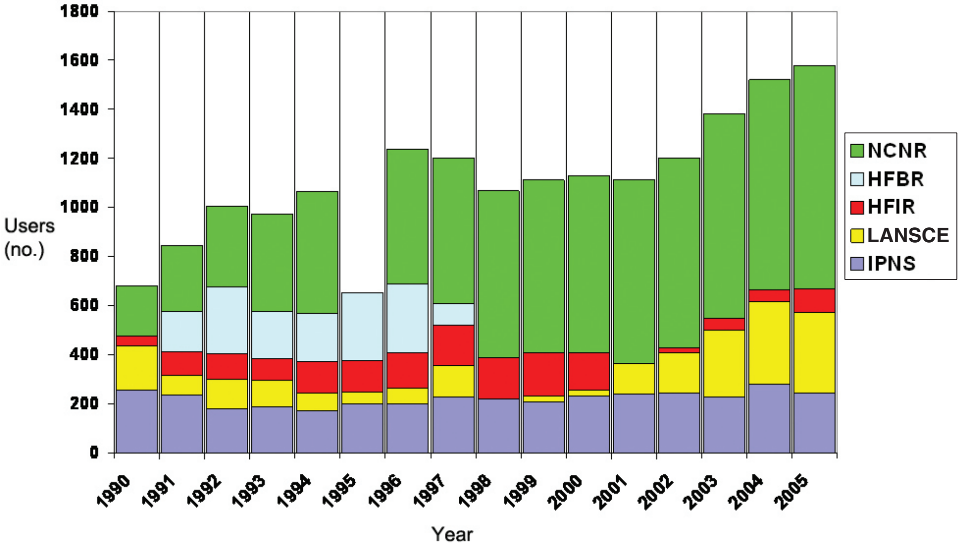

FIGURE 11.11 Growth of the U.S. neutron user community between 1990 and 2005. NOTE: NCNR, National Institute of Standards and Technology (NIST) Center for Neutron Research; HFBR, High Flux Beam Reactor; HFIR, High Flux Isotope Reactor; IPNS, Intense Pulsed Neutron Source. SOURCE: Patrick Gallagher, National Institute of Standards and Technology.

in 2005. The data in Figure 11.11 also show the negative impact of the closure of HFBR in 1997, from which it took the community 6 years to recover. The graph also shows the impressive growth since 2000 of the user base at LANSCE and the huge impact of the NIST Center for Neutron Research.

The other significant development over the past decade has been the changing pattern of industrial use of neutrons. The data are partly anecdotal, but the numbers of primary industrial users have diminished as the amount of basic research at some of the major industrial laboratories, such as at IBM research laboratories and at Bell Laboratories, has been reduced. In addition, there is some evidence that more work is being done in industry through university collaborators.

Looking to the future, if the funding agencies pursue full utilization of the available U.S. sources, which will require increased operating funds as well as capital investments (see the following subsection), the size of the U.S. neutron user base is expected to approach that of Europe today over the next 15 years. These projections assume that the second target station will be built at SNS, that IPNS will remain open, and that all the facilities will have a full complement of instruments (see two subsections below).

### *Medium-Term Developments*

A number of important upgrades to the existing facilities have already been approved but not yet funded: the SNS Power Upgrade ($160 million), a second cold source/guide hall at NIST ($100 million), and the LANSCE accelerator refurbishment ($170 million, funded by the National Nuclear Security Administration). In addition, a number of other major projects are in the advanced stages of planning—specifically, the second target station at SNS (the Long Wavelength Target Station [LWTS], $500 million)—and a second guide hall at HFIR ($150 million) has also been under discussion. SNS is designed to accommodate a second target station fed from the same accelerator complex, while operating at a lower repetition rate than that at the existing High Power Target Station (HPTS). This would double the number of beam lines that can be supported, enabling a much broader scientific program and providing the optimal route to a significant number of additional high-flux beam lines (about 25) without the expense of building an entirely new source. More importantly, a lower repetition rate would lend itself to optimizing the target station environment and its instruments for long-wavelength (cold) neutrons. In the long term, the LWTS would more than double the scientific capability of SNS for about 25 percent of the capital cost while providing space for enough additional instruments to double the user community at SNS.

The proposed LWTS will be a nanoscience neutron source with an order-of-magnitude better performance in many applications compared with the HPTS. The use and sophistication of neutron diffraction and crystallography are growing strongly in the study of complex materials having both atomic scale and nanoscale features. These include hybrid organic-inorganic materials for sensors, mesoporous solids for chemical separations and catalysis, and supramolecular complexes of biomolecules. The LWTS will be ideal for neutron reflectometry, which strongly impacts the study of polymer thin films and interfaces, magnetic films and multilayers, liquid surfaces, biological membranes, bilayers, and in situ corrosion studies. In addition, neutron spectroscopy using long-wavelength neutrons is increasingly being applied to the study of the low-energy dynamics of complex systems, such as polymer (reptation), proteins, and molecules in confined geometries or adsorbed on surfaces.

The cold source for the second guide hall at HFIR would be placed in a region of very high flux leading to the highest steady-state cold neutron source in the world (by a factor of about two to three). The science opportunities for the second guide hall would eventually fall into the same realm as the SNS second target but would be tailored to the complementary strengths of a continuous versus pulsed source.

In addition to these major capital projects, a number of other developments will be required in order to achieve the full potential of the source capabilities. These developments, which are interdependent and therefore not prioritized in the list below, are as follows:

- Robust funding of research programs; *neutron science is single-investigator driven.* In order for projects that involve the use of neutrons to be carried out, faculty must have their own grants to support graduate students and postdoctoral assistants;
- Full staffing of beam lines; the current level of three to four staff scientists per instrument needs to increase to at least five to better utilize the investment in the instrumentation;
- Continued funding to permit full operating time of facilities in order to accommodate all very highly rated proposals;
- Significant investment in ancillary equipment or sample environments, for example, samples in extreme environments of temperature, pressure, and magnetic field; and
- Substantial investment in software development, including data analysis, visualization, modeling, and so on. The project on Distributed Data Analysis for Neutron Scattering Experiments (DANSE) is an excellent start and may provide the basis for a future coordinated national effort in this area.

It is also important to recognize that the quality of the science emerging from the facilities will be severely compromised if the instruments are not state of the art. This will require an investment of approximately $100 million per year, compared with about $25 million that is being spent at present.

Beyond the full-utilization scenario described above, the United States will need a new national facility, driven by the age of some of the existing facilities and the intriguing new concepts that are developing, such as very cold neutron sources for ultralong neutron wavelengths, long pulsed sources, and novel continuous sources. The committee emphasizes that the long-term strategy must be planned during the coming decade, based on experience with the current facilities, bearing in mind the needs of individual investigators working in CMMP and the instrumentation and facilities they need to carry out state-of-the-art research.

*Recommendations for Neutron Sources in CMMP Research*

**Recommendation:** DOE should complete the instrument suite for the SNS at Oak Ridge National Laboratory, together with provision of state-of-the-art ancillary equipment for these instruments, in order to gain the maximum benefit from the recent investment in the SNS.

**Recommendation:** DOE should construct the second target station at SNS as the top priority for major capital investment for neutron sources, since it will facilitate a wide range of new science and will provide qualitatively different capabilities for cold neutron studies.

**Recommendation:** DOE, NSF, and the Department of Commerce should sustain commitments to the existing neutron facilities at Los Alamos National Laboratory and the National Institute of Standards and Technology as needed to meet the growing demand for neutron studies and to train new users in neutron-scattering techniques.

**Recommendation:** With support from the funding agencies and in the next 5 years, the research community should begin to make longer-term plans for a future neutron source.

## Electron Microscopy

Electron microscopy is an integral part of the discovery and development of new materials. Of all CMMP papers produced each year, a significant fraction contains data relying on some type of electron microscopy. The two major types of electron microscopy are scanning electron microscopy (SEM), which images the reflected beam, and transmission electron microscopy, which detects the transmitted beam. While the fundamental principles underlying electron microscopy have been known for at least half a century, the recent rate of instrumental advance is the highest since the invention of the electron microscope, with enormous potential to solve key questions of CMMP. Traditional areas of success include studies of crystalline solids as well as solid interfaces. More recently, new technology has enabled new directions in nanomaterials, soft matter such as (bio-) polymers, organic/inorganic composites, and dynamic processes at the atomic scale. New techniques include tomography as well as holography for magnetic materials and dopant profiles.

Electron microscopy is well positioned to address a wide range of important, upcoming characterization challenges in CMMP. These include tomography and the three-dimensional mapping of electronic structure at the atomic level; local structure-property determination for individual, embedded nanophases and their interaction with the surrounding matrix; and the three-dimensional imaging of magnetic fields at the nanoscale (Figure 11.12).

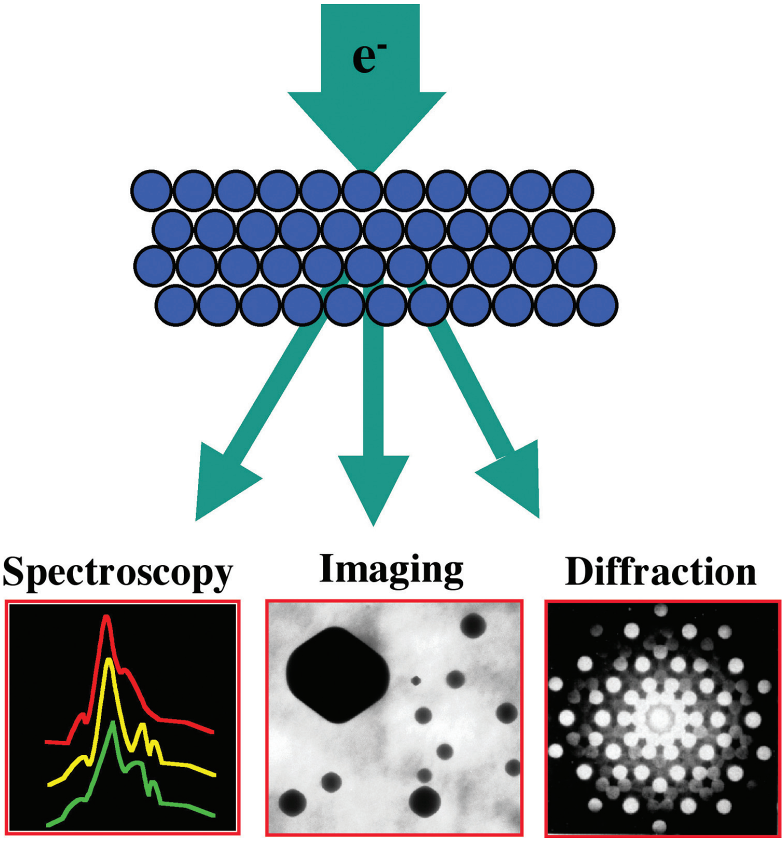

FIGURE 11.12 After the electron beam penetrates a sufficiently thin sample, the three principal modalities of a transmission electron microscope provide complementary information. SOURCE: Ulrich Dahmen, Lawrence Berkeley National Laboratory.

### *Current Status of Electron Microscopy Facilities*

DOE supports three electron beam sources: one each at Argonne, Lawrence Berkeley, and Oak Ridge National Laboratories (ANL, LBNL, and ORNL). The number of users of these sources has grown somewhat over the past two decades to approximately 500 in 2006 from 350 in 1985. The smaller base of users of electron-beam sources reflects the fact that electron microscopes are comparatively widespread, and the national facilities offer significant opportunities to the more sophisticated users: atomic resolution imaging at LBNL, in situ studies such as radiation effects at ANL, and microanalysis and spectroscopy at ORNL. Yet the largest usage, perhaps as high as 80 to 90 percent of the aggregate workload, of electron microscopy takes place at smaller, local facilities or in the laboratories of individual PIs, because of the ubiquitous use of electron microscopy for CMMP materials characterization. Nevertheless, there is an increasing gap, in terms of both the initial cost of systems and the continued upkeep and support for technical staff, between the more standard yet highly used characterization facilities on the one hand and the highest-end facilities that advance the forefront of the field on the other hand.

Currently, electron microscopy happens at three levels of sophistication. "Workhorse" microscopes typically are commercial instruments for routine microscopy, sample preparation, and user training. High-end machines are leading-edge commercial instruments that typically are found at local or regional facilities, operating in support of area universities, national laboratories, and industry. High-end machines play an important educational role for the use and design of microscopes, techniques, and associated instrumentation, and they provide for training of the next generation of microscopists in CMMP. Finally, at the cutting edge there are one-of-a-kind, next-generation instruments, optimized for specific electron-optical beam line applications. Support at all three levels will be a key for the continued success of this type of experimental facility within the general CMMP framework.

The main hurdle for reaching the highest spatial resolution has not been the electron's wavelength but limitations, such as aberration, associated with the design of the focusing lens. As a consequence, with traditional approaches it has not been possible to go below the 1 angstrom (0.1 nanometer) level and reach true subatomic resolution. The recent advent of aberration-corrected instruments has been a breakthrough for electron microscopy (in fact, providing a leap for TEM as well as for SEM performance; see Figure 11.13). These new instruments hold promise of enabling entirely new insights into areas such as the subsurface mapping of electron distributions, quantum confinement, spintronics, real-time flux bundle imaging, nanomagnetism, catalysis, and electrochemistry.

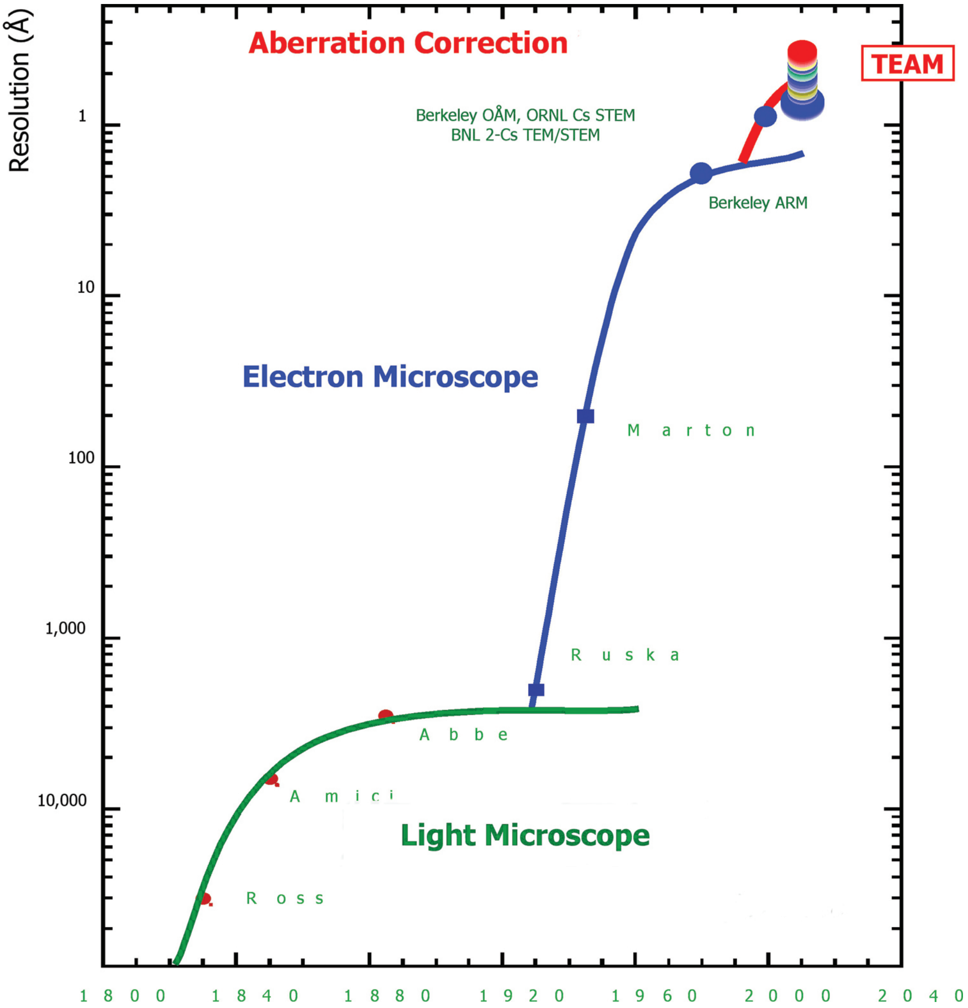

FIGURE 11.13 The evolution of microscopy resolution over time. The Department of Energy Transmission Electron Aberration-corrected Microscope (TEAM) array could break through the 0.1 nanometer resolution barrier. NOTE: OÅM, One-Angstrom Microscope; ORNL, Oak Ridge National Laboratory; STEM, Scanning Transmission Electron Microscope; BNL, Brookhaven National Laboratory; TEM, Transmission Electron Microscope; ARM, Atomic Resolution Microscope. SOURCE: Ulrich Dahmen, Lawrence Berkeley National Laboratory. Adapted from H. Rose, "Correction of Aberrations, A Promising Means for Improving the Spatial and Energy Resolution of Energy-Filtering Electron Microscopes," *Ultramicroscopy* **56**, 11-25 (1994).

### *Medium-Term Developments*

Two research directions were identified as being particularly promising for advancing electron microscopy during the next 10 years: the imaging of phenomena far from equilibrium and the imaging of a material's response to direct, in situ manipulation. Currently, almost all work is done on static samples at or near equilibrium. With the development of faster detectors and emitters, a goal is to achieve high temporal resolution (down to picoseconds). Coupled with millivolt spectral resolution, this will make it possible to track atomic-scale dynamics in real time, including phase-transformation kinetics and chemical reactions. The further development of in situ manipulation systems for TEM will open up a host of opportunities for studies of nanomechanics, in situ deposition and growth of samples, and the interaction of materials with applied electric, magnetic, strain, and photon fields.

For high-end instruments, further developments will likely combine highly focused electron beams with other types of probes, turning electron microscopes into more complex probe stations. At the forefront level, a completely different approach to overcoming aberration issues may be to do away with lenses altogether. Lensless, aberration-free imaging might be achieved if the full information (that is, both amplitude and phase) contained in the scattered wave function can be recovered.

### *The DOE Transmission Electron Aberration-corrected Microscope (TEAM) Project*

The current leading effort that capitalizes on aberration-correcting electron optics is the Transmission Electron Aberration-corrected Microscope (TEAM) project, bringing together five leading microscopy groups supported by DOE to jointly design and construct a new-generation microscope with extraordinary capabilities. The project is part of DOE's 20-year roadmap of Facilities for the Future of Science, and after its completion in 2009, the instrument will be made available to the scientific user community at the National Center for Electron Microscopy.

The vision for the TEAM project is the idea of providing a sample space for electron-scattering experiments in a tunable electron optical environment by removing some of the constraints that have limited electron microscopy until now. The resulting improvements in spatial, spectral, and temporal resolution, the increased space around the sample, and the possibility of exotic electron-optical settings will enable new types of experiments. The TEAM microscope will feature unique corrector elements for spherical and chromatic aberrations, a novel atomic force microscopy-inspired specimen stage, a high-brightness gun, and numerous other innovations that will extend resolution down to the half-angstrom level. The improvement in sensitivity, brightness, signal to noise, and stability will make it possible to address major challenges such as single-atom spectroscopy and atomic-resolution tomography.

The machine is being designed as a platform for a sequence of instruments, each optimized for different performance goals that were identified in a series of workshops.[7] The most important scientific driving force that emerged from these workshops is the need for in situ experiments to observe directly the relationship between structure and properties of individual nanoscale objects. Successive instruments built on the TEAM platform would provide unique experimental capabilities to probe the dynamics and mechanisms of reactions, such as catalysis in a gaseous environment, or the effects of gradients in temperature, composition, stress, and magnetic or electric fields on the structure of materials at the atomic level. The ability to probe nanoscale volumes of materials with atomic resolution meets one of the important scientific challenges in CMMP. The United States has not been a leader in the field of electron microscopy for considerable time, with much of the cutting-edge development taking place in Asia and Europe. If fully funded, the TEAM array will be an opportunity for the United States to reclaim a forefront position and will provide best-in-class instrumentation at the international level.

### *Recommendations for Electron Microscopy in CMMP Research*

> **Recommendation:** DOE and NSF should support the CMMP community's needs for electron microscopy instrumentation at universities on a competitive basis. Cutting-edge electron microscopy technique development (such as the DOE TEAM project) should be continued in order to fully reestablish U.S. competitiveness in developing the next generation of electron microscopes.
>
> **Recommendation:** *Revitalize U.S. electron microscopy.* Integrated support across all three facility levels (standard, high end, forefront) is urgently required to realize the full benefit to the CMMP community of recent technical achievements in the field of electron optics. This support includes not only capital investment in new instruments on a competitive basis, but also the support of career instrument scientists and operating costs at electron microscopy facilities.
>
> **Recommendation:** *Fund technique development.* At present, technique development typically is a by-product of other research projects. To stimulate technical innovation in the field, programs dedicated to electron microscopy technique development will make a significant difference.

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[7] For more information on the TEAM workshops, see the reports at http://ncem.lbl.gov/team3.htm; last accessed September 17, 2007.

**Recommendation:** *Hold crosscutting workshops.* There are major opportunities to reach out and connect with communities that use other, yet related techniques to image nanoscale phenomena, such as atom-probe and ion microscopes for three-dimensional imaging at the atomic scale, and x-ray nanoprobes. All of these communities, from electron microscopy to x-ray nanoprobe, are now gearing up to study similar materials problems and will face many similar scientific as well as technique-related challenges; yet the communities operate in parallel. Interdisciplinary, broadly based, and forward-looking workshops to address such common issues should be encouraged.

### High-Magnetic-Field Facilities

Magnetic fields interact with moving charges. Because the typical length scales associated with this interaction scale decrease with increasing magnetic-field strength, high magnetic fields can probe small spatial features and the associated fast processes. In order to achieve magnetic lengths comparable to the size of a quantum dot of 6-nanometer diameter, fields of about 20 tesla (T) are required; 80 T are necessary to shrink this length by another factor of two. As a consequence, the study of magnetic phenomena on the scale of a few nanometers, and from there on down to atomic dimensions, necessitates pushing the limits of what is possible with current magnet technology.

Traditional areas of success for high-field research have been the study of fundamental mechanisms in correlated quantum systems such as low-dimensional magnetism, the quantum Hall effect, and superconductivity, as well as the investigation of the properties of interacting magnetic flux bundles (“vortex matter”) inside superconductors. Separately, high-field research has enabled magnetic resonance studies in organic materials, providing important insights into membrane protein structures, hemoglobin, and the underpinnings of photosynthesis. Furthermore, CMMP research provides advanced materials, including superconductors with better performance, special conductors, and high-strength alloys. These materials form the critical components for magnets used in applications ranging from atomic particle accelerators to medical magnetic resonance imaging (MRI).

Two recent studies have looked into the current status and the potential for future developments of high-field magnet research. For more detailed information and discussions of the various technical issues, the committee refers to these reports.[8,9]

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[8] National Research Council, *Opportunities in High Magnetic Field Science*, Washington, D.C.: The National Academies Press, 2005.

[9] Report of the International Union of Pure and Applied Physics working group on Facilities for Condensed Matter Physics: High Magnetic Fields, 2004. Available at http://www.iupap.org/wg/fcmp/hmff/highmagneticreport.pdf; last accessed September 17, 2007.

### *Current Status of High-Magnetic-Field Facilities*

Magnet facilities fall into two categories, delineated by magnet technology and, thus, by the maximum achievable magnet field strength. Smaller high-field magnets (<20 T) are currently based on technology using superconducting niobium compounds and are available commercially. These magnets are found in single PI laboratories as well as in local multiuser facilities. Costs rise steeply with increasing field. Niobium-titanium magnets deliver up to 11 T, while $Nb_3Sn$ goes up to 20 T in driven magnets (at a cost of $1 million to $2 million) and up to ~22 T in persistent-mode NMR magnets (at a cost of $5 million to $15 million per system). For these smaller magnet systems there have been no major technological advances in recent years.

Large magnets (>30 T) comprise both continuous-field (direct current [dc]) and pulsed systems, are typically unique in design, and, because of their complexity and costs, are mostly located at dedicated high-field facilities, such as the National High Magnetic Field Laboratory (NHMFL) in the United States. At U.S. national facilities, large magnets are currently available that can reach up to 45 T in continuous mode (hybrid superconducting/resistive magnets), and up to 60 T for 100 microseconds in pulsed mode. As pointed out in the reports mentioned above, the value of the maximum achievable field is not the only important parameter for high-field research. Depending on the application, the quality and usefulness of a facility are determined also by factors such as the homogeneity of the field, the diameter of the magnet bore, or the availability of an environment amenable to low-noise measurements. Furthermore, for much of CMMP research, another important factor is the simultaneous access to low sample temperatures, that is, a large ratio of magnetic-field strength to temperature. In this area, the NHMFL has been a leader with its High B/T Facility.

With high-field magnet user facilities come challenges of energy costs in the face of increasing magnet hours driven by user demand. This challenge motivates higher-efficiency magnets, but they involve larger capital investment. As each magnet technology becomes more broadly used (for example, resistive magnets for nuclear and electron resonance), the issues shift toward addressing and integrating different magnet specifications (for example, peak field, time at fixed field, and field homogeneity) desired by the CMMP, chemistry, and biology user communities.

### *Medium-Term Developments*

High-magnetic-field research in CMMP is driven by the prospect of using the field as an exquisitely sensitive tuning parameter to explore emergent quantum phases of matter and by being able to perform precision spectroscopy using techniques such as NMR. In the area of complex fluids, the same spectroscopic methods can be used to track trace elements, while quadrupolar NMR opens up almost the entire periodic table as candidate nuclei. This capability will allow for a new level of structure-function correlation in glasses, ceramics, catalysts, and porous materials (for example, zeolites and batteries).

Technological challenges for the coming decade center on the development of new magnet technology beyond niobium. The recent report *Opportunities in High Magnetic Field Science*[10] identified a 30-T high-resolution NMR magnet, a 60-T dc hybrid magnet, and a 100-T long-pulse magnet as grand challenges. All of these require conductor materials in forms that are not yet commercially available, which in itself poses a materials research and development challenge. The NHMFL has been taking the lead in meeting these challenges and, furthermore, has embarked on developing additional magnet systems for low power consumption, complex fluids research, and ultrahigh fields (200 T/1 microsecond pulsed magnet).

New superconducting materials, such as $MgB_2$ or high-$T_c$ materials such as yttrium barium copper oxide (YBCO) or bismuth strontium calcium copper oxide (BSCCO), offer several advantages in terms of larger upper critical field strength and higher operating temperatures (eliminating the need to cool with cryogens such as liquid helium). Mulifilament $MgB_2$-based technology currently can go as high as 10 T, but 30 T or more appear eventually achievable. Commercial magnets based on this new technology are around the corner, with MRI applications as a major driver. Bi-2212 magnet wires promise greater than 50-T fields, among other advantages, while YBCO offers the highest fields. However, there are still many research and development challenges in terms of fabricating sufficiently long wires or tapes out of these materials and in improving their tensile strength, as required to withstand the forces generated in high-field magnets. Successful development of these materials could lead to relatively low cost and easy-to-operate magnets and would broaden the accessibility of high fields to small groups. Special pulsed and hybrid magnets also will benefit from the integration of high-$T_c$ components. Resistive plus high-$T_c$ technology should get well beyond 50 T. For pulsed magnets, multishot 100-T fields are within reach.

An important direction besides magnet development will be the integration of high fields with beam lines. This would allow the investigation of the neutron and x-ray scattering properties of materials in high magnetic fields. Currently, there are interesting design proposals to add hybrid magnets of fields of about 30 T to beam lines at the SNS at ORNL, and at the APS at ANL. Another plan, involving a collaboration of NHMFL, Jefferson Laboratory, and the University of California at Santa Barbara, envisions combining advanced magnet technology with an infrared free-electron laser. This would allow access to the terahertz regime that is resonant with magnetic-field energy scales.

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[10] National Research Council, *Opportunities in High Magnetic Field Science*, Washington, D.C.: The National Academies Press, 2005.

*Recommendations for High-Magnetic-Field Facilities in CMMP Research*

> **Recommendation:** NSF should continue the support of the National High Magnetic Field Laboratory and high-magnetic-field instrumentation development following the priorities recommended by the recent National Research Council report *Opportunities in High Magnetic Field Science.*[11]
>
> **Recommendation:** The research community, with support from the federal agencies, should exploit the opportunities for superconducting magnets provided by the recent and imminent high-$T_c$ conductor forms. This will benefit small-scale users and high-field NMR users, and will allow for more powerful hybrid magnets.

## Nanocenters and Materials Synthesis

The past decade has given rise to significant investment in the establishment of a diverse portfolio of nanoscience research centers. This development was made possible by the stewardship of the multiagency National Nanotechnology Initiative (NNI). The centers complement traditional major neutron and photon sources for CMMP research and include strong user support in their mission statements. The centers differ in character from one another according to the directives of their sponsoring agencies. But, more significantly, they are in many ways distinct in character from large-scale facilities such as neutron and photon sources. The primary focus of the nanocenters is on the *creation of new materials* as well as on the advanced characterization of materials, while the other major facilities deal primarily with advanced characterizations. This focus represents a turning point, an acknowledgment of the central importance of the need for new materials in order to invigorate CMMP. This is a theme that needs to be extended and broadened in the next decade in order for the United States to recapture its leadership in the area of the discovery of new materials. In this subsection, nanocenters are discussed and the model is considered for the design and discovery of new materials of interest to CMMP researchers, such as bulk crystals, novel thin films, and superlattices.

### *Current Status of Nanocenters and Materials Synthesis*

Researchers at many institutions face challenges associated with the availability of materials. They may lack the expertise or the appropriate equipment

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[11] National Research Council, *Opportunities in High Magnetic Field Science*, Washington, D.C.: The National Academies Press, 2005.

for the synthesis or growth of new or high-quality materials. The NSF National Nanotechnology Infrastructure Network (NNIN) program is intended to address these issues. The NNIN program is largely directed at providing capabilities for the synthesis and fabrication of materials and for providing computational and theoretical tools and expertise. A network of 13 universities around the country (see Figure 11.14) participates in this program to provide and share facilities for nanoscience and engineering research.

In addition to the NSF NNIN program, DOE has established Nanoscale Science Research Centers at five national laboratories: the Center for Nanophase Materials Sciences at ORNL, the Molecular Foundry at LBNL, the Center for Integrated Nanotechnologies jointly operated by Sandia National Laboratories and Los Alamos National Laboratory, the Center for Nanoscale Materials at ANL, and the Center for Functional Nanomaterials at Brookhaven National Laboratory. These centers are largely dedicated to materials synthesis, fabrication, and characterization. They provide access to electron-beam nanowriters, lithography and stamping for nanofabrication; x-ray nanoprobes and facilities for complex materials formation and soft hybrid materials; and infrastructure for theory simulations.

The nanocenters are distributed facilities that embrace interdisciplinary approaches to solving nanoscience and nanotechnology problems using a full suite of modern instrumentation. At many of the nanocenters, theory and simulation

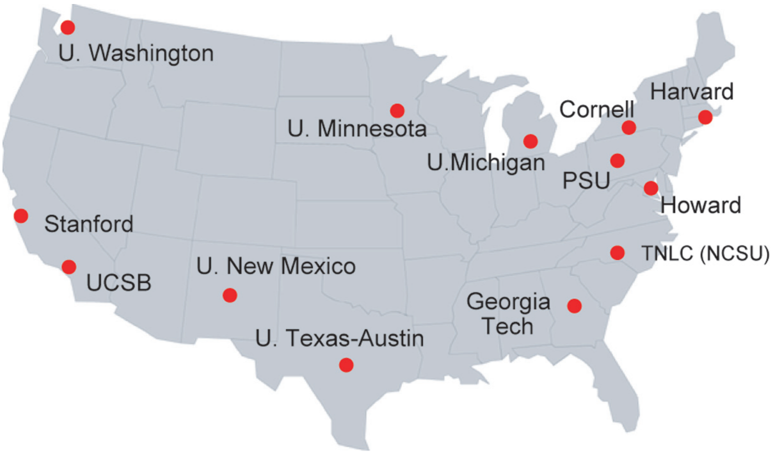

FIGURE 11.14 Institutions participating in the National Nanotechnology Infrastructure Network program. NOTE: UCSB, University of California at Santa Barbara; PSU, Pennsylvania State University; TNLC (NCSU), Triangle National Lithography Center (North Carolina State University). SOURCE: See http://www.nnin.org.

are on a similar footing with experimental science. Also, the pursuit of world-class, in-house scientific research programs is on a similar footing with user support services. The nanocenters provide a pathway from fundamental science to applications with the possibility of commercialization and the creation of new start-up companies.

The balance between science and user-service programs at the nanocenters is approached differently, depending on the sponsoring agency. For example, the DOE NSRCs encourage a model whereby each Ph.D. staff member pursues basic science research *and* user-support services. The NIST Center for Nanoscale Science and Technology has separate divisions that emphasize scientific programs and user support. The NIST scientific programs focus on solving major measurement-related obstacles in the path from discovery to production. The Department of Defense (DOD) supports an in-house, mission-oriented Institute for Nanoscience at the Naval Research Laboratory.

### *Medium-Term Developments*

The challenge ahead is to learn how to sustain the progress of the nanoscience era and to optimize accessibility to a diverse range of instruments and facilities. In cases where nanocenters are co-located with other major facilities, the planning of one-stop shopping needs to be perfected so that newly created nanosystems can be interrogated with electrons, neutrons, and x-rays in a single visit. Metrics need to be refined for monitoring the success of the new nanocenters. The funding for operations needs to support the diverse suite of equipment at the nanocenters. Models need to be evaluated for a balance of in-house science and user support. Barriers will need to be lowered to facilitate the transition from science to commercialization.

The nanocenters have addressed a gap in research culture by acknowledging the importance of synthesis, processing, and fabrication of new materials and systems. Recognizing this, it is imperative to accelerate the momentum and to energize other areas of new-materials exploration and discovery of vital interest to CMMP. The design and synthesis of novel systems are the foundation to address all of the CMMP grand challenges. The energy challenge needs new materials for storing hydrogen, thermoelectrics, organic light-emitting diode (LED) crystals, and high-performance superconductors and ferromagnetics. Information technology needs new materials for spintronic, organic, and molecular electronics that exhibit quantum coherence properties suitable for quantum computation prototyping. Multiferroics, magnetic semiconductors, and half-metallic ferromagnets are specific systems also of great interest to spintronics. As the art of crystal growth matures into a science, the resulting insights might apply to the understanding of the physics of soft-matter crystallization. Protein crystallography data collection at photon sources would benefit immensely from such a development. This example highlights the multidisciplinary nature of the quest that brings together chemists, biologists, engineers, and physicists. The new crystal discovery centers of the future can be distributed, as are the nanocenters. The models for creating and operating them might also benefit from examining the NSF NNIN and DOE NSRC models. Presumably viable hybrid organizational structures will evolve that best serve the particular materials missions of these future efforts. A target budgetary level per year might be similar to that for NSF of its NNIN program, and for DOE a level of the equivalent of one or two of its five NSRC facilities (for further discussion, see Chapter 9).

Why is it imperative to move forward on a new-materials discovery agenda now? The United States is not in a lead role in the creation of new materials. It needs to recapture its lost status, because the consequences of delay and neglect are long-term erosion of the U.S. competitive edge and a loss of intellectual property. New materials invigorate all of the CMMP grand challenges. While new-materials discovery is cross-disciplinary, at present there is no obvious academic home for new-materials initiatives. This problem needs to be remedied. New-materials discovery embraces theory and simulation in the sense of virtual fabrication. New materials created via computer models, including electronic band structure codes, provide insights and guidelines to direct the design of new materials in the laboratory. The new-materials discovery centers of the future will also provide fertile training grounds for future generations of graduate students. The nanocenters started the culture change by emphasizing the creation of new materials. The transformation needs to be extended to embrace the larger landscape of new-materials discovery beyond the nano-realm. The time is ripe to focus on this strategic scientific goal, to plan multidisciplinary team approaches, and to identify visionary management, scientific advisers, and stakeholders, as stated above. Balance must be sought between support of the individual investigators and small groups of investigators relative to centers, instrumentation, and major facilities investments.

### *Recommendations for Materials Synthesis and Nanocenters in CMMP Research*

Nanoscience is a core discipline whose advances will affect all of the other challenges, from emergent phenomena (Chapter 2) to information technology (Chapter 7). The past decade has already seen significant federal investment in nanotechnology infrastructure. Notable are the NSF-funded Nanoscale Science and Engineering Centers and the National Nanotechnology Infrastructure Network, as well as the new DOE-funded Nanoscale Science Research Centers at the national laboratories. These facilities serve a critical need and deserve continued support. Nanoscience by its very nature spans an enormously wide variety of disciplines, from condensed-matter physics to engineering to chemistry and biology. This makes it all the more critical to develop an intellectual resource network that allows scientists from one discipline to have access to the knowledge of all of the others. There is need for training opportunities for students, postdoctoral researchers, and faculty that allow them to reach beyond the standard disciplinary boxes. There is also need to develop knowledge repositories like those that exist in biology, where genomes and so on are stored and made widely available. The NSF and DOE-funded nanoscience centers should take the lead in meeting these needs, teaching short courses on particular techniques and subfields, as well as providing repositories of information.

> **Recommendation:** DOE and NSF should develop distributed national facilities in support of the design, discovery, and growth of new materials for both fundamental and applied CMMP research.[12]

> **Recommendation:** DOE should evaluate the new NSRCs by metrics described in Chapter 9. The National Nanotechnology Coordination Office (NNCO), in its arrangement of the triennial review of the NNI, should evaluate all NNI-funded centers and networks of centers by similar metrics.

## Large-Scale High-Performance Computing Facilities

High-performance computing is well recognized as a prerequisite for scientific and technological preeminence. High-priority, significant resources at the federal level are therefore directed toward the ongoing development and maintenance of state-of-the-art computational facilities for general scientific research, including CMMP. In understanding how such resources address the needs of CMMP researchers, it is important to note that large-scale computation is an important component of many scientific fields that share these resources. Below, the committee describes the major U.S. high-performance computing facilities and shows data as to how the available resources are shared among disciplines.

### *Current Status of Computing Facilities*

The largest and most powerful systems define the limits of the types of computational studies that can be carried out at present. For the U.S. CMMP community, these computational facilities are supported by NSF, DOE, and DOD.

Building on the system of NSF supercomputing centers of the 1990s, the devel-

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[12] The National Research Council study *Assessment of and Outlook for New Materials Synthesis and Crystal Growth* will make detailed recommendations on how best to support this need. The report is expected to be released in the summer of 2008.

opment of the TeraGrid began in 2000 as the world's largest, most comprehensive distributed cyberinfrastructure for open scientific research. Partners in this distributed framework include the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign, the San Diego Supercomputer Center (SDSC) at the University of California at San Diego, Argonne National Laboratory, the Center for Advanced Computing Research (CACR) at the California Institute of Technology, Pittsburgh Supercomputing Center, Indiana and Purdue Universities, Oak Ridge National Laboratory, and the Texas Advanced Computing Center at the University of Texas at Austin. As of 2005, the TeraGrid had about 1600 users. A relatively small fraction is used for materials and (all of) physics research (see Figure 11.15).

DOE supports scientific computing primarily through the National Energy Research Scientific Computing Center (NERSC) and through Leadership Computing Facilities (LCF) at the national laboratories. NERSC is described by DOE as "one of the largest facilities in the world devoted to providing computational resources and expertise for basic scientific research," with 2677 users in 2005. Reflecting the broad DOE mission, a relatively small fraction of resources (about 9 percent) is devoted to computation for materials research (see Figure 11.15).

At national laboratories, such as ORNL where materials are a larger component of research, the fraction of resources at the LCF is correspondingly higher.

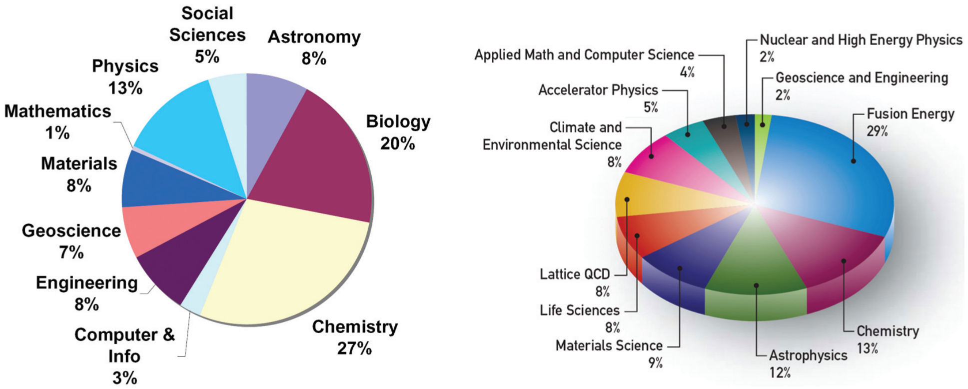

FIGURE 11.15 (Left) National Science Foundation TeraGrid usage, by discipline, in FY 2005. NOTE: "Computer & Info," computer science and information technology. (Right) Department of Energy National Energy Research Scientific Computing Center usage, by discipline, in 2005. NOTE: "Lattice QCD," lattice quantum chromodynamics. SOURCES: (Left) National Science Foundation TeraGrid. (Right) National Energy Research Scientific Computing Center, Lawrence Berkeley National Laboratory.

At ORNL's National Center for Computational Sciences, about 25 percent of the center's resources are used for materials computations. A number of the LCFs are also partners in the NSF TeraGrid.

DOD has a large network of supercomputer centers (the High Performance Computing Modernization Program) to support the computing needs of DOD researchers, with 4550 users in 2005. Materials research falls in the category "CCM" (Computational Chemistry, Biology, and Materials Science). The share for this category can be seen in Figure 11.16.

While the focus of this discussion has been on high-performance computing, there is much interesting and innovative work done in computational materials that does not demand computational resources at the highest available level, but where accessibility and throughput are key considerations. Much valuable work is done at computing facilities at the state level, at individual universities, in departments, and by research groups. Support for computational facilities from sources such as the NSF Major Research Instrumentation program should be encouraged, and budgeting for computer equipment in theoretical and computational CMMP

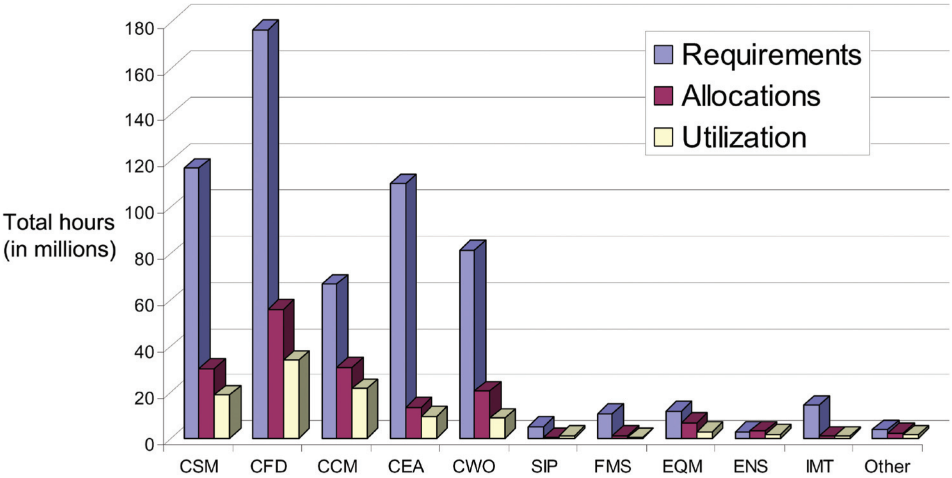

FIGURE 11.16 FY 2006 Department of Defense high-performance computing requirements, allocations, and utilization breakdown for individual "computational technology areas." Computational Chemistry, Biology, and Materials Science (CCM) is third from the left; other areas are Computational Structural Mechanics (CSM), Computational Fluid Dynamics (CFD), Computational Electromagnetics and Acoustics (CEA), Climate/Weather/Ocean Modeling and Simulation (CWO), Signal/Image Processing (SIP), Forces Modeling and Simulation (FMS), Environmental Quality Modeling and Simulation (EQM), Electronics, Networking and Systems (ENS), and Integrated Modeling and Test Environments (IMT). SOURCE: C.J. Henry, Department of Defense High Performance Computing Modernization Program.

individual and small-group proposals should be considered the norm. However, this hierarchical structure, while it evolved largely to meet the needs of researchers, does come with problems of its own. As computational power increases, issues of professional systems administration and user support personnel for computing clusters become increasingly important. The diversity of facilities can make the system hard to navigate for researchers seeking resources. This latter challenge is particularly common for computational junior faculty members starting careers in computational CMMP.

## CONCLUSIONS

The need for sophisticated tools (experimental, computational, and theoretical) to probe the structure and properties of materials over a wide range of length scales is essential for continued progress in CMMP research. The new-generation facilities (light and neutron sources, magnetic-field facilities, and electron microscopes), which offer higher fluxes and energies, provide significant advantages with regard to resolution, sensitivity, and data acquisition. Two additional challenges will continue to be important in the future: the simultaneous measurement of structure and dynamics over various time and length scales and dimensions, and the simultaneous measurement of structure and dynamics while the system is perturbed independently by an external field (magnetic, stress, electric, and so on).

The synthesis, structure, and properties of materials are all intimately connected, so researchers will increasingly need to be intimately familiar with this entire spectrum of activities. Lessons learned from one class of materials will increasingly be used to understand the behavior of seemingly different classes of materials. For the first time in history, the complexity of CMMP is such that new advances in the field will depend on strong support for large-scale facilities, mid-scale facilities, interdisciplinary research centers, and individual investigators who actually carry out the research. Students will have to understand computational methods, together with the full spectrum of experimental endeavors (synthesis, fabrication, and measurement) to become successful researchers.

# Concluding Remarks

Moving into the 21st century, CMMP faces exciting scientific and technological opportunities, summarized in the six grand challenges identified in this report. These and other challenges will drive the continued vitality and growth of CMMP, as well as its continuing impact on the U.S. economy and society. The fundamental scientific questions, the close interplay between theoretical and experimental research, and the technological applications that will contribute to solving important societal problems all drive enthusiasm for the field. Attracted by such compelling research opportunities, more starting graduate students in U.S. programs choose CMMP than any other single subfield of physics. These young minds are the future of CMMP and of its role in society.

However, the Committee on CMMP 2010 also concluded that there are danger signs on the horizon. U.S. leadership in fundamental CMMP research is seriously threatened by the low success rates in proposals submitted for government funding of research, the precipitous decline of involvement of industrial laboratories in fundamental CMMP research, and the increasing competition from other countries for the best scientists. Due to tremendous momentum in the research establishment, the ill effects of these structural problems are only just starting to manifest themselves in measurable terms, such as publication rates, and in the ability to attract the best young scientists to research positions in the United States. The Committee on CMMP 2010 therefore urges that action be taken now. Prompt attention to these structural problems is needed to ensure U.S. leadership in CMMP research and technological innovation now and for the future.

# Appendixes

# A

# Statement of Task

A comprehensive assessment of the current status and future prospects of the field of condensed-matter and materials physics (CMMP) and its connections to other areas of science and technology is proposed. This assessment, CMMP 2010, is part of a broader study, Physics 2010, the latest decadal assessment and future outlook of the field of physics, conducted by the Board on Physics and Astronomy under the auspices of the National Research Council (NRC). This proposed study identifies fundamental theoretical and experimental challenges in CMMP and their relationship with other areas of physics. Because CMMP has proven to have great societal benefit, the potential applications of CMMP and its strong connections to fields that are closer to technology will also be explored.

The committee will be charged to produce a comprehensive report on the status of CMMP. The committee's report shall:

1. Review the field of CMMP, emphasize recent accomplishments, and identify new opportunities and compelling scientific questions, connecting to other recent studies where appropriate.
2. Identify the potential future impact of CMMP on other scientific fields and current and emerging technologies.
3. Consider how CMMP has contributed and will likely contribute to meeting national societal needs such as in education, workforce, and healthcare.
4. Identify, discuss, and suggest priorities for construction, purchase, and operation of tools and facilities ranging from instrumentation for the individual investigator to the national user facilities.

5. Make recommendations on how the U.S. research enterprise might realize the full potential of condensed-matter and materials physics research.
6. Examine the structure and level of the current research effort in condensed-matter and materials physics. Obtain objective information on current status and trends in the following areas: (1) the performing institutions: government, universities, and industry; (2) different levels of aggregation of researchers ranging from principal investigators through small groups and large teams at centers; (3) the role of the research community and performing institutions in initiating research; and (4) the relationship between research opportunities and the current structure of the research effort. Analyze this information, make comparisons internationally, and draw relevant conclusions.

# B

# Agendas of Committee Meetings

## FIRST MEETING
## IRVINE, CALIFORNIA
## FEBRUARY 12-13, 2006

### Sunday, February 12, 2006

OPEN SESSION

| | |
|---|---|
| 8:30 a.m. | Welcome and Introductions<br>—Mildred Dresselhaus and William Spencer, *Co-Chairs* |
| 8:45 | Introduction to the National Research Council (NRC)<br>—Natalia Melcer, NRC |
| 9:00 | CMMP 2010 Context: History, Charge, and Scope<br>—James Eisenstein, California Institute of Technology |
| 9:30 | Perspectives from the Solid State Sciences Committee<br>—Marc Kastner, Massachusetts Institute of Technology |
| 10:30 | Perspectives from the Last Decadal Survey<br>—Venkatesh Narayanamurti, Harvard University |
| 11:15 | Discussion |
| Noon | Lunch |
| 1:00 p.m. | CMMP in Context<br>—Malcolm Beasley, Stanford University |
| 1:45 | Data Gathering<br>—Natalia Melcer, NRC |

| | |
|---|---|
| 2:30 | Town Hall Meetings and Focus Groups: Topics, Dates, Attendance |
| 3:30 | Discussion |
| 5:00 | Adjourn |

### Monday, February 13, 2006

OPEN SESSION

| | |
|---|---|
| 8:00 a.m. | Setting Scientific Priorities<br>—Rob Dimeo, Office of Science and Technology Policy, and Joel Parriott, Office of Management and Budget |
| 8:30 | Perspectives from the Department of Energy Basic Energy Sciences<br>—Harriet Kung, Department of Energy (by videoconference) |
| 9:00 | Perspectives from the National Science Foundation Division of Materials Research<br>—Lance Haworth, NSF (by videoconference) |
| 9:30 | Perspectives from the NSF Division of Physics<br>—Joseph Dehmer, NSF (by videoconference) |
| 10:00 | Perspectives from the Department of Defense Air Force Office of Scientific Research<br>—Brendan Godfrey, Air Force Office of Scientific Research (by videoconference) |

CLOSED SESSION

| | |
|---|---|
| 10:45 a.m. | Committee Discussion |
| Noon | Lunch |
| 1:00 p.m. | Committee Discussion |
| 3:00 | Adjourn |

## SECOND MEETING
## WASHINGTON, D.C.
## MAY 25-26, 2006

### Thursday, May 25, 2006

CLOSED SESSION

| | |
|---|---|
| 8:30 a.m. | Welcome and Plans for the Meeting<br>—Mildred Dresselhaus and William Spencer, *Co-Chairs* |
| 8:45 | Committee Discussion |

OPEN SESSION

| | |
|---|---|
| 11:00 a.m. | Department of Energy User Facilities<br>—Pedro Montano, Department of Energy |
| 11:45 | Lunch |
| 12:45 p.m. | National Laboratories and Innovation<br>—Robert Rosner, Argonne National Laboratory |
| 1:30 | AMO 2010: Lessons Learned<br>—Philip Bucksbaum, Stanford University (by videoconference) |

CLOSED SESSION

| | |
|---|---|
| 2:30 p.m. | Committee Discussion |
| 5:30 | Adjourn for the Day |

### Friday, May 26, 2006

CLOSED SESSION

| | |
|---|---|
| 8:30 a.m. | Committee Discussion |
| Noon | Lunch and Adjourn |

## THIRD MEETING
## IRVINE, CALIFORNIA
## AUGUST 31-SEPTEMBER 1, 2006

### Thursday, August 31, 2006

CLOSED SESSION

| | |
|---|---|
| 8:00 a.m. | Welcome and Plans for the Meeting<br>—Mildred Dresselhaus and William Spencer, *Co-Chairs* |
| 8:10 | Interim Report |
| 9:00 | Data Subgroup<br>—Natalia Melcer, NRC |
| 10:15 | Industrial Laboratories Subgroup<br>—William Spencer, *Co-Chai*r |
| 11:15 | Final Report: Outline of Challenge Sections<br>—Mildred Dresselhaus, *Co-Chair* |
| 12:15 p.m. | Lunch |

OPEN SESSION

| | |
|---|---|
| 1:15 p.m. | AMO 2010: Lessons Learned<br>—Philip Bucksbaum, Stanford University (by videoconference) |

CLOSED SESSION

| | |
|---|---|
| 2:00 p.m. | Final Report: Outline of Remaining Sections, Format, Assignments |
| 3:15 | Final Report: Discussion of Findings, Conclusions, and Recommendations |
| 5:00 | Short Booklet |
| 5:30 | Adjourn for the Day |

**Friday, September 1, 2006**

OPEN SESSION

| | |
|---|---|
| 8:25 a.m. | Reconvene<br>—Mildred Dresselhaus and William Spencer, C*o-Chairs* |
| 8:30 | Economic Role of Science<br>—Nathan Rosenberg, Stanford University |
| 9:30 | Comments and Perspective on CMMP<br>—Steven Chu, Lawrence Berkeley National Laboratory (by videoconference) |

CLOSED SESSION

| | |
|---|---|
| 10:45 a.m. | Facilities Subgroup Report |
| 11:45 | Final Report Discussion |
| 12:30 p.m. | Lunch and Adjourn |

### FOURTH MEETING
### WASHINGTON, D.C.
### JANUARY 30-31, 2007

**Tuesday, January 30, 2007**

CLOSED SESSION

| | |
|---|---|
| 8:00 a.m. | Welcome and Plans for the Meeting<br>—William Spencer, *Co-Chair* |
| 8:15 | Committee Discussion: Challenges 1, 2, 3 |
| 10:00 | Committee Discussion: Challenges 4, 5, 6, 7 |
| Noon | Lunch |
| 1:00 p.m. | Reconvene<br>—Mildred Dresselhaus, *Co-Chair* |
| 1:05 | Committee Discussion: Societal and Scientific Impact, Data, National and Industrial Laboratories, Facilities |
| 3:15 | Committee Discussion: Findings and Recommendations |
| 5:30 | Adjourn for the Day |

### Wednesday, January 31, 2007

CLOSED SESSION
8:00 a.m. Reconvene and Review of First Day
—William Spencer, *Co-Chair*
8:15 Committee Discussion: Findings and Recommendations
9:45 Committee Discussion: Executive Summary
—Mildred Dresselhaus, *Co-Chair*
11:30 Committee Discussion: Time Line for Completion, Assignments
Noon Lunch and Adjourn

# C

# Agenda and Participants at Facilities Workshop

## AGENDA

### Sunday, January 28, 2007

| | |
|---|---|
| 8:30 a.m. | Welcome, Challenges for CMMP, Purpose of Workshop<br>—Mildred Dresselhaus and William Spencer, *Co-Chairs*, Committee on CMMP 2010 |
| 9:00 | National Science Foundation Perspective<br>—Lance Haworth, National Science Foundation |
| 9:30 | Department of Energy Perspective<br>—Patricia Dehmer, Department of Energy (by videoconference) |
| 10:30 | Light Sources<br>—David Moncton, Massachusetts Institute of Technology |
| 10:50 | Neutron Sources<br>—Sunil Sinha, University of California at San Diego |
| 11:10 | Magnetic Fields<br>—Peter Littlewood, University of Cambridge (by videoconference) |
| 11:30 | Electron Microscopy<br>—David Muller, Cornell University |
| 11:50 | Nanoscience/Nanotechnology Facilities<br>—Julia Phillips, Sandia National Laboratories |
| 12:10 p.m. | Lunch |
| 1:30 | Concurrent Breakout Sessions |

Light Sources
—Steven Dierker, Brookhaven National Laboratory
—Roger Falcone, Lawrence Berkeley National Laboratory
—J. Murray Gibson, Argonne National Laboratory
—Sol Gruner, Cornell University
—Franz Himpsel, University of Wisconsin at Madison
—Zhi-Xun Shen, Stanford University
Neutron Sources
—Patrick Gallagher, National Institute of Standards and Technology
—Ramanan Krishnamoorti, University of Houston
—Douglas MacLaughlin, University of California at Riverside
—Thomas Mason, Oak Ridge National Laboratory
—James Rhyne, Los Alamos National Laboratory
Magnetic Fields/Electron Microscopy
—Gregory Boebinger, National High Magnetic Field Laboratory
—Ulrich Dahmen, Lawrence Berkeley National Laboratory
—David Larbalestier, Florida State University
—Stephen Pennycook, Oak Ridge National Laboratory
—Amanda Petford-Long, Argonne National Laboratory
—Michael Treacy, Arizona State University
Crosscutting Facilities
—Paul Canfield, Ames Laboratory
—Robert Celotta, National Institute of Standards and Technology
—Richard Colton, Naval Research Laboratory
—Linda Horton, Oak Ridge National Laboratory
—Arthur Ramirez, Alcatel-Lucent
—Sandip Tiwari, Cornell University

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|---|---|
| 3:00 | Break |
| 3:30 | Reconvene Breakout Sessions |
| 5:00 | Reception |
| 6:00 | Adjourn |

**Monday, January 29, 2007**

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|---|---|
| 8:00 a.m. | Convening Remarks<br>Mildred Dresselhaus and William Spencer, *Co-Chairs,* Committee on CMMP 2010 |
| 8:30 | Reconvene Breakout Sessions |
| 10:30 | Breakout Session Reports, Meeting Wrap-Up, and Summary |
| Noon | Adjourn and Lunch |

## PARTICIPANTS

### Members of Committee on CMMP 2010

Mildred S. Dresselhaus, *Co-Chair*, Massachusetts Institute of Technology
William J. Spencer, *Co-Chair*, SEMATECH (retired)
Gabriel Aeppli, University College London
Samuel D. Bader, Argonne National Laboratory
William Bialek, Princeton University
Anthony K. Cheetham, University of California, Santa Barbara
James P. Eisenstein, California Institute of Technology
Heinrich M. Jaeger, University of Chicago

### Invited Speakers

Gregory Boebinger, National High Magnetic Field Laboratory
Paul Canfield, Ames Laboratory
Robert Celotta, National Institute of Standards and Technology
Richard Colton, Naval Research Laboratory
Ulrich Dahmen, Lawrence Berkeley National Laboratory
Patricia Dehmer, Department of Energy (Videoconferencing)
Steven Dierker, Brookhaven National Laboratory
Roger Falcone, Lawrence Berkeley National Laboratory
Patrick Gallagher, National Institute of Standards and Technology
J. Murray Gibson, Argonne National Laboratory
Sol M. Gruner, Cornell University
Lance Haworth, National Science Foundation
Franz Himpsel, University of Wisconsin at Madison
Linda Horton, Oak Ridge National Laboratory
Ramanan Krishnamoorti, University of Houston
David Larbalestier, Florida State University
Peter Littlewood, University of Cambridge (Videoconferencing)
Douglas MacLaughlin, University of California at Riverside
Thomas Mason, Oak Ridge National Laboratory
David E. Moncton, Massachusetts Institute of Technology
David A. Muller, Cornell University
Stephen Pennycook, Oak Ridge National Laboratory
Amanda Petford-Long, Argonne National Laboratory
Julia Phillips, Sandia National Laboratories
Arthur Ramirez, Alcatel-Lucent
James Rhyne, Los Alamos National Laboratory

Zhi-Xun Shen, Stanford University
Sunil Sinha, University of California at San Diego
Sandip Tiwari, Cornell University
Michael Treacy, Arizona State University

## Registered Attendees

Hamad Alyahyaei, California State University at Los Angeles
Ara Apkarian, University of California at Irvine
Joseph Bisognano, University of Wisconsin at Madison
Robert Cauble, Lawrence Livermore National Laboratory
John Corlett, Lawrence Berkeley National Laboratory
Thomas Earnest, Lawrence Berkeley National Laboratory
David Ederer, Louisiana State University
Giulia Galli, University of California, Davis
Martin Greven, Stanford University
John Hemminger, University of California at Irvine
Zahid Hussain, Lawrence Berkeley National Laboratory
Fatima Ibrahim, University of California at Irvine
Chi-Chang Kao, Brookhaven National Laboratory
Andrew Lankford, University of California at Irvine
Bennett Larson, Oak Ridge National Laboratory
Chun Ning (Jeanie) Lau, University of California at Riverside
Jeffrey Lindemuth, Lake Shore Cryotronics
Gabrielle Long, Argonne National Laboratory
Christian Mailhiot, Lawrence Livermore National Laboratory
Thomas Mason, University of California at Los Angeles
John Miao, University of California at Los Angeles
John Mitchell, Argonne National Laboratory
Pedro Montano, Department of Energy
W.J. (Bill) Nellis, Harvard University
Patricia Oddone, Lawrence Berkeley National Laboratory
Raymond Osborn, Argonne National Laboratory
Won-Kyu Rhim, California Institute of Technology
Robert Schoenlein, Lawrence Berkeley National Laboratory
Adam Schwartz, Lawrence Livermore National Laboratory
Qun Shen, Argonne National Laboratory
Gopal Shenoy, Argonne National Laboratory
George Srajer, Argonne National Laboratory
David Tanner, University of Florida
Richard Weber, Materials Development, Inc.

Gwyn Williams, Thomas Jefferson National Laboratory
Clare Yu, University of California at Irvine
Nestor J. Zaluzec, Argonne National Laboratory
Alexander Zholents, Lawrence Berkeley National Laboratory

## Staff

Donald Shapero, Board on Physics and Astronomy, National Research Council
Natalia Melcer, Board on Physics and Astronomy, National Research Council

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# Biographies of Committee Members

**Mildred S. Dresselhaus, *Co-Chair***

Mildred Dresselhaus is Institute Professor of Electrical Engineering and Physics at the Massachusetts Institute of Technology. Her recent research interests range broadly over condensed-matter and materials physics, with a particular focus on carbon science, nanoscience, and their intersection as well as the role of nanoscience in energy-related research. Dr. Dresselhaus is a member of the National Academy of Sciences, the National Academy of Engineering, and the American Philosophical Society and a fellow of the American Academy of Arts and Sciences, the American Physical Society (APS), the Institute of Electrical and Electronics Engineers (IEEE), the Materials Research Society, the Society of Women Engineers, and the American Association for the Advancement of Science (AAAS). She has served as president of the APS, treasurer of the National Academy of Sciences, president of the AAAS, and as a member of numerous advisory committees and councils. She served as the director of the Office of Science at the U.S. Department of Energy in 2000-2001. She was elected foreign fellow of the National Academy of Sciences, India, in 2006. She is now chair of the governing board of the American Institute of Physics. Dr. Dresselhaus has received numerous awards, including the National Medal of Science and 22 honorary doctorates. She is the coauthor of four books on carbon science.

**William J. Spencer, *Co-Chair***

William Spencer is chairman emeritus of the International SEMATECH Board. He served as chairman of the SEMATECH and International SEMATECH boards and president and chief executive officer of SEMATECH. Dr. Spencer has held key research positions at Xerox Corporation, Bell Laboratories, and Sandia National Laboratories. He received the Regents Meritorious Service Medal from the University of New Mexico in 1981; the C.B. Sawyer Award for contribution to "The Theory and Development of Piezoelectric Devices" in 1972; and a citation for achievement from William Jewell College in 1969, where he also received a doctor of science degree in 1990. Dr. Spencer is a member of the National Academy of Engineering, a fellow of IEEE, and he serves on numerous advisory groups and boards. He was the Regents Professor at the University of California in the spring of 1998. He has been a visiting professor at the University of California, Berkeley, School of Engineering and the Haas School of Business since the fall of 1998. He is a research professor of medicine at the University of New Mexico. Dr. Spencer received an A.B. degree from William Jewell College in Liberty, Missouri, and an M.S. degree in mathematics and a Ph.D. in physics from Kansas State University.

**Gabriel Aeppli**

Gabriel Aeppli is the Quain Professor of Physics at University College London and the director of the London Centre for Nanotechnology. Prior to taking up these posts in the fall of 2002, he was a senior research scientist for NEC Labs America and a Distinguished Member of Technical Staff at Bell Laboratories. He obtained a B.Sc. in mathematics and Ph.D., M.Sc., and B.Sc. in electrical engineering from the Massachusetts Institute of Technology. His main research interests are quantum information processing, nanotechnology (including especially its manifestations in the life sciences), and particle and x-ray beam-based probes of condensed matter. Dr. Aeppli's honors include the 2005 Buckley Prize of the APS, 2003 International Union of Pure and Applied Physics Magnetism Prize/Neel Medal, 2002 Royal Society Wolfson Research Merit Award, and the 2002 Mildner Lecturer, Department of Electronic and Electrical Engineering, University College London. He is a fellow of Riso National Laboratory, the American Physical Society, and the Japan Society for the Promotion of Science. In addition, he has been a member and chair of many panels, sponsored by the Department of Energy, American Physical Society, and the National Research Council, among others.

**Samuel D. Bader**

Samuel Bader is an Argonne Distinguished Fellow and serves as group leader for magnetic films and an associate director of Argonne National Laboratory's Materials Science Division, and as chief scientist for the Center for Nanoscale Materials. Dr. Bader received his B.S. and Ph.D. in chemistry from the University of California, Berkeley. His current research interests include employing nanotechnology to create novel permanent magnets and exploring laterally confined nanomagnets in order to develop magnetic electronics and bio-inspired, self-assembled magnetic nanostructures. He is a fellow of the American Physical Society and of the American Vacuum Society. His honors include the DOE Basic Energy Sciences Award for Outstanding Achievement in Solid State Physics, the University of Chicago Award for Distinguished Performance at Argonne, the AVS John A. Thornton Memorial Award, and the APS David Adler Lectureship Award. He is an adjunct professor in the Department of Materials Science and Engineering at the University of Illinois at Urbana-Champaign, and in the Department of Physics and Astronomy at Northwestern University, and a senior fellow of the University of Chicago-Argonne Consortium for Nanoscience Research. He chaired the Scientific Advisory Committee of the Advanced Light Source at Lawrence Berkeley National Laboratory and serves on the Scientific Advisory Board of the National Nanotechnology Infrastructure Network.

**William Bialek**

William Bialek is the John Archibald Wheeler/Battelle Professor in Physics at Princeton University. He also is an associated faculty member in the Department of Molecular Biology and a member of the multidisciplinary Lewis–Sigler Institute. He attended the University of California, Berkeley, receiving the A.B. (1979) and Ph.D. (1983) degrees in biophysics. Dr. Bialek's research interests have ranged from the dynamics of individual biological molecules to learning and cognition. Best known for contributions to the understanding of coding and computation in the brain, Dr. Bialek and collaborators have shown that aspects of brain function can be described as essentially optimal strategies for adapting to the complex dynamics of the world, making the most of the available signals in the face of fundamental physical constraints and limitations. He is a fellow of the American Physical Society and was a Presidential Young Investigator and Miller Research Fellow and Regents' Junior Faculty Fellow. He recently completed a term as chair of the advisory board for the Kavli Institute for Theoretical Physics, and he recently received the President's Award for Distinguished Teaching at Princeton.

**David J. Bishop**

David Bishop is the chief technology officer and chief operating officer of LGS, the wholly owned subsidiary of Alcatel-Lucent dedicated to serving the U.S. federal government market. Most recently he was president of government research and security solutions for Bell Laboratories/Lucent Technologies. Dr. Bishop was a Bell Laboratories Fellow, and in his previous positions with Lucent, he served as nanotechnology research vice president for Bell Laboratories/Lucent Technologies, president of the New Jersey Nanotechnology Consortium, and the physical sciences research vice president. In 1988 he was made a Distinguished Member of the Technical Staff, and later that same year was promoted to department head, Bell Laboratories. Dr. Bishop joined AT&T Bell Laboratories in 1978 as a postdoctoral member of the staff and in 1979 became a member of the technical staff. He graduated magna cum laude with honors from Syracuse University in 1973 with a B.S. in physics. In 1977 he received an M.S. in physics from Cornell University and in 1978 a Ph.D. in physics from Cornell.

**Anthony K. Cheetham**

Anthony Cheetham is a professor of solid state chemistry, materials, and chemistry and director of the International Center for Materials Research at the University of California at Santa Barbara. He received his B.A. in 1969 from St. Catherine's College in Oxford, U.K., and his M.A. and D.Phil. from Wadham College, also in Oxford. His research interests include nanoporous and open-framework materials, novel phosphors for solid-state lighting, magnetic properties of mixed metal manganates, and new methods for materials characterization. His honors include a 1977 Fulbright Scholarship (Arizona State University), and 1982 Corday-Morgan Medal, 1988 Solid State Chemistry Award, and 1996 Structural Chemistry Award, all from the Royal Society of Chemistry, London, as well as the 2003 Professor C.N.R. Rao Lecture Award from the Chemical Research Society of India, 2003 Humphry Davy Prize Lectureship of the Royal Society, and the 2004 Somiya Award of the International Union of Materials Research Societies (with Professor C.N.R. Rao). He is a fellow of the Royal Society, London; associate fellow of the Third World Academy of Sciences; and honorary fellow of the Indian Academy of Sciences. Dr. Cheetham is a member of the European Academy of Arts, Sciences and Humanities and a foreign member of both the Pakistan Academy of Sciences and the National Academy of Sciences of India. He has served on advisory and planning committees for the Spallation Neutron Source, European Synchrotron Radiation Facility and Argonne, Brookhaven, Oak Ridge, and Los Alamos National Laboratories.

**James P. Eisenstein**

James Eisenstein is the Frank J. Roshek Professor of Physics and Applied Physics at the California Institute of Technology (Caltech) and is an expert in low-dimensional condensed-matter physics. His research focuses on experimental studies of correlated electron systems in semiconductors with particular interest in the physics of single- and multi-layer two-dimensional electron systems; his laboratory uncovered several new exotic electron states over the years. He spent a number of years working at Bell Laboratories before going to Caltech. Dr. Eisenstein is a fellow of the American Physical Society and a member of the National Academy of Sciences. He was awarded the 2003 Associated Students of the California Institute of Technology award for excellence in teaching, the 2007 Buckley Prize of the APS, and was a Loeb Lecturer at Harvard University in 2003. He has served on several NRC committees, including National Institute of Standards and Technology review panels, and he is a member of the Solid State Sciences Committee.

**Hidetoshi Fukuyama**

Hidetoshi Fukuyama is professor emeritus of Tokyo University and is currently professor of Tokyo University of Science. He received his B.S., M.S., and Ph.D. in physics from Tokyo University. He was director of the Institute for Solid State Physics, Tokyo University (1999-2003) and director of the International Frontier Center for Advanced Materials (IFCAM) of the Institute of Materials Research, Tohoku University (2004-2006). His research interests include theoretical studies of quantum transport phenomena in solids in general, including orbital magnetism, spin-Peierls phenomena, Anderson localization, high-temperature superconductivity, and electronic properties of molecular solids. His honors include the 1987 Japan IBM Science Award, the 1998 Superconductivity Science and Technology Award, and the 2003 National Medal with Purple Ribbon. He is a fellow of the American Physical Society. He served as a vice president of IUPAP (2002-2005) and currently serves on the international advisory committee for J-PARC.

**Laura Garwin**

Laura Garwin is a postgraduate student in trumpet performance at the Royal College of Music in London, U.K. Until August 2006 she was executive director of the Bauer Center for Genomics Research at Harvard University, and before that she was the North American editor of *Nature*. Dr. Garwin received her A.B. in physics from Harvard University, M.A. in geology from the University of Oxford, and Ph.D. in earth sciences from the University of Cambridge. She is a fellow of the American Physical Society and the British–American Project, a Rhodes Scholar, and editor, with Tim Lincoln, of *A Century of Nature: Twenty-One Discoveries That Changed Science and the World*. Dr. Garwin served on the American Physical Society's Publications Oversight Committee and on the steering committee for the American Physical Society's topical conferences, "Opportunities in Biology for Physicists."

**Peter F. Green**

Peter Green is a professor of materials science and engineering and chair of the department at the University of Michigan. He also has appointments in applied physics and macromolecular science. He received his Ph.D. in materials science and engineering from Cornell University in 1985. Dr. Green was a member of the technical staff at Sandia National Laboratories working on the physical properties of polymers and from 1991 to 1996 he served as the department manager of the Glass and Electronic Ceramics Research Department at Sandia. In 1996 he joined the faculty at the University of Texas, Department of Chemical Engineering, and was appointed the Paul D. and Betty Robertson Meek Centennial Professor in Chemical Engineering in 2000 before moving to the University of Michigan in 2005. Dr. Green's current research includes studies of polymer blends, block copolymers, thin-film polymer interfaces, polymer melt dynamics, and relaxation processes in organic glasses. He is a fellow of the American Physical Society and the American Ceramic Society. He was elected to the Materials Research Society (MRS) board of directors in 2000 and has served on the executive committee of the Polymer Science Division of the American Chemical Society. He was the 2006 president of the MRS and is as a member-at-large to the Council on Gordon Research Conferences. Dr. Green has served on the external advisory board of the Division of Math and Physical Science at the National Science Foundation.

**Frances Hellman**

Frances Hellman is a professor of physics and of materials science and engineering at the University of California, Berkeley, and a member of the Materials Science Division of Lawrence Berkeley National Laboratory. She received her B.A. in physics from Dartmouth College in 1978 and her Ph.D. in applied physics from Stanford University in 1985. Her current research includes the properties of novel magnetic and semiconducting materials especially in thin-film form. Her research group uses specific heat, magnetic susceptibility, electrical resistivity, and other measurements as a function of temperature in order to test and develop models for materials that challenge our understanding of metallic behavior. She specializes in using Si microfabrication techniques to develop calorimeters capable of measuring thin films and tiny crystals, work for which she won the 2006 APS Keithley Instrumentation Prize. In addition, she is interested in the materials science of growing thin films by vapor deposition processes. Dr. Hellman is a fellow of the American Physical Society, past-chair of both the Topical Group on Magnetism and its Applications (GMAG) and the Division of Materials Physics (DMP). She has served on the APS Panel on Public Affairs, the NSF Mathematical and Physical Sciences Advisory Committee, and the Board on Physics and Astronomy. She also is on the board of the San Francisco Exploratorium and the California State Summer School for Mathematics and Science.

**Randall G. Hulet**

Randall Hulet is a professor of physics at Rice University. He received his B.S. in physics from Stanford University and Ph.D. from Massachusetts Institute of Technology. Dr. Hulet investigates atoms at temperatures of a few nano-kelvin. At such temperatures, the effects of quantum mechanics dominate, greatly altering normal atomic behavior. Dr. Hulet and his group have used laser-cooling and atom-trapping techniques to explore this regime of matter, investigating ultracold atom collisions and quantum statistical effects, such as Bose-Einstein condensation. His honors include the I.I. Rabi Prize from the American Physical Society, a Presidential Young Investigators Award, a research fellowship from the Alfred P. Sloan Foundation, and the NASA Exceptional Scientific Achievement Medal. Dr. Hulet is a fellow of the American Physical Society, American Association for the Advancement of Science, and the American Academy of Arts and Sciences.

**Heinrich M. Jaeger**

Heinrich Jaeger is a professor of physics in the Department of Physics and James Franck Institute at the University of Chicago. He is also director of both the University of Chicago Materials Research Science and Engineering Center and the University of Chicago/Argonne Consortium for Nanoscience Research. He received his undergraduate degree in physics from the University of Kiel, Germany, and his M.S. and Ph.D., both in physics, from the University of Minnesota. In his research, he studies the interactions between many, more or less identical “building blocks” that make up larger, complex structures or show collective effects. This includes studies on nonlinear dynamics of (macroscopic) granular materials, self-assembly and transport properties of nanostructures, and vortex dynamics in superconductors. Dr. Jaeger’s honors include the Outstanding Achievement Award from the University of Minnesota, Research Corporation Cottrell Scholarship, Alfred P. Sloan Research Fellowship, David and Lucile Packard Fellowship, James Franck Fellowship, and a Fulbright Scholarship. He is a fellow of the American Physical Society.

**Steven A. Kivelson**

Steven Kivelson is a professor of physics at Stanford University and is associate director of the Stanford Institute for Theoretical Physics. He received his Ph.D. from Harvard University in 1979. He was a postdoctoral fellow at the University of Pennsylvania and the Institute for Theoretical Physics at the University of California, Santa Barbara. Following that, he was a professor of physics at the State University of New York, Stony Brook, and at the University of California, Los Angeles. He is interested in the qualitative understanding of the macroscopic collective properties, especially equilibrium properties, of condensed-matter systems, and in how these properties arise from the interactions between microscopic degrees of freedom. Recently, his focus has been on the theory of high-temperature superconductivity, the quantum Hall effect, and on conducting phases with novel patterns of broken spatial symmetries in highly correlated electronic fluids. Dr. Kivelson has received an Alfred P. Sloan Foundation Fellowship, a John Simon Guggenheim Fellowship, and a Miller Fellowship. He is a fellow of the American Physical Society and the American Academy of Arts and Sciences.

**Andrea J. Liu**

Andrea Liu is a professor of physics in the Department of Physics and Astronomy at the University of Pennsylvania. She received her B.A. from the University of California, Berkeley, and Ph.D. from Cornell University. Dr. Liu is a condensed-matter theorist who specializes in soft condensed-matter physics. She has done seminal work in several areas, including electrostatic self-assembly and jamming. Dr. Liu's current research focuses on jamming and on the biophysics of cell crawling. She is a fellow of the American Physical Society.

**Paul McEuen**

Paul McEuen is a professor of physics at Cornell University and principal investigator at Lawrence Berkeley National Laboratory (LBNL). Dr. McEuen received his B.S. in engineering physics from the University of Oklahoma and his Ph.D. in applied physics from Yale University. His research interests are in the science and technology of nanostructures, particularly carbon-based systems such as nanotubes and $C_{60}$ molecules; novel fabrication techniques at the nanometer scale; scanned probe microscopy of nanostructures; and assembly and measurement of chemical and biological nanostructures. His honors include Office of Naval Research Young Investigator, Alfred P. Sloan Foundation Fellow, Packard Foundation Fellow, National Young Investigator, LBNL Outstanding Performance Award, Packard Foundation Interdisciplinary Fellow, and Agilent Technologies Europhysics Prize in Condensed Matter Physics. Dr. McEuen is a fellow of the American Physical Society.

**Karin M. Rabe**

Karin Rabe is a professor of physics in the Department of Physics and Astronomy at the State University of New Jersey, Rutgers. She received her A.B. in physics from Princeton University and a Ph.D. in physics from the Massachusetts Institute of Technology. The research in her group currently centers on the theoretical investigation of ferroelectrics and related materials and of magnetic and nonmagnetic martensites. First-principles density-functional methods are used both directly and in the construction of first-principles effective Hamiltonians for theoretical prediction and analysis of properties of materials, both real and as-yet hypothetical, in bulk and thin-film forms. Dr. Rabe's honors include the Arthur Greer Memorial Prize, Alfred P. Sloan Research Fellowship, Junior Faculty Fellowship in the Natural Sciences, Presidential Young Investigator, and Clare Boothe Luce Professorship. She is a fellow of the American Physical Society.

**Thomas N. Theis**

Thomas Theis is the director of physical sciences at IBM T.J. Watson Research Center. He received a B.S. degree in physics from Rensselaer Polytechnic Institute in 1972, and M.S. and Ph.D. degrees from Brown University in 1974 and 1978, respectively. A portion of his Ph.D. research was done at the Technical University of Munich, where he completed a postdoctoral year before joining IBM Research in 1979. Dr. Theis joined the Department of Semiconductor Science and Technology at the IBM T.J. Watson Research Center to study electronic properties of two-dimensional systems. Among his many accomplishments, Dr. Theis coordinated the transfer of copper interconnection technology from IBM Research to the IBM Microelectronics Division. The replacement of aluminum chip wiring by copper was an industry first, the biggest change in chip wiring technology in 30 years, and involved close collaboration between research, product development, and manufacturing organizations. Dr. Theis assumed his current position in February 1998. He is a member of IEEE, the Materials Research Society, a fellow of the American Physical Society, and currently serves on advisory boards for the American Institute of Physics Corporate Associates and the National Nanofabrication Users Network, and the advisory committee for the NIST Advanced Technology Program.